# MinervaLab

*Release 0.1*

**Jun 18, 2020**

# Contents

CHAPTER 1

# Applications

## 1.1 Mathematical analysis of the van der Waals isotherms

**Code:** #118-000

**File:** `apps/van_der_waals/mathematical_analysis.ipynb`

**Run it online:**

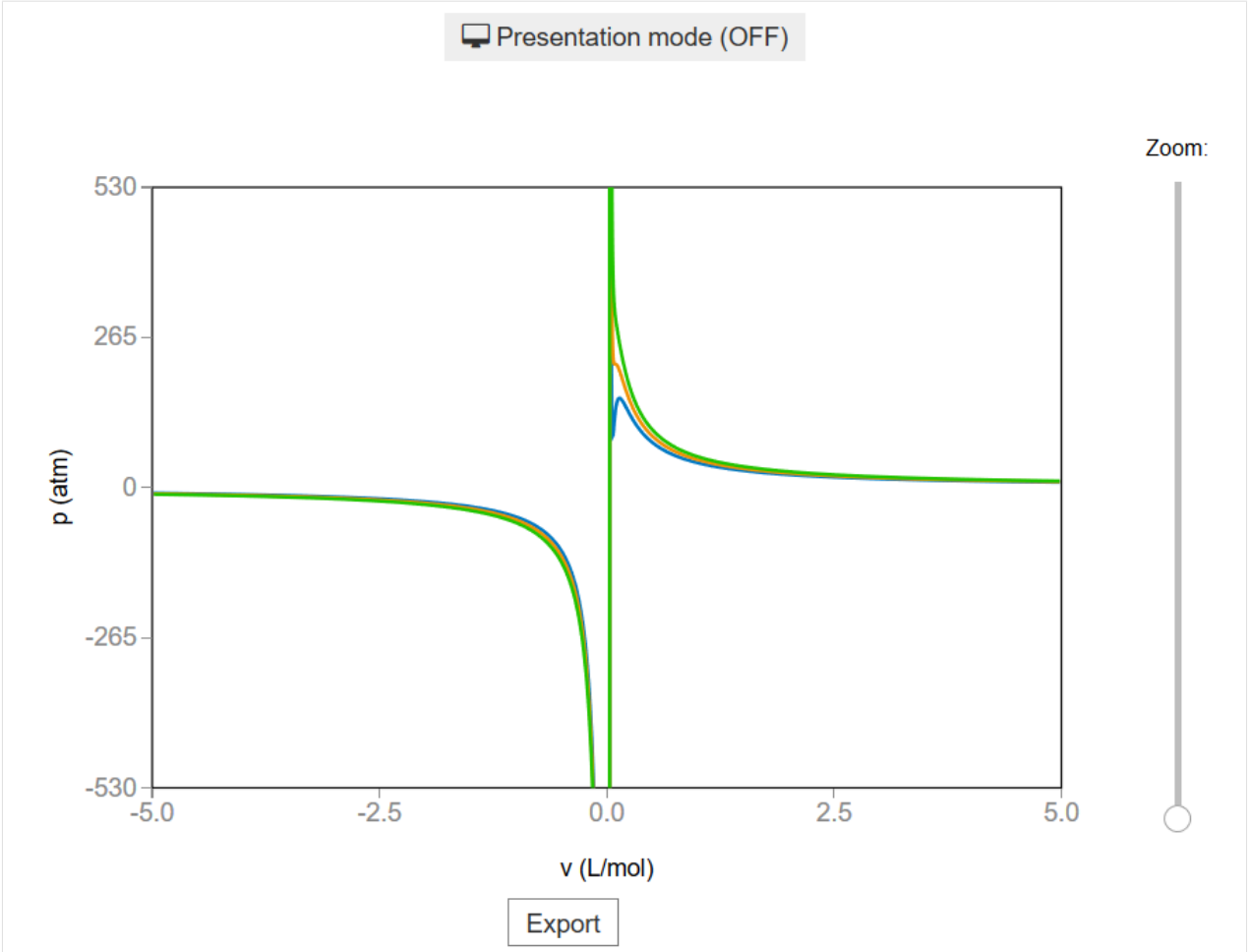
The aim of this notebook is to show the mathematical function of van der Waals isotherms.

### 1.1.1 Interface

The main interface (`main_block_118_000`) is divided in two HBox: `top_block_118_000` and `bottom_block_118_000`. `top_block_118_000` contains of a bqplot Figure (`fig_118_001`) and `bottom_block_118_000` contains 4 bqplot Figures: `fig_118_003`, `fig_118_004`, `fig_118_005` and `fig_118_006`. The slider `zoom_slider` controls the zoom of `fig_118_001`.

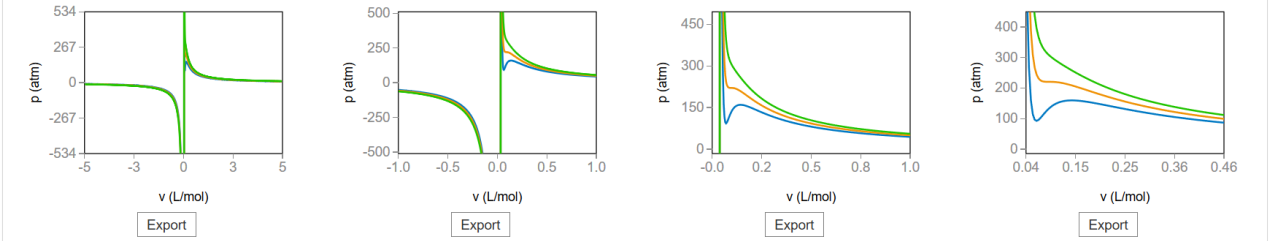
[1]:
```
from IPython.display import Image
Image(filename='../../static/images/apps/118-000_1.png')
```

[1]:




[2]:
```
Image(filename='../../static/images/apps/118-000_2.png')
```

[2]:




### 1.1.2 CSS

A custom `css` file is used to improve the interface of this application. It can be found here.

[1]:
```
from IPython.display import HTML
display(HTML("<head><link rel='stylesheet' type='text/css' href='./../../static/
↪custom.css'></head>"))
display(HTML("<style>.container { width:100% !important; }</style>"))
```

```
<IPython.core.display.HTML object>
```

```
<IPython.core.display.HTML object>
```

### 1.1.3 Packages

[2]:
```
from bqplot import *
import bqplot as bq
import bqplot.marks as bqm
import bqplot.scales as bqs
import bqplot.axes as bqa

import ipywidgets as widgets

import urllib.parse
import webbrowser

import sys
```

### 1.1.4 Physical functions

This are the functions that have a physical meaning:

- `calculate_critic`
- `get_absolute_isotherms`
- `bar_to_atm`

[3]:
```
def calculate_critic(a, b):

    """
        This function calculates the critic point
        (p_c, v_c, T_c) from given a and b parameters of
        the Van der Waals equation of state for real gases.

        :math:`(P + a \\frac{n^2}{V^2})(V - nb) = nRT`

        :math:`p_c = \\frac{a}{27 b^2}`
        :math:`v_c = 3b`
        :math:`T_c = \\frac{8a}{27 b R}`

    Args:
        a: Term related with the attraction between particles in
        L^2 bar/mol^2.\n
        b: Term related with the volume that is occupied by one
        mole of the molecules in L/mol.\n

    Returns:
        p_c: Critical pressure in bar.\n
        v_c: Critical volume in L/mol.\n
        T_c: Critical tenperature in K.\n

    """

    if b == 0.0:
        return None
```

(continues on next page)

(continued from previous page)

```
    k_B = 1.3806488e-23 #m^2 kg s^-2 K^-1
    N_A = 6.02214129e23
    R = 0.082 * 1.01325 #bar L mol^-1 K^-1

    p_c = a/27.0/(b**2)
    v_c = 3.0*b
    T_c = 8.0*a/27.0/b/R

    return p_c, v_c, T_c
```

[4]:
```
def get_absolute_isotherms(a, b, v_values, T_values):
    """This function calculates the theoretical p(v, T) plane
        (in absolute coordinates) according to van der Waals
        equation of state from a given range of volumes
        and tenperatures.

    Args:
        a: Term related with the attraction between particles in
           L^2 bar/mol^2.\n
        b: Term related with the volume that is occupied by one
        mole of the molecules in L/mol.\n
        v_values: An array containing the values of v
        for which the isotherms must be calculated.\n
        T_values: An array containing the values of T for which
        the isotherms must be calculated.\n


    Returns:
        isotherms: A list consisted of numpy arrays containing the
        pressures of each isotherm.
    """
    isotherms = []

    R = 0.082 * 1.01325 #bar L mol^-1 K^-1

    for T in T_values:

        isot = []

        for v in v_values:

            p = R*T/(v - b) - (a/v**2)
            isot = np.append(isot, p)

        isotherms.append(isot)

    return isotherms
```

[5]:
```
def bar_to_atm(p_values):
    """This function changes the pressures of an array
    form bars to atm.

    Args:
        p_values: List consisted of pressures in bars.\n
```

(continues on next page)

(continued from previous page)

```
    Returns:
        p_values: List consisted of pressures in atm.\n
    """

    p_values = np.array(p_values) * 0.9869

    return p_values
```

### 1.1.5 Functions related to the interaction

[6]:
```
def update_scales(change):
    """This function updates the scales of fig_118_001 (and its marks)
    when the value of zoom_slider is changed.\n
    """
    index = change.owner.value

    new_scale_x = bqs.LinearScale(min = x_min[index], max = x_max[index])
    new_scale_y = bqs.LinearScale(min = y_min[index], max = y_max[index])


    # if the scales are not updated in this order the transition
    # is a bit laggy

    for mark in fig_118_001.marks:

        mark.scales = {
            'x' : new_scale_x,
            'y' : new_scale_y
        }

    axis_x_118_001.scale = new_scale_x
    axis_y_118_001.scale = new_scale_y
```

[7]:
```
def change_view(change):
    """This function changes the visualization of all the
    components of the application so they are suitable for
    a projection.\n
    """

    obj = change.owner

    if obj.value:

        obj.description = 'Presentation mode (ON)'

        display(HTML(
            "<style>" \
            ".widget-readout { font-size: 30px ; }" \
            ".widget-label-basic {font-size: 30px;}" \
            "option {font-size: 25px;}" \
            ".p-Widget.jupyter-widgets.widget-slider.widget-vslider.widget-inline-
↪vbox {width: auto}" \
            ".p-Widget .jupyter-widgets .widgets-label {width: auto; height: auto;␣
↪font-size: 30px;}" \
```

(continues on next page)

(continued from previous page)

```
            ".widget-label {font-size: 30px ; height: auto !important;}" \
            ".p-Widget .bqplot .figure .jupyter-widgets {height: auto !important;}" \
            ".widget-text input[type='number'] {font-size: 30px;height: auto;}" \
            ".option { font-size: 30px ;}" \
            ".p-Widget .jupyter-widgets .jupyter-button.widget-button {font-size:␣
↪30px ; width: auto; height: auto;}" \
            ".p-Widget.jupyter-widgets.jupyter-button.widget-toggle-button{font-size:␣
↪30px ; width: auto; height: auto;}" \
            ".p-Widget.p-Panel.jupyter-widgets.widget-container.widget-box.widget-
↪vbox {padding-bottom: 30px}" \
            ".bqplot > svg .axis text.axislabel, .bqplot > svg .axis tspan.axislabel
↪{font-size: 30px;}" \
            ".q-grid .slick-cell {font-size: 30px;}" \
            ".slick-column-name {font-size: 30px;}"
            "</style>"
            )
        )

        for figure in figures:

            figure.legend_text = {'font-size': '30px'}
            figure.title_style = {'font-size': '30px'}

            for axis in figure.axes:
                axis.tick_style = {'font-size': '30px'}
                axis.label_style = {'font-size': '30px'}

    else:

        obj.description = 'Presentation mode (OFF)'

        display(HTML(
            "<style>" \
            ".widget-readout { font-size: 14px ;}" \
            ".widget-label-basic {font-size: 14px;}" \
            "option {font-size: 12px;}" \
            ".p-Widget .jupyter-widgets .widgets-label {font-size: 14px;}" \
            ".widget-label {font-size: 14px ;}" \
            ".widget-text input[type='number'] {font-size: 14px;}" \
            ".option { font-size: 14px ;}" \
            ".p-Widget .jupyter-widgets .jupyter-button.widget-button {font-size:␣
↪14px;}" \
            ".p-Widget.jupyter-widgets.jupyter-button.widget-toggle-button {font-size:
↪ 14px;}" \
            ".bqplot > svg .axis text.axislabel, .bqplot > svg .axis tspan.axislabel
↪{font-size: 14px;}" \
            ".q-grid .slick-cell {font-size: 14px;}" \
            ".slick-column-name {font-size: 14px;}"
            "</style>"
            )
        )

        for figure in figures:

            figure.legend_text = {'font-size': '14px'}
            figure.title_style = {'font-size': '20px'}
```

(continues on next page)

(continued from previous page)

```
            for axis in figure.axes:
                axis.tick_style = {'font-size': '14px'}
                axis.label_style = {'font-size': '14px'}
```

[8]:
```
def prepare_export(button):
    """This function sends the selected plot to the 'export_plot'
    function.
    """

    if button is prepare_export_fig_118_001_button:

        export_plot(fig_118_001)

    elif button is prepare_export_fig_118_003_button:

        export_plot(fig_118_003)

    elif button is prepare_export_fig_118_004_button:

        export_plot(fig_118_004)

    elif button is prepare_export_fig_118_005_button:

        export_plot(fig_118_005)

    elif button is prepare_export_fig_118_006_button:

        export_plot(fig_118_006)
```

[9]:
```
def export_plot(plot):
    """This function sends the selected plot to the export module.
    """

    global data

    text_lines = []

    np.set_printoptions(threshold=sys.maxsize)

    for mark in plot.marks:
        mark.tooltip = None

    data =  repr((plot, text_lines))

    %store data

    rel_url = "../../../apps/modules/export_module.ipynb"
    abs_url = urllib.parse.urljoin(notebook_url, rel_url)

    if not webbrowser.open(abs_url):
        go_to_export_button.value = "<form action=" + abs_url + " target='_blank'>
↪<button type=''submit''>Open in export module</button></form>"
```

[ ]:
```
%%javascript
```

(continues on next page)

(continued from previous page)

```
//Get the URL of the current notebook

var kernel = Jupyter.notebook.kernel;
var command = ["notebook_url = ",
               "'", window.location.href, "'" ].join('')

kernel.execute(command)
```

### 1.1.6 Main interface

[ ]:
```
#In this program we are going to use water's parameters
a = 5.536 #L^2 bar mol^-2
b = 0.03049 #L mol^-1

colors = ['#0079c4','#f09205','#21c400', '#850082']

p_c, v_c, T_c = calculate_critic(a, b)

p_c = p_c * 0.9869 #unit change from bar to atm

v_values = np.linspace(-5.0, 5.0, 3000) #L/mol
T_values = [0.9*T_c, 1.0*T_c, 1.1*T_c]

p_values = get_absolute_isotherms(a, b, v_values, T_values)
p_values = bar_to_atm(p_values)

v_values_hd = np.linspace(-20, 20, 10000)
p_values_hd = get_absolute_isotherms(a, b, v_values_hd, T_values)

######################
######TOP BLOCK######
######################

top_block_118_000 = widgets.VBox(
    [],
    layout=widgets.Layout(align_items='center')
)

scale_x_118_001 = bqs.LinearScale(min = min(v_values), max = max(v_values))
scale_y_118_001 = bqs.LinearScale(min =-500.0, max = 500.0)

axis_x_118_001 = bqa.Axis(
    scale=scale_x_118_001,
    tick_format='.1f',
    tick_style={'font-size': '15px'},
    num_ticks=5,
    grid_lines = 'none',
    grid_color = '#8e8e8e',
    label='v (L/mol)',
    label_location='middle',
    label_style={'stroke': 'black', 'default-size': 35},
    label_offset='50px'
)

axis_y_118_001 = bqa.Axis(
```

(continues on next page)

(continued from previous page)

```
    scale=scale_y_118_001,
    tick_format='.0f',
    tick_style={'font-size': '15px'},
    num_ticks=5,
    grid_lines = 'none',
    grid_color = '#8e8e8e',
    orientation='vertical',
    label='p (atm)',
    label_location='middle',
    label_style={'stroke': 'red', 'default_size': 35},
    label_offset='50px'
)

fig_118_001 = Figure(
    title='',
    marks=[],
    axes=[axis_x_118_001, axis_y_118_001],
    animation_duration=500,
    legend_location='top-right',
    background_style= {'fill': 'white',  'stroke': 'black'},
    min_aspect_ratio=1.0,
    fig_margin=dict(top=70, bottom=60, left=80, right=30),
    toolbar = True,
    layout = widgets.Layout(),
)

marks = [
    bqm.Lines(
        x = [v_values for elem in p_values],
        y = p_values,
        scales = {'x': scale_x_118_001, 'y': scale_y_118_001},
        opacities = [1.0],
        visible = True,
        colors = colors,
    )
]

fig_118_001.marks = marks

prepare_export_fig_118_001_button = widgets.Button(
    description='Export',
    disabled=False,
    button_style='',
    tooltip='',
    layout=widgets.Layout(
        width='initial',
        align_self='center'
    )
)

prepare_export_fig_118_001_button.on_click(prepare_export)


zoom_slider = widgets.IntSlider(
    value=0,
    min=0,
    max=30,
```

(continues on next page)

(continued from previous page)

```
    step=1,
    description='Zoom:',
    disabled=False,
    continuous_update=True,
    orientation='vertical',
    readout=False,
    readout_format='d',
    layout = widgets.Layout(margin='35px 0 0 0', height='80%')
)

zoom_slider.observe(update_scales, 'value')


# Calculate the values of the scales
x_min = np.linspace(scale_x_118_001.min, 0.0, zoom_slider.max+1)
x_max = np.linspace(scale_x_118_001.max, 5.0*v_c, zoom_slider.max+1)

y_min = np.linspace(scale_y_118_001.min, 0.0, zoom_slider.max+1)
y_max = np.linspace(scale_y_118_001.max, 456.0, zoom_slider.max+1)


change_view_button = widgets.ToggleButton(
    value=False,
    description='Presentation mode (OFF)',
    disabled=False,
    button_style='',
    tooltip='',
    icon='desktop',
    layout=widgets.Layout(
        width='initial',
        align_self='center'
    )
)

change_view_button.observe(change_view, 'value')

top_block_118_000.children = [
    change_view_button,
    widgets.HBox([
        widgets.VBox([
            fig_118_001,
            prepare_export_fig_118_001_button,
        ]),
        zoom_slider
    ])
]


#####################
####BOTTOM BLOCK#####
#####################

bottom_block_118_000 = widgets.HBox(
    [],
    layout=widgets.Layout(
        height='300px',
        width='100%'
```

(continues on next page)

(continued from previous page)

```
    )
)

scale_x_118_003 = bqs.LinearScale(
    min = scale_x_118_001.min,
    max = scale_x_118_001.max
)

scale_y_118_003 = bqs.LinearScale(
    min = scale_y_118_001.min,
    max = scale_y_118_001.max
)

axis_x_118_003 = bqa.Axis(
    scale=scale_x_118_003,
    tick_format='.0f',
    tick_style={'font-size': '15px'},
    num_ticks=5,
    grid_lines = 'none',
    grid_color = '#8e8e8e',
    label='v (L/mol)',
    label_location='middle',
    label_style={'stroke': 'black', 'default-size': 35},
    label_offset='50px'
)

axis_y_118_003 = bqa.Axis(
    scale=scale_y_118_003,
    tick_format='.0f',
    tick_style={'font-size': '15px'},
    num_ticks=5,
    grid_lines = 'none',
    grid_color = '#8e8e8e',
    orientation='vertical',
    label='p (atm)',
    label_location='middle',
    label_style={'stroke': 'red', 'default_size': 35},
    label_offset='50px'
)

marks = [
    bqm.Lines(
        x = [v_values for elem in p_values],
        y = p_values,
        scales = {'x': scale_x_118_003, 'y': scale_y_118_003},
        opacities = [1.0],
        visible = True,
        colors = colors
    )
]

fig_118_003 = Figure(
    title='',
    marks=marks,
    axes=[axis_x_118_003, axis_y_118_003],
    animation_duration=0,
    legend_location='top-right',
```

(continues on next page)

(continued from previous page)

```
    background_style= {'fill': 'white',  'stroke': 'black'},
    min_aspect_ratio=1.0,
    fig_margin=dict(top=50, bottom=60, left=80, right=30),
    toolbar = False,
    layout = widgets.Layout(height='90%', width='95%')
)

scale_x_118_004 = bqs.LinearScale(min = -2.0, max = 2.0)
scale_y_118_004 = bqs.LinearScale(min = -2.2*p_c, max = 2.2*p_c)

axis_x_118_004 = bqa.Axis(
    scale=scale_x_118_004,
    tick_format='.0f',
    tick_style={'font-size': '15px'},
    num_ticks=5,
    grid_lines = 'none',
    grid_color = '#8e8e8e',
    label='v (L/mol)',
    label_location='middle',
    label_style={'stroke': 'black', 'default-size': 35},
    label_offset='50px'
)

axis_y_118_004 = bqa.Axis(
    scale=scale_y_118_004,
    tick_format='.0f',
    tick_style={'font-size': '15px'},
    tick_values = [-500, -250, 0, 250, 500],
    grid_lines = 'none',
    grid_color = '#8e8e8e',
    orientation='vertical',
    label='p (atm)',
    label_location='middle',
    label_style={'stroke': 'red', 'default_size': 35},
    label_offset='50px'
)

marks = [
    bqm.Lines(
        x = [v_values_hd for elem in p_values_hd],
        y = p_values_hd,
        scales = {'x': scale_x_118_004, 'y': scale_y_118_004},
        opacities = [1.0],
        visible = True,
        colors = colors,
    )
]

fig_118_004 = Figure(
    title='',
    marks=marks,
    axes=[axis_x_118_004, axis_y_118_004],
    animation_duration=0,
    legend_location='top-right',
    background_style= {'fill': 'white',  'stroke': 'black'},
    min_aspect_ratio=1.0,
    fig_margin=dict(top=50, bottom=60, left=80, right=30),
```

(continues on next page)

(continued from previous page)

```
    toolbar = True,
    layout = widgets.Layout(height='90%', width='95%')
)



scale_x_118_005 = bqs.LinearScale(min = 0.0, max = 2.0)
scale_y_118_005 = bqs.LinearScale(min = 0.0, max = 2.2*p_c)

axis_x_118_005 = bqa.Axis(
    scale=scale_x_118_005,
    tick_format='.1f',
    tick_style={'font-size': '15px'},
    num_ticks=5,
    grid_lines = 'none',
    grid_color = '#8e8e8e',
    label='v (L/mol)',
    label_location='middle',
    label_style={'stroke': 'black', 'default-size': 35},
    label_offset='50px'
)

axis_y_118_005 = bqa.Axis(
    scale=scale_y_118_005,
    tick_format='.0f',
    tick_style={'font-size': '15px'},
    tick_values = [0, 150, 300, 450],
    grid_lines = 'none',
    grid_color = '#8e8e8e',
    orientation='vertical',
    label='p (atm)',
    label_location='middle',
    label_style={'stroke': 'red', 'default_size': 35},
    label_offset='50px'
)

marks = [
    bqm.Lines(
        x = [v_values_hd for elem in p_values_hd],
        y = p_values_hd,
        scales = {'x': scale_x_118_005, 'y': scale_y_118_005},
        opacities = [1.0],
        visible = True,
        colors = colors,
    )
]

fig_118_005 = Figure(
    title='',
    marks=marks,
    axes=[axis_x_118_005, axis_y_118_005],
    animation_duration=0,
    legend_location='top-right',
    background_style= {'fill': 'white',  'stroke': 'black'},
    min_aspect_ratio=1.0,
    fig_margin=dict(top=50, bottom=60, left=80, right=30),
    toolbar = True,
```

(continues on next page)

(continued from previous page)

```
    layout = widgets.Layout(height='90%', width='95%')
)

scale_x_118_006 = bqs.LinearScale(min = 0.5*v_c, max = 5.0*v_c)
scale_y_118_006 = bqs.LinearScale(min = 0.0, max = 2.0*p_c)

axis_x_118_006 = bqa.Axis(
    scale=scale_x_118_006,
    tick_format='.2f',
    tick_style={'font-size': '15px'},
    num_ticks=5,
    grid_lines = 'none',
    grid_color = '#8e8e8e',
    label='v (L/mol)',
    label_location='middle',
    label_style={'stroke': 'black', 'default-size': 35},
    label_offset='50px'
)

axis_y_118_006 = bqa.Axis(
    scale=scale_y_118_006,
    tick_format='.0f',
    tick_style={'font-size': '15px'},
    tick_values = [0, 100, 200, 300, 400],
    grid_lines = 'none',
    grid_color = '#8e8e8e',
    orientation='vertical',
    label='p (atm)',
    label_location='middle',
    label_style={'stroke': 'red', 'default_size': 35},
    label_offset='50px'
)

marks = [
    bqm.Lines(
        x = [v_values_hd for elem in p_values_hd],
        y = p_values_hd,
        scales = {'x': scale_x_118_006, 'y': scale_y_118_006},
        opacities = [1.0],
        visible = True,
        colors = colors,
    )
]

fig_118_006 = Figure(
    title='',
    marks=marks,
    axes=[axis_x_118_006, axis_y_118_006],
    animation_duration=0,
    legend_location='top-right',
    background_style= {'fill': 'white',  'stroke': 'black'},
    min_aspect_ratio=1.0,
    fig_margin=dict(top=50, bottom=60, left=80, right=30),
    toolbar = True,
    layout = widgets.Layout(height='90%', width='95%')
)
```

(continues on next page)

(continued from previous page)

```
prepare_export_fig_118_003_button = widgets.Button(
    description='Export',
    disabled=False,
    button_style='',
    tooltip='',
    layout=widgets.Layout(
        width='initial',
        align_self='center'
    )
)

prepare_export_fig_118_003_button.on_click(prepare_export)

prepare_export_fig_118_004_button = widgets.Button(
    description='Export',
    disabled=False,
    button_style='',
    tooltip='',
    layout=widgets.Layout(
        width='initial',
        align_self='center'
    )
)

prepare_export_fig_118_004_button.on_click(prepare_export)

prepare_export_fig_118_005_button = widgets.Button(
    description='Export',
    disabled=False,
    button_style='',
    tooltip='',
    layout=widgets.Layout(
        width='initial',
        align_self='center'
    )
)

prepare_export_fig_118_005_button.on_click(prepare_export)

prepare_export_fig_118_006_button = widgets.Button(
    description='Export',
    disabled=False,
    button_style='',
    tooltip='',
    layout=widgets.Layout(
        width='initial',
        align_self='center'
    )
)

prepare_export_fig_118_006_button.on_click(prepare_export)

bottom_block_118_000.children = [
    widgets.VBox([
        fig_118_003,
        prepare_export_fig_118_003_button,
        ],
```

(continues on next page)

(continued from previous page)

```
        layout=widgets.Layout(
            width='25%',
        )
    ),
    widgets.VBox([
        fig_118_004,
        prepare_export_fig_118_004_button,
    ],
        layout=widgets.Layout(
            width='25%',
        )
    ),
    widgets.VBox([
        fig_118_005,
        prepare_export_fig_118_005_button,
    ],
        layout=widgets.Layout(
            width='25%',
        )
    ),
    widgets.VBox([
        fig_118_006,
        prepare_export_fig_118_006_button,
    ],
        layout=widgets.Layout(
            width='25%',
        )
    ),
]

######################
####MAIN BLOCK#####
######################

main_block_118_000 = widgets.VBox(
    [],
    layout=widgets.Layout(align_items='center')
)

main_block_118_000.children = [
    top_block_118_000,
    bottom_block_118_000
]

figures = [
    fig_118_001,
    fig_118_003,
    fig_118_004,
    fig_118_005,
    fig_118_006,
]

main_block_118_000
```

## 1.2 Mathematical analysis of the effect of a and b parameters

**Code:** #119-000

**File:** `apps/van_der_waals/parameters_analysis.ipynb`

**Run it online:**

---

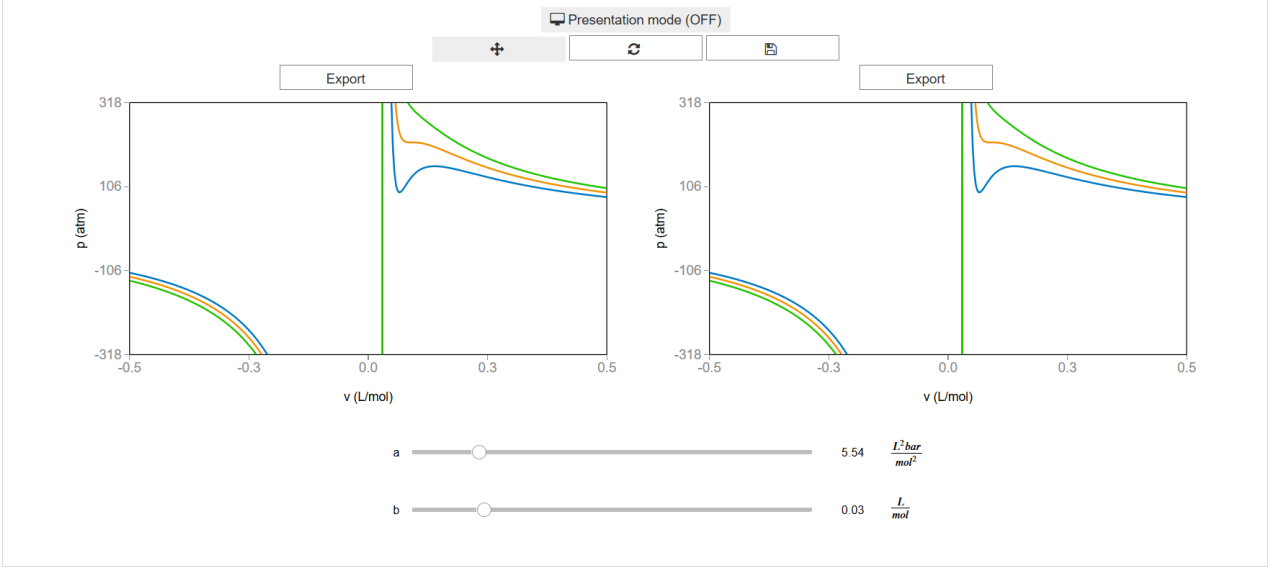
The aim of this notebook is to visualize the effect of a and b parameters on van der Waals' isotherms.

### 1.2.1 Interface

The main interface (`main_block_119_000`) is divided in two HBox: `top_block_119_000` and `bottom_block_119_000`. `top_block_119_000` contains of 2 bqplot Figures: `fig_119_001` and `fig_119_002`.

[1]:
```
from IPython.display import Image
Image(filename='../../static/images/apps/119-000_1.png')
```

[1]:




The sliders `a_slider` and `b_slider` update the values of $a$ and $b$ which updates the isotherms of `fig_119_001` and `fig_119_002`.

[2]:
```
Image(filename='../../static/images/apps/119-000_2.png')
```

[2]:

### 1.2.2 CSS

A custom `css` file is used to improve the interface of this application. It can be found here.

[1]:
```
from IPython.display import HTML
display(HTML("<head><link rel='stylesheet' type='text/css' href='./../../static/
↪custom.css'></head>"))
display(HTML("<style>.container { width:100% !important; }</style>"))
```

```
<IPython.core.display.HTML object>
```

```
<IPython.core.display.HTML object>
```

### 1.2.3 Packages

[2]:
```
from bqplot import *
import bqplot as bq
import bqplot.marks as bqm
import bqplot.scales as bqs
import bqplot.axes as bqa

import ipywidgets as widgets

import urllib.parse
import webbrowser

import sys
```

### 1.2.4 Physical functions

This are the functions that have a physical meaning:

- `get_absolute_isotherms`
- `calculate_critic`
- `bar_to_atm`

[3]:
```
def get_absolute_isotherms(a, b, v_values, T_values):
    """This function calculates the theoretical p(v, T) plane
        (in absolute coordinates) according to van der Waals
        equation of state from a given range of volumes
        and tenperatures.

    Args:
        a: Term related with the attraction between particles in
           L^2 bar/mol^2.\n
        b: Term related with the volume that is occupied by one
        mole of the molecules in L/mol.\n
        v_values: An array containing the values of v
        for which the isotherms must be calculated.\n
        T_values: An array containing the values of T for which
        the isotherms must be calculated.\n


    Returns:
```

(continues on next page)

(continued from previous page)

```
        isotherms: A list consisted of numpy arrays containing the
        pressures of each isotherm.
    """
    isotherms = []

    R = 0.082 * 1.01325 #bar L mol^-1 K^-1

    for T in T_values:

        isot = []

        for v in v_values:

            p = R*T/(v - b) - (a/v**2)
            isot = np.append(isot, p)

        isotherms.append(isot)

    return isotherms
```

[4]:
```
def calculate_critic(a, b):

    """
        This function calculates the critic point
        (p_c, v_c, T_c) from given a and b parameters of
        the Van der Waals equation of state for real gases.

        :math:`(P + a \\frac{n^2}{V^2})(V - nb) = nRT`

        :math:`p_c = \\frac{a}{27 b^2}`
        :math:`v_c = 3b`
        :math:`T_c = \\frac{8a}{27 b R}`

    Args:
        a: Term related with the attraction between particles in
        L^2 bar/mol^2.\n
        b: Term related with the volume that is occupied by one
        mole of the molecules in L/mol.\n

    Returns:
        p_c: Critical pressure in bar.\n
        v_c: Critical volume in L/mol.\n
        T_c: Critical tenperature in K.\n

    """

    if b == 0.0:
        return None

    k_B = 1.3806488e-23 #m^2 kg s^-2 K^-1
    N_A = 6.02214129e23
    R = 0.082 * 1.01325 #bar L mol^-1 K^-1

    p_c = a/27.0/(b**2)
    v_c = 3.0*b
    T_c = 8.0*a/27.0/b/R
```

(continues on next page)

(continued from previous page)

```
    return p_c, v_c, T_c
```

[5]:
```
def bar_to_atm(p_values):
    """This function changes the pressures of an array
    form bars to atm.

    Args:
        p_values: List consisted of pressures in bars.\n

    Returns:
        p_values: List consisted of pressures in atm.\n
    """

    p_values = np.array(p_values) * 0.9869

    return p_values
```

### 1.2.5 Functions related to interaction

[6]:
```
def get_zoom_arrays(initial_x_range, final_x_range, initial_y_range, final_y_range,␣
↪size):
    """This function calculates the arrays of the max/min values of
    x/y for some given limits.

    Args:
        initial_x_range: List consisted of initial values of x.\n
        final_x_range: List consisted of final values of x.\n
        initial_y_range: List consisted of initial values of y.\n
        final_y_range: List consisted of final values of y.\n

    Returns:
        x_min: Array consisted of minimun values of x.\n
        x_max: Array consisted of maximun values of x.\n
        y_min: Array consisted of minimun values of y.\n
        y_max: Array consisted of maximun values of y.\n
    """

    x_min = np.linspace(min(initial_x_range), min(final_x_range), size)
    x_max = np.linspace(max(initial_x_range), max(final_x_range), size)

    y_min = np.linspace(min(initial_y_range), min(final_y_range), size)
    y_max = np.linspace(max(initial_y_range), max(final_y_range), size)

    return x_min, x_max, y_min, y_max
```

[7]:
```
def update_isotherms(change):
    """This function updates the isotherms of bqplot Figure
    'fig_119_002' when 'a_slider' of 'b_slider' are updated.
    """

    p_values = get_absolute_isotherms(
        a_slider.value,
        b_slider.value,
```

(continues on next page)

(continued from previous page)

```
        v_values,
        T_values
    )

    p_values = bar_to_atm(p_values)

    marks = [
        bqm.Lines(
            x = [v_values for elem in p_values],
            y = p_values,
            scales = {'x': scale_x_119_001, 'y': scale_y_119_001},
            opacities = [1.0],
            visible = True,
            colors = colors,
        )
    ]

    fig_119_002.marks = marks
```

[8]:
```
def change_view(change):
    """This function changes the visualization of all the
    components of the application so they are suitable for
    a projection.\n
    """

    obj = change.owner

    if obj.value:

        obj.description = 'Presentation mode (ON)'

        display(HTML(
            "<style>" \
            ".widget-readout { font-size: 30px ; }" \
            ".widget-label-basic {font-size: 30px;}" \
            "option {font-size: 25px;}" \
            ".p-Widget.jupyter-widgets.widget-slider.widget-vslider.widget-inline-
↪vbox {width: auto}" \
            ".p-Widget .jupyter-widgets .widgets-label {width: auto; height: auto;␣
↪font-size: 30px;}" \
            ".widget-label {font-size: 30px ; height: auto !important;}" \
            ".p-Widget .bqplot .figure .jupyter-widgets {height: auto !important;}" \
            ".widget-text input[type='number'] {font-size: 30px;height: auto;}" \
            ".option { font-size: 30px ;}" \
            ".p-Widget .jupyter-widgets .jupyter-button.widget-button {font-size:␣
↪30px ; width: auto; height: auto;}" \
            ".p-Widget.jupyter-widgets.jupyter-button.widget-toggle-button{font-size:␣
↪30px ; width: auto; height: auto;}" \
            ".p-Widget.p-Panel.jupyter-widgets.widget-container.widget-box.widget-
↪vbox {padding-bottom: 30px}" \
            ".bqplot > svg .axis text.axislabel, .bqplot > svg .axis tspan.axislabel
↪{font-size: 30px;}" \
            ".q-grid .slick-cell {font-size: 30px;}" \
            ".slick-column-name {font-size: 30px;}" \
            ".widget-html-content {font-size: 30px;}"
            "</style>"
```

(continues on next page)

(continued from previous page)

```
            )
        )

        for figure in figures:

            figure.legend_text = {'font-size': '30px'}
            figure.title_style = {'font-size': '30px'}

            for axis in figure.axes:
                axis.tick_style = {'font-size': '30px'}
                axis.label_style = {'font-size': '30px'}

    else:

        obj.description = 'Presentation mode (OFF)'

        display(HTML(
            "<style>" \
            ".widget-readout { font-size: 14px ;}" \
            ".widget-label-basic {font-size: 14px;}" \
            "option {font-size: 12px;}" \
            ".p-Widget .jupyter-widgets .widgets-label {font-size: 14px;}" \
            ".widget-label {font-size: 14px ;}" \
            ".widget-text input[type='number'] {font-size: 14px;}" \
            ".option { font-size: 14px ;}" \
            ".p-Widget .jupyter-widgets .jupyter-button.widget-button {font-size:
↪14px;}" \
            ".p-Widget.jupyter-widgets.jupyter-button.widget-toggle-button {font-size:
↪ 14px;}" \
            ".bqplot > svg .axis text.axislabel, .bqplot > svg .axis tspan.axislabel
↪{font-size: 14px;}" \
            ".q-grid .slick-cell {font-size: 14px;}" \
            ".slick-column-name {font-size: 14px;}" \
            ".widget-html-content {font-size: 14px;}"
            "</style>"
            )
        )

        for figure in figures:

            figure.legend_text = {'font-size': '14px'}
            figure.title_style = {'font-size': '20px'}

            for axis in figure.axes:
                axis.tick_style = {'font-size': '14px'}
                axis.label_style = {'font-size': '14px'}
```

[9]:
```
def prepare_export(button):
    """This function sends the selected plot to the 'export_plot'
    function.
    """

    if button is prepare_export_fig_119_001_button:

        export_plot(fig_119_001)
```

(continues on next page)

(continued from previous page)

```
    elif button is prepare_export_fig_119_002_button:

        export_plot(fig_119_002)
```

[10]:
```
def export_plot(plot):
    """This function sends the selected plot to the export module.
    """

    global data

    text_lines = []

    np.set_printoptions(threshold=sys.maxsize)

    tooltips = []

    for mark in plot.marks:
        tooltips.append(mark.tooltip)
        mark.tooltip = None

    data =  repr((plot, text_lines))

    %store data

    rel_url = "../../../apps/modules/export_module.ipynb"
    abs_url = urllib.parse.urljoin(notebook_url, rel_url)

    if not webbrowser.open(abs_url):
        go_to_export_button.value = "<form action=" + abs_url + " target='_blank'>
↪<button type=''submit''>Open in export module</button></form>"

    for i in range(len(plot.marks)):
        mark = plot.marks[i]
        mark.tooltip = tooltips[i]
```

[ ]:
```
%%javascript

//Get the URL of the current notebook

var kernel = Jupyter.notebook.kernel;
var command = ["notebook_url = ",
               "'", window.location.href, "'" ].join('')

kernel.execute(command)
```

### 1.2.6 Main interface

[ ]:
```
#In this program we are going to use water's parameters
a = 5.536 #L^2 bar mol^-2
b = 0.03049 #L mol^-1

colors = ['#0079c4','#f09205','#21c400', '#850082']

p_c, v_c, T_c = calculate_critic(a, b)
```

(continues on next page)

(continued from previous page)

```
p_c = p_c * 0.9869 #unit change from bar to atm

v_values = np.linspace(-5, 5, 3000) #L/mol
T_values = [0.9*T_c, 1.0*T_c, 1.1*T_c]

p_values = get_absolute_isotherms(a, b, v_values, T_values)
p_values = bar_to_atm(p_values)

######################
######TOP BLOCK######
######################

top_block_119_000 = widgets.VBox(
    [],
    layout=widgets.Layout(
        align_items='center',
    )
)

scale_x_119_001 = bqs.LinearScale(min = -0.5, max = 0.5)
scale_y_119_001 = bqs.LinearScale(min = -300, max = 300)

axis_x_119_001 = bqa.Axis(
    scale=scale_x_119_001,
    tick_format='.1f',
    tick_style={'font-size': '15px'},
    num_ticks=5,
    grid_lines = 'none',
    grid_color = '#8e8e8e',
    label='v (L/mol)',
    label_location='middle',
    label_style={'stroke': 'black', 'default-size': 35},
    label_offset='50px'
)

axis_y_119_001 = bqa.Axis(
    scale=scale_y_119_001,
    tick_format='.0f',
    tick_style={'font-size': '15px'},
    num_ticks=4,
    grid_lines = 'none',
    grid_color = '#8e8e8e',
    orientation='vertical',
    label='p (atm)',
    label_location='middle',
    label_style={'stroke': 'red', 'default_size': 35},
    label_offset='50px'
)

fig_119_001 = Figure(
    title='',
    marks=[],
    axes=[axis_x_119_001, axis_y_119_001],
    animation_duration=0,
    legend_location='top-right',
    background_style= {'fill': 'white',  'stroke': 'black'},
```

(continues on next page)

(continued from previous page)

```
    min_aspect_ratio=1.0,
    fig_margin=dict(top=10, bottom=60, left=80, right=30),
    toolbar = True,
    layout=widgets.Layout(
        height='350px',
    )
)

marks = [
    bqm.Lines(
        x = [v_values for elem in p_values],
        y = p_values,
        scales = {'x': scale_x_119_001, 'y': scale_y_119_001},
        opacities = [1.0],
        visible = True,
        colors = colors,
    )
]

fig_119_001.marks = marks


tb_119_001 = Toolbar(figure=fig_119_001, layout=widgets.Layout(align_self='center'))

fig_119_002 = Figure(
    title='',
    marks=[],
    axes=[axis_x_119_001, axis_y_119_001],
    animation_duration=0,
    legend_location='top-right',
    background_style= {'fill': 'white',  'stroke': 'black'},
    min_aspect_ratio=1.0,
    fig_margin=dict(top=10, bottom=60, left=80, right=30),
    toolbar = True,
    layout=widgets.Layout(
        height='350px',
    )
)

fig_119_002.marks = marks

change_view_button = widgets.ToggleButton(
    value=False,
    description='Presentation mode (OFF)',
    disabled=False,
    button_style='',
    tooltip='',
    icon='desktop',
    layout=widgets.Layout(
        width='initial',
        align_self='center'
    )
)

change_view_button.observe(change_view, 'value')

prepare_export_fig_119_001_button = widgets.Button(
```

(continues on next page)

(continued from previous page)

```
    description='Export',
    disabled=False,
    button_style='',
    tooltip='',
    layout=widgets.Layout(
        align_self='center'
    )
)

prepare_export_fig_119_001_button.on_click(prepare_export)

prepare_export_fig_119_002_button = widgets.Button(
    description='Export',
    disabled=False,
    button_style='',
    tooltip='',
    layout=widgets.Layout(
        align_self='center'
    )
)

prepare_export_fig_119_002_button.on_click(prepare_export)

top_block_119_000.children = [
    change_view_button,
    tb_119_001,
    widgets.HBox([
        widgets.VBox([
            prepare_export_fig_119_001_button,
            fig_119_001
        ]),
        widgets.VBox([
            prepare_export_fig_119_002_button,
            fig_119_002
        ])
    ])
]

####################
######BOTTOM BLOCK###
####################

bottom_block_119_000 = widgets.VBox(
    [],
    layout=widgets.Layout(
        align_items='center',
        width='100%',
        margin='30px 0 0 0'
    )
)

a_slider = widgets.FloatSlider(
    min=0,
    max=34.0,
    step=0.001,
    value=a,
    description='a',
```

(continues on next page)

(continued from previous page)

```
    disabled=False,
    continuous_update=False,
    orientation='horizontal',
    readout=True,
    layout=widgets.Layout(width='90%'),
)

a_slider.observe(update_isotherms, 'value')

b_slider = widgets.FloatSlider(
    min=0,
    max=0.1735,
    step=0.0001,
    value=b,
    description='b',
    disabled=False,
    continuous_update=False,
    orientation='horizontal',
    readout=True,
    layout=widgets.Layout(width='90%'),
)

b_slider.observe(update_isotherms, 'value')

bottom_block_119_000.children = [
    widgets.HBox([
        a_slider,
        widgets.HTMLMath(
            value=r"\( \frac{L^2 bar}{mol^2} \)",
            layout=widgets.Layout(height='60px')
        )],
        layout=widgets.Layout(
            width='50%',
            height='100%'
        )
    ),
    widgets.HBox([
        b_slider,
        widgets.HTMLMath(
            value=r"\( \frac{L}{mol} \)",
            layout=widgets.Layout(height='60px')
        )],
        layout=widgets.Layout(
            width='50%',
            height='100%'
        )
    )
]

######################
####MAIN BLOCK#####
######################

main_block_119_000 = widgets.VBox(
    [],
    layout=widgets.Layout(align_items='center')
)
```

(continues on next page)

(continued from previous page)

```
main_block_119_000.children = [
    top_block_119_000,
    bottom_block_119_000
]

figures = [
    fig_119_001,
    fig_119_002
]

main_block_119_000
```

## 1.3 Effect of a and b in van der Waals isotherms

**Code:** #114-000

**File:** `apps/van_der_waals/effect_of_a_and_b.ipynb`

**Run it online:**

---

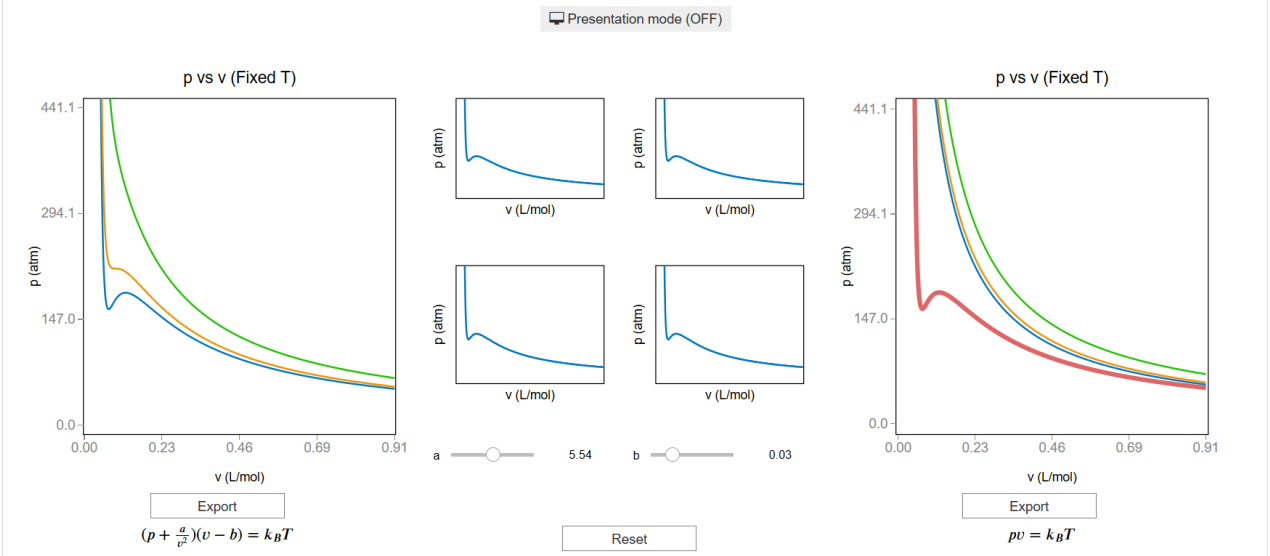
The aim of this notebook is to visualize the effect of a and b parameters on van der Waals' isotherms.

### 1.3.1 Interface

The main interface (`main_block_114_000`) is divided in two HBox: `top_block_114_000` and `bottom_block_114_000`. `top_block_114_000` contains of 5 bqplot Figures: `fig_114_001`, `fig_114_002`, `fig_114_003`, `fig_114_004` and `fig_114_005`.

[1]:
```
from IPython.display import Image
Image(filename='../../static/images/apps/114-000_1.png')
```

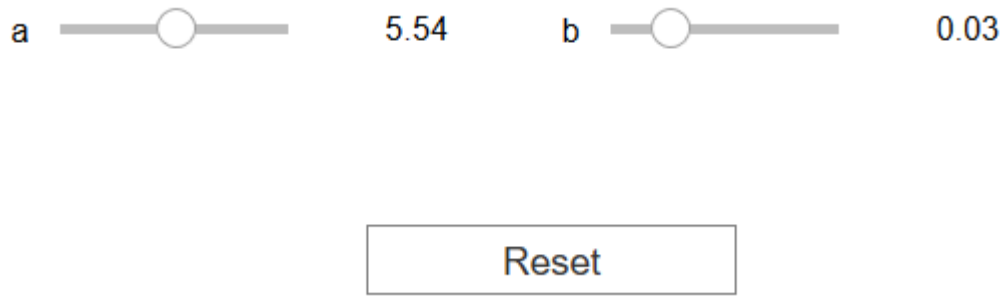
[1]:



The sliders `a_slider_114_003` and `b_slider_114_004` update the values of $a$ and $b$ which updates the isotherms of `fig_114_003`, `fig_114_004` and `fig_114_005`. The button `reset_button` resets the values of $a$ and $b$.

[2]:
```
Image(filename='../../static/images/114-000_2.png')
```

[2]:




### 1.3.2 CSS

A custom `css` file is used to improve the interface of this application. It can be found here.

[3]:
```
from IPython.display import HTML
display(HTML("<head><link rel='stylesheet' type='text/css' href='./../../static/
↪custom.css'></head>"))
display(HTML("<style>.container { width:100% !important; }</style>"))
display(HTML("<style>.widget-label { display: contents !important; }</style>"))
display(HTML("<style>.slider-container { margin: 12px !important; }</style>"))
```

```
<IPython.core.display.HTML object>
```

```
<IPython.core.display.HTML object>
```

```
<IPython.core.display.HTML object>
```

```
<IPython.core.display.HTML object>
```

### 1.3.3 Packages

[4]:
```
from bqplot import *
import bqplot as bq
import bqplot.marks as bqm
import bqplot.scales as bqs
import bqplot.axes as bqa

import ipywidgets as widgets

import urllib.parse
import webbrowser

import sys
```

### 1.3.4 Physical functions

This are the functions that have a physical meaning:

- get_absolute_isotherms
- calculate_critic
- bar_to_atm

[5]:
```
def get_absolute_isotherms(a, b, v_values, T_values):
    """This function calculates the theoretical p(v, T) plane
        (in absolute coordinates) according to van der Waals
        equation of state from a given range of volumes
        and tenperatures.

    Args:
        a: Term related with the attraction between particles in
           L^2 bar/mol^2.\n
        b: Term related with the volume that is occupied by one
        mole of the molecules in L/mol.\n
        v_values: An array containing the values of v
        for which the isotherms must be calculated.\n
        T_values: An array containing the values of T for which
        the isotherms must be calculated.\n


    Returns:
        isotherms: A list consisted of numpy arrays containing the
        pressures of each isotherm.
    """
    isotherms = []

    R = 0.082 * 1.01325 #bar L mol^-1 K^-1

    for T in T_values:

        isot = []

        for v in v_values:

            p = R*T/(v - b) - (a/v**2)
            isot = np.append(isot, p)

        isotherms.append(isot)

    return isotherms
```

[6]:
```
def calculate_critic(a, b):

    """
        This function calculates the critic point
        (p_c, v_c, T_c) from given a and b parameters of
        the Van der Waals equation of state for real gases.

        :math:`(P + a \\frac{n^2}{V^2})(V - nb) = nRT`

        :math:`p_c = \\frac{a}{27 b^2}`
        :math:`v_c = 3b`
        :math:`T_c = \\frac{8a}{27 b R}`

   Args:
```

(continues on next page)

(continued from previous page)

```
        a: Term related with the attraction between particles in
        L^2 bar/mol^2.\n
        b: Term related with the volume that is occupied by one
        mole of the molecules in L/mol.\n

    Returns:
        p_c: Critical pressure in bar.\n
        v_c: Critical volume in L/mol.\n
        T_c: Critical tenperature in K.\n

    """

    if b == 0.0:
        return None

    k_B = 1.3806488e-23 #m^2 kg s^-2 K^-1
    N_A = 6.02214129e23
    R = 0.082 * 1.01325 #bar L mol^-1 K^-1

    p_c = a/27.0/(b**2)
    v_c = 3.0*b
    T_c = 8.0*a/27.0/b/R

    return p_c, v_c, T_c
```

[7]:
```
def bar_to_atm(p_values):
    """This function changes the pressures of an array
    form bars to atm.

    Args:
        p_values: List consisted of pressures in bars.\n

    Returns:
        p_values: List consisted of pressures in atm.\n
    """

    p_values = np.array(p_values) * 0.9869

    return p_values
```

### 1.3.5 Functions related to interaction

[8]:
```
def update_isotherms(change):
    """This function update the lines a_line, b_line and
    unique_isotherm when a_slider_114_003 or b_slider_114_004 are
    updated.
    """

    obj = change.owner
    T_values = [0.95*T_c]

    if obj is a_slider_114_003:

        v_values = np.linspace(1.2*b_initial, 10*v_c, 500)
```

(continues on next page)

(continued from previous page)

```
        isotherms = get_absolute_isotherms(
            a_slider_114_003.value,
            b_initial,
            v_values,
            T_values
        )

        a_line.y = bar_to_atm(isotherms)[0]

    elif obj is b_slider_114_004:

        v_values = np.linspace(1.2*b_slider_114_004.value, 10*v_c, 500)

        if b_slider_114_004.value == 0.0:

            v_values = np.linspace(0.0001, 10*v_c, 500)

        isotherms = get_absolute_isotherms(
            a_initial,
            b_slider_114_004.value,
            v_values,
            T_values
        )

        b_line.x = v_values
        b_line.y = bar_to_atm(isotherms)[0]

    if b_slider_114_004.value == 0.0:

        v_values = np.linspace(0.0001, 10*v_c, 500)

    isotherms = get_absolute_isotherms(
        a_slider_114_003.value,
        b_slider_114_004.value,
        v_values,
        T_values
    )

    unique_isotherm.x = v_values
    unique_isotherm.y = bar_to_atm(isotherms)[0]
```

[9]:
```
def restart(a):
    """This function sets the values of a_slider_114_003
    and b_slider_114_004 to their initial ones.
    """

    a_slider_114_003.value, b_slider_114_004.value = a_initial, b_initial
```

[10]:
```
def change_view(change):
    """This function changes the visualization of all the
    components of the application so they are suitable for
    a projection.\n
    """

    obj = change.owner
```

(continues on next page)

(continued from previous page)

```
    if obj.value:

        obj.description = 'Presentation mode (ON)'

        display(HTML(
            "<style>" \
            ".widget-readout { font-size: 30px ; }" \
            ".widget-label-basic {font-size: 30px;}" \
            "option {font-size: 25px;}" \
            ".p-Widget.jupyter-widgets.widget-slider.widget-vslider.widget-inline-
↪vbox {width: auto}" \
            ".p-Widget .jupyter-widgets .widgets-label {width: auto; height: auto;␣
↪font-size: 30px;}" \
            ".widget-label {font-size: 30px ; height: auto !important;}" \
            ".p-Widget .bqplot .figure .jupyter-widgets {height: auto !important;}" \
            ".widget-text input[type='number'] {font-size: 30px;height: auto;}" \
            ".option { font-size: 30px ;}" \
            ".p-Widget .jupyter-widgets .jupyter-button.widget-button {font-size:␣
↪30px ; width: auto; height: auto;}" \
            ".p-Widget.jupyter-widgets.jupyter-button.widget-toggle-button{font-size:␣
↪30px ; width: auto; height: auto;}" \
            ".p-Widget.p-Panel.jupyter-widgets.widget-container.widget-box.widget-
↪vbox {padding-bottom: 30px}" \
            ".bqplot > svg .axis text.axislabel, .bqplot > svg .axis tspan.axislabel
↪{font-size: 30px;}" \
            ".q-grid .slick-cell {font-size: 30px;}" \
            ".slick-column-name {font-size: 30px;}" \
            ".widget-html-content {font-size: 30px;}"
            "</style>"
            )
        )

        for figure in figures:

            figure.legend_text = {'font-size': '30px'}
            figure.title_style = {'font-size': '30px'}

            for axis in figure.axes:
                axis.tick_style = {'font-size': '30px'}
                axis.label_style = {'font-size': '30px'}

    else:

        obj.description = 'Presentation mode (OFF)'

        display(HTML(
            "<style>" \
            ".widget-readout { font-size: 14px ;}" \
            ".widget-label-basic {font-size: 14px;}" \
            "option {font-size: 12px;}" \
            ".p-Widget .jupyter-widgets .widgets-label {font-size: 14px;}" \
            ".widget-label {font-size: 14px ;}" \
            ".widget-text input[type='number'] {font-size: 14px;}" \
            ".option { font-size: 14px ;}" \
            ".p-Widget .jupyter-widgets .jupyter-button.widget-button {font-size:␣
↪14px;}" \
```

(continues on next page)

(continued from previous page)

```
            ".p-Widget.jupyter-widgets.jupyter-button.widget-toggle-button {font-size:
↪ 14px;}" \
            ".bqplot > svg .axis text.axislabel, .bqplot > svg .axis tspan.axislabel
↪{font-size: 14px;}" \
            ".q-grid .slick-cell {font-size: 14px;}" \
            ".slick-column-name {font-size: 14px;}" \
            ".widget-html-content {font-size: 14px;}"
            "</style>"
            )
        )

        for figure in figures:

            figure.legend_text = {'font-size': '14px'}
            figure.title_style = {'font-size': '20px'}

            for axis in figure.axes:
                axis.tick_style = {'font-size': '14px'}
                axis.label_style = {'font-size': '14px'}
```

[11]:
```
def prepare_export(button):
    """This function sends the selected plot to the 'export_plot'
    function.
    """

    if button is prepare_export_fig_114_001_button:

        export_plot(fig_114_001)

    elif button is prepare_export_fig_114_005_button:

        export_plot(fig_114_005)
```

[12]:
```
def export_plot(plot):
    """This function sends the selected plot to the export module.
    """

    global data

    text_lines = []

    np.set_printoptions(threshold=sys.maxsize)

    tooltips = []

    for mark in plot.marks:
        tooltips.append(mark.tooltip)
        mark.tooltip = None

    data =  repr((plot, text_lines))

    %store data

    rel_url = "../../../apps/modules/export_module.ipynb"
    abs_url = urllib.parse.urljoin(notebook_url, rel_url)
```

(continues on next page)

(continued from previous page)

```
    if not webbrowser.open(abs_url):
        go_to_export_button.value = "<form action=" + abs_url + " target='_blank'>
↪<button type=''submit''>Open in export module</button></form>"

    for i in range(len(plot.marks)):
        mark = plot.marks[i]
        mark.tooltip = tooltips[i]
```

[ ]:
```
%%javascript

//Get the URL of the current notebook

var kernel = Jupyter.notebook.kernel;
var command = ["notebook_url = ",
               "'", window.location.href, "'" ].join('')

kernel.execute(command)
```

### 1.3.6 Main interface

[ ]:
```
a_initial = 5.536 #L^2 bar/mol^2
b_initial = 0.03049 #L/mol

a, b = a_initial, b_initial

p_c, v_c, T_c = calculate_critic(a, b)

T_values = [0.95*T_c, T_c, 1.2*T_c]
v_values = np.linspace(1.2*b, 10*v_c, 500)
colors = ['#0079c4','#f09205','#21c400']

p_values = get_absolute_isotherms(a, b, v_values, T_values)
p_values = bar_to_atm(p_values)

########################################
###############FIGURES#################
########################################


fig_114_001 = bq.Figure(
    title='p vs v (Fixed T)',
    marks=[],
    axes=[],
    animation_duration=0,
    legend_location='top-right',
    background_style= {'fill': 'white',  'stroke': 'black'},
    fig_margin=dict(top=70, bottom=60, left=80, right=30),
    toolbar = True,
    layout = widgets.Layout(width='100%', height='500px')
)

fig_114_002 = bq.Figure(
    title='',
    marks=[],
```

(continues on next page)

(continued from previous page)

```
    axes=[],
    animation_duration=0,
    legend_location='top-right',
    background_style= {'fill': 'white',  'stroke': 'black'},
    fig_margin=dict(top=30, bottom=60, left=25, right=10),
    toolbar = True,
    layout = widgets.Layout(width='90%', height='40%')
)

fig_114_003 = bq.Figure(
    title='',
    marks=[],
    axes=[],
    animation_duration=0,
    legend_location='top-right',
    background_style= {'fill': 'white',  'stroke': 'black'},
    fig_margin=dict(top=10, bottom=60, left=25, right=10),
    toolbar = True,
    layout = widgets.Layout(width='90%', height='40%')
)

fig_114_004 = bq.Figure(
    title='',
    marks=[],
    axes=[],
    animation_duration=0,
    legend_location='top-right',
    background_style= {'fill': 'white',  'stroke': 'black'},
    fig_margin=dict(top=10, bottom=60, left=25, right=10),
    toolbar = True,
    layout = widgets.Layout(width='90%', height='40%')
)

fig_114_005 = bq.Figure(
    title='p vs v (Fixed T)',
    marks=[],
    axes=[],
    animation_duration=0,
    legend_location='top-right',
    background_style= {'fill': 'white',  'stroke': 'black'},
    fig_margin=dict(top=70, bottom=60, left=80, right=30),
    toolbar = True,
    layout = widgets.Layout(width='100%', height='500px')
)

scale_x = bqs.LinearScale(min = 0.0, max = max(v_values))
scale_y = bqs.LinearScale(min = 0, max = 2.0*p_c)

axis_x = bqa.Axis(
    scale=scale_x,
    tick_format='.2f',
    tick_style={'font-size': '15px'},
    tick_values = np.linspace(0, max(v_values), 5),
    grid_lines = 'none',
    grid_color = '#8e8e8e',
    label='v (L/mol)',
    label_location='middle',
```

(continues on next page)

(continued from previous page)

```
    label_style={'stroke': 'black', 'default-size': 35},
    label_offset='50px'
)

axis_y = bqa.Axis(
    scale=scale_y,
    tick_format='.1f',
    tick_style={'font-size': '15px'},
    tick_values = np.linspace(0, 2.0*p_c, 4),
    grid_lines = 'none',
    grid_color = '#8e8e8e',
    orientation='vertical',
    label='p (atm)',
    label_location='middle',
    label_style={'stroke': 'red', 'default_size': 35},
    label_offset='50px'
)

axis_x_no_ticks = bqa.Axis(
    scale=scale_x,
    tick_format='.2f',
    tick_style={'font-size': '15px'},
    num_ticks=0,
    grid_lines = 'none',
    grid_color = '#8e8e8e',
    label='v (L/mol)',
    label_location='middle',
    label_style={'stroke': 'black', 'default-size': 35},
    label_offset='15px'
)

axis_y_no_ticks = bqa.Axis(
    scale=scale_y,
    tick_format='.0f',
    tick_style={'font-size': '15px'},
    num_ticks=0,
    grid_lines = 'none',
    grid_color = '#8e8e8e',
    orientation='vertical',
    label='p (atm)',
    label_location='middle',
    label_style={'stroke': 'red', 'default_size': 35},
    label_offset='15px'
)

fig_114_001.axes = [axis_x, axis_y]
fig_114_002.axes = [axis_x_no_ticks, axis_y_no_ticks]
fig_114_003.axes = [axis_x_no_ticks, axis_y_no_ticks]
fig_114_004.axes = [axis_x_no_ticks, axis_y_no_ticks]
fig_114_005.axes = [axis_x, axis_y]

#####################################
###############MARKS#################
#####################################

x_values = [ v_values for i in range(len(p_values))]
y_values = []
```

(continues on next page)

(continued from previous page)

```
color_values = []
label_values = []

for i in range(len(p_values)):

    y_values.append(p_values[i])
    color_values.append(colors[i])
    label_values.append(str(T_values[i]))

new_state = bqm.Lines(
    x = x_values,
    y = y_values,
    scales = {'x': scale_x, 'y': scale_y},
    opacities = [1.0 for elem in p_values],
    visible = True,
    colors = color_values,
    labels = label_values,
)

old_state = bqm.Lines(
    x = x_values,
    y = y_values,
    scales = {'x': scale_x, 'y': scale_y},
    opacities = [1.0 for elem in p_values],
    visible = True,
    colors = color_values,
    labels = label_values,
)

current_state = bqm.Lines(
    x = x_values[0],
    y = y_values[0],
    scales = {'x': scale_x, 'y': scale_y},
    opacities = [1.0 for elem in p_values],
    visible = True,
    colors = color_values,
    labels = label_values,
)

a_line = bqm.Lines(
    x = x_values[0],
    y = y_values[0],
    scales = {'x': scale_x, 'y': scale_y},
    opacities = [1.0 for elem in p_values],
    visible = True,
    colors = color_values,
    labels = label_values,
)

b_line = bqm.Lines(
    x = x_values[0],
    y = y_values[0],
    scales = {'x': scale_x, 'y': scale_y},
    opacities = [1.0 for elem in p_values],
    visible = True,
    colors = color_values,
    labels = label_values,
```

(continues on next page)

(continued from previous page)

```
)

ideal_isotherms = get_absolute_isotherms(0, 0, v_values, T_values)
ideal_isotherms = bar_to_atm(ideal_isotherms)

ideal_line = bqm.Lines(
    x = x_values,
    y = ideal_isotherms,
    scales = {'x': scale_x, 'y': scale_y},
    opacities = [1.0 for elem in p_values],
    visible = True,
    colors = color_values,
    labels = label_values,
)

unique_isotherm = bqm.Lines(
    x = x_values[0],
    y = y_values[0],
    scales = {'x': scale_x, 'y': scale_y},
    opacities = [0.6],
    visible = True,
    colors = ['#c90000'],
    labels = [label_values[0]],
    stroke_width = 5
)

fig_114_001.marks = [old_state]
fig_114_002.marks = [current_state]
fig_114_003.marks = [a_line]
fig_114_004.marks = [b_line]
fig_114_005.marks = [ideal_line, unique_isotherm]

############################
##########WIDGETS###########
############################

a_slider_114_003 = widgets.FloatSlider(
    min=0.0,
    max=2.0*a,
    step=0.1,
    value=a,
    description='a',
    disabled=False,
    continuous_update=True,
    orientation='horizontal',
    readout=True,
    layout=widgets.Layout(width='90%')
)

a_slider_114_003.observe(update_isotherms, 'value')

b_slider_114_004 = widgets.FloatSlider(
    min=0.0,
    max=4.0*b,
    step=0.001,
    value=b,
    description='b',
```

(continues on next page)

(continued from previous page)

```
    disabled=False,
    continuous_update=True,
    orientation='horizontal',
    readout=True,
    layout=widgets.Layout(width='90%')
)

b_slider_114_004.observe(update_isotherms, 'value')

reset_button = widgets.Button(
    description='Reset',
    disabled=False,
    button_style='',
    tooltip='Return to the original state',
)

reset_button.on_click(restart)

change_view_button = widgets.ToggleButton(
    value=False,
    description='Presentation mode (OFF)',
    disabled=False,
    button_style='',
    tooltip='',
    icon='desktop',
    layout=widgets.Layout(
        width='initial',
        align_self='center'
    )
)

change_view_button.observe(change_view, 'value')

prepare_export_fig_114_001_button = widgets.Button(
    description='Export',
    disabled=False,
    button_style='',
    tooltip='',
)

prepare_export_fig_114_001_button.on_click(prepare_export)

prepare_export_fig_114_005_button = widgets.Button(
    description='Export',
    disabled=False,
    button_style='',
    tooltip='',
)

prepare_export_fig_114_005_button.on_click(prepare_export)

############################
#########BLOCKS#############
############################

top_block_114_000 = widgets.HBox(
    [],
```

(continues on next page)

(continued from previous page)

```
    layout=widgets.Layout(
        width='100%',
        align_self='center'
    )
)

top_block_114_000.children = [
    widgets.VBox([
        fig_114_001,
        prepare_export_fig_114_001_button
    ],
        layout=widgets.Layout(
            width='33%',
            align_items='center'
        )
    ),
    widgets.VBox([
        fig_114_002,
        fig_114_003,
        a_slider_114_003
    ],
        layout=widgets.Layout(
            width='16%',
            height='500px',
            align_items='center',
            margin='40px 0 0 0'
        )
    ),
    widgets.VBox([
        fig_114_002,
        fig_114_004,
        b_slider_114_004
    ],
        layout=widgets.Layout(
            width='16%',
            height='500px',
            align_items='center',
            margin='40px 0 0 0'
        )
    ),
    widgets.VBox([
        fig_114_005,
        prepare_export_fig_114_005_button
    ],
        layout=widgets.Layout(
            width='33%',
            align_items='center'
        )
    ),
]

bottom_block_114_000 = widgets.HBox(
    [],
    layout=widgets.Layout(
        width='100%',
        height='60px',
        align_self='center'
```

(continues on next page)

(continued from previous page)

```
    )
)

bottom_block_114_000.children = [
    widgets.VBox([
        widgets.HTMLMath(
            value=r"\( (p + \frac{a}{v^2})(v - b) = k_B T \)"
        )
    ],
        layout=widgets.Layout(
            width='33%',
            align_items='center'
        )
    ),
    widgets.VBox(
        [reset_button],
        layout=widgets.Layout(
            width='33%',
            align_items='center'
        )
    ),
    widgets.VBox([
        widgets.HTMLMath(
            value=r"\( p v = k_B T \)"
        )
    ],
        layout=widgets.Layout(
            width='33%',
            align_items='center'
        )
    )
                        ]

main_block_114_000 = widgets.VBox(
    [],
    layout=widgets.Layout(
        width='100%',
        align_items='center'
    )
)

main_block_114_000.children = [
    change_view_button,
    top_block_114_000,
    bottom_block_114_000
]

figures = [
    fig_114_001,
    fig_114_002,
    fig_114_003,
    fig_114_004,
    fig_114_005,
]

main_block_114_000
```

## 1.4 Effect of a and b in van der Waals isotherms (reduced variables)

**Code:** #11C-000

**File:** `apps/van_der_waals/effect_of_a_and_b_reduces.ipynb`

**Run it online:**

---

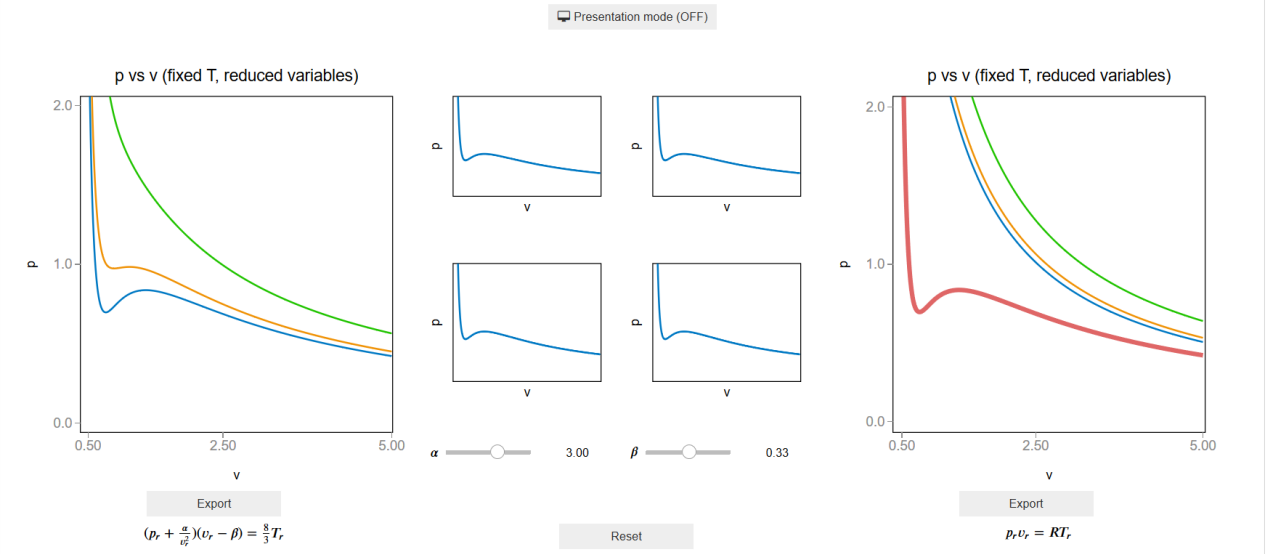
The aim of this notebook is to visualize the effect of a and b parameters on van der Waals' isotherms (reduced variables).

### 1.4.1 Interface

The main interface (`main_block_11C_000`) is divided in two HBox: `top_block_11C_000` and `bottom_block_11C_000`. `top_block_11C_000` contains of 5 bqplot Figures: `fig_11C_001`, `fig_11C_002`, `fig_11C_003`, `fig_11C_004` and `fig_11C_005`.

[1]:
```
from IPython.display import Image
Image(filename='../../static/images/apps/11C-000_1.png')
```

[1]:




### 1.4.2 CSS

A custom `css` file is used to improve the interface of this application. It can be found here.

[2]:
```
from IPython.display import HTML
display(HTML("<head><link rel='stylesheet' type='text/css' href='./../../static/
↪custom.css'></head>"))
display(HTML("<style>.container { width:100% !important; }</style>"))
display(HTML("<style>.widget-label { display: contents !important; }</style>"))
display(HTML("<style>.slider-container { margin: 12px !important; }</style>"))
```

```
<IPython.core.display.HTML object>
```

```
<IPython.core.display.HTML object>
```

```
<IPython.core.display.HTML object>
```

```
<IPython.core.display.HTML object>
```

### 1.4.3 Packages

[3]:
```
from bqplot import *
import bqplot as bq
import bqplot.marks as bqm
import bqplot.scales as bqs
import bqplot.axes as bqa

import ipywidgets as widgets

import urllib.parse
import webbrowser

import sys
```

### 1.4.4 Physical functions

This are the functions that have a physical meaning:

- `get_relative_isotherms_params`

[4]:
```
def get_relative_isotherms_params(alpha, beta, v_range, T_range):
    """This function calculates the theoretical p(v, T) plane
        (in reduced coordinates) according to van der Waals
        equation of state from a given range of volumes
        and tenperatures and taking into account the values
        of alpha and beta.

    Args:
        alpha: The value of the a parameter.\n
        alpha: The value of the b parameter.\n
        v_range: An array containing the values of v
        (in reduced coordinates)for which the isotherms must be
        calculated.\n
        T_range: An array containing the values of T
        (in reduced coordinates)for which the isotherms must be
        calculated.\n


    Returns:
        isotherms: A list consisted of numpy arrays containing the
        pressures of each isotherm.
    """

    isotherms = []

    for T in T_range:
        p_R = []
        for v in v_range:
```

(continues on next page)

(continued from previous page)

```
            val = (8.0/3.0*T/(v - beta) - alpha/v**2)
            p_R = np.append(p_R, val)

        isotherms.append(p_R)

    return isotherms
```

### 1.4.5 Functions related to interaction

[5]:
```
def update_isotherms(change):
    """This function update the lines 'alpha_line', 'beta_line' and
    'unique_isotherm' when 'alpha_slider_11C_003' or 'beta_slider_11C_004' are
    updated.
    """

    obj = change.owner
    T_values = [0.95]

    if obj is alpha_slider_11C_003:

        v_values = np.linspace(0.4, 5.0, 500)
        isotherms = get_relative_isotherms_params(
            alpha_slider_11C_003.value,
            beta_initial,
            v_values,
            T_values
        )

        alpha_line.y = isotherms[0]

    elif obj is beta_slider_11C_004:

        v_values = np.linspace(0.4, 5.0, 500)

        if beta_slider_11C_004.value == 0.0:

            v_values = np.linspace(0.4, 5.0, 500)

        isotherms = get_relative_isotherms_params(
            alpha_initial,
            beta_slider_11C_004.value,
            v_values,
            T_values
        )

        beta_line.x = v_values
        beta_line.y = isotherms[0]

    if beta_slider_11C_004.value == 0.0:
        v_values = np.linspace(0.4, 5.0, 500)

    isotherms = get_relative_isotherms_params(
        alpha_slider_11C_003.value,
        beta_slider_11C_004.value,
        v_values,
```

(continues on next page)

(continued from previous page)

```
        T_values
    )

    unique_isotherm.x = v_values
    unique_isotherm.y = isotherms[0]
```

[6]:
```
def restart(a):
    """This function sets the values of 'alpha_slider_11C_003'
    and 'beta_slider_11C_004' to their initial ones.
    """

    alpha_slider_11C_003.value, beta_slider_11C_004.value = alpha_initial, beta_
↪initial
```

[7]:
```
def change_view(change):
    """This function changes the visualization of all the
    components of the application so they are suitable for
    a projection.\n
    """

    obj = change.owner

    if obj.value:

        obj.description = 'Presentation mode (ON)'

        display(HTML(
            "<style>" \
            ".widget-readout { font-size: 30px ; }" \
            ".widget-label-basic {font-size: 30px;}" \
            "option {font-size: 25px;}" \
            ".p-Widget.jupyter-widgets.widget-slider.widget-vslider.widget-inline-
↪vbox {width: auto}" \
            ".p-Widget .jupyter-widgets .widgets-label {width: auto; height: auto;␣
↪font-size: 30px;}" \
            ".widget-label {font-size: 30px ; height: auto !important;}" \
            ".p-Widget .bqplot .figure .jupyter-widgets {height: auto !important;}" \
            ".widget-text input[type='number'] {font-size: 30px;height: auto;}" \
            ".option { font-size: 30px ;}" \
            ".p-Widget .jupyter-widgets .jupyter-button.widget-button {font-size:␣
↪30px ; width: auto; height: auto;}" \
            ".p-Widget.jupyter-widgets.jupyter-button.widget-toggle-button{font-size:␣
↪30px ; width: auto; height: auto;}" \
            ".p-Widget.p-Panel.jupyter-widgets.widget-container.widget-box.widget-
↪vbox {padding-bottom: 30px}" \
            ".bqplot > svg .axis text.axislabel, .bqplot > svg .axis tspan.axislabel
↪{font-size: 30px;}" \
            ".q-grid .slick-cell {font-size: 30px;}" \
            ".slick-column-name {font-size: 30px;}" \
            ".widget-html-content {font-size: 30px;}"
            "</style>"
            )
        )

        for figure in figures:
```

(continues on next page)

(continued from previous page)

```
            figure.legend_text = {'font-size': '30px'}
            figure.title_style = {'font-size': '30px'}

            for axis in figure.axes:
                axis.tick_style = {'font-size': '30px'}
                axis.label_style = {'font-size': '30px'}

    else:

        obj.description = 'Presentation mode (OFF)'

        display(HTML(
            "<style>" \
            ".widget-readout { font-size: 14px ;}" \
            ".widget-label-basic {font-size: 14px;}" \
            "option {font-size: 12px;}" \
            ".p-Widget .jupyter-widgets .widgets-label {font-size: 14px;}" \
            ".widget-label {font-size: 14px ;}" \
            ".widget-text input[type='number'] {font-size: 14px;}" \
            ".option { font-size: 14px ;}" \
            ".p-Widget .jupyter-widgets .jupyter-button.widget-button {font-size:
↪14px;}" \
            ".p-Widget.jupyter-widgets.jupyter-button.widget-toggle-button {font-size:
↪ 14px;}" \
            ".bqplot > svg .axis text.axislabel, .bqplot > svg .axis tspan.axislabel
↪{font-size: 14px;}" \
            ".q-grid .slick-cell {font-size: 14px;}" \
            ".slick-column-name {font-size: 14px;}" \
            ".widget-html-content {font-size: 14px;}"
            "</style>"
            )
        )

        for figure in figures:

            figure.legend_text = {'font-size': '14px'}
            figure.title_style = {'font-size': '20px'}

            for axis in figure.axes:
                axis.tick_style = {'font-size': '14px'}
                axis.label_style = {'font-size': '14px'}
```

[8]:
```
def prepare_export(button):
    """This function sends the selected plot to the 'export_plot'
    function.
    """

    if button is prepare_export_fig_11C_001_button:

        export_plot(fig_11C_001)

    elif button is prepare_export_fig_11C_005_button:

        export_plot(fig_11C_005)
```

[9]:
```
def export_plot(plot):
    """This function sends the selected plot to the export module.
    """

    global data

    text_lines = []

    np.set_printoptions(threshold=sys.maxsize)

    tooltips = []

    for mark in plot.marks:
        tooltips.append(mark.tooltip)
        mark.tooltip = None

    data =  repr((plot, text_lines))

    %store data

    rel_url = "../../../apps/modules/export_module.ipynb"
    abs_url = urllib.parse.urljoin(notebook_url, rel_url)

    if not webbrowser.open(abs_url):
        go_to_export_button.value = "<form action=" + abs_url + " target='_blank'>
↪<button type=''submit''>Open in export module</button></form>"

    for i in range(len(plot.marks)):
        mark = plot.marks[i]
        mark.tooltip = tooltips[i]
```

[ ]:
```
%%javascript

//Get the URL of the current notebook

var kernel = Jupyter.notebook.kernel;
var command = ["notebook_url = ",
               "'", window.location.href, "'" ].join('')

kernel.execute(command)
```

### 1.4.6 Main interface

[ ]:
```
alpha_initial = 3.0 #0.0 < alpha < 3.0
beta_initial = 0.33 #0.0 < beta < 0.33

a, b = 5.536, 0.03049 #L^2 bar/mol^2, L/mol

T_values = [0.95, 1.0, 1.2]
v_values = np.linspace(0.4, 5.0, 500)
colors = ['#0079c4','#f09205','#21c400']

p_values = get_relative_isotherms_params(
    alpha_initial,
    beta_initial,
```

(continues on next page)

(continued from previous page)

```
    v_values,
    T_values
)

#######################################
#######CREATE THE FIGURES##############
#######################################


fig_11C_001 = bq.Figure(
    title='p vs v (fixed T, reduced variables)',
    marks=[],
    axes=[],
    animation_duration=0,
    legend_location='top-right',
    background_style= {'fill': 'white',  'stroke': 'black'},
    fig_margin=dict(top=70, bottom=60, left=80, right=30),
    toolbar = True,
    layout = widgets.Layout(
        width='100%',
        height='500px'
    )
)

fig_11C_002 = bq.Figure(
    title='',
    marks=[],
    axes=[],
    animation_duration=0,
    legend_location='top-right',
    background_style= {'fill': 'white',  'stroke': 'black'},
    fig_margin=dict(top=30, bottom=60, left=25, right=10),
    toolbar = True,
    layout = widgets.Layout(
        width='90%',
        height='40%'
    )
)

fig_11C_003 = bq.Figure(
    title='',
    marks=[],
    axes=[],
    animation_duration=0,
    legend_location='top-right',
    background_style= {'fill': 'white',  'stroke': 'black'},
    fig_margin=dict(top=10, bottom=60, left=25, right=10),
    toolbar = True,
    layout = widgets.Layout(
        width='90%',
        height='40%'
    )
)

fig_11C_004 = bq.Figure(
    title='',
    marks=[],
```

(continues on next page)

(continued from previous page)

```
    axes=[],
    animation_duration=0,
    legend_location='top-right',
    background_style= {'fill': 'white',  'stroke': 'black'},
    fig_margin=dict(top=10, bottom=60, left=25, right=10),
    toolbar = True,
    layout = widgets.Layout(
        width='90%',
        height='40%'
    )
)

fig_11C_005 = bq.Figure(
    title='p vs v (fixed T, reduced variables)',
    marks=[],
    axes=[],
    animation_duration=0,
    legend_location='top-right',
    background_style= {'fill': 'white',  'stroke': 'black'},
    fig_margin=dict(top=70, bottom=60, left=80, right=30),
    toolbar = True,
    layout = widgets.Layout(
        width='100%',
        height='500px'
    )
)

scale_x = bqs.LinearScale(min = 0.4, max = 5.0)
scale_y = bqs.LinearScale(min = 0, max = 2.0)

axis_x = bqa.Axis(
    scale=scale_x,
    tick_format='.2f',
    tick_style={'font-size': '15px'},
    tick_values = [0.5, 2.5, 5.0],
    grid_lines = 'none',
    grid_color = '#8e8e8e',
    label='v',
    label_location='middle',
    label_style={'stroke': 'black', 'default-size': 35},
    label_offset='50px'
)

axis_y = bqa.Axis(
    scale=scale_y,
    tick_format='.1f',
    tick_style={'font-size': '15px'},
    tick_values = [0, 1, 2],
    grid_lines = 'none',
    grid_color = '#8e8e8e',
    orientation='vertical',
    label='p',
    label_location='middle',
    label_style={'stroke': 'red', 'default_size': 35},
    label_offset='50px'
)
```

(continues on next page)

(continued from previous page)

```
axis_x_no_ticks = bqa.Axis(
    scale=scale_x,
    tick_format='.2f',
    tick_style={'font-size': '15px'},
    num_ticks=0,
    grid_lines = 'none',
    grid_color = '#8e8e8e',
    label='v',
    label_location='middle',
    label_style={'stroke': 'black', 'default-size': 35},
    label_offset='15px'
)

axis_y_no_ticks = bqa.Axis(
    scale=scale_y,
    tick_format='.0f',
    tick_style={'font-size': '15px'},
    num_ticks=0,
    grid_lines = 'none',
    grid_color = '#8e8e8e',
    orientation='vertical',
    label='p',
    label_location='middle',
    label_style={'stroke': 'red', 'default_size': 35},
    label_offset='15px'
)

fig_11C_001.axes = [axis_x, axis_y]
fig_11C_002.axes = [axis_x_no_ticks, axis_y_no_ticks]
fig_11C_003.axes = [axis_x_no_ticks, axis_y_no_ticks]
fig_11C_004.axes = [axis_x_no_ticks, axis_y_no_ticks]
fig_11C_005.axes = [axis_x, axis_y]


########################################
##############MARKS#####################
########################################

x_values = [v_values for i in range(len(p_values))]
y_values = []
color_values = []
label_values = []

for i in range(len(p_values)):

    y_values.append(p_values[i])
    color_values.append(colors[i])
    label_values.append(str(T_values[i]))

new_state = bqm.Lines(
    x = x_values,
    y = y_values,
    scales = {'x': scale_x, 'y': scale_y},
    opacities = [1.0 for elem in p_values],
    visible = True,
    colors = color_values,
    labels = label_values,
```

(continues on next page)

(continued from previous page)

```
)

old_state = bqm.Lines(
    x = x_values,
    y = y_values,
    scales = {'x': scale_x, 'y': scale_y},
    opacities = [1.0 for elem in p_values],
    visible = True,
    colors = color_values,
    labels = label_values,
)

current_state = bqm.Lines(
    x = x_values[0],
    y = y_values[0],
    scales = {'x': scale_x, 'y': scale_y},
    opacities = [1.0 for elem in p_values],
    visible = True,
    colors = color_values,
    labels = label_values,
)

alpha_line = bqm.Lines(
    x = x_values[0],
    y = y_values[0],
    scales = {'x': scale_x, 'y': scale_y},
    opacities = [1.0 for elem in p_values],
    visible = True,
    colors = color_values,
    labels = label_values,
)

beta_line = bqm.Lines(
    x = x_values[0],
    y = y_values[0],
    scales = {'x': scale_x, 'y': scale_y},
    opacities = [1.0 for elem in p_values],
    visible = True,
    colors = color_values,
    labels = label_values,
)

ideal_isotherms = get_relative_isotherms_params(
    0,
    0,
    v_values,
    T_values
)

ideal_line = bqm.Lines(
    x = x_values,
    y = ideal_isotherms,
    scales = {'x': scale_x, 'y': scale_y},
    opacities = [1.0 for elem in p_values],
    visible = True,
    colors = color_values,
    labels = label_values,
```

(continues on next page)

(continued from previous page)

```
)

unique_isotherm = bqm.Lines(
    x = x_values[0],
    y = y_values[0],
    scales = {'x': scale_x, 'y': scale_y},
    opacities = [0.6],
    visible = True,
    colors = ['#c90000'],
    labels = [label_values[0]],
    stroke_width = 5
)

fig_11C_001.marks = [old_state]
fig_11C_002.marks = [current_state]
fig_11C_003.marks = [alpha_line]
fig_11C_004.marks = [beta_line]
fig_11C_005.marks = [ideal_line, unique_isotherm]

alpha_slider_11C_003 = widgets.FloatSlider(
    min=0.0,
    max=5.0,
    step=0.01,
    value=alpha_initial,
    description=r"\( \alpha \)",
    disabled=False,
    continuous_update=True,
    orientation='horizontal',
    readout=True,
    layout=widgets.Layout(width='90%')
)

alpha_slider_11C_003.observe(update_isotherms, 'value')

beta_slider_11C_004 = widgets.FloatSlider(
    min=0.0,
    max=0.66,
    step=0.001,
    value=beta_initial,
    description=r"\( \beta \)",
    disabled=False,
    continuous_update=True,
    orientation='horizontal',
    readout=True,
    layout=widgets.Layout(width='90%')
)

beta_slider_11C_004.observe(update_isotherms, 'value')

return_button = widgets.Button(
    description='Reset',
    disabled=False,
    button_style='',
    tooltip='Return to the original state',
)

return_button.on_click(restart)
```

(continues on next page)

(continued from previous page)

```
change_view_button = widgets.ToggleButton(
    value=False,
    description='Presentation mode (OFF)',
    disabled=False,
    button_style='',
    tooltip='',
    icon='desktop',
    layout=widgets.Layout(
        width='initial',
        align_self='center'
    )
)

change_view_button.observe(change_view, 'value')

prepare_export_fig_11C_001_button = widgets.Button(
    description='Export',
    disabled=False,
    button_style='',
    tooltip='',
)

prepare_export_fig_11C_001_button.on_click(prepare_export)

prepare_export_fig_11C_005_button = widgets.Button(
    description='Export',
    disabled=False,
    button_style='',
    tooltip='',
)

prepare_export_fig_11C_005_button.on_click(prepare_export)

top_block_11C_000 = widgets.HBox(
    [],
    layout=widgets.Layout(
        width='100%',
        align_self='center'
    )
)

top_block_11C_000.children = [
    widgets.VBox([
        fig_11C_001,
        prepare_export_fig_11C_001_button
    ],
        layout=widgets.Layout(
            width='33%',
            align_items='center'
        )
    ),
    widgets.VBox([
        fig_11C_002,
        fig_11C_003,
        alpha_slider_11C_003
    ],
```

(continues on next page)

(continued from previous page)

```
        layout=widgets.Layout(
            width='16%',
            height='500px',
            align_items='center',
            margin='40px 0 0 0'
        )
    ),
    widgets.VBox([
        fig_11C_002,
        fig_11C_004,
        beta_slider_11C_004
    ],
        layout=widgets.Layout(
            width='16%',
            height='500px',
            align_items='center',
            margin='40px 0 0 0'
        )
    ),
    widgets.VBox([
        fig_11C_005,
        prepare_export_fig_11C_005_button
    ],
        layout=widgets.Layout(
            width='33%',
            align_items='center'
        )
    ),
]

bottom_block_11C_000 = widgets.HBox(
    [],
    layout=widgets.Layout(
        width='100%',
        height='60px',
        align_self='center'
    )
)

bottom_block_11C_000.children = [
    widgets.VBox([
        widgets.HTMLMath(
            value=r"\( (p_r + \frac{\alpha}{v_r^2})(v_r - \beta) = \frac{8}{3} T_r \)"
        )],
            layout=widgets.Layout(
                width='33%',
                align_items='center'
            )
    ),
    widgets.VBox(
        [return_button],
        layout=widgets.Layout(
            width='33%',
            align_items='center'
        )
    ),
    widgets.VBox([
```

(continues on next page)

(continued from previous page)

```
        widgets.HTMLMath(
            value=r"\( p_r v_r = R T_r \)"
        )],
            layout=widgets.Layout(
                width='33%',
                align_items='center'
            )
    )
]

main_block_11C_000 = widgets.VBox(
    [],
    layout=widgets.Layout(
        width='100%',
        align_items='center'
    )
)

main_block_11C_000.children = [
    change_view_button,
    top_block_11C_000,
    bottom_block_11C_000
]

figures = [
    fig_11C_001,
    fig_11C_002,
    fig_11C_003,
    fig_11C_004,
    fig_11C_005,
]

main_block_11C_000
```

## 1.5 Critical points for various fluids

**Code:** #113-000

**File:** `apps/van_der_waals/critical_points.ipynb`

**Run it online:**

---

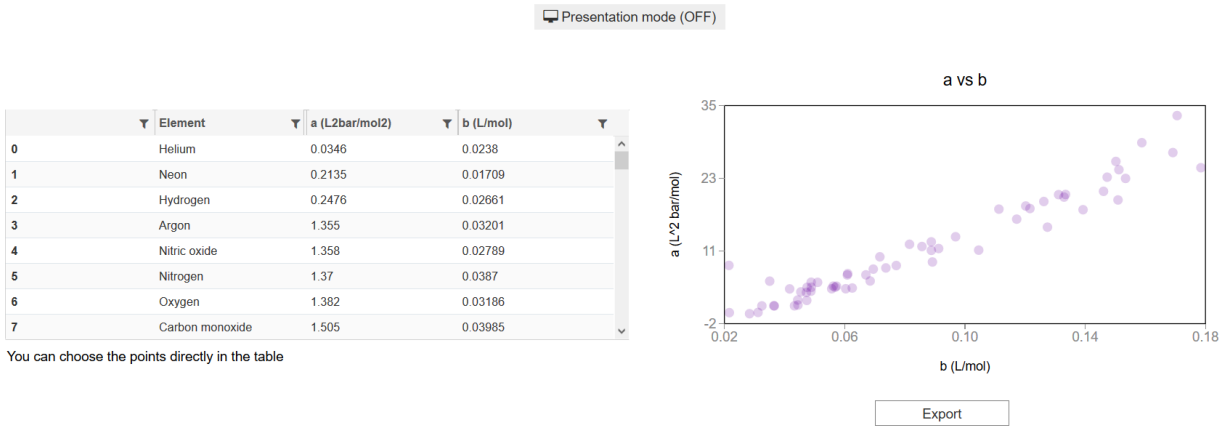
The aim of this notebook is to visualize the critical points of various fluids.

### 1.5.1 Interface

The main interface (`main_block_113_000`) is divided in three VBox: `top_block_113_000`, `middle_block_113_000` and `bottom_block_113_000`. `top_block_113_000` contains a bqplot Figure (`fig_113_001`) and a qgrid chart (`qgrid_table`). `middle_block_113_000` contains of 3 bqplot Figures: `fig_113_002`, `fig_113_003` and `fig_113_005`.

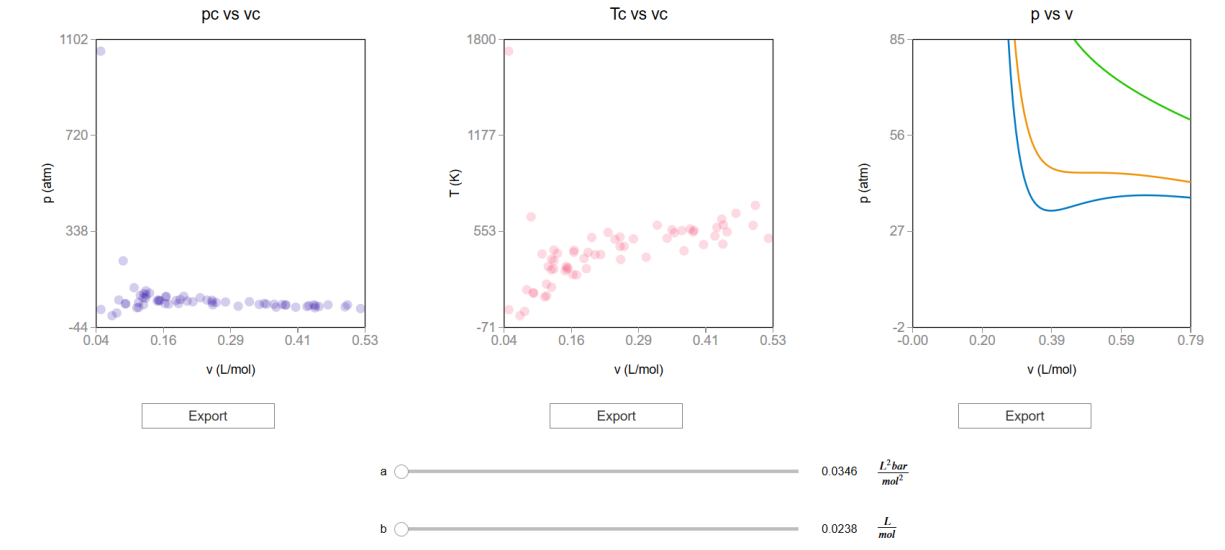
[1]:
```
from IPython.display import Image
Image(filename='../../static/images/apps/113-000_1.png')
```

[1]:




[2]:
```
Image(filename='../../static/images/apps/113-000_2.png')
```

[2]:




## 1.5.2 CSS

A custom `css` file is used to improve the interface of this application. It can be found here.

[1]:
```
from IPython.display import HTML
display(HTML("<head><link rel='stylesheet' type='text/css' href='./../../static/
↪custom.css'></head>"))
display(HTML("<style>.container { width:100% !important; }</style>"))
```

```
<IPython.core.display.HTML object>
```

```
<IPython.core.display.HTML object>
```

### 1.5.3 Packages

[2]:
```
from bqplot import *
import bqplot as bq
import bqplot.marks as bqm
import bqplot.scales as bqs
import bqplot.axes as bqa

import ipywidgets as widgets

import scipy

import qgrid
import pandas as pd

import urllib.parse
import webbrowser

import sys
```

### 1.5.4 Physical functions

This are the functions that have a physical meaning:

- `calculate_critic`
- `get_absolute_isotherms`
- `bar_to_atm`

[3]:
```
def calculate_critic(a, b):

    """
        This function calculates the critic point
        (p_c, v_c, T_c) from given a and b parameters of
        the Van der Waals equation of state for real gases.

        :math:`(P + a \\frac{n^2}{V^2})(V - nb) = nRT`

        :math:`p_c = \\frac{a}{27 b^2}`
        :math:`v_c = 3b`
        :math:`T_c = \\frac{8a}{27 b R}`

    Args:
        a: Term related with the attraction between particles in
        L^2 bar/mol^2.\n
        b: Term related with the volume that is occupied by one
        mole of the molecules in L/mol.\n

    Returns:
        p_c: Critical pressure in bar.\n
        v_c: Critical volume in L/mol.\n
        T_c: Critical tenperature in K.\n

    """

    if b == 0.0:
```

(continues on next page)

(continued from previous page)

```
        return None

    k_B = 1.3806488e-23 #m^2 kg s^-2 K^-1
    N_A = 6.02214129e23
    R = 0.082 * 1.01325 #bar L mol^-1 K^-1

    p_c = a/27.0/(b**2)
    v_c = 3.0*b
    T_c = 8.0*a/27.0/b/R

    return p_c, v_c, T_c
```

[4]:
```
def get_absolute_isotherms(a, b, v_values, T_values):
    """This function calculates the theoretical p(v, T) plane
        (in absolute coordinates) according to van der Waals
        equation of state from a given range of volumes
        and tenperatures.

    Args:
        a: Term related with the attraction between particles in
           L^2 bar/mol^2.\n
        b: Term related with the volume that is occupied by one
        mole of the molecules in L/mol.\n
        v_values: An array containing the values of v
        for which the isotherms must be calculated.\n
        T_values: An array containing the values of T for which
        the isotherms must be calculated.\n


    Returns:
        isotherms: A list consisted of numpy arrays containing the
        pressures of each isotherm.
    """
    isotherms = []

    R = 0.082 * 1.01325 #bar L mol^-1 K^-1

    for T in T_values:

        isot = []

        for v in v_values:

            p = R*T/(v - b) - (a/v**2)
            isot = np.append(isot, p)

        isotherms.append(isot)

    return isotherms
```

[5]:
```
def bar_to_atm(p_values):
    """This function changes the pressures of an array
    form bars to atm.

    Args:
        p_values: List consisted of pressures in bars.\n
```

(continues on next page)

(continued from previous page)

```
    Returns:
        p_values: List consisted of pressures in atm.\n
    """

    p_values = np.array(p_values) * 0.9869

    return p_values
```

[6]:
```
def generate_critical_points(df):
    """This function takes a Pandas dataframe containing three
    columns (element, a, b) and returns four lists: pc, vc, Tc and names

    Args:
        df: Pandas dataframe consisted of three columns: element, a, b.\n

    Returns:
        pc: A numpy array consisted of the values of the critical pressures.\n
        vc: A numpy array consisted of the values of the critical volumes.\n
        Tc: A numpy array consisted of the values of the critical tenperatures.\n
        names: A list consisted of the names of the elements.\n
    """

    pc = []
    vc = []
    Tc = []

    names = []

    name_values = df.iloc[:,0]
    a_values, b_values, names_sorted = get_a_b_names(df)

    for i in range(len(a_values)):

        names.append(names_sorted[i])

        a = float(a_values[i])
        b = float(b_values[i])
        p, v, T = calculate_critic(a, b)

        pc = np.append(pc, p)
        vc = np.append(vc, v)
        Tc = np.append(Tc, T)

    return pc, vc, Tc, names
```

[7]:
```
def get_a_b_names(df):
    """This function takes a pandas dataframe containing the
    columns 'a (L2bar/mol2)', 'b (L/mol)' and 'Element' and return the
    lists of the colums sorted by the values of 'a (L2bar/mol2)'.

    Args:
        df: Pandas dataframe consisted of three columns: 'a (L2bar/mol2)',
        'b (L/mol)' and 'Element'.\n

    Returns:
```

(continues on next page)

(continued from previous page)

```
        a_values_sorted: A list array consisted of the sorted values of 'a (L2bar/
↪mol2)'.\n
        b_values_sorted: A list array consisted of the sorted values of 'b (L/mol)'.\n
        names_sorted: A list consisted of the names of the sorted values of 'Element'.
↪\n
    """

    a_values = list(df['a (L2bar/mol2)'])
    b_values = list(df['b (L/mol)'])
    names = list(df['Element'])

    a_values_sorted = sorted(a_values)

    #Sort values of b depending on the order of a
    b_values_sorted = [y for _,y in sorted(zip(a_values, b_values))]
    names_sorted = [y for _,y in sorted(zip(a_values, names))]

    return a_values_sorted, b_values_sorted, names_sorted
```

### 1.5.5 Functions related to the interaction

[8]:
```
def change_visible_points(event, QGridWidget):
    """This function changes the visible points in
    fig_113_002, fig_113_003 and fig_113_004 according to
    the values filtered in qgrid_table.
    """

    i = QGridWidget.get_changed_df().index

    new_pc = pc[i]
    new_vc = vc[i]
    new_Tc = Tc[i]

    new_names = np.asarray(names_sorted)[i].tolist()

    new_a_values = np.asarray(a_values)[i].tolist()
    new_b_values = np.asarray(b_values)[i].tolist()

    scale_x_v = bqs.LinearScale(min = min(new_vc), max = max(new_vc))
    scale_y_p = bqs.LinearScale(min = min(new_pc), max = max(new_pc))
    scale_y_T = bqs.LinearScale(min = min(new_Tc), max = max(new_Tc))

    scale_x_004 = bqs.LinearScale(min = min(new_b_values), max = max(new_b_values))
    scale_y_004 = bqs.LinearScale(min = min(new_a_values), max = max(new_a_values))

    axis_x_v.scale = scale_x_v
    axis_y_p.scale = scale_y_p
    axis_y_T.scale = scale_y_T

    axis_x_004.scale = scale_x_004
    axis_y_004.scale = scale_y_004

    fig_113_002.axes = [axis_x_v, axis_y_p]
    fig_113_003.axes = [axis_x_v, axis_y_T]
    fig_113_004.axes = [axis_x_004, axis_y_004]
```

(continues on next page)

(continued from previous page)

```
    for mark in fig_113_002.marks:

        mark.scales = {
            'x': scale_x_v,
            'y': scale_y_p
        }

    for mark in fig_113_003.marks:

        mark.scales = {
            'x': scale_x_v,
            'y': scale_y_T
        }

    fig_113_002.marks[0].x, fig_113_002.marks[0].y = new_vc, new_pc
    fig_113_002.marks[0].names = new_names

    fig_113_003.marks[0].x, fig_113_003.marks[0].y = new_vc, new_Tc
    fig_113_003.marks[0].names = new_names

    for mark in fig_113_004.marks:

        mark.scales = {
            'x': scale_x_004,
            'y': scale_y_004
        }

    update_slider_options(new_a_values, new_b_values)
```

[9]:
```
def change_selected_points(event, QGridWidget):
    """This function changes the selected points in
    fig_113_002 and fig_113_003 according to
    the values selected in qgrid_table.
    """

    i = QGridWidget.get_changed_df().index

    new_pc = pc[i]
    new_vc = vc[i]
    new_Tc = Tc[i]

    new_names = np.asarray(names_sorted)[i].tolist()

    selected_113_002.x, selected_113_002.y = new_vc, new_pc
    selected_113_002.names = new_names

    selected_113_003.x, selected_113_003.y = new_vc, new_Tc
    selected_113_003.names = new_names
```

[10]:
```
def update_slider_options(a_values, b_values):
    """This function changes the options of
    a_slider and b_slider sliders.

    Args:
        a_values: List consisted of a_slider's new options.\n
```

(continues on next page)

(continued from previous page)

```
        b_values: List consisted of b_slider's new options.\n
    """

    a_slider.options = a_values
    b_slider.options = b_values

    a_slider.value = a_values[0]
    b_slider.value = b_values[0]
```

[11]:
```
def update_sliders(change):
    """This function updates the visible mark in
    fig_113_005 and the tracers tracer_113_002 and
    tracer_113_003.\n
    """

    index = change.get('owner').index
    name = change.get('owner').description

    if name == 'a':

        b_slider.value = b_slider.options[index]

    elif name == 'b':

        a_slider.value = a_slider.options[index]

    tracer_113_002.x = np.array([scatter_113_002.x[index]])
    tracer_113_002.y = np.array([scatter_113_002.y[index]])

    tracer_113_003.x = np.array([scatter_113_003.x[index]])
    tracer_113_003.y = np.array([scatter_113_003.y[index]])

    i = a_values.index(a_slider.value)
    element_name = fig_113_005.marks[i].labels[0]

    tracer_113_002.names = [element_name]
    tracer_113_003.names = [element_name]

    for mark in fig_113_005.marks:

        if mark.labels[0] == element_name:

            mark.visible = True

        else:

            mark.visible = False
```

[12]:
```
tt = widgets.Label("")

def hover_handler(self, content):
    tt.value = str(content.get('data').get('name'))
```

[13]:
```
def change_view(change):
    """This function changes the visualization of all the
```

(continues on next page)

(continued from previous page)

```
    components of the application so they are suitable for
    a projection.\n
    """

    obj = change.owner

    if obj.value:

        obj.description = 'Presentation mode (ON)'

        display(HTML(
            "<style>" \
            ".widget-readout { font-size: 30px ; }" \
            ".widget-label-basic {font-size: 30px;}" \
            "option {font-size: 25px;}" \
            ".p-Widget.jupyter-widgets.widget-slider.widget-vslider.widget-inline-
↪vbox {width: auto}" \
            ".p-Widget .jupyter-widgets .widgets-label {width: auto; height: auto;␣
↪font-size: 30px;}" \
            ".widget-label {font-size: 30px ; height: auto !important;}" \
            ".p-Widget .bqplot .figure .jupyter-widgets {height: auto !important;}" \
            ".widget-text input[type='number'] {font-size: 30px;height: auto;}" \
            ".option { font-size: 30px ;}" \
            ".p-Widget .jupyter-widgets .jupyter-button.widget-button {font-size:␣
↪30px ; width: auto; height: auto;}" \
            ".p-Widget.jupyter-widgets.jupyter-button.widget-toggle-button{font-size:␣
↪30px ; width: auto; height: auto;}" \
            ".p-Widget.p-Panel.jupyter-widgets.widget-container.widget-box.widget-
↪vbox {padding-bottom: 30px}" \
            ".bqplot > svg .axis text.axislabel, .bqplot > svg .axis tspan.axislabel
↪{font-size: 30px;}" \
            ".q-grid .slick-cell {font-size: 30px;}" \
            ".slick-column-name {font-size: 30px;}"
            "</style>"
            )
        )

        for figure in figures:

            figure.legend_text = {'font-size': '30px'}
            figure.title_style = {'font-size': '30px'}

            for axis in figure.axes:
                axis.tick_style = {'font-size': '30px'}
                axis.label_style = {'font-size': '30px'}

    else:

        obj.description = 'Presentation mode (OFF)'

        display(HTML(
            "<style>" \
            ".widget-readout { font-size: 14px ;}" \
            ".widget-label-basic {font-size: 14px;}" \
            "option {font-size: 12px;}" \
            ".p-Widget .jupyter-widgets .widgets-label {font-size: 14px;}" \
            ".widget-label {font-size: 14px ;}" \
```

(continues on next page)

(continued from previous page)

```
            ".widget-text input[type='number'] {font-size: 14px;}" \
            ".option { font-size: 14px ;}" \
            ".p-Widget .jupyter-widgets .jupyter-button.widget-button {font-size:
↪14px;}" \
            ".p-Widget.jupyter-widgets.jupyter-button.widget-toggle-button {font-size:
↪ 14px;}" \
            ".bqplot > svg .axis text.axislabel, .bqplot > svg .axis tspan.axislabel
↪{font-size: 14px;}" \
            ".q-grid .slick-cell {font-size: 14px;}" \
            ".slick-column-name {font-size: 14px;}"
            "</style>"
            )
        )

        for figure in figures:

            figure.legend_text = {'font-size': '14px'}
            figure.title_style = {'font-size': '20px'}

            for axis in figure.axes:
                axis.tick_style = {'font-size': '14px'}
                axis.label_style = {'font-size': '14px'}
```

[14]:
```
def prepare_export(button):
    """This function sends the selected plot to the 'export_plot'
    function.
    """

    if button is prepare_export_fig_113_002_button:

        export_plot(fig_113_002)

    elif button is prepare_export_fig_113_003_button:

        export_plot(fig_113_003)

    elif button is prepare_export_fig_113_004_button:

        export_plot(fig_113_004)

    elif button is prepare_export_fig_113_005_button:

        export_plot(fig_113_005)
```

[15]:
```
def export_plot(plot):
    """This function sends the selected plot to the export module.
    """

    global data

    text_lines = []

    np.set_printoptions(threshold=sys.maxsize)

    tooltips = []
```

(continues on next page)

(continued from previous page)

```
    for mark in plot.marks:
        tooltips.append(mark.tooltip)
        mark.tooltip = None

    data =  repr((plot, text_lines))

    %store data

    rel_url = "../../../apps/modules/export_module.ipynb"
    abs_url = urllib.parse.urljoin(notebook_url, rel_url)

    if not webbrowser.open(abs_url):
        go_to_export_button.value = "<form action=" + abs_url + " target='_blank'>
↪<button type=''submit''>Open in export module</button></form>"

    for i in range(len(plot.marks)):
        mark = plot.marks[i]
        mark.tooltip = tooltips[i]
```

[ ]:
```
%%javascript

//Get the URL of the current notebook

var kernel = Jupyter.notebook.kernel;
var command = ["notebook_url = ",
               "'", window.location.href, "'" ].join('')

kernel.execute(command)
```

### 1.5.6 Main interface

[17]:
```
#data taken from https://en.wikipedia.org/wiki/Van_der_Waals_constants_(data_page)␣
↪using https://wikitable2csv.ggor.de/
#format: Element, a (L2bar/mol2), b (L/mol)

raw_data = [
"Acetic acid",17.71,0.1065,
"Acetic anhydride",20.158,0.1263,
"Acetone",16.02,0.1124,
"Acetonitrile",17.81,0.1168,
"Acetylene",4.516,0.0522,
"Ammonia",4.225,0.0371,
"Argon",1.355,0.03201,
"Benzene",18.24,0.1154,
"Bromobenzene",28.94,0.1539,
"Butane",14.66,0.1226,
"Carbon dioxide",3.640,0.04267,
"Carbon disulfide",11.77,0.07685,
"Carbon monoxide",1.505,0.03985,
"Carbon tetrachloride",19.7483,0.1281,
"Chlorine",6.579,0.05622,
"Chlorobenzene",25.77,0.1453,
"Chloroethane",11.05,0.08651,
"Chloromethane",7.570,0.06483,
```

(continues on next page)

(continued from previous page)

```
"Cyanogen",7.769,0.06901,
"Cyclohexane",23.11,0.1424,
"Diethyl ether",17.61,0.1344,
"Diethyl sulfide",19.00,0.1214,
"Dimethyl ether",8.180,0.07246,
"Dimethyl sulfide",13.04,0.09213,
"Ethane",5.562,0.0638,
"Ethanethiol",11.39,0.08098,
"Ethanol",12.18,0.08407,
"Ethyl acetate",20.72,0.1412,
"Ethylamine",10.74,0.08409,
"Fluorobenzene",20.19,0.1286,
"Fluoromethane",4.692,0.05264,
"Freon",10.78,0.0998,
"Germanium tetrachloride",22.90,0.1485,
"Helium",0.0346,0.0238,
"Hexane",24.71,0.1735,
"Hydrogen",0.2476,0.02661,
"Hydrogen bromide",4.510,0.04431,
"Hydrogen chloride",3.716,0.04081,
"Hydrogen selenide",5.338,0.04637,
"Hydrogen sulfide",4.490,0.04287,
"Iodobenzene",33.52,0.1656,
"Krypton",2.349,0.03978,
"Mercury",8.200,0.01696,
"Methane",2.283,0.04278,
"Methanol",9.649,0.06702,
"Neon",0.2135,0.01709,
"Nitric oxide",1.358,0.02789,
"Nitrogen",1.370,0.0387,
"Nitrogen dioxide",5.354,0.04424,
"Nitrous oxide",3.832,0.04415,
"Oxygen",1.382,0.03186,
"Pentane",19.26,0.146,
"Phosphine",4.692,0.05156,
"Propane",8.779,0.08445,
"Radon",6.601,0.06239,
"Silane",4.377,0.05786,
"Silicon tetrafluoride",4.251,0.05571,
"Sulfur dioxide",6.803,0.05636,
"Tin tetrachloride",27.27,0.1642,
"Toluene",24.38,0.1463,
"Water",5.536,0.03049,
"Xenon",4.250,0.05105
]
```

[ ]:
```
"""

.. module:: critical_points.ipynb
    :sypnopsis: This module creates an interface to interact with the
    critical points of different fluids.\n

.. moduleauthor:: Jon Gabirondo López (jgabirondo001@ikasle.ehu.eus)

"""
```

(continues on next page)

(continued from previous page)

```
# Prepare the database

data_array = np.array(raw_data)
data_reshaped = np.reshape(data_array, (-1,3)); #reshape in three columns

database = pd.DataFrame(
    data=data_reshaped,
    columns=["Element", "a (L2bar/mol2)", "b (L/mol)"]
)

# numpy converts all elements to 'object' and
# pandas interprets them as string, but I want a and b values to be float
database["a (L2bar/mol2)"] = np.round(
    pd.to_numeric(database["a (L2bar/mol2)"]),
    4
)

database["b (L/mol)"] = np.round(
    pd.to_numeric(database["b (L/mol)"]),
    5
)

a_values, b_values, names_sorted = get_a_b_names(database)

database["Element"] = names_sorted
database["a (L2bar/mol2)"] = a_values
database["b (L/mol)"] = b_values

# Show the database in QGrid chart.

grid_options = {
    # SlickGrid options
    'fullWidthRows': True,
    'syncColumnCellResize': True,
    'forceFitColumns': True,
    'defaultColumnWidth': 150,
    'rowHeight': 28,
    'enableColumnReorder': False,
    'enableTextSelectionOnCells': True,
    'editable': False, #lehen True
    'autoEdit': False,
    'explicitInitialization': True,

    # Qgrid options
    'maxVisibleRows': 7, #we have changed it to 5 (default = 15)
    'minVisibleRows': 7, #we have changed it to 5 (default = 8)
    'sortable': True,
    'filterable': True,
    'highlightSelectedCell': False,
    'highlightSelectedRow': True
}

qgrid_table = qgrid.show_grid(database, grid_options=grid_options)

qgrid_table.on(['filter_changed'], change_visible_points)
qgrid_table.on(['selection_changed'], change_selected_points)
```

(continues on next page)

(continued from previous page)

```
# QGrid triggering actions
#[
#    'cell_edited',
#    'selection_changed',
#    'viewport_changed',
#    'row_added',
#    'row_removed',
#    'filter_dropdown_shown',
#    'filter_changed',
#    'sort_changed',
#    'text_filter_viewport_changed',
#    'json_updated'
#]

########################################
###########TOP BLOCK###################
########################################

top_block_113_000 = widgets.VBox(
    [],
    layout=widgets.Layout(
        width='100%',
        align_self='center',
    )
)

fig_113_004 = bq.Figure(
    title='a vs b',
    marks=[],
    axes=[],
    animation_duration=0,
    legend_location='top-right',
    background_style= {'fill': 'white',  'stroke': 'black'},
    fig_margin=dict(top=80, bottom=80, left=80, right=30),
    toolbar = True,
    layout = widgets.Layout(height='400px')
)

scale_x_004 = bqs.LinearScale(min = min(b_values), max = max(b_values))
scale_y_004 = bqs.LinearScale(min = min(a_values), max = max(a_values))

axis_x_004 = bqa.Axis(
    scale=scale_x_004,
    tick_format='.2f',
    tick_style={'font-size': '15px'},
    num_ticks=5,
    grid_lines = 'none',
    grid_color = '#8e8e8e',
    label='b (L/mol)',
    label_location='middle',
    label_style={'stroke': 'black', 'default-size': 35},
    label_offset='50px'
)

axis_y_004 = bqa.Axis(
    scale=scale_y_004,
    tick_format='.0f',
```

(continues on next page)

(continued from previous page)

```
    tick_style={'font-size': '15px'},
    num_ticks=4,
    grid_lines = 'none',
    grid_color = '#8e8e8e',
    orientation='vertical',
    label='a (L^2 bar/mol)',
    label_location='middle',
    label_style={'stroke': 'red', 'default_size': 35},
    label_offset='50px'
)

fig_113_004.axes = [axis_x_004, axis_y_004]

scatter_113_004 = bqm.Scatter(
    name = '',
    x = b_values,
    y = a_values,
    scales = {'x': scale_x_004, 'y': scale_y_004},
    default_opacities = [0.2],
    visible = True,
    colors = ['#6a03a1'],
    names = names_sorted,
    display_names = False,
    labels=[],
    tooltip = tt
)

scatter_113_004.on_hover(hover_handler)

fig_113_004.marks = [scatter_113_004]

message1 = widgets.HTML(value='<p>You can choose the points directly in the table</p>
↪')

change_view_button = widgets.ToggleButton(
    value=False,
    description='Presentation mode (OFF)',
    disabled=False,
    button_style='',
    tooltip='',
    icon='desktop',
    layout=widgets.Layout(
        width='initial',
        align_self='center'
    )
)

change_view_button.observe(change_view, 'value')

prepare_export_fig_113_004_button = widgets.Button(
    description='Export',
    disabled=False,
    button_style='',
    tooltip='',
)

prepare_export_fig_113_004_button.on_click(prepare_export)
```

(continues on next page)

(continued from previous page)

```
top_block_113_000.children = [
    change_view_button,
    widgets.HBox([
        widgets.VBox([
            qgrid_table,
            message1
        ],
            layout=widgets.Layout(
                width='50%',
                margin='80px 0 0 0'
            )
        ),
        widgets.VBox([
            fig_113_004,
            prepare_export_fig_113_004_button
        ],
            layout=widgets.Layout(
                width='50%',
                align_items='center',
            )
        )
    ])
]


########################################
###########MIDDLE BLOCK#################
########################################

middle_block_113_000 = widgets.HBox(
    [],
    layout=widgets.Layout(
        width='100%',
        align_self='center',
        align_content='center'
    )
)

fig_113_002 = bq.Figure(
    title='pc vs vc',
    marks=[],
    axes=[],
    animation_duration=0,
    legend_location='top-right',
    background_style= {'fill': 'white',  'stroke': 'black'},
    fig_margin=dict(top=80, bottom=80, left=80, right=30),
    toolbar = True,
    layout = widgets.Layout(width='90%')
)

fig_113_003 = bq.Figure(
    title='Tc vs vc',
    marks=[],
    axes=[],
    animation_duration=0,
    legend_location='top-right',
```

(continues on next page)

(continued from previous page)

```
    background_style= {'fill': 'white',  'stroke': 'black'},
    fig_margin=dict(top=80, bottom=80, left=80, right=30),
    toolbar = True,
    layout = widgets.Layout(width='90%')
)


pc, vc, Tc, names = generate_critical_points(database)

scale_x_v = bqs.LinearScale(min = min(vc), max = max(vc))
scale_y_p = bqs.LinearScale(min = min(pc), max = max(pc))
scale_y_T = bqs.LinearScale(min = min(Tc), max = max(Tc))


axis_x_v = bqa.Axis(
    scale=scale_x_v,
    tick_format='.2f',
    tick_style={'font-size': '15px'},
    num_ticks=5,
    grid_lines = 'none',
    grid_color = '#8e8e8e',
    label='v (L/mol)',
    label_location='middle',
    label_style={'stroke': 'black', 'default-size': 35},
    label_offset='50px'
)

axis_y_p = bqa.Axis(
    scale=scale_y_p,
    tick_format='.0f',#'0.2f',
    tick_style={'font-size': '15px'},
    num_ticks=4,
    grid_lines = 'none',
    grid_color = '#8e8e8e',
    orientation='vertical',
    label='p (atm)',
    label_location='middle',
    label_style={'stroke': 'red', 'default_size': 35},
    label_offset='50px'
)

axis_y_T = bqa.Axis(
    scale=scale_y_T,
    tick_format='.0f',#'0.2f',
    tick_style={'font-size': '15px'},
    num_ticks=4,
    grid_lines = 'none',
    grid_color = '#8e8e8e',
    orientation='vertical',
    label='T (K)',
    label_location='middle',
    label_style={'stroke': 'red', 'default_size': 35},
    label_offset='50px'
)
```

(continues on next page)

(continued from previous page)

```
fig_113_002.axes = [axis_x_v, axis_y_p]
fig_113_003.axes = [axis_x_v, axis_y_T]

scatter_113_002 = bqm.Scatter(
    name = '',
    x = vc,
    y = pc,
    scales = {'x': scale_x_v, 'y': scale_y_p},
    default_opacities = [0.2],
    visible = True,
    colors = ['#2807a3'],
    names = names,
    display_names = False,
    labels=[],
    tooltip = tt
)

scatter_113_002.on_hover(hover_handler)

scatter_113_003 = bqm.Scatter(
    name = '',
    x = vc,
    y = Tc,
    scales = {'x': scale_x_v, 'y': scale_y_T},
    default_opacities = [0.2 for v in vc],
    visible = True,
    colors = ['#f5426c'],
    names = names,
    display_names = False,
    labels=[],
    tooltip = tt
)

scatter_113_003.on_hover(hover_handler)


tracer_113_002 = bqm.Scatter(
    name = 'tracer_113_002',
    x = [1.0],
    y = [1.0],
    scales = {'x': scale_x_v, 'y': scale_y_p},
    default_opacities = [1.0],
    visible = True,
    colors=['black'],
)

tracer_113_003 = bqm.Scatter(
    name = 'tracer_113_003',
    x = [1.0],
    y = [1.0],
    scales = {'x': scale_x_v, 'y': scale_y_T},
    default_opacities = [1.0],
    visible = True,
    colors=['black'],
)

selected_113_002 = bqm.Scatter(
```

(continues on next page)

(continued from previous page)

```
    name = 'selected_113_002',
    x = [],
    y = [],
    scales = {'x': scale_x_v, 'y': scale_y_p},
    default_opacities = [1.0],
    visible = True,
    display_names = False,
    colors = scatter_113_002.colors,
    tooltip = tt
)

selected_113_002.on_hover(hover_handler)

selected_113_003 = bqm.Scatter(
    name = 'selected_113_003',
    x = [],
    y = [],
    scales = {'x': scale_x_v, 'y': scale_y_T},
    default_opacities = [1.0],
    visible = True,
    display_names = False,
    colors = scatter_113_003.colors,
    tooltip = tt
)

selected_113_002.on_hover(hover_handler)

fig_113_002.marks = [
    scatter_113_002,
    selected_113_002,
    tracer_113_002
]

fig_113_003.marks = [
    scatter_113_003,
    selected_113_003,
    tracer_113_003
]

colors = ['#0079c4','#f09205','#21c400']

fig_113_005 = bq.Figure(
    title='p vs v',
    marks=[],
    axes=[],
    animation_duration=500,
    legend_location='top-right',
    background_style= {'fill': 'white',  'stroke': 'black'},
    fig_margin=dict(top=80, bottom=80, left=80, right=20),
    toolbar = True,
    layout = widgets.Layout(width='90%')
)

p_values = []
v_values = []

for i in range(len(a_values)):
```

(continues on next page)

(continued from previous page)

```
    a = a_values[i]
    b = b_values[i]


    p_c, v_c, T_c = calculate_critic(a, b)

    v = np.linspace(0.45*v_c, 5.0*v_c, 300)
    T_values = [0.95*T_c, T_c, 1.2*T_c]

    p = get_absolute_isotherms(a, b, v, T_values)

    p_values.append(bar_to_atm(p))
    v_values.append(v)

v_mean = np.mean(v_values)
v_min = np.min(v_values)

p_mean = np.mean(p_values)
p_min = np.min(p_values)

scale_x_005 = bqs.LinearScale(min = 0.0, max = 1.2*v_mean)
scale_y_005 = bqs.LinearScale(min = 0.0, max = 1.2*p_mean)

axis_x_005 = bqa.Axis(
    scale=scale_x_005,
    tick_format='.2f',
    tick_style={'font-size': '15px'},
    num_ticks=5,
    grid_lines = 'none',
    grid_color = '#8e8e8e',
    label='v (L/mol)',
    label_location='middle',
    label_style={'stroke': 'black', 'default-size': 35},
    label_offset='50px'
)


axis_y_005 = bqa.Axis(
    scale=scale_y_005,
    tick_format='.0f',
    tick_style={'font-size': '15px'},
    num_ticks=4,
    grid_lines = 'none',
    grid_color = '#8e8e8e',
    orientation='vertical',
    label='p (atm)',
    label_location='middle',
    label_style={'stroke': 'red', 'default_size': 35},
    label_offset='50px'
)

fig_113_005.axes = [axis_x_005, axis_y_005]

marks = []

for i in range(len(a_values)):
```

(continues on next page)

(continued from previous page)

```
    marks.append(bqm.Lines(
        x = v_values[i],
        y = p_values[i],
        scales = {'x': scale_x_005, 'y': scale_y_005},
        opacities = [1.0 for elem in p_values],
        visible = a == a_values[i],
        colors = colors,
        labels = [names_sorted[i]]
        )
    )

fig_113_005.marks = marks

prepare_export_fig_113_002_button = widgets.Button(
        description='Export',
        disabled=False,
        button_style='',
        tooltip='',
    )

prepare_export_fig_113_002_button.on_click(prepare_export)

prepare_export_fig_113_003_button = widgets.Button(
        description='Export',
        disabled=False,
        button_style='',
        tooltip='',
    )

prepare_export_fig_113_003_button.on_click(prepare_export)

prepare_export_fig_113_005_button = widgets.Button(
        description='Export',
        disabled=False,
        button_style='',
        tooltip='',
    )

prepare_export_fig_113_005_button.on_click(prepare_export)

middle_block_113_000.children = [
    widgets.VBox([
        fig_113_002,
        prepare_export_fig_113_002_button
    ],
        layout=widgets.Layout(
            width='33%',
            align_items='center',
        )
    ),
    widgets.VBox([
        fig_113_003,
        prepare_export_fig_113_003_button
    ],
        layout=widgets.Layout(
            width='33%',
```

(continues on next page)

(continued from previous page)

```
            align_items='center',
        )
    ),
    widgets.VBox([
        fig_113_005,
        prepare_export_fig_113_005_button
    ],
        layout=widgets.Layout(
            width='33%',
            align_items='center',
        )
    )
]

########################################
##########BOTTOM BLOCK#################
########################################
bottom_block_113_000 = widgets.VBox(
    [],
    layout=widgets.Layout(
        align_items='center',
        width='100%',
        margin='30px 0 0 0'
    )
)

a_slider = widgets.SelectionSlider(
    options=a_values,
    value=a_values[0],
    description='a',
    disabled=False,
    continuous_update=True,
    orientation='horizontal',
    readout=True,
    layout=widgets.Layout(width='90%'),
)

a_slider.observe(update_sliders, 'value')

b_slider = widgets.SelectionSlider(
    options=b_values,
    value=b_values[0],
    description='b',
    disabled=False,
    continuous_update=True,
    orientation='horizontal',
    readout=True,
    layout=widgets.Layout(width='90%'),
)

b_slider.observe(update_sliders, 'value')

bottom_block_113_000.children = [
    widgets.HBox([
        a_slider,
        widgets.HTMLMath(
            value=r"\( \frac{L^2 bar}{mol^2} \)",
```

(continues on next page)

(continued from previous page)

```
            layout=widgets.Layout(height='60px')
        )],
        layout=widgets.Layout(
            width='50%',
            height='100%'
        )
    ),
    widgets.HBox([
        b_slider,
        widgets.HTMLMath(
            value=r"\( \frac{L}{mol} \)",
            layout=widgets.Layout(height='60px')
        )],
        layout=widgets.Layout(width='50%', height='100%')
    )
]

########################################
###########MAIN BLOCK###################
########################################

main_block_113_000 = widgets.VBox(
    [],
    layout=widgets.Layout(align_content='center')
)

main_block_113_000.children = [
    top_block_113_000,
    middle_block_113_000,
    bottom_block_113_000
]

figures = [
    fig_113_002,
    fig_113_003,
    fig_113_004,
    fig_113_005
]

main_block_113_000
```

## 1.6 Compare elements' isotherms

**Code:** #115-000

**File:** `apps/van_der_waals/compare_elements.ipynb`

**Run it online:**

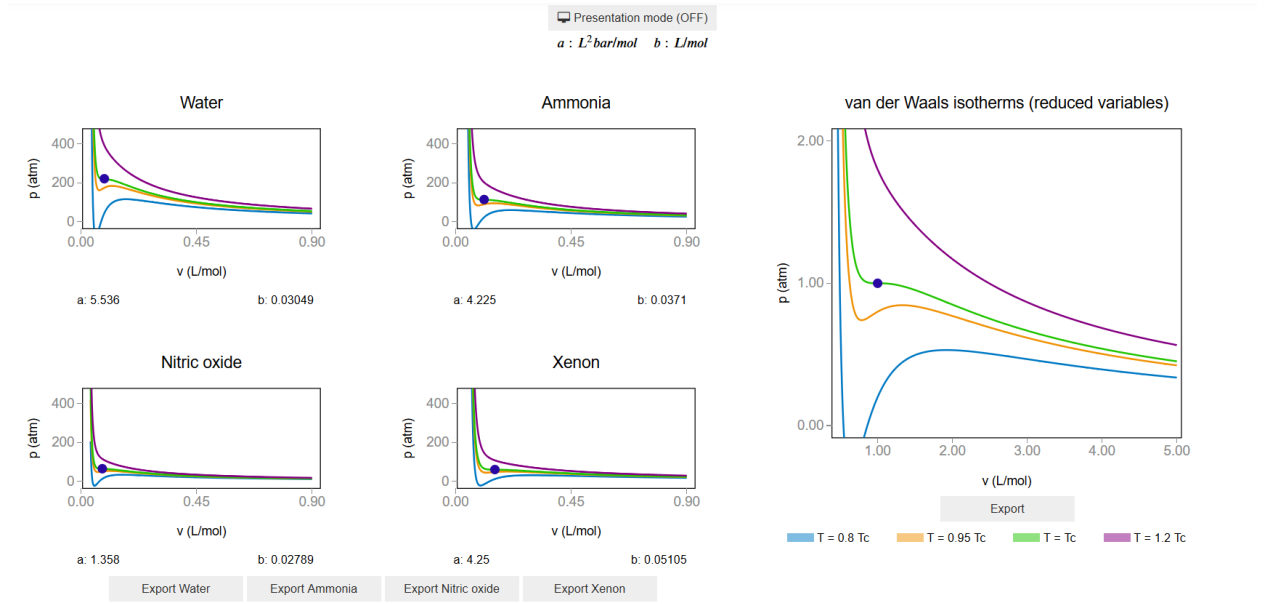
---

The aim of this Notebook is to compare the isotherms of different elements.

### 1.6.1 Interface

The main interface (`main_block_115_000`) is divided in two VBox: `left_block` and `right_block`. `left_block` consists of four bqplot Figures and `right_block` contains `fig_115_001`.

[1]:
```
from IPython.display import Image
Image(filename='../../static/images/apps/115-000_1.png')
```

[1]:



### 1.6.2 CSS

A custom `css` file is used to improve the interface of this application. It can be found here.

[2]:
```
from IPython.display import HTML
display(HTML("<head><link rel='stylesheet' type='text/css' href='./../../static/
↪custom.css'></head>"))
display(HTML("<style>.container { width:100% !important; }</style>"))
```

```
<IPython.core.display.HTML object>
```

```
<IPython.core.display.HTML object>
```

### 1.6.3 Packages

[3]:
```
from bqplot import *
import bqplot as bq
import bqplot.marks as bqm
import bqplot.scales as bqs
import bqplot.axes as bqa

import ipywidgets as widgets

import urllib.parse
import webbrowser
```

(continues on next page)

(continued from previous page)

```
import sys
```

### 1.6.4 Physical functions

This are the functions that have a physical meaning:

- `calculate_critic`
- `get_absolute_isotherms`
- `get_relative_isotherms`
- `bar_to_atm`

[4]:
```
def calculate_critic(a, b):

    """
        This function calculates the critic point
        (p_c, v_c, T_c) from given a and b parameters of
        the Van der Waals equation of state for real gases.

        :math:`(P + a \\frac{n^2}{V^2})(V - nb) = nRT`

        :math:`p_c = \\frac{a}{27 b^2}`
        :math:`v_c = 3b`
        :math:`T_c = \\frac{8a}{27 b R}`

    Args:
        a: Term related with the attraction between particles in
        L^2 bar/mol^2.\n
        b: Term related with the volume that is occupied by one
        mole of the molecules in L/mol.\n

    Returns:
        p_c: Critical pressure in bar.\n
        v_c: Critical volume in L/mol.\n
        T_c: Critical tenperature in K.\n

    """

    if b == 0.0:
        return None

    k_B = 1.3806488e-23 #m^2 kg s^-2 K^-1
    N_A = 6.02214129e23
    R = 0.082 * 1.01325 #bar L mol^-1 K^-1

    p_c = a/27.0/(b**2)
    v_c = 3.0*b
    T_c = 8.0*a/27.0/b/R

    return p_c, v_c, T_c
```

[5]:
```
def get_absolute_isotherms(a, b, v_values, T_values):
    """This function calculates the theoretical p(v, T) plane
```

(continues on next page)

(continued from previous page)

```
        (in absolute coordinates) according to van der Waals
        equation of state from a given range of volumes
        and tenperatures.

    Args:
        a: Term related with the attraction between particles in
           L^2 bar/mol^2.\n
        b: Term related with the volume that is occupied by one
        mole of the molecules in L/mol.\n
        v_values: An array containing the values of v
        for which the isotherms must be calculated.\n
        T_values: An array containing the values of T for which
        the isotherms must be calculated.\n


    Returns:
        isotherms: A list consisted of numpy arrays containing the
        pressures of each isotherm.
    """
    isotherms = []

    R = 0.082 * 1.01325 #bar L mol^-1 K^-1

    for T in T_values:

        isot = []

        for v in v_values:

            p = R*T/(v - b) - (a/v**2)
            isot = np.append(isot, p)

        isotherms.append(isot)

    return isotherms
```

[6]:
```
def get_relative_isotherms(v_range, T_range):
    """This function calculates the theoretical p(v, T) plane
        (in reduced coordinates) according to van der Waals
        equation of state from a given range of volumes
        and tenperatures.

    Args:
        v_range: An array containing the values of v
        (in reduced coordinates)for which the isotherms must be
        calculated.\n
        T_range: An array containing the values of T
        (in reduced coordinates)for which the isotherms must be
        calculated.\n


    Returns:
        isotherms: A list consisted of numpy arrays containing the
        pressures of each isotherm.
    """
```

(continues on next page)

(continued from previous page)

```
    isotherms = []

    for T in T_range:
        p_R = []
        for v in v_range:
            val = (8.0/3.0*T/(v - 1.0/3.0) - 3.0/v**2)
            p_R = np.append(p_R, val)

        isotherms.append(p_R)

    return isotherms
```

[7]:
```
def bar_to_atm(p_values):
    """This function changes the pressures of an array
    form bars to atm.

    Args:
        p_values: List consisted of pressures in bars.\n

    Returns:
        p_values: List consisted of pressures in atm.\n
    """

    p_values = np.array(p_values) * 0.9869

    return p_values
```

### 1.6.5 Functions related to interaction

[8]:
```
def change_view(change):
    """This function changes the visualization of all the
    components of the application so they are suitable for
    a projection.\n
    """

    obj = change.owner

    if obj.value:

        obj.description = 'Presentation mode (ON)'

        display(HTML(
            "<style>" \
            ".widget-readout { font-size: 30px ; }" \
            ".widget-label-basic {font-size: 30px;}" \
            "option {font-size: 25px;}" \
            ".p-Widget.jupyter-widgets.widget-slider.widget-vslider.widget-inline-
↪vbox {width: auto}" \
            ".p-Widget .jupyter-widgets .widgets-label {width: auto; height: auto;␣
↪font-size: 30px;}" \
            ".widget-label {font-size: 30px ; height: auto !important;}" \
            ".p-Widget .bqplot .figure .jupyter-widgets {height: auto !important;}" \
            ".widget-text input[type='number'] {font-size: 30px;height: auto;}" \
            ".option { font-size: 30px ;}" \
```

(continues on next page)

(continued from previous page)

```
            ".p-Widget .jupyter-widgets .jupyter-button.widget-button {font-size:␣
↪30px ; width: auto; height: auto;}" \
            ".p-Widget.jupyter-widgets.jupyter-button.widget-toggle-button{font-size:␣
↪30px ; width: auto; height: auto;}" \
            ".p-Widget.p-Panel.jupyter-widgets.widget-container.widget-box.widget-
↪vbox {padding-bottom: 30px}" \
            ".bqplot > svg .axis text.axislabel, .bqplot > svg .axis tspan.axislabel
↪{font-size: 30px;}" \
            ".q-grid .slick-cell {font-size: 30px;}" \
            ".slick-column-name {font-size: 30px;}" \
            ".widget-html-content {font-size: 30px;}"
            "</style>"
            )
        )

        for figure in figures:

            figure.legend_text = {'font-size': '30px'}
            figure.title_style = {'font-size': '30px'}

            for axis in figure.axes:
                axis.tick_style = {'font-size': '30px'}
                axis.label_style = {'font-size': '30px'}

    else:

        obj.description = 'Presentation mode (OFF)'

        display(HTML(
            "<style>" \
            ".widget-readout { font-size: 14px ;}" \
            ".widget-label-basic {font-size: 14px;}" \
            "option {font-size: 12px;}" \
            ".p-Widget .jupyter-widgets .widgets-label {font-size: 14px;}" \
            ".widget-label {font-size: 14px ;}" \
            ".widget-text input[type='number'] {font-size: 14px;}" \
            ".option { font-size: 14px ;}" \
            ".p-Widget .jupyter-widgets .jupyter-button.widget-button {font-size:␣
↪14px;}" \
            ".p-Widget.jupyter-widgets.jupyter-button.widget-toggle-button {font-size:
↪ 14px;}" \
            ".bqplot > svg .axis text.axislabel, .bqplot > svg .axis tspan.axislabel
↪{font-size: 14px;}" \
            ".q-grid .slick-cell {font-size: 14px;}" \
            ".slick-column-name {font-size: 14px;}" \
            ".widget-html-content {font-size: 14px;}"
            "</style>"
            )
        )

        for figure in figures:

            figure.legend_text = {'font-size': '14px'}
            figure.title_style = {'font-size': '20px'}

            for axis in figure.axes:
                axis.tick_style = {'font-size': '14px'}
```

(continues on next page)

(continued from previous page)

```
                axis.label_style = {'font-size': '14px'}
```

[9]:
```
def prepare_export(button):
    """This function sends the selected plot to the 'export_plot'
    function.
    """

    if button is prepare_export_fig_0_button:

        export_plot(figures[0])

    elif button is prepare_export_fig_1_button:

        export_plot(figures[1])

    elif button is prepare_export_fig_2_button:

        export_plot(figures[2])

    elif button is prepare_export_fig_3_button:

        export_plot(figures[3])

    elif button is prepare_export_fig_115_001_button:

        export_plot(fig_115_001)
```

[10]:
```
def export_plot(plot):
    """This function sends the selected plot to the export module.
    """

    global data

    text_lines = []

    np.set_printoptions(threshold=sys.maxsize)

    tooltips = []

    for mark in plot.marks:
        tooltips.append(mark.tooltip)
        mark.tooltip = None

    data =  repr((plot, text_lines))

    %store data

    rel_url = "../../../apps/modules/export_module.ipynb"
    abs_url = urllib.parse.urljoin(notebook_url, rel_url)

    if not webbrowser.open(abs_url):
        go_to_export_button.value = "<form action=" + abs_url + " target='_blank'>
↪<button type=''submit''>Open in export module</button></form>"

    for i in range(len(plot.marks)):
        mark = plot.marks[i]
```

(continues on next page)

(continued from previous page)

```
        mark.tooltip = tooltips[i]
```

[ ]:
```
%%javascript

//Get the URL of the current notebook

var kernel = Jupyter.notebook.kernel;
var command = ["notebook_url = ",
               "'", window.location.href, "'" ].join('')

kernel.execute(command)
```

### 1.6.6 Main interface

[ ]:
```
#(a, b, element's name)
parameters = [(5.536, 0.03049, 'Water'),
              (4.225, 0.0371, 'Ammonia'),
              (1.358, 0.02789, 'Nitric oxide'),
              (4.25, 0.05105, 'Xenon')]

colors = ['#0079c4','#f09205','#21c400', '#850082']

#I want to show the same range in v so you can compare the isotherms of all the␣
↪elements
#so, let's calculate the critic point of the first one and use as a reference for the␣
↪rest

p_c1, v_c1, T_c1 = calculate_critic(parameters[0][0], parameters[0][1])
v_values = np.linspace(0.8*parameters[0][1], 10*v_c1, 500)

scale_x = bqs.LinearScale(min = min(v_values), max = max(v_values))
scale_y = bqs.LinearScale(min = 0.0, max = 2.0*p_c1)

axis_x = bqa.Axis(
    scale=scale_x,
    tick_format='.2f',
    tick_style={'font-size': '15px'},
    tick_values=[0, 0.45, 0.9],
    grid_lines = 'none',
    grid_color = '#8e8e8e',
    label='v (L/mol)',
    label_location='middle',
    label_style={'stroke': 'black', 'default-size': 35},
    label_offset='50px'
)

axis_y = bqa.Axis(
    scale=scale_y,
    tick_format='.0f',
    tick_style={'font-size': '15px'},
    tick_values=[0, 200, 400],
    grid_lines = 'none',
    grid_color = '#8e8e8e',
    orientation='vertical',
```

(continues on next page)

(continued from previous page)

```
    label='p (atm)',
    label_location='middle',
    label_style={'stroke': 'red', 'default_size': 35},
    label_offset='50px'
)

main_block_115_000 = widgets.VBox(
    [],
    layout=widgets.Layout(width='100%')
)

left_block = widgets.VBox(
    [],
    layout=widgets.Layout(width='60%')
)

right_block = widgets.VBox(
    [],
    layout=widgets.Layout(width='40%')
)

h_block_1 = widgets.HBox([])
left_block.children = [h_block_1]

if len(parameters) > 3:

    h_block_2 = widgets.HBox([])
    left_block.children = [
        h_block_1,
        h_block_2
    ]

figures = []

for i in range(len(parameters)):

    elem = parameters[i]

    a = elem[0]
    b = elem[1]
    name = elem[2]

    p_c, v_c, T_c = calculate_critic(a, b)

    T_values = [0.8*T_c, 0.95*T_c, T_c, 1.2*T_c]
    T_values_str = [str(t) for t in T_values]
    v_values = np.linspace(b+0.01, 0.9, 500)

    isotherms = get_absolute_isotherms(a, b, v_values, T_values)
    isotherms = bar_to_atm(isotherms)

    block = widgets.VBox(
        [],
        layout=widgets.Layout(width='100%')
    )

    marks = []
```

(continues on next page)

(continued from previous page)

```
    lines = bqm.Lines(
        x = [v_values for elem in isotherms],
        y = isotherms,
        scales = {'x': scale_x, 'y': scale_y},
        opacities = [1.0],
        visible = True, #True, #t == '1.00',
        colors = colors,
        labels = T_values_str,
    )

    critical_point = bqm.Scatter(
        name = '',
        x = [v_c],
        y = [p_c],
        scales = {'x': scale_x, 'y': scale_y},
        default_opacities = [1.0],
        visible = True,
        colors = ['#2807a3'],
    )

    marks = [
        lines,
        critical_point
    ]

    fig = Figure(
        title=name,
        marks=marks,
        axes=[axis_x, axis_y],
        animation_duration=0,
        legend_location='top-right',
        background_style= {'fill': 'white',  'stroke': 'black'},
        min_aspect_ratio=1.0,
        fig_margin=dict(top=80, bottom=60, left=80, right=30),
        toolbar = True,
        layout = widgets.Layout(width='90%', height='250px')
    )

    figures.append(fig)

    block.children = [
        fig,
        widgets.HBox([
            widgets.HTML(value='a: '+str(a)),
            widgets.HTML(value='b: '+str(b)),
        ],
            layout=widgets.Layout(
                    align_self='center',
                    justify_content='space-around',
                    width='100%'
                )
        )

    ]

    if i > 1:
```

(continues on next page)

(continued from previous page)

```
        h_block_2.children = h_block_2.children + (block,)

    else:
        h_block_1.children = h_block_1.children + (block,)

v_values = np.linspace(0.45, 5.0, 500)
T_values = [0.8, 0.95, 1.0, 1.2]
T_values_str = [str(t) for t in T_values]
relative_isotherms = get_relative_isotherms(v_values, T_values)

scale_x = bqs.LinearScale(min = 0.45, max = 5.0)
scale_y = bqs.LinearScale(min = 0.0, max = 2.0)

axis_x = bqa.Axis(
    scale=scale_x,
    tick_format='0.2f',
    tick_style={'font-size': '15px'},
    tick_values=[1,2,3,4,5],
    grid_lines = 'none',
    grid_color = '#8e8e8e',
    label='v (L/mol)',
    label_location='middle',
    label_style={'stroke': 'black', 'default-size': 35},
    label_offset='50px'
)

axis_y = bqa.Axis(
    scale=scale_y,
    tick_format='0.2f',
    tick_style={'font-size': '15px'},
    tick_values=[0,1,2],
    grid_lines = 'none',
    grid_color = '#8e8e8e',
    orientation='vertical',
    label='p (atm)',
    label_location='middle',
    label_style={'stroke': 'red', 'default_size': 35},
    label_offset='50px'
)

fig_115_001 = Figure(
    title='van der Waals isotherms (reduced variables)',
    marks=[],
    axes=[axis_x, axis_y],
    animation_duration=0,
    legend_location='top-right',
    background_style= {'fill': 'white',  'stroke': 'black'},
    min_aspect_ratio=1.0,
    fig_margin=dict(top=80, bottom=60, left=80, right=30),
    toolbar = True,
    layout = widgets.Layout(width='90%')
)

lines = bqm.Lines(
    x = [v_values for elem in relative_isotherms],
    y = relative_isotherms,
    scales = {'x': scale_x, 'y': scale_y},
```

(continues on next page)

(continued from previous page)

```
    opacities = [1.0],
    visible = True,
    colors = colors,
    labels = T_values_str,
)

critical_point = bqm.Scatter(
    name = '',
    x = [1.0],
    y = [1.0],
    scales = {'x': scale_x, 'y': scale_y},
    default_opacities = [1.0],
    visible = True,
    colors = ['#2807a3'],
)

fig_115_001.marks = [
    lines,
    critical_point
]

right_block.children = [fig_115_001]

change_view_button = widgets.ToggleButton(
    value=False,
    description='Presentation mode (OFF)',
    disabled=False,
    button_style='',
    tooltip='',
    icon='desktop',
    layout=widgets.Layout(
        width='initial',
        align_self='center'
    )
)

change_view_button.observe(change_view, 'value')

prepare_export_fig_0_button = widgets.Button(
    description='Export '+parameters[0][2],
    disabled=False,
    button_style='',
    tooltip='',
)

prepare_export_fig_0_button.on_click(prepare_export)

prepare_export_fig_1_button = widgets.Button(
    description='Export '+parameters[1][2],
    disabled=False,
    button_style='',
    tooltip='',
)

prepare_export_fig_1_button.on_click(prepare_export)

prepare_export_fig_2_button = widgets.Button(
```

(continues on next page)

(continued from previous page)

```
    description='Export '+parameters[2][2],
    disabled=False,
    button_style='',
    tooltip='',
)

prepare_export_fig_2_button.on_click(prepare_export)

prepare_export_fig_3_button = widgets.Button(
    description='Export '+parameters[3][2],
    disabled=False,
    button_style='',
    tooltip='',
)

prepare_export_fig_3_button.on_click(prepare_export)

prepare_export_fig_115_001_button = widgets.Button(
    description='Export',
    disabled=False,
    button_style='',
    tooltip='',
    layout=widgets.Layout(
        align_self = 'center',
    )
)

prepare_export_fig_115_001_button.on_click(prepare_export)

tenperatures_text =  widgets.HTML(
    value="<div style='width:30px;text-align:left;display:inline-block;margin-left:
↪30px;" \
        + "border: 5px solid #0079c4;opacity: 0.5'> </div>" \
        + "  T = 0.8 Tc" \
        + "<div style='width:30px;text-align:left;display:inline-block;margin-left:
↪30px;" \
        + "border: 5px solid #f09205;opacity: 0.5'> </div>" \
        + "  T = 0.95 Tc" \
        + "<div style='width:30px;text-align:left;display:inline-block;margin-left:
↪30px;" \
        + "border: 5px solid #21c400;opacity: 0.5'> </div>" \
        + "  T = Tc" \
        + "<div style='width:30px;text-align:left;display:inline-block;margin-left:
↪30px;" \
        + "border: 5px solid #850082;opacity: 0.5'> </div>" \
        + "  T = 1.2 Tc" \
)

left_block.children = left_block.children + (
    widgets.HBox([
        prepare_export_fig_0_button,
        prepare_export_fig_1_button,
        prepare_export_fig_2_button,
        prepare_export_fig_3_button
    ],
    layout=widgets.Layout(
        align_self = 'center',
```

(continues on next page)

(continued from previous page)

```
    )
    ),
)

right_block.children = right_block.children + (
    prepare_export_fig_115_001_button,
    tenperatures_text
)

main_block_115_000.children = [
    change_view_button,
    widgets.HTMLMath(
        '$a: L^2 bar / mol \quad b: L/mol$',
        layout=widgets.Layout(
            align_self = 'center',
        )
    ),
    widgets.HBox([
        left_block,
        right_block,
    ])
]

figures.append(fig_115_001)

main_block_115_000
```

## 1.7 Maxwell's construction on van der Waals isotherms

**Code:** #111-000

**File:** `apps/van_der_waals/p_v_2D.ipynb`

**Run it online:**

---

### 1.7.1 Interface

The main interface (`main_block_111_000`) is divided in two Box: `top_block_111_000` and `middle_block_111_000`.

`top_block_111_000` contains the widgets to control the tenperatute range shown and the toggles of the different areas and isother types.

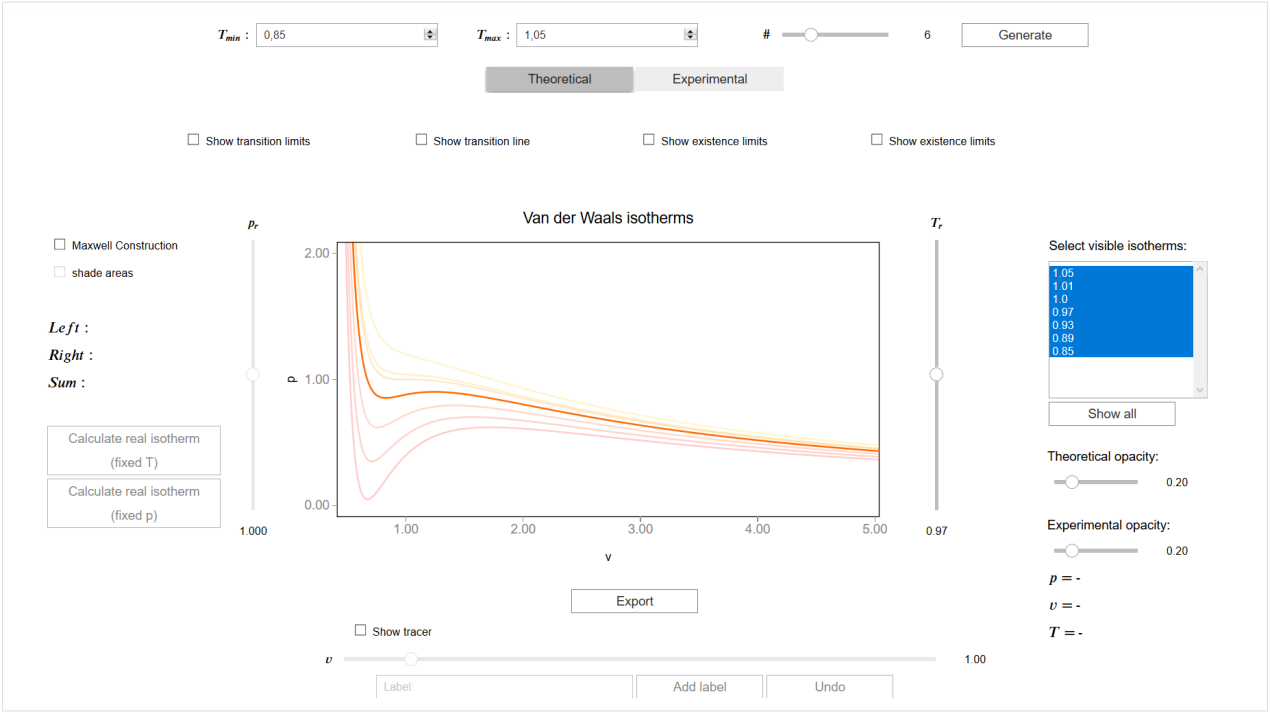
`middle_block_111_000` contains the main figure (`fig_111_000`) and the different controlers to implement Maxwell's construction: `T_slider` changes the selected isotherm and `p_slider` controls the isobaric line.

Some buttons are only available if `maxwell_construction_checkbox` is activated.

`v_slider` controls the position of the mark `tracer` and it is only available if `show_tracer_checkbox` is activated.

[1]:
```
from IPython.display import Image
Image(filename='../../static/images/apps/111-000_1.png')
```

[1]:




## 1.7.2 CSS

A custom `css` file is used to improve the interface of this application. It can be found here.

[2]:
```
from IPython.display import HTML
display(HTML("<head><link rel='stylesheet' type='text/css' href='./../../static/
↪custom.css'></head>"))
display(HTML("<style>.container { width:100% !important; } .jupyter-button {white-
↪space: normal !important;}</style>"))
```

```
<IPython.core.display.HTML object>
```

```
<IPython.core.display.HTML object>
```

## 1.7.3 Packages

[3]:
```
from bqplot import *
import bqplot as bq
import bqplot.marks as bqm
import bqplot.scales as bqs
import bqplot.axes as bqa

import ipywidgets as widgets

from scipy import interpolate
from scipy.signal import argrelextrema

import urllib.parse
import webbrowser
```

(continues on next page)

(continued from previous page)

```
import sys
```

### 1.7.4 Physical functions

This are the functions that have a physical meaning:

- `get_relative_isotherms`
- `experimetal_isotherms`
- `get_roots`
- `p_indefinite_integral`
- `p_definite_integral`
- `find_real_fixed_p`
- `find_real_fixed_T`

[4]:
```
def get_relative_isotherms(v_range, T_range):
    """This function calculates the theoretical p(v, T) plane
        (in reduced coordinates) according to van der Waals
        equation of state from a given range of volumes
        and tenperatures.

    Args:
        v_range: An array containing the values of v
        (in reduced coordinates)for which the isotherms must be
        calculated.\n
        T_range: An array containing the values of T
        (in reduced coordinates)for which the isotherms must be
        calculated.\n


    Returns:
        isotherms: A list consisted of numpy arrays containing the
        pressures of each isotherm.
    """

    isotherms = []

    for T in T_range:
        p_R = []
        for v in v_range:
            val = (8.0/3.0*T/(v - 1.0/3.0) - 3.0/v**2)
            p_R = np.append(p_R, val)

        isotherms.append(p_R)

    return isotherms
```

[5]:
```
def experimental_isotherms(p_range, v_range, T_range, fixed_p, fixed_T):
    """This function calculates the experimental p(v, T) plane
        (in reduced coordinates) according to van der Waals
        equation of state for a given range of volumes
```

(continues on next page)

(continued from previous page)

```
        and tenperatures or for a given range of volumes
        and pressures.

    Args:
        p_range: An array containing the values of p
        (in reduced coordinates)for which the isotherms must be
        calculated. Only used if fixed_p == True.\n
        v_range: An array containing the values of v
        (in reduced coordinates)for which the isotherms must be
        calculated.\n
        T_range: An array containing the values of v
        (in reduced coordinates)for which the isotherms must be
        calculated. Only used if fixed_T == True.\n
        fixed_p: Boolean variable which represents if the isotherms
        must be calculated for a given pressures.\n
        fixed_T: Boolean variable which represents if the isotherms
        must be calculated for a given pressures.\n


    Returns:
        expe_data: A list consisted of numpy arrays containing the
        pressures of each theoretical isotherm.\n
        theo_data: A list consisted of numpy arrays containing the
        pressures of each theoretical isotherm.\n
        v_limits: A list consisted of arrays of the volume limits of
        the phase-transition of each subcritical isotherm.\n
        p_limits: A list consisted of arrays of the pressure limits of
        the phase-transition of each subcritical isotherm.\n
        tenperatures: A list consisted of the tenperatures of the
        isotherms.\n
    """

    if fixed_T:

        theo_data = get_relative_isotherms(v_range, T_range)
        expe_data = []

        v_limits = []
        p_limits = []

        p_range = np.linspace(0.001, 1.0, num=10000)
        pressures, v_isobaric_limits = find_real_fixed_T(p_range, T_range)

        for i in range(len(theo_data)):

            p_expe = []

            if i < len(v_isobaric_limits):

                    v_lim = v_isobaric_limits[i]

                    if len(v_lim) > 1: #check if there is only one point
                        for j in range(len(v_range)):

                            if v_range[j] > v_lim[0] and v_range[j] < v_lim[1]:
                                p_expe.append(pressures[i])
```

(continues on next page)

(continued from previous page)

```
                        else:
                            p_expe.append(theo_data[i][j])

                    v_limits = np.append(v_limits, [v_lim[0], v_lim[1]])
                    p_limits = np.append(p_limits, [pressures[i], pressures[i]])

                else:
                    p_expe = theo_data[i]
                    v_limits = np.append(v_limits, [1.0])
                    p_limits = np.append(p_limits, [1.0])

            else:

                p_expe = theo_data[i]

            expe_data.append(p_expe)

        tenperatures = T_range

        return expe_data, theo_data, p_limits, v_limits, tenperatures

    elif fixed_p:

        tenperatures, v_isobaric_limits = find_real_fixed_p(p_range, T_range)

        theo_data = get_relative_isotherms(v_range, tenperatures)
        expe_data = []

        v_limits = []
        p_limits = []

        for i in range(len(theo_data)):

            p_expe = []

            if i < len(v_isobaric_limits):

                    v_lim = v_isobaric_limits[i]

                    if len(v_lim) > 1: #check if there is only one point

                        for j in range(len(v_range)):

                            if v_range[j] > v_lim[0] and v_range[j] < v_lim[1]:
                                p_expe.append(p_range[i])

                            else:
                                p_expe.append(theo_data[i][j])

                        v_limits = np.append(
                            v_limits,
                            [v_lim[0],
                             v_lim[1]]
                        )
                        p_limits = np.append(
                            p_limits,
                            [p_range[i],
```

(continues on next page)

(continued from previous page)

```
                            p_range[i]]
                        )

                    else:
                        p_expe = theo_data[i]
                        v_limits = np.append(v_limits, [1.0])
                        p_limits = np.append(p_limits, [1.0])

            else:

                p_expe = theo_data[i]

            expe_data.append(p_expe)

        return expe_data, theo_data, p_limits, v_limits, tenperatures
```

[6]:
```
def get_roots(p, T):
    """This function calculates the roots of a van der Waals
    isotherm of a given T and set of pressures.

    Args:
        p: Numpy array consisted of the pressures of the isotherm.\n
        T: Value of the tenperature.\n

    Returns:
        roots_in_range: A list consisted of the real roots.\n
    """


    roots = np.roots([1.0, - 1.0/3.0*(1.0 + 8.0*T/p), 3.0/p, -1.0/p])
    roots_in_range = []

    for root in roots:
        if np.isreal(root):
            root = np.real(root)
            if root > 0:
                roots_in_range.append(root)
    roots_in_range.sort()

    return roots_in_range
```

[7]:
```
def p_indefinite_integral(p_0, v_0, T):
    """This function calculates the indefinite integral between
    a van der Waals isotherm and a isobaric line.

    Args:
        p0: Isobaric line's pressure.\n
        v0: Value of the volume.\n
        T: Value of the tenperature.\n

    Returns:
        integral: Value of the indefinite integral between a
        van der Waals isotherm at T and a isobaric line of p0 at a
        volume v0.\n
    """
```

(continues on next page)

(continued from previous page)

```
    integral = 8.0/3.0 * T *np.log(v_0 - 1.0/3.0) + 3.0/v_0 - p_0*v_0

    return integral
```

[8]:
```
def definite_integral(p_0, v_range, T):
    """This function 'p_indefinite_integral' function to calculate
    the definite integral between a van der Waals isotherm and a
    isobaric line.

    Args:
        p0: Isobaric line's pressure.\n
        v_range: Tuple or list consisted of volume limits.\n
        T: Value of the tenperature.\n

    Returns:
        integral: Value of the definite integral between a
        van der Waals isotherm at T and a isobaric line of p0 in a
        volume range v_range.\n
    """

    v_0, v_1 = v_range[0], v_range[1]

    integral = p_indefinite_integral(p_0, v_1, T) - p_indefinite_integral(p_0, v_0, T)

    return integral
```

[9]:
```
def find_real_fixed_T(p_values, T_values):
    """This function uses Maxwell's construction to find the
       pressures in which phase transition happens given some
       fixed tenperatures.\n

    Args:
        p_values: List of pressures in which the real isotherm is
        searched.\n
        T_values: List of tenperatures of the isotherms.\n


    Returns:
        pressures: List of pressures in which phase transition
        happens.\n
        v_range: Volume limits of phase transition zones.
    """

    eps = 1e-3

    pressures = []
    v_ranges = []

    for T in T_values:

        if T < 1.0:

            for p in p_values:

                roots = get_roots(p, T)
```

(continues on next page)

(continued from previous page)

```
                if len(roots) == 3:

                    v_range = [roots[0], roots[2]]
                    area = definite_integral(p, v_range, T)

                    if abs(area) < eps:

                        pressures.append(p)
                        v_ranges.append(v_range)

                        break

        elif T == 1.0:

            pressures.append(1.0)
            v_ranges.append([1.0])

    return pressures, v_ranges
```

[10]:
```
def find_real_fixed_p(p_values, T_values):
    """This function uses Maxwell's construction to find the
       tenperatures in which phase transition happens given some
       fixed pressures.\n

    Args:
        p_values: List of pressures of the isotherms.\n
        T_values: List of tenperatures in which the real isotherm is
        searched.\n


    Returns:
        tenperatures: List of tenperatures in which phase transition
        happens.\n
        v_range: Volume limits of phase transition zones.
    """

    eps = 1e-3

    tenperatures = []
    v_ranges = []

    for p in p_values:

        if p < 1.0:

            for T in T_values:

                roots = get_roots(p, T)

                if len(roots) == 3:

                    v_range = [roots[0], roots[2]]
                    area = definite_integral(p, v_range, T)

                    if abs(area) < eps:
```

(continues on next page)

(continued from previous page)

```
                        tenperatures.append(T)
                        v_ranges.append(v_range)

                        break

        elif p == 1.0:

            tenperatures.append(1.0)
            v_ranges.append([1.0])

    return tenperatures, v_ranges
```

### 1.7.5 Functions related to the interaction

[11]:
```
def get_t_range(t_min_input, t_max_input, num_input):
    """This function calculates the set of N values between the
    values of the t_min_input and t_max_input widgets.

    Args:
        t_min_input: IPython widget which values represents the
        lower limit of the range.\n
        t_max_input:  IPython widget which values represents the
        upper limit of the range.\n
        num_input: IPython widget which values represents the
        number of values calculated.\n

    Returns:
        t_range: Numpy array containing the calculated values
        rounded to 3 decimals.
    """

    t_min = t_min_input.value
    t_max = t_max_input.value
    num = num_input.value

    t_range = []

    if t_min > t_max:
        t_range = np.linspace(start=t_max, stop=t_min, num=num)

    elif t_min == t_max:
        t_range = [t_min]

    else:
        t_range = np.linspace(start=t_min, stop=t_max, num=num)

    if 1.0 not in t_range:
        t_range = np.append(t_range, 1.0)
        t_range = np.sort(t_range)

    t_range = np.round(t_range, 3)

    return t_range
```

[12]:
```
def find_nearest_index(array, value):
    """This function find index of the element in an array which
    value is the nearest to the given one.

    Args:
        array: A list or numpy array containing the elements.\n
        value: Float number.\n

    Returns:
        idx: Index of the element in array which value is the nearest
        to value.
    """

    array = np.asarray(array)
    idx = (np.abs(array - value)).argmin()
    return idx
```

[13]:
```
def show_tracer(change):
    """This function controls if the bqplot mark 'tracer' of
    the bqplot figure 'fig_111_000' is visible or not.\n
    """

    if show_tracer_checkbox.value:
        tracer.visible = True
        v_slider.disabled = False
        update_tracer(change)

        label_input.disabled = False
        add_label_button.disabled = False
        undo_label_button.disabled = False

    else:
        tracer.visible = False
        v_slider.disabled = True

        label_input.disabled = True
        add_label_button.disabled = True
        undo_label_button.disabled = True
```

[14]:
```
def update_tracer(change):
    """This function updates the position of the bqplot mark 'tracer'
    of the bqplot figure 'fig_111_000' and the representation of the position
    of the tracer.\n
    """

    v = v_slider.value
    T = T_slider.value

    for mark in fig_111_000.marks:

        if str(T) in mark.labels:

            i = mark.labels.index(str(T))
            x_values = mark.x
            y_values = mark.y[i]

            break
```

(continues on next page)

(continued from previous page)

```
    i_v = find_nearest_index(x_values, v)
    tracer.x = np.array([x_values[i_v]])
    tracer.y = np.array([y_values[i_v]])

    tracer_p.value = " " + str(np.round(tracer.y, 3)[0])
    tracer_v.value = " " + str(np.round(tracer.x, 3)[0])
    tracer_T.value = " " + str(T_slider.value)
```

[15]:
```
def add_label(x, y, label):
    """This function adds a point and a name to the bqplot mark
    'labels_points' of the bqplot figure 'fig_111_000'.\n
    """

    x_labels = [elem for elem in labels_points.x]
    y_labels = [elem for elem in labels_points.y]

    x_labels.append(tracer.x[0])
    y_labels.append(tracer.y[0])

    labels_points.x, labels_points.y = x_labels, y_labels
    labels_points.names = np.append(labels_points.names, label)
```

[16]:
```
def get_new_label(labels):
    """This function returns an alphabetical label different
    from the ones given in the 'labels' list.

    Args:
        labels: A list consisted of the current labels.\n

    Returns:
        elem: A string with a new label which is not in 'labels'.\n
    """


    alpha = 'ABCDEFGHIJKLMNOPQRSTUVWXYZ'
    alpha2 = 'ABCDEFGHIJKLMNOPQRSTUVWXYZ'
    count = 0
    i = 0
    while i < len(alpha):

        elem = alpha[i]

        if not np.isin(elem,labels):
            break

        if i == (len(alpha) - 1):
            alpha = [alpha2[count] + elem for elem in alpha2]
            i = 0
            count = count + 1

        i = i + 1

    return elem
```

[17]:
```
def add_label_button_clicked(a):
    """This function is called when 'add_label_button' is clicked
    and calls 'add_label' function.\n
    """

    label = label_input.value

    if label == '':
        label = get_new_label(labels_points.names)

    add_label(tracer.x[0], tracer.y[0], label)
    label_input.value = ''
```

[18]:
```
def undo_label_button_clicked(a):
    """This function removes the last label added to the bqplot
    mark 'labels_points' of the bqplot figure 'fig_111_000'.\n
    """

    if len(labels_points.x) > 0:

        labels_points.x, labels_points.y = labels_points.x[:-1], labels_points.y[:-1]
        labels_points.names = labels_points.names[:-1]
```

[19]:
```
def update_isobaric(change):
    """This function updates the bqplot mark 'isobaric' of the bqplot figure
    'fig_111_000' when the slider 'p_slider' is moved. Also updates the value
    of the integrals.\n
    """

    p = p_slider.value
    T = T_slider.value

    for mark in fig_111_000.marks:

        if str(T) in mark.labels:

            i = mark.labels.index(str(T))

            x_values = mark.x
            y_values = mark.y[i]
            break

    roots = get_roots(p, T)

    if len(roots) == 3:

        isobaric.fill = 'between'
        shade_areas(change)

        #find where the isobaric curve intersects the isotherm
        i_min = find_nearest_index(x_values, roots[0])
        i_max = find_nearest_index(x_values, roots[2])
        x_real = x_values.tolist()[i_min:i_max]

        #we have two lines: one for the isobaric and the other for the isotherm
        x = [x_real, x_real]
        y = [[p for elem in x_real], y_values[i_min:i_max]]
```

(continues on next page)

(continued from previous page)

```
        v_range_1 = (roots[0], roots[1])
        v_range_2 = (roots[1], roots[2])

        left_integral = definite_integral(p, v_range_1, T)
        right_integral = definite_integral(p, v_range_2, T)

        integral_value_left_text.value = '%.2f' % left_integral
        integral_value_right_text.value = '%.2f' % right_integral

        integral_value_text.value = '%.2f' % (left_integral + right_integral)

    else:
        isobaric.fill = 'none'
        x = [x_values, x_values]
        y = [[p for elem in x_values], y_values]

        integral_value_left_text.value = '-'
        integral_value_right_text.value = '-'
        integral_value_text.value = '-'

    isobaric.x, isobaric.y = x, y
```

[20]:
```
def shade_areas(change):
    """This function shades the area between the bqplot mark
    'isobaric' and the isotherm mark of the bqplot figure
    'fig_111_000'.\n
    """

    if shade_areas_checkbox.value:

        isobaric.fill_opacities = [0.35]

    else:

        isobaric.fill_opacities = [0.0]
```

[21]:
```
def find_real_isotherm(a):
    """This function moves p_slider to find the real isotherm
    where both areas value is equal.\n
    """

    if T_slider.value < 1.0:

        p_min = p_slider.min
        p_max = 1.0
        step = p_slider.step

        p_range = np.arange(p_max, p_min, -step)

        for p in p_range:
            p_slider.value = p
            if integral_value_text.value == '0.00':
                break
```

[22]:
```
def generate_isotherm_marks(p_range, v_range, T_range, fixed_T, fixed_p, scale_x,␣
↪scale_y):
    """This function generates the marks of the experimental and
       theoretical isotherms (in reduced variables) and of the limits
       of the phase transition and the non-existence zones for a given
       range of volumes and tenperatures or for a given range of
       volumes and pressures.

    Args:
        p_range: An array containing the values of p
        (in reduced coordinates)for which the isotherms must be
        calculated. Only used if fixed_p == True.\n
        v_range: An array containing the values of v
        (in reduced coordinates)for which the isotherms must be
        calculated.\n
        T_range: An array containing the values of v
        (in reduced coordinates)for which the isotherms must be
        calculated. Only used if fixed_T == True.\n
        fixed_p: Boolean variable which represents if the isotherms
        must be calculated for a given pressures.\n
        fixed_T: Boolean variable which represents if the isotherms
        must be calculated for a given pressures.\n


    Returns:
        marks: The marks of the experimental and
        theoretical isotherms (in reduced variables) and of the limits
        of the phase transition and the non-existence zones.\n
        T_limits: A list consisted of the tenperatures of the
        isotherms.\n
    """

    data = experimental_isotherms(
        p_range=p_range,
        v_range=v_range,
        T_range=T_range,
        fixed_T = fixed_T,
        fixed_p = fixed_p
    )

    expe_p_values = data[0]
    theo_p_values = data[1]

    p_limits = data[2]
    v_limits = data[3]
    T_limits = data[4]

    marks = []

    #generate a gradient from red to yellow
    colors = generate_gradient('#FF0000', '#FFfa00', len(T_limits))
    opacities = [opacity_theo_slider.value for t in T_limits]
    opacities[int(len(T_limits)/2)] = 1.0

    #theoretical isotherms
    marks.append(bqm.Lines(
        x = v_range,
```

(continues on next page)

(continued from previous page)

```
        y = np.array([theo_p_values]),
        scales = {'x': scale_x, 'y': scale_y},
        opacities = opacities,
        visible = True,
        colors = colors,
        labels = [str(t) for t in T_limits],
        name = 'theo'
        ))

    p_values_real = []
    v_values_real = []

    #experimental isotherms
    marks.append(bqm.Lines(
        x = v_range,
        y = np.array([expe_p_values]),
        scales = {'x': scale_x, 'y': scale_y},
        opacities = opacities,
        visible = experimental_toggle.value,
        colors = colors,
        labels = [str(t) for t in T_limits],
        line_style = 'solid'
        ))

    scatter_colors = []

    for color in colors:

        scatter_colors.append(color)
        scatter_colors.append(color)

    #maxwell limits
    marks.append(
        bqm.Scatter(
            x = v_limits,
            y = p_limits,
            scales = {'x': scale_x, 'y': scale_y},
            opacities = [opacity_theo_slider.value],
            visible = show_transition_limits_checkbox.value,
            colors = ['blue'],
            names = [],
            labels = ['maxwell_limits'],
            default_size = 15,
            tooltip = tt
        )
    )

    try:

        # If there is only one point the interpolation
        # can't be done.

        f_maxwell = interpolate.interp1d(
            v_limits,
            p_limits,
            kind = 'cubic',
            fill_value = 'extrapolate'
```

(continues on next page)

(continued from previous page)

```
        )

        maxwell_v = np.linspace(0.45, v_limits[1], 1000)
        maxwell_interp = f_maxwell(maxwell_v)

    except:

        maxwell_v = []
        maxwell_interp = []


    marks.append(bqm.Lines(
        x = maxwell_v,
        y = maxwell_interp,
        scales = {'x': scale_x, 'y': scale_y},
        opacities = [0.4],
        visible = show_transition_line_checkbox.value,
        colors = ['blue'],
        labels = ['maxwell_limits_interpolated'],
        line_style = 'solid',
        stroke_width = 3,
        fill = 'bottom',
        fill_opacities = [0.1]
        )
    )

    #non-existence limits
    non_e_min, non_e_max = find_local_extrema(theo_p_values)

    non_e_v_limits = []
    non_e_p_limits = []

    for i in range(len(non_e_min)):

        idx = non_e_min[i]
        non_e_p_limits = np.append(non_e_p_limits, np.take(theo_p_values[i],idx))
        non_e_v_limits = np.append(non_e_v_limits, np.take(v_range, idx))

    for i in range(len(non_e_max)):

        idx = non_e_max[i]
        non_e_p_limits = np.append(non_e_p_limits, np.take(theo_p_values[i],idx))
        non_e_v_limits = np.append(non_e_v_limits, np.take(v_range,idx))

    non_e_p_limits = np.append(non_e_p_limits, 1.0)
    non_e_v_limits = np.append(non_e_v_limits, 1.0)

    marks.append(
        bqm.Scatter(
            x = non_e_v_limits,
            y = non_e_p_limits,
            scales = {'x': scale_x, 'y': scale_y},
            opacities = [opacity_expe_slider.value],
            visible = show_existence_limits_checkbox.value,
            colors = ['green'],
            names = [],
            labels = ['non-existence limits'],
```

(continues on next page)

(continued from previous page)

```
            default_size = 15,
            tooltip = tt
        )
    )

    try:

        # If there is only one point the interpolation
        # can't be done.

        f_non_e = interpolate.interp1d(
            non_e_v_limits,
            non_e_p_limits,
            kind='cubic'
        )



        non_e_v = np.linspace(min(non_e_v_limits), max(non_e_v_limits), 1000)
        non_e_interp = f_non_e(non_e_v)

    except:

        non_e_v = []
        non_e_interp = []


    marks.append(bqm.Lines(
        x = non_e_v,
        y = non_e_interp,
        scales = {'x': scale_x, 'y': scale_y},
        opacities = [0.4],
        visible = show_existence_line_checkbox.value,
        colors = ['green'],
        labels = ['non_existence_limits_interpolated'],
        line_style = 'solid',
        stroke_width = 3,
        fill = 'bottom',
        fill_opacities = [0.1]
        )
    )

    return marks, T_limits
```

[23]:
```
def change_isotherms(a):
    """This function replaces the marks from the figure with
    the new calculated ones.
    """



    v_range = np.linspace(start=0.45, stop=5.2, num=500)
    t_range = get_t_range(t_min_input, t_max_input, num_input)

    marks, T_limits = generate_isotherm_marks(
        p_range=[],
        v_range=v_range,
```

(continues on next page)

(continued from previous page)

```
        T_range=t_range,
        fixed_T=True,
        fixed_p=False,
        scale_x=scale_x,
        scale_y=scale_y
    )

    marks.append(tracer)
    marks.append(labels_points)
    marks.append(isobaric)

    fig_111_000.marks = marks

    T_slider.options = t_range

    str_t_range = [str(t) for t in reversed(t_range)]

    select_visible.options = str_t_range
    select_visible.value = str_t_range

    T_slider.value = t_range[0]
    T_slider.value = t_range[int(t_range.size/2)]
```

[24]:
```
def select_isotherm(change):
    """This function selects a isotherm from the figure using
    T_slider.
    """

    # an error is generated in that case
    if len(T_slider.options) == len(select_visible.options):

        indexes = []

        for index in select_visible.index:

            indexes.append(len(select_visible.options)-1 - index)

        theo_opacities = [0.0 for t in T_slider.options]
        expe_opacities = [0.0 for t in T_slider.options]

        for i in indexes:

            theo_opacities[i] = opacity_theo_slider.value
            expe_opacities[i] = opacity_expe_slider.value

        if T_slider.index in indexes:

            if theoretical_toggle.value:

                theo_opacities[T_slider.index] = 1.0

            elif experimental_toggle.value:

                expe_opacities[T_slider.index] = 1.0

        for i in range(len(fig_111_000.marks)):
```

(continues on next page)

(continued from previous page)

```
            mark = fig_111_000.marks[i]
            label = mark.labels[0]

            if str(T_slider.value) in mark.labels:

                if i%3 == 0 and label in select_visible.value:

                    mark.opacities = theo_opacities

                elif i%3 == 1 and label in select_visible.value:

                    mark.opacities = expe_opacities

        if maxwell_construction_checkbox.value:

            update_isobaric(change)

        if show_tracer_checkbox.value:

            update_tracer(change)
```

[25]:
```
def show_isotherm(change):
    """This function changes the visibility of the isotherms
    according to the ones which are selected in 'select_visible'.
    """

    # an error is generated in that case
    if len(T_slider.options) == len(select_visible.options):

        indexes = []

        for index in select_visible.index:

            indexes.append(len(select_visible.options)-1 - index)

        theo_opacities = [0.0 for t in T_slider.options]
        expe_opacities = [0.0 for t in T_slider.options]

        for i in indexes:

            theo_opacities[i] = opacity_theo_slider.value
            expe_opacities[i] = opacity_expe_slider.value

        if T_slider.index in indexes:

            if theoretical_toggle.value:

                theo_opacities[T_slider.index] = 1.0

            elif experimental_toggle.value:

                expe_opacities[T_slider.index] = 1.0

        for i in range(len(fig_111_000.marks)):
```

(continues on next page)

(continued from previous page)

```
            mark = fig_111_000.marks[i]
            label = mark.labels[0]

            if str(T_slider.value) in mark.labels:

                if i%3 == 0:

                    mark.opacities = theo_opacities

                elif i%3 == 1:

                    mark.opacities = expe_opacities

            elif label not in ('isobaric', 'labels', 'tracer'):

                if i%3 == 0 and label in select_visible.value:

                    mark.visible = theoretical_toggle.value

                elif i%3 == 1 and label in select_visible.value:

                    mark.visible = experimental_toggle.value

                elif i%3 == 2 and label in select_visible.value:

                    mark.visible = show_limits_checkbox.value
```

[26]:
```
def show_all(a):
    """This function makes all isotherms visible.
    """

    select_visible.value = [str(t) for t in T_slider.options]
```

[27]:
```
def show_maxwell(change):
    """This function enables the buttons related to
    Maxwell's construction.
    """

    if maxwell_construction_checkbox.value:

        p_slider.disabled = False
        shade_areas_checkbox.disabled = False
        fixed_T_button.disabled = False
        fixed_p_button.disabled = False

        isobaric.visible = True
        update_isobaric(change)

    else:

        p_slider.disabled = True
        shade_areas_checkbox.disabled = True
        isobaric.visible = False
        fixed_T_button.disabled = True
        fixed_p_button.disabled = True
```

[28]:
```
def show_limits(change):
    """This function controls the visibility of the limits
    of the phase transition and non-existence zones.
    """

    fig_111_000.marks[2].visible = show_transition_limits_checkbox.value
    fig_111_000.marks[3].visible = show_transition_line_checkbox.value
    fig_111_000.marks[4].visible = show_existence_limits_checkbox.value
    fig_111_000.marks[5].visible = show_existence_line_checkbox.value
```

[29]:
```
def change_isotherm_type(change):
    """This function controls the visibility of the theoretical
    and experimental isotherms.
    """

    t_options = [str(t) for t in T_slider.options]

    for i in range(len(fig_111_000.marks)):

        mark = fig_111_000.marks[i]

        if i == 0:

            mark.visible = theoretical_toggle.value

        elif i == 1:

            mark.visible = experimental_toggle.value
```

[30]:
```
def find_local_extrema(array):
    """This function fidn the local maxima and minima of a given
    array.

    Args:
        array: Numpy array containing the values.\n


    Returns:
        local_min_ind: List consisted of the indexes of the local
        minima.\n
        local_max_ind: List consisted of the indexes of the local
        maxima.\n
    """


    local_min_ind = []
    local_max_ind = []

    for a in array:

        local_min_ind.append(argrelextrema(a, np.less))
        local_max_ind.append(argrelextrema(a, np.greater))

    return local_min_ind, local_max_ind
```

[31]:
```
def add_isotherm_mark_fixed_p(a):
```

(continues on next page)

(continued from previous page)

```
    """This function adds a isotherm which real isotherm has a phase
    transition at pressure p to the figure.\n
    """

    if p_slider.value < 1.0:

        v_values = np.linspace(start=0.45, stop=5.2, num=500)
        p_values = [p_slider.value]
        T_values = np.linspace(0.01, 1.0, 10000)

        new_marks, new_T_values = generate_isotherm_marks(
            p_range = p_values,
            v_range = v_values,
            T_range = T_values,
            fixed_T = False,
            fixed_p = True,
            scale_x = scale_x,
            scale_y = scale_y
        )

        #only take first three decimals
        new_T_values = [float(str(T)[:5]) for T in new_T_values]

        #calculate new tenperature range including new isotherms
        t_range = np.append(T_slider.options, new_T_values)
        new_t_range = np.sort(t_range)

        #get where the new marks should be inserted
        indexes, = np.where(new_t_range == new_T_values)

        #add data from the new isotherm to the old ones
        old_marks = fig_111_000.marks

        for i in range(2):

            try:
                old_marks[i].y = np.insert(
                    old_marks[i].y,
                    indexes,
                    new_marks[i].y,
                    axis=0
                )

            except:
                old_marks[i].y = np.insert(
                    old_marks[i].y,
                    indexes,
                    [new_marks[i].y],
                    axis=0
                )

            for label in new_marks[i].labels:
                new_labels = np.insert(
                    old_marks[i].labels,
                    indexes,
                    label
                )
```

(continues on next page)

(continued from previous page)

```
            old_marks[i].labels = new_labels.tolist()

        for i in range(2, 4):

            old_marks[i].x = np.append(
                old_marks[i].x,
                new_marks[i].x,
                axis=0
            )

            old_marks[i].y = np.append(
                old_marks[i].y,
                new_marks[i].y,
                axis=0
            )

        #update colors
        colors = generate_gradient(
            '#FF0000',
            '#FFfa00',
            len(new_t_range)
        )

        old_marks[0].colors = colors
        old_marks[1].colors = colors

        fig_111_000.marks = old_marks

        #update tenperature slider and visible selector
        T_slider.options = new_t_range
        T_slider.value = new_t_range[0]

        T_slider.value = T_slider.options[indexes[0]]

        select_visible.options = [
            str(t) for t in T_slider.options[::-1]
        ]
        select_visible.value = [
            str(t) for t in T_slider.options[::-1]
        ]
```

[32]:
```
def prepare_export(button):
    """This function sends the selected plot to the 'export_plot'
    function.
    """

    if button is prepare_export_fig_111_000_button:

        export_plot(fig_111_000)
```

[33]:
```
def change_view(change):
    """This function changes the visualization of all the
    components of the application so they are suitable for
    a projection.\n
    """
```

(continues on next page)

(continued from previous page)

```
    obj = change.owner

    if obj.value:

        obj.description = 'Presentation mode (ON)'

        display(HTML(
            "<style>" \
            ".widget-readout { font-size: 30px ; }" \
            ".widget-label-basic {font-size: 30px;}" \
            "option {font-size: 25px;}" \
            ".p-Widget.jupyter-widgets.widget-slider.widget-vslider.widget-inline-
↪vbox {width: auto}" \
            ".p-Widget .jupyter-widgets .widgets-label {width: auto; height: auto;␣
↪font-size: 30px;}" \
            ".widget-label {font-size: 30px ; height: auto !important;}" \
            ".p-Widget .bqplot .figure .jupyter-widgets {height: auto !important;}" \
            ".widget-text input[type='number'] {font-size: 30px;height: auto;}" \
            ".option { font-size: 30px ;}" \
            ".p-Widget .jupyter-widgets .jupyter-button.widget-button {font-size:␣
↪30px ; width: auto; height: auto;}" \
            ".p-Widget.jupyter-widgets.jupyter-button.widget-toggle-button{font-size:␣
↪30px ; width: auto; height: auto;}" \
            ".p-Widget.p-Panel.jupyter-widgets.widget-container.widget-box.widget-
↪vbox {padding-bottom: 30px}" \
            ".bqplot > svg .axis text.axislabel, .bqplot > svg .axis tspan.axislabel
↪{font-size: 30px;}"
            "</style>"
            )
        )

        for figure in figures:

            figure.legend_text = {'font-size': '30px'}
            figure.title_style = {'font-size': '30px'}

            for axis in figure.axes:
                axis.tick_style = {'font-size': '30px'}
                axis.label_style = {'font-size': '30px'}

    else:

        obj.description = 'Presentation mode (OFF)'

        display(HTML(
            "<style>" \
            ".widget-readout { font-size: 14px ;}" \
            ".widget-label-basic {font-size: 14px;}" \
            "option {font-size: 12px;}" \
            ".p-Widget .jupyter-widgets .widgets-label {font-size: 14px;}" \
            ".widget-label {font-size: 14px ;}" \
            ".widget-text input[type='number'] {font-size: 14px;}" \
            ".option { font-size: 14px ;}" \
            ".p-Widget .jupyter-widgets .jupyter-button.widget-button {font-size:␣
↪14px;}" \
            ".p-Widget.jupyter-widgets.jupyter-button.widget-toggle-button {font-size:
↪ 14px;}" \
```

(continues on next page)

(continued from previous page)

```
            ".bqplot > svg .axis text.axislabel, .bqplot > svg .axis tspan.axislabel
↪{font-size: 14px;}"
            "</style>"
            )
        )

        for figure in figures:

            figure.legend_text = {'font-size': '14px'}
            figure.title_style = {'font-size': '20px'}

            for axis in figure.axes:
                axis.tick_style = {'font-size': '14px'}
                axis.label_style = {'font-size': '14px'}
```

[34]:
```
def export_plot(plot):
    """This function sends the selected plot to the export module.
    """

    global data

    text_lines = []

    np.set_printoptions(threshold=sys.maxsize)
    data =  repr((plot, text_lines))

    %store data

    rel_url = "../../../apps/modules/export_module.ipynb"
    abs_url = urllib.parse.urljoin(notebook_url, rel_url)

    if not webbrowser.open(abs_url):
        go_to_export_button.value = "<form action=" + abs_url + " target='_blank'>
↪<button type=''submit''>Open in export module</button></form>"
```

[ ]:
```
%%javascript

//Get the URL of the current notebook

var kernel = Jupyter.notebook.kernel;
var command = ["notebook_url = ",
               "'", window.location.href, "'" ].join('')

kernel.execute(command)
```

### 1.7.6 Functions related to visualization

[36]:
```
def hex_to_rgb(number_hex):
    """This function converts a hexadecimal color to its rgb
    equivalent.

    Args:
        number_hex: String containing the hexadecimal representation
        of the color.\n
```

(continues on next page)

(continued from previous page)

```
    Returns:
        number_rgb: Tuple consisted of the 3 numbers of the rgb
        representation of the color.\n
    """

    if '#' in number_hex:
        number_hex = number_hex[1:]

    number_rgb = (int(number_hex[0:2], 16), \
                  int(number_hex[2:4], 16), \
                  int(number_hex[4:], 16))

    return number_rgb
```

[37]:
```
def rgb_to_hex(number_rgb):
    """This function converts a rgb color to its hexadecimal
    equivalent.

    Args:
        number_rgb: Tuple consisted of the 3 numbers of the rgb
        representation of the color.\n

    Returns:
        number_hex: String containing the hexadecimal representation
        of the color.\n
    """

    number_rgb = '#' \
    + format(number_rgb[0], '02x') \
    + format(number_rgb[1], '02x') \
    + format(number_rgb[2], '02x')

    return number_rgb
```

[38]:
```
def generate_gradient(initial, final, length):
    """This function generates a color gradient consisted of N
    colors from the initial to the final.

    Args:
        initial: String of the hexadecimal representation of the
        initial color.\n
        final: String of the hexadecimal representation of the
        final color.\n
        length: Number of colors.\n

    Returns:
        colors: List consisted of strings of the hexadecimal
        colors.\n
    """

    i_r, i_g, i_b = hex_to_rgb(initial)
    f_r, f_g, f_b = hex_to_rgb(final)

    r_step = (f_r - i_r)/length
    g_step = (f_g - i_g)/length
```

(continues on next page)

(continued from previous page)

```
    b_step = (f_b - i_b)/length

    r, g, b = i_r, i_g, i_b
    colors = []

    for i in range(length):

        h = rgb_to_hex((int(round(r)),int(round(g)),int(round(b))))

        colors.append(h)

        r = r + r_step
        g = g + g_step
        b = b + b_step

    return colors
```

### 1.7.7 Main interface

[ ]:
```
"""

.. module:: p_v_2D.ipynb
    :sypnopsis: This module creates an interface to interact with the
    van der Waals isotherms in the p(v, T) plane.\n

.. moduleauthor:: Jon Gabirondo López (jgabirondo001@ikasle.ehu.eus)

"""

saved = []

##############################
######TOP BLOCK###############
##############################

top_block_111_000 = widgets.VBox(
    [],
    layout=widgets.Layout(align_items='center')
)

change_view_button = widgets.ToggleButton(
    value=False,
    description='Presentation mode (OFF)',
    disabled=False,
    button_style='',
    tooltip='',
    icon='desktop',
    layout=widgets.Layout(
        width='auto'
    )
)

change_view_button.observe(change_view, 'value')

t_min_input = widgets.BoundedFloatText(
```

(continues on next page)

(continued from previous page)

```
    value=0.85,
    min=0.5,
    max=3.0,
    step=0.005,
    description=r'\( T_{min}: \)',
    disabled=False
)

t_max_input = widgets.BoundedFloatText(
    value=1.05,
    min=0.5,
    max=3.0,
    step=0.005,
    description=r'\( T_{max}: \)',
    disabled=False
)

num_input = widgets.IntSlider(
    value=6,
    min=1,
    max=20,
    description=r'\( \# \)',
    disabled=False,
    continuous_update=True,
    orientation='horizontal',
    readout=True,
)

generate_button = widgets.Button(
    description='Generate',
    disabled=False,
    button_style='',
    tooltip='Generate isotherms in the selected T range.',
)

generate_button.on_click(change_isotherms)

############################
#isotherm_type_block
############################

theoretical_toggle = widgets.ToggleButton(
    value=True,
    description='Theoretical',
    disabled=False,
    button_style='',
    tooltip='Show theoretical isotherms',
    style = {'description_width': 'initial'},
    layout = widgets.Layout(
        align_self='center',
        width='100%'
    )
)

experimental_toggle = widgets.ToggleButton(
    value=False,
    description='Experimental',
```

(continues on next page)

(continued from previous page)

```
    disabled=False,
    button_style='',
    tooltip='Show experimental isotherms',
    style = {'description_width': 'initial'},
    layout = widgets.Layout(
        align_self='center',
        width='100%'
    ),
)

theoretical_toggle.observe(change_isotherm_type, 'value')
experimental_toggle.observe(change_isotherm_type, 'value')

show_transition_limits_checkbox = widgets.Checkbox(
    value=False,
    description='Show transition limits',
    disabled=False,
    layout = widgets.Layout(width='148px !important')
)

show_transition_line_checkbox = widgets.Checkbox(
    value=False,
    description='Show transition line',
    disabled=False,
    layout = widgets.Layout(width='148px !important')
)

show_existence_limits_checkbox = widgets.Checkbox(
    value=False,
    description='Show existence limits',
    disabled=False,
    layout = widgets.Layout(width='148px !important')
)

show_existence_line_checkbox = widgets.Checkbox(
    value=False,
    description='Show existence line',
    disabled=False,
    layout = widgets.Layout(width='148px !important')
)

show_transition_limits_checkbox.observe(show_limits, 'value')
show_transition_line_checkbox.observe(show_limits, 'value')
show_existence_limits_checkbox.observe(show_limits, 'value')
show_existence_line_checkbox.observe(show_limits, 'value')

isotherm_type_block = widgets.HBox(
    [],
    layout = widgets.Layout(
        align_self='center',
        margin='10px 0 0 0'
    )
)

top_block_111_000.children = [
    change_view_button,
    widgets.HTML('</br>'),
```

(continues on next page)

(continued from previous page)

```
    widgets.HBox([
        t_min_input,
        t_max_input,
        num_input,
        generate_button
    ]),
    widgets.HBox([
        theoretical_toggle,
        experimental_toggle,
    ],
        layout = widgets.Layout(
            margin='20px 0 20px 0',
            width='33%')
    ),
    widgets.HBox([
        show_transition_limits_checkbox,
        show_transition_line_checkbox,
        show_existence_limits_checkbox,
        show_existence_line_checkbox
    ],
        layout = widgets.Layout(
            margin='20px 0 20px 0',
            width='100%')
    )
]

##############################
############MIDDLE BLOCK#####
##############################

middle_block_111_000 = widgets.HBox(
    [],
    layout=widgets.Layout(width='100%')
)

T_values = get_t_range(t_min_input, t_max_input, num_input)

############################
#FIGURE
############################

scale_x = bqs.LinearScale(min = 0.45, max = 5.0)
scale_y = bqs.LinearScale(min = 0.0, max = 2.0)

fig_111_000 = bq.Figure(
    title='Van der Waals isotherms',
    marks=[],
    axes=[],
    animation_duration=0,
    layout = widgets.Layout(
        align_self='center',
        width='75%'
    ),
    legend_location='top-right',
    background_style= {'fill': 'white','stroke': 'black'},
    fig_margin=dict(top=80,bottom=80,left=60,right=30),
    toolbar = True
```

(continues on next page)

(continued from previous page)

```
    )

axis_x = bqa.Axis(
    scale=scale_x,
    tick_format='0.2f',
    tick_style={'font-size': '15px'},
    tick_values=[1.0, 2.0, 3.0, 4.0, 5.0],
    grid_lines = 'none',
    grid_color = '#8e8e8e',
    label='v',
    label_location='middle',
    label_style={'stroke': 'black', 'default-size': 35},
    label_offset='50px'
)

axis_y = bqa.Axis(
    scale=scale_y,
    tick_format='0.2f',
    tick_style={'font-size': '15px'},
    tick_values=[0.0, 1.0, 2.0],
    grid_lines = 'none',
    grid_color = '#8e8e8e',
    orientation='vertical',
    label='p',
    label_location='middle',
    label_style={'stroke': 'red', 'default_size': 35},
    label_offset='50px'
)

fig_111_000.axes = [axis_x, axis_y]


tt = bq.Tooltip(
    fields = ['y', 'x'],
    formats = ['.3f', '.3f'],
    labels = ['p', 'v']
)

marks = []

tracer = bqm.Scatter(
    name = 'tracer',
    x = [1.0],
    y = [1.0],
    scales = {'x': scale_x, 'y': scale_y},
    visible = False,
    colors = ['black'],
    names = [],
    labels=['tracer'],
    tooltip = tt
)

marks.append(tracer)

labels_points = bqm.Scatter(
    name = 'labels',
    x = [],
```

(continues on next page)

(continued from previous page)

```
    y = [],
    scales = {'x': scale_x, 'y': scale_y},
    #opacities = [1.0],
    visible = True,
    colors = ['black'],
    names = [],
    labels=['labels'],
    tooltip = tt,
)

marks.append(labels_points)


isobaric = bqm.Lines(
    x = [],
    y = [],
    scales = {'x': scale_x, 'y': scale_y},
    opacities = [1.0, 0.0],
    visible = False,
    colors = ['green'],
    fill_opacities = [0.35],
    fill = 'none',
    labels = ['isobaric'],
)

marks.append(isobaric)

################################
#LEFT BLOCK
################################

left_block_111_000 = widgets.VBox(
    [],
    layout = widgets.Layout(
        width='15%',
        margin = '70px 0 0 0'
    )
)

maxwell_construction_checkbox = widgets.Checkbox(
    value=False,
    description='Maxwell Construction',
    disabled=False
)

maxwell_construction_checkbox.observe(show_maxwell, 'value')

p_slider = widgets.FloatSlider(
    value=1.0,
    min=0.001,
    max=scale_y.max,
    step=0.001,
    description=r'\( p_r \)',
    disabled=True,
    continuous_update=True,
    orientation='vertical',
    readout=True,
```

(continues on next page)

(continued from previous page)

```
    readout_format='.3f',
    layout = widgets.Layout(
        height = '80%',
        margin = '45px 0 0 0'
    )
)

p_slider.observe(update_isobaric, 'value')

shade_areas_checkbox = widgets.Checkbox(
    value=False,
    description='shade areas',
    disabled=True
)

shade_areas_checkbox.observe(shade_areas, 'value')

integral_value_text = widgets.HTML(
    value="",
)

integral_value_left_text = widgets.HTML(
    value="",
)

integral_value_right_text = widgets.HTML(
    value="",
)

fixed_T_button = widgets.Button(
    description='Calculate real isotherm (fixed T)',
    disabled=True,
    button_style='',
    tooltip="Use Maxwell's construction to" \
            "calculate real isotherm (fixed T)",
    layout = {
        'width' : 'auto',
        'height' : 'auto',
    }
)

fixed_T_button.on_click(find_real_isotherm)

fixed_p_button = widgets.Button(
    description='Calculate real isotherm (fixed p)',
    disabled=True,
    button_style='',
    tooltip="Use Maxwell's construction to" \
            "calculate real isotherm (fixed p)",
    layout = {
        'width' : 'auto',
        'height' : 'auto',
    }
)

fixed_p_button.on_click(add_isotherm_mark_fixed_p)
```

(continues on next page)

(continued from previous page)

```
left_block_111_000.children = [
    maxwell_construction_checkbox,
    shade_areas_checkbox,
    widgets.HTML(value="</br>"),
    widgets.HBox([
        widgets.Label(value="$Left:$"),
        integral_value_left_text,
    ]),
    widgets.HBox([
        widgets.Label(value="$Right:$"),
        integral_value_right_text,
    ]),
    widgets.HBox([
        widgets.Label(value="$Sum:$"),
        integral_value_text,
    ]),
    widgets.HTML(value="</br>"),
    fixed_T_button,
    fixed_p_button
]

################################
#RIGHT BLOCK
################################

right_block_111_000 = widgets.VBox(
    [],
    layout = widgets.Layout(
        width='15%',
        margin = '70px 0 0 0'
    )
)

T_slider = widgets.SelectionSlider(
    options=T_values,
    value=T_values[int(T_values.size/2)],
    description=r'\( T_r \)',
    disabled=False,
    continuous_update=True,
    orientation='vertical',
    readout=True,
    layout = widgets.Layout(
        height = '80%',
        margin = '45px 0 0 0'
    )
)

T_slider.observe(select_isotherm, 'value')

select_visible = widgets.SelectMultiple(
    options=[str(t) for t in T_values],
    value=[str(t) for t in T_values],
    rows=10,
    description='',
    disabled=False,
    layout = widgets.Layout(width = '90%')
)
```

(continues on next page)

(continued from previous page)

```
select_visible.observe(show_isotherm, 'value')

show_all_button = widgets.Button(
    description='Show all',
    disabled=False,
    button_style='',
    tooltip='Show all isotherms',
)

show_all_button.on_click(show_all)

opacity_theo_slider = widgets.FloatSlider(
    value=0.2,
    min=0.0,
    max=1.0,
    step=0.05,
    description="",
    disabled=False,
    continuous_update=True,
    orientation='horizontal',
    readout=True,
    layout = widgets.Layout(width = '90%')
)

opacity_theo_slider.observe(select_isotherm, 'value')

opacity_expe_slider = widgets.FloatSlider(
    value=0.2,
    min=0.0,
    max=1.0,
    step=0.05,
    description="",
    disabled=False,
    continuous_update=True,
    orientation='horizontal',
    readout=True,
    layout = widgets.Layout(width = '90%')
)

opacity_expe_slider.observe(select_isotherm, 'value')

tracer_p = widgets.Label(value=" - ")
tracer_p_base = widgets.Label(value="$p =$")

tracer_v = widgets.Label(value=" - ")
tracer_v_base = widgets.Label(value="$v =$")

tracer_T = widgets.Label(value=" - ")
tracer_T_base = widgets.Label(value="$T =$")

right_block_111_000.children = [
    widgets.Label(value="Select visible isotherms:"),
    select_visible,
    show_all_button,
    widgets.Label(
        value="Theoretical opacity:",
```

(continues on next page)

(continued from previous page)

```
        layout=widgets.Layout(
            margin='20px 0 0 0'
        )
    ),
    opacity_theo_slider,
    widgets.Label(
        value="Experimental opacity:",
        layout=widgets.Layout(
            margin='20px 0 0 0'
        )
    ),
    opacity_expe_slider,
    widgets.HBox([
        tracer_p_base,
        tracer_p,
    ]),
    widgets.HBox([
        tracer_v_base,
        tracer_v,
    ]),
    widgets.HBox([
        tracer_T_base,
        tracer_T,
    ]),
]

################################
#tracer_block
################################

tracer_block_111_000 = widgets.VBox(
    [],
    layout=widgets.Layout(
        align_items="center",
        width="100%"
    )
)

show_tracer_checkbox = widgets.Checkbox(
    value=False,
    description='Show tracer',
    disabled=False,
    layout=widgets.Layout(width='40%')
)

show_tracer_checkbox.observe(show_tracer, 'value')


v_slider = widgets.FloatSlider(
    value=1.0,
    min=0.5,
    max=5.0,
    step=0.001,
    description=r'\( v \)',
    disabled=True,
    continuous_update=True,
    orientation='horizontal',
```

(continues on next page)

(continued from previous page)

```
    readout=True,
    readout_format='.2f',
    layout = widgets.Layout(width = '90%')
)

v_slider.observe(update_tracer, 'value')

label_input = widgets.Text(
    value='',
    placeholder="Label:",
    disabled = True,
)

add_label_button = widgets.Button(
        description='Add label',
        disabled=True,
        button_style='',
        tooltip="Add label in tracer's position",
    )

add_label_button.on_click(add_label_button_clicked)

undo_label_button = widgets.Button(
        description='Undo',
        disabled=True,
        button_style='',
        tooltip="Remove last added label",
    )

undo_label_button.on_click(undo_label_button_clicked)

tracer_block_111_000.children = [
    widgets.HBox([
        show_tracer_checkbox,
    ],
        layout=widgets.Layout(
            align_items="center",
            width="70%")
    ),
    v_slider,
    widgets.HBox([
        label_input,
        add_label_button,
        undo_label_button
    ],
        layout=widgets.Layout(
            align_items="center"
        )
    )
]

############################
#FIGURE BLOCK
############################
change_isotherms(None)

figure_block_111_000 = widgets.VBox(
```

(continues on next page)

(continued from previous page)

```
    [],
    layout = widgets.Layout(width='70%')
)

prepare_export_fig_111_000_button = widgets.Button(
        description='Export',
        disabled=False,
        button_style='',
        tooltip='',
    )

prepare_export_fig_111_000_button.on_click(prepare_export)

go_to_export_button = widgets.HTML()

figure_block_111_000.children = [
    widgets.HBox([
        p_slider,
        fig_111_000,
        T_slider
    ]),
    widgets.VBox([
        prepare_export_fig_111_000_button,
        go_to_export_button
        ],
        layout=widgets.Layout(
            align_items="center",
            width="100%"
        )
    ),
    tracer_block_111_000
]

middle_block_111_000.children = [
    left_block_111_000,
    figure_block_111_000,
    right_block_111_000
]

############################
########MAIN BLOCK##########
############################

main_block_111_000 = widgets.VBox(
    [],
    layout=widgets.Layout(
        width='100%',
        align_items='center'
    )
)


main_block_111_000.children = [
    top_block_111_000,
    middle_block_111_000,
]
```

(continues on next page)

(continued from previous page)

```
figures = [
    fig_111_000
]

main_block_111_000
```

## 1.8 p-T plane and Gibbs free energy

**Code:** #11B-000

**File:** `apps/van_der_waals/p_T_2D.ipynb`

**Run it online:**

---

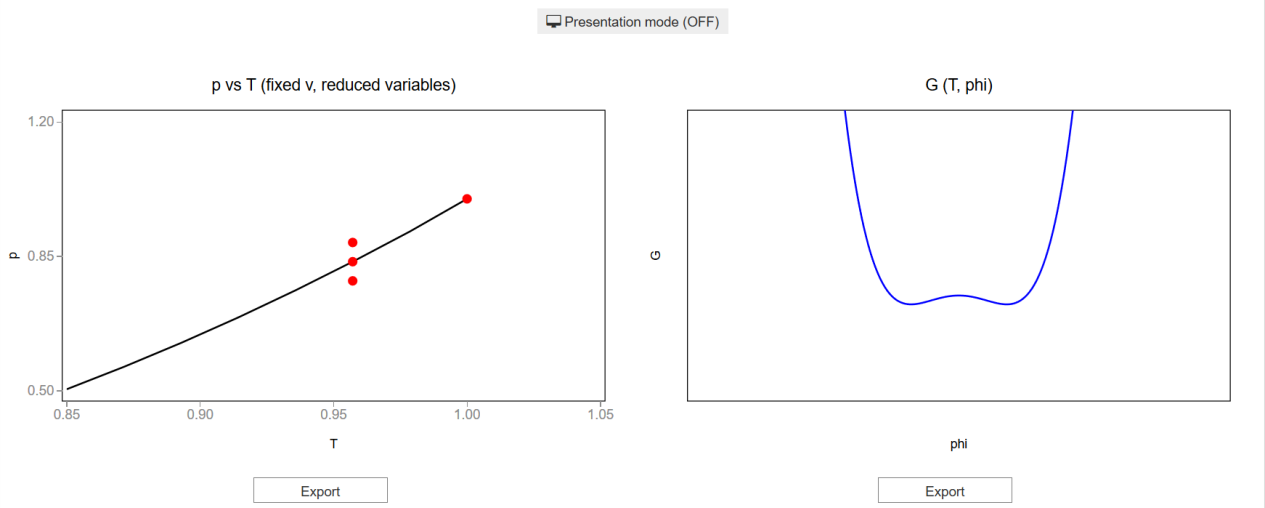
The aim of this Notebook is to visualize the Gibbs energy in different points of the p-T plane.

### 1.8.1 Interface

The main interface (`main_block_11B_000`) is divided in two VBox containing two bqplot Figures and `fig_11B_001` and `fig_11B_001`.

[1]:
```
from IPython.display import Image
Image(filename='../../static/images/apps/11B-000_1.png')
```

[1]:




### 1.8.2 CSS

A custom `css` file is used to improve the interface of this application. It can be found here.

[2]:
```
from IPython.display import HTML
display(HTML("<head><link rel='stylesheet' type='text/css' href='./../../static/
↪custom.css'></head>"))
display(HTML("<style>.container { width:100% !important; }</style>"))
```

```
<IPython.core.display.HTML object>
```

```
<IPython.core.display.HTML object>
```

### 1.8.3 Packages

[3]:
```
from bqplot import *
import bqplot as bq
import bqplot.marks as bqm
import bqplot.scales as bqs
import bqplot.axes as bqa

import ipywidgets as widgets

import urllib.parse
import webbrowser

import sys
```

### 1.8.4 Physical functions

This are the functions that have a physical meaning:

- `get_relative_isotherms`
- `experimental_isotherms`
- `find_real_fixed_T`
- `get_roots`
- `p_indefinite_integral`
- `definite_integral`
- `get_gibbs_energy`

[4]:
```
def get_relative_isotherms(v_range, T_range):
    """This function calculates the theoretical p(v, T) plane
        (in reduced coordinates) according to van der Waals
        equation of state from a given range of volumes
        and tenperatures.

    Args:
        v_range: An array containing the values of v
        (in reduced coordinates)for which the isotherms must be
        calculated.\n
        T_range: An array containing the values of T
        (in reduced coordinates)for which the isotherms must be
        calculated.\n


    Returns:
        isotherms: A list consisted of numpy arrays containing the
        pressures of each isotherm.
    """
```

(continues on next page)

(continued from previous page)

```
    isotherms = []

    for T in T_range:
        p_R = []
        for v in v_range:
            val = (8.0/3.0*T/(v - 1.0/3.0) - 3.0/v**2)
            p_R = np.append(p_R, val)

        isotherms.append(p_R)

    return isotherms
```

[5]:
```
def experimental_isotherms(p_range, v_range, T_range, fixed_p, fixed_T):
    """This function calculates the experimental p(v, T) plane
        (in reduced coordinates) according to van der Waals
        equation of state for a given range of volumes
        and tenperatures or for a given range of volumes
        and pressures.

    Args:
        p_range: An array containing the values of p
        (in reduced coordinates)for which the isotherms must be
        calculated. Only used if fixed_p == True.\n
        v_range: An array containing the values of v
        (in reduced coordinates)for which the isotherms must be
        calculated.\n
        T_range: An array containing the values of v
        (in reduced coordinates)for which the isotherms must be
        calculated. Only used if fixed_T == True.\n
        fixed_p: Boolean variable which represents if the isotherms
        must be calculated for a given pressures.\n
        fixed_T: Boolean variable which represents if the isotherms
        must be calculated for a given pressures.\n


    Returns:
        expe_data: A list consisted of numpy arrays containing the
        pressures of each theoretical isotherm.\n
        theo_data: A list consisted of numpy arrays containing the
        pressures of each theoretical isotherm.\n
        v_limits: A list consisted of arrays of the volume limits of
        the phase-transition of each subcritical isotherm.\n
        p_limits: A list consisted of arrays of the pressure limits of
        the phase-transition of each subcritical isotherm.\n
        tenperatures: A list consisted of the tenperatures of the
        isotherms.\n
    """

    if fixed_T:

        theo_data = get_relative_isotherms(v_range, T_range)
        expe_data = []

        v_limits = []
        p_limits = []
```

(continues on next page)

(continued from previous page)

```
        p_range = np.linspace(0.001, 1.0, num=10000)
        pressures, v_isobaric_limits = find_real_fixed_T(p_range, T_range)

        for i in range(len(theo_data)):

            p_expe = []

            if i < len(v_isobaric_limits):

                    v_lim = v_isobaric_limits[i]

                    if len(v_lim) > 1: #check if there is only one point
                        for j in range(len(v_range)):

                            if v_range[j] > v_lim[0] and v_range[j] < v_lim[1]:
                                p_expe.append(pressures[i])

                            else:
                                p_expe.append(theo_data[i][j])

                        v_limits = np.append(v_limits, [v_lim[0], v_lim[1]])
                        p_limits = np.append(p_limits, [pressures[i], pressures[i]])

                    else:
                        p_expe = theo_data[i]
                        v_limits = np.append(v_limits, [1.0])
                        p_limits = np.append(p_limits, [1.0])

            else:

                p_expe = theo_data[i]

            expe_data.append(p_expe)

        tenperatures = T_range

        return expe_data, theo_data, p_limits, v_limits, tenperatures

    elif fixed_p:

        tenperatures, v_isobaric_limits = find_real_fixed_p(p_range, T_range)

        theo_data = get_relative_isotherms(v_range, tenperatures)
        expe_data = []

        v_limits = []
        p_limits = []

        for i in range(len(theo_data)):

            p_expe = []

            if i < len(v_isobaric_limits):

                    v_lim = v_isobaric_limits[i]

                    if len(v_lim) > 1: #check if there is only one point
```

(continues on next page)

(continued from previous page)

```
                    for j in range(len(v_range)):

                        if v_range[j] > v_lim[0] and v_range[j] < v_lim[1]:
                            p_expe.append(p_range[i])

                        else:
                            p_expe.append(theo_data[i][j])

                    v_limits = np.append(v_limits, [v_lim[0], v_lim[1]])
                    p_limits = np.append(p_limits, [p_range[i], p_range[i]])

                else:
                    p_expe = theo_data[i]
                    v_limits = np.append(v_limits, [1.0])
                    p_limits = np.append(p_limits, [1.0])

            else:

                p_expe = theo_data[i]

            expe_data.append(p_expe)

        return expe_data, theo_data, p_limits, v_limits, tenperatures
```

[6]:
```
def get_roots(p, T):
    """This function finds the intersection between an isobaric curve
       and Van der Waals equation of state for a given T.\n
       Values of v with no physical meaning are dismissed
       (v < 0 or complex).

    Args:
        p: Pressure of the isobaric curve.\n
        T: Tenperature of the isotherm.\n


    Returns:
        roots_in_range: A sorted list of the volumes in which the
        isobaric curve intersects the isotherm.\n
    """

    roots = np.roots([1.0, - 1.0/3.0*(1.0 + 8.0*T/p), 3.0/p, -1.0/p])
    roots_in_range = []

    for root in roots:

        # A third degree polynomial has 3 complex roots,
        # but we are only interested in the ones which are
        # purely real.

        if np.isreal(root):

            root = np.real(root)

            if root > 0:
```

(continues on next page)

(continued from previous page)

```
                roots_in_range.append(root)

    roots_in_range.sort()

    return roots_in_range
```

[7]:
```
def p_indefinite_integral(p_0, v_0, T):
    """This function calculates the indefinite integral between
    a van der Waals isotherm and a isobaric line.

    Args:
        p0: Isobaric line's pressure.\n
        v0: Value of the volume.\n
        T: Value of the tenperature.\n

    Returns:
        integral: Value of the indefinite integral between a
        van der Waals isotherm at T and a isobaric line of p0 at a
        volume v0.\n
    """

    integral = 8.0/3.0 * T *np.log(v_0 - 1.0/3.0) + 3.0/v_0 - p_0*v_0

    return integral
```

[8]:
```
def definite_integral(p_0, v_range, T):
    """This function 'p_indefinite_integral' function to calculate
    the definite integral between a van der Waals isotherm and a
    isobaric line.

    Args:
        p0: Isobaric line's pressure.\n
        v_range: Tuple or list consisted of volume limits.\n
        T: Value of the tenperature.\n

    Returns:
        integral: Value of the definite integral between a
        van der Waals isotherm at T and a isobaric line of p0 in a
        volume range v_range.\n
    """

    v_0, v_1 = v_range[0], v_range[1]

    integral = p_indefinite_integral(p_0, v_1, T) - p_indefinite_integral(p_0, v_0, T)

    return integral
```

[9]:
```
def find_real_fixed_T(p_values, T_values):
    """This function uses Maxwell's construction to find the
       pressures in which phase transition happens given some
       fixed tenperatures.\n

    Args:
        p_values: List of pressures in which the real isotherm is
        searched.\n
```

(continues on next page)

(continued from previous page)

```
        T_values: List of tenperatures of the isotherms.\n


    Returns:
        pressures: List of pressures in which phase transition
        happens.\n
        v_range: Volume limits of phase transition zones.
    """

    eps = 1e-3

    pressures = []
    v_ranges = []

    for T in T_values:

        if T < 1.0:

            for p in p_values:

                roots = get_roots(p, T)

                if len(roots) == 3:

                    v_range = [roots[0], roots[2]]
                    area = definite_integral(p, v_range, T)

                    if abs(area) < eps:

                        pressures.append(p)
                        v_ranges.append(v_range)

                        break

        elif T == 1.0:

            pressures.append(1.0)
            v_ranges.append([1.0])

    return pressures, v_ranges
```

[10]:
```
def get_gibbs_energy(G_1, G_2, G_3, G_4, phi):
    """This function calculates the representation of Gibbs energy
    for a given constants.\n

    G = G_1*phi + G_2*phi**2 + G_3*phi**3 + G_4*phi**4

    Args:
        G_1, G_2, G_3, G_4: Values of the parameters.
        phi: Array consisted of the values where Gibbs energy
        must be calculated.

    Returns:
        gibbs: Array containing the values of Gibbs energy.

    """
```

(continues on next page)

(continued from previous page)

```
    gibbs = []

    for f in phi:
        gibbs = np.append(gibbs, G_1*f + G_2*f**2 + G_3*f**3 + G_4*f**4)

    return gibbs
```

### 1.8.5 Functions related to interaction

[11]:
```
def hover_handler(self, content):
    """This function update the line 'gibbs_lines' from
    'fig_11B_002' when the cursor goes over 'scatter_points'.
    """

    g = {0:[-40, -40, 1.0, 20],
         1:[0, -40, 0, 40],
         2:[40, -40, -1.0, 20],
         3:[0, 40, 0, 20]}

    params = g.get(content.get('data').get('index'))

    gibbs = get_gibbs_energy(
        G_1=params[0],
        G_2=params[1],
        G_3=params[2],
        G_4=params[3],
        phi = phi
    )

    scale_y_11B_002.min = min(gibbs) - 100
    scale_y_11B_002.max = 200

    gibbs_lines.y = gibbs
    #tt_box.children = [fig_11B_002,]
```

[12]:
```
def change_view(change):
    """This function changes the visualization of all the
    components of the application so they are suitable for
    a projection.\n
    """

    obj = change.owner

    if obj.value:

        obj.description = 'Presentation mode (ON)'

        display(HTML(
            "<style>" \
            ".widget-readout { font-size: 30px ; }" \
            ".widget-label-basic {font-size: 30px;}" \
            "option {font-size: 25px;}" \
            ".p-Widget.jupyter-widgets.widget-slider.widget-vslider.widget-inline-
↪vbox {width: auto}" \
```

(continues on next page)

(continued from previous page)

```
            ".p-Widget .jupyter-widgets .widgets-label {width: auto; height: auto;␣
↪font-size: 30px;}" \
            ".widget-label {font-size: 30px ; height: auto !important;}" \
            ".p-Widget .bqplot .figure .jupyter-widgets {height: auto !important;}" \
            ".widget-text input[type='number'] {font-size: 30px;height: auto;}" \
            ".option { font-size: 30px ;}" \
            ".p-Widget .jupyter-widgets .jupyter-button.widget-button {font-size:␣
↪30px ; width: auto; height: auto;}" \
            ".p-Widget.jupyter-widgets.jupyter-button.widget-toggle-button{font-size:␣
↪30px ; width: auto; height: auto;}" \
            ".p-Widget.p-Panel.jupyter-widgets.widget-container.widget-box.widget-
↪vbox {padding-bottom: 30px}" \
            ".bqplot > svg .axis text.axislabel, .bqplot > svg .axis tspan.axislabel
↪{font-size: 30px;}" \
            ".q-grid .slick-cell {font-size: 30px;}" \
            ".slick-column-name {font-size: 30px;}" \
            ".widget-html-content {font-size: 30px;}"
            "</style>"
            )
        )

        for figure in figures:

            figure.legend_text = {'font-size': '30px'}
            figure.title_style = {'font-size': '30px'}

            for axis in figure.axes:
                axis.tick_style = {'font-size': '30px'}
                axis.label_style = {'font-size': '30px'}

    else:

        obj.description = 'Presentation mode (OFF)'

        display(HTML(
            "<style>" \
            ".widget-readout { font-size: 14px ;}" \
            ".widget-label-basic {font-size: 14px;}" \
            "option {font-size: 12px;}" \
            ".p-Widget .jupyter-widgets .widgets-label {font-size: 14px;}" \
            ".widget-label {font-size: 14px ;}" \
            ".widget-text input[type='number'] {font-size: 14px;}" \
            ".option { font-size: 14px ;}" \
            ".p-Widget .jupyter-widgets .jupyter-button.widget-button {font-size:␣
↪14px;}" \
            ".p-Widget.jupyter-widgets.jupyter-button.widget-toggle-button {font-size:
↪ 14px;}" \
            ".bqplot > svg .axis text.axislabel, .bqplot > svg .axis tspan.axislabel
↪{font-size: 14px;}" \
            ".q-grid .slick-cell {font-size: 14px;}" \
            ".slick-column-name {font-size: 14px;}" \
            ".widget-html-content {font-size: 14px;}"
            "</style>"
            )
        )

        for figure in figures:
```

(continues on next page)

(continued from previous page)

```
            figure.legend_text = {'font-size': '14px'}
            figure.title_style = {'font-size': '20px'}

            for axis in figure.axes:
                axis.tick_style = {'font-size': '14px'}
                axis.label_style = {'font-size': '14px'}
```

[13]:
```
def prepare_export(button):
    """This function sends the selected plot to the 'export_plot'
    function.
    """

    if button is prepare_export_fig_11B_001_button:

        export_plot(fig_11B_001)

    elif button is prepare_export_fig_11B_002_button:

        export_plot(fig_11B_002)
```

[14]:
```
def export_plot(plot):
    """This function sends the selected plot to the export module.
    """

    global data

    text_lines = []

    np.set_printoptions(threshold=sys.maxsize)

    tooltips = []

    for mark in plot.marks:
        tooltips.append(mark.tooltip)
        mark.tooltip = None

    data =  repr((plot, text_lines))

    %store data

    rel_url = "../../../apps/modules/export_module.ipynb"
    abs_url = urllib.parse.urljoin(notebook_url, rel_url)

    if not webbrowser.open(abs_url):
        go_to_export_button.value = "<form action=" + abs_url + " target='_blank'>
↪<button type=''submit''>Open in export module</button></form>"

    for i in range(len(plot.marks)):
        mark = plot.marks[i]
        mark.tooltip = tooltips[i]
```

[ ]:
```
%%javascript

//Get the URL of the current notebook
```

(continues on next page)

(continued from previous page)

```
var kernel = Jupyter.notebook.kernel;
var command = ["notebook_url = ",
               "'", window.location.href, "'" ].join('')

kernel.execute(command)
```

### 1.8.6 Main interface

[ ]:
```
v_values = np.linspace(start=0.4, stop=5, num=1000)
T_values = np.linspace(start=0.85, stop=1.0, num=8)

expe_data, theo_data, trans_pressures, v_limits, trans_tenperatures = experimental_
↪isotherms(
     p_range = [],
     v_range = v_values,
     T_range = T_values,
     fixed_p = False,
     fixed_T = True
)

trans_pressures = np.unique(trans_pressures)

j = 5

scatter_pres = [
    trans_pressures[j]-0.05,
    trans_pressures[j],
    trans_pressures[j]+0.05,
    1.0
]

scatter_tenp = [T_values[j], T_values[j], T_values[j], 1.0]

phi = np.linspace(-12, 5, 500)

scale_x_11B_001 = bqs.LinearScale(min = min(T_values), max = 1.05)
scale_y_11B_001 = bqs.LinearScale(min = min(trans_pressures), max = 1.2)

fig_11B_001 = bq.Figure(
    title='p vs T (fixed v, reduced variables)',
    marks=[],
    axes=[],
    animation_duration=0,
    layout = widgets.Layout(width='100%'),
    legend_location='top-right',
    background_style= {'fill': 'white',  'stroke': 'black'},
    fig_margin=dict(top=80, bottom=80, left=60, right=30),
    toolbar = True,
)

axis_x_11B_001 = bqa.Axis(
    scale=scale_x_11B_001,
    tick_format='0.2f',
    tick_style={'font-size': '15px'},
```

(continues on next page)

(continued from previous page)

```
    tick_values=[0.85, 0.9, 0.95, 1, 1.05],
    grid_lines = 'none',
    grid_color = '#8e8e8e',
    label='T',
    label_location='middle',
    label_style={'stroke': 'black', 'default-size': 35},
    label_offset='50px'
)

axis_y_11B_001 = bqa.Axis(
    scale=scale_y_11B_001,
    tick_format='0.2f',
    tick_style={'font-size': '15px'},
    tick_values=[0.5, 0.85, 1.2],
    grid_lines = 'none',
    grid_color = '#8e8e8e',
    orientation='vertical',
    label='p',
    label_location='middle',
    label_style={'stroke': 'red', 'default_size': 35},
    label_offset='50px'
)

fig_11B_001.axes = [
    axis_x_11B_001,
    axis_y_11B_001
]

pressures_lines = bqm.Lines(
    name = '',
    x = T_values,
    y = trans_pressures,
    scales = {'x': scale_x_11B_001, 'y': scale_y_11B_001},
    visible = True,
    colors = ['black'],
    names = [],
    labels=['labels']
)

critic_point = bqm.Scatter(
    name = '',
    x = [1.0],
    y = [1.0],
    scales = {'x': scale_x_11B_001, 'y': scale_y_11B_001},
    visible = True,
    colors = ['red'],
    names = [],
    labels=[]
)

tt_box = widgets.HBox([])

scatter_points = bqm.Scatter(
    name = '',
    x = scatter_tenp,
    y = scatter_pres,
    scales = {'x': scale_x_11B_001, 'y': scale_y_11B_001},
```

(continues on next page)

(continued from previous page)

```
    visible = True,
    colors = ['red'],
    names = [],
    labels=[],
)

scatter_points.on_hover(hover_handler)

fig_11B_001.marks = [
    pressures_lines,
    scatter_points
]

scale_x_11B_002 = bqs.LinearScale(min = -4, max = 4)
scale_y_11B_002 = bqs.LinearScale()

fig_11B_002 = bq.Figure(
    title='G (T, phi)',
    marks=[],
    axes=[],
    animation_duration=0,
    layout = widgets.Layout(width='100%'),
    legend_location='top-right',
    background_style= {'fill': 'white',  'stroke': 'black'},
    fig_margin=dict(top=80, bottom=80, left=60, right=30),
    toolbar = True
)

axis_x_11B_002 = bqa.Axis(
    scale=scale_x_11B_002,
    tick_format='0.2f',
    tick_style={'font-size': '15px'},
    num_ticks=0,
    grid_lines = 'none',
    grid_color = '#8e8e8e',
    label='phi',
    label_location='middle',
    label_style={'stroke': 'black', 'default-size': 35},
    label_offset='50px'
)

axis_y_11B_002 = bqa.Axis(
    scale=scale_y_11B_002,
    tick_format='0.2f',
    tick_style={'font-size': '15px'},
    num_ticks=0,
    grid_lines = 'none',
    grid_color = '#8e8e8e',
    orientation='vertical',
    label='G',
    label_location='middle',
    label_style={'stroke': 'red', 'default_size': 35},
    label_offset='30px'
)

fig_11B_002.axes = [
    axis_x_11B_002,
```

(continues on next page)

(continued from previous page)

```
    axis_y_11B_002
]

gibbs_lines = bqm.Lines(
    name = '',
    x = phi,
    y = [],
    scales = {'x': scale_x_11B_002, 'y': scale_y_11B_002},
    visible = True,
    colors = ['blue'],
    names = [],
    labels=['']
)

fig_11B_002.marks = [gibbs_lines]

change_view_button = widgets.ToggleButton(
    value=False,
    description='Presentation mode (OFF)',
    disabled=False,
    button_style='',
    tooltip='',
    icon='desktop',
    layout=widgets.Layout(
        width='initial',
        align_self='center'
    )
)

change_view_button.observe(change_view, 'value')

prepare_export_fig_11B_001_button = widgets.Button(
    description='Export',
    disabled=False,
    button_style='',
    tooltip='',
)

prepare_export_fig_11B_001_button.on_click(prepare_export)

prepare_export_fig_11B_002_button = widgets.Button(
    description='Export',
    disabled=False,
    button_style='',
    tooltip='',
)

prepare_export_fig_11B_002_button.on_click(prepare_export)

main_block_11B_000 = widgets.VBox(
    [],
    layout = widgets.Layout(
        align_items='center',
        width='100%'
    )
)
```

(continues on next page)

(continued from previous page)

```
main_block_11B_000.children = [
    change_view_button,
    widgets.HBox([
        widgets.VBox([
            fig_11B_001,
            prepare_export_fig_11B_001_button
        ],
            layout = widgets.Layout(
                align_items='center',
                width='100%'
            )
        ),
        widgets.VBox([
            fig_11B_002,
            prepare_export_fig_11B_002_button
        ],
            layout = widgets.Layout(
                align_items='center',
                width='100%'
            )
        ),
    ],
        layout = widgets.Layout(
                align_items='center',
                width='100%'
            )
    )
]

figures = [
    fig_11B_001,
    fig_11B_002
]

main_block_11B_000
```

## 1.9 Chemical potential of a van der Waals real gas

**Code:** #117-000

**File:** `apps/van_der_waals/chemical_potential.ipynb`

**Run it online:**

---

The aim of this notebook is to show the contruction of the chemical potential based in van der Waals' isotherms.

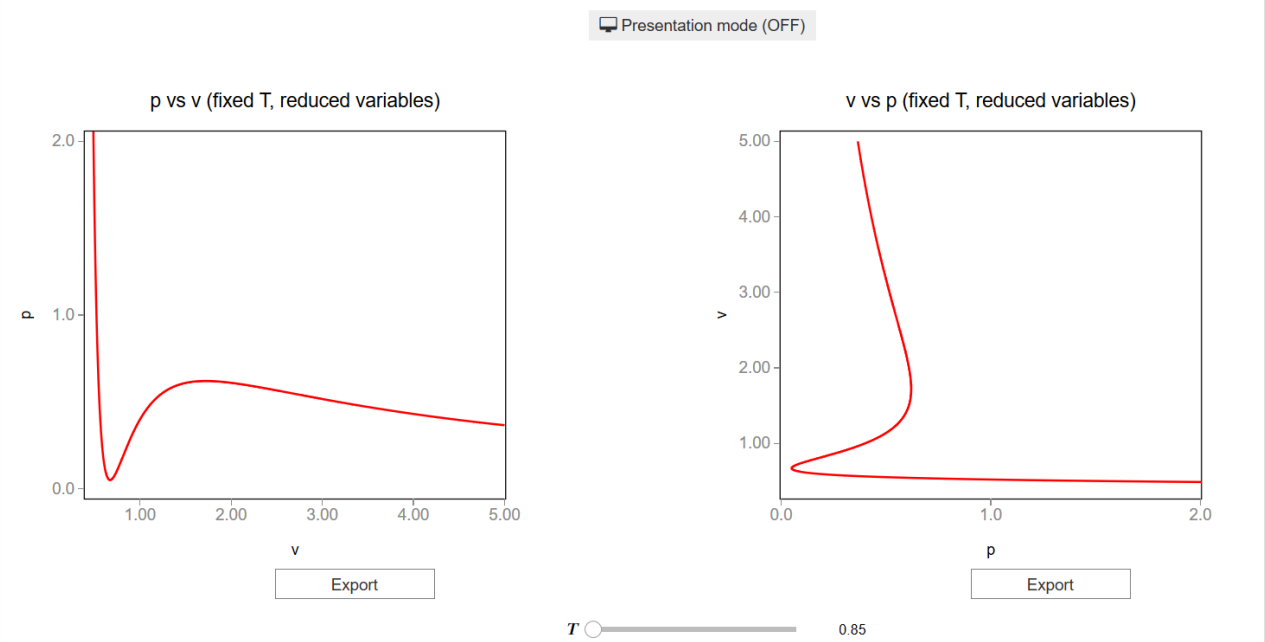
### 1.9.1 Interface

The main interface (`main_block_117_000`) is divided in five VBox: `block_1`, `block_2`, `block_3`, `block_4` and `block_5`. `block_1` contains two bqplot Figures: `fig_117_001` and `fig_117_002`. `block_2` contains the `T_slider` widget which controls the isotherms and chemical potentials shown in `fig_117_001`, `fig_117_002`, `fig_117_003` and `fig_117_004`. `block_3` contains two bqplot Figures: `fig_117_003`

and `fig_117_004`. `block_4` contains two bqplot Figures: `fig_117_005` and `fig_117_006`. `block_5` contains two bqplot Figures: `fig_117_007` and `fig_117_008`.

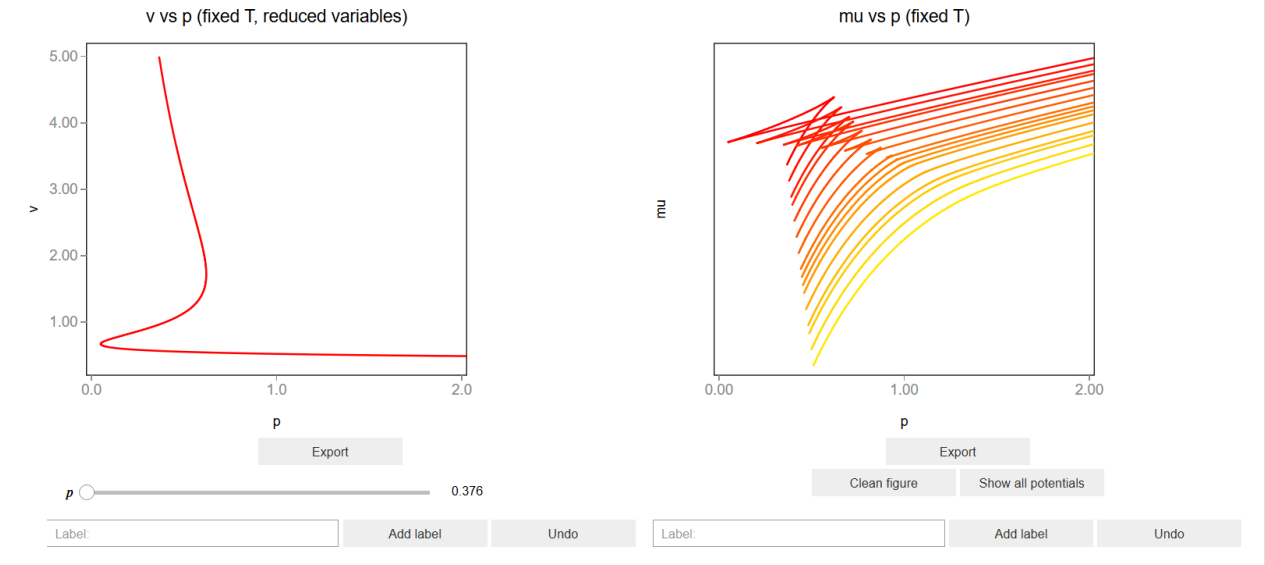
[1]:
```
from IPython.display import Image
Image(filename='../../static/images/apps/117-000_1.png')
```

[1]:



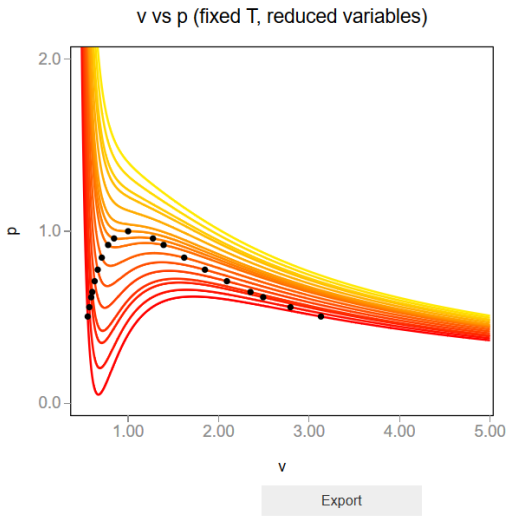

[2]:
```
Image(filename='../../static/images/apps/117-000_2.png')
```

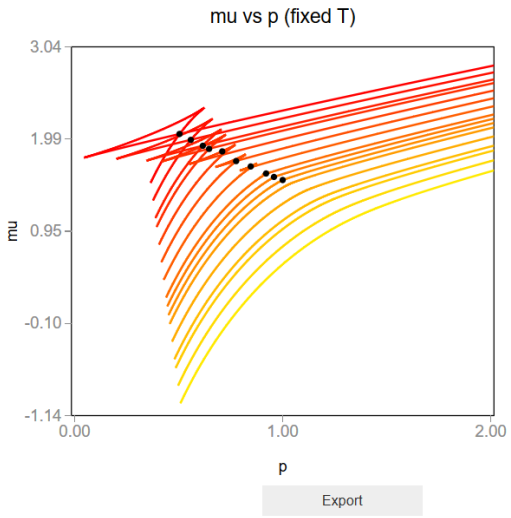
[2]:




[3]:
```
Image(filename='../../static/images/apps/117-000_3.png')
```

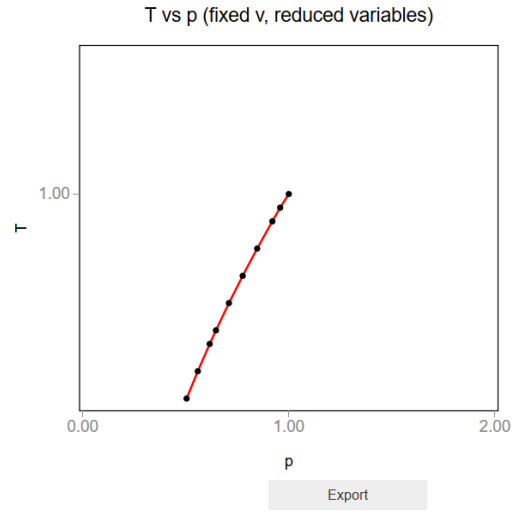
[3]:

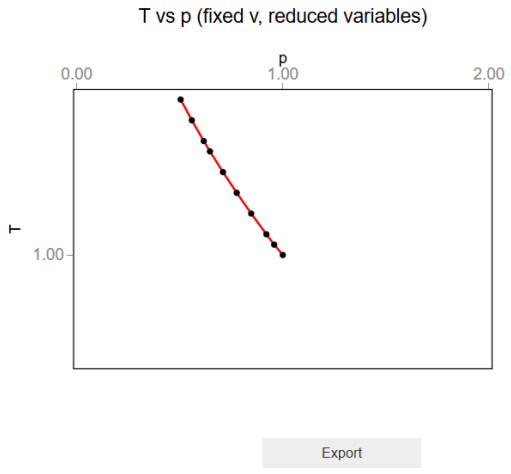



[4]:
```
Image(filename='../../static/images/apps/117-000_4.png')
```

[4]:




### 1.9.2 CSS

A custom `css` file is used to improve the interface of this application. It can be found here.

[5]:
```
from IPython.display import HTML
display(HTML("<head><link rel='stylesheet' type='text/css' href='./../../static/
↪custom.css'></head>"))
display(HTML("<style>.container { width:100% !important; }</style>"))
display(HTML("<style>.widget-label { display: contents !important; }</style>"))
display(HTML("<style>.slider-container { margin: 12px !important; }</style>"))
display(HTML("<style>.jupyter-widgets { overflow: auto !important; }</style>"))
```

```
<IPython.core.display.HTML object>
```

```
<IPython.core.display.HTML object>
<IPython.core.display.HTML object>
<IPython.core.display.HTML object>
<IPython.core.display.HTML object>
```

### 1.9.3 Packages

[6]:
```
from bqplot import *
import bqplot as bq
import bqplot.marks as bqm
import bqplot.scales as bqs
import bqplot.axes as bqa

import ipywidgets as widgets

import urllib.parse
import webbrowser

import sys
```

### 1.9.4 Physical functions

This are the functions that have a physical meaning:

- get_relative_isotherms
- experimetal_isotherms
- get_roots
- p_indefinite_integral
- p_definite_integral
- find_real_fixed_p
- find_real_fixed_T
- get_chemical_potential

[7]:
```
def get_relative_isotherms(v_range, T_range):
    """This function calculates the theoretical p(v, T) plane
        (in reduced coordinates) according to van der Waals
        equation of state from a given range of volumes
        and tenperatures.

    Args:
        v_range: An array containing the values of v
        (in reduced coordinates)for which the isotherms must be
        calculated.\n
        T_range: An array containing the values of v
        (in reduced coordinates)for which the isotherms must be
        calculated.\n
```

(continues on next page)

(continued from previous page)

```
    Returns:
        isotherms: A list consisted of numpy arrays containing the
        pressures of each isotherm.
    """

    isotherms = []

    for T in T_range:
        p_R = []
        for v in v_range:
            val = (8.0/3.0*T/(v - 1.0/3.0) - 3.0/v**2)
            p_R = np.append(p_R, val)

        isotherms.append(p_R)

    return isotherms

    return isotherms
```

[8]:
```
def experimental_isotherms(p_range, v_range, T_range, fixed_p, fixed_T):
    """This function calculates the experimental p(v, T) plane
        (in reduced coordinates) according to van der Waals
        equation of state for a given range of volumes
        and tenperatures or for a given range of volumes
        and pressures.

    Args:
        p_range: An array containing the values of p
        (in reduced coordinates)for which the isotherms must be
        calculated. Only used if fixed_p == True.\n
        v_range: An array containing the values of v
        (in reduced coordinates)for which the isotherms must be
        calculated.\n
        T_range: An array containing the values of v
        (in reduced coordinates)for which the isotherms must be
        calculated. Only used if fixed_T == True.\n
        fixed_p: Boolean variable which represents if the isotherms
        must be calculated for a given pressures.\n
        fixed_T: Boolean variable which represents if the isotherms
        must be calculated for a given pressures.\n


    Returns:
        expe_data: A list consisted of numpy arrays containing the
        pressures of each theoretical isotherm.\n
        theo_data: A list consisted of numpy arrays containing the
        pressures of each theoretical isotherm.\n
        v_limits: A list consisted of arrays of the volume limits of
        the phase-transition of each subcritical isotherm.\n
        p_limits: A list consisted of arrays of the pressure limits of
        the phase-transition of each subcritical isotherm.\n
        tenperatures: A list consisted of the tenperatures of the
        isotherms.\n
    """

    if fixed_T:
```

(continues on next page)

(continued from previous page)

```
        theo_data = get_relative_isotherms(v_range, T_range)
        expe_data = []

        v_limits = []
        p_limits = []

        p_range = np.linspace(0.001, 1.0, num=10000)
        pressures, v_isobaric_limits = find_real_fixed_T(p_range, T_range)

        for i in range(len(theo_data)):

            p_expe = []

            if i < len(v_isobaric_limits):

                    v_lim = v_isobaric_limits[i]

                    if len(v_lim) > 1: #check if there is only one point
                        for j in range(len(v_range)):

                            if v_range[j] > v_lim[0] and v_range[j] < v_lim[1]:
                                p_expe.append(pressures[i])

                            else:
                                p_expe.append(theo_data[i][j])

                        v_limits = np.append(v_limits, [v_lim[0], v_lim[1]])
                        p_limits = np.append(p_limits, [pressures[i], pressures[i]])

                    else:
                        p_expe = theo_data[i]
                        v_limits = np.append(v_limits, [1.0])
                        p_limits = np.append(p_limits, [1.0])

            else:

                p_expe = theo_data[i]

            expe_data.append(p_expe)

        tenperatures = T_range

        return expe_data, theo_data, p_limits, v_limits, tenperatures

    elif fixed_p:

        tenperatures, v_isobaric_limits = find_real_fixed_p(p_range, T_range)

        theo_data = get_relative_isotherms(v_range, tenperatures)
        expe_data = []

        v_limits = []
        p_limits = []

        for i in range(len(theo_data)):
```

(continues on next page)

(continued from previous page)

```
            p_expe = []

            if i < len(v_isobaric_limits):

                    v_lim = v_isobaric_limits[i]

                    if len(v_lim) > 1: #check if there is only one point

                        for j in range(len(v_range)):

                            if v_range[j] > v_lim[0] and v_range[j] < v_lim[1]:
                                p_expe.append(p_range[i])

                            else:
                                p_expe.append(theo_data[i][j])

                        v_limits = np.append(v_limits, [v_lim[0], v_lim[1]])
                        p_limits = np.append(p_limits, [p_range[i], p_range[i]])

                    else:
                        p_expe = theo_data[i]
                        v_limits = np.append(v_limits, [1.0])
                        p_limits = np.append(p_limits, [1.0])

            else:

                p_expe = theo_data[i]

            expe_data.append(p_expe)

        return expe_data, theo_data, p_limits, v_limits, tenperatures
```

[9]:
```
def get_roots(p, T):
    """This function finds the intersection between an isobaric curve
       and Van der Waals equation of state for a given T.\n
       Values of v with no physical meaning are dismissed
       (v < 0 or complex).

    Args:
        p: Pressure of the isobaric curve.\n
        T: Tenperature of the isotherm.\n


    Returns:
        roots_in_range: A sorted list of the volumes in which the
        isobaric curve intersects the isotherm.\n
    """

    roots = np.roots([1.0, - 1.0/3.0*(1.0 + 8.0*T/p), 3.0/p, -1.0/p])
    roots_in_range = []

    for root in roots:

        # A third degree polynomial has 3 complex roots,
        # but we are only interested in the ones which are
        # purely real.
```

(continues on next page)

(continued from previous page)

```
        if np.isreal(root):

            root = np.real(root)

            if root > 0:

                roots_in_range.append(root)

    roots_in_range.sort()

    return roots_in_range
```

[10]:
```
def p_indefinite_integral(p_0, v_0, T):
    """This function calculates the indefinite integral between
    a van der Waals isotherm and a isobaric line.

    Args:
        p0: Isobaric line's pressure.\n
        v0: Value of the volume.\n
        T: Value of the tenperature.\n

    Returns:
        integral: Value of the indefinite integral between a
        van der Waals isotherm at T and a isobaric line of p0 at a
        volume v0.\n
    """

    integral = 8.0/3.0 * T *np.log(v_0 - 1.0/3.0) + 3.0/v_0 - p_0*v_0

    return integral
```

[11]:
```
def definite_integral(p_0, v_range, T):
    """This function 'p_indefinite_integral' function to calculate
    the definite integral between a van der Waals isotherm and a
    isobaric line.

    Args:
        p0: Isobaric line's pressure.\n
        v_range: Tuple or list consisted of volume limits.\n
        T: Value of the tenperature.\n

    Returns:
        integral: Value of the definite integral between a
        van der Waals isotherm at T and a isobaric line of p0 in a
        volume range v_range.\n
    """

    v_0, v_1 = v_range[0], v_range[1]

    integral = p_indefinite_integral(p_0, v_1, T) - p_indefinite_integral(p_0, v_0, T)

    return integral
```

[12]:
```
def find_real_fixed_T(p_values, T_values):
```

(continues on next page)

(continued from previous page)

```
    """This function uses Maxwell's construction to find the
       pressures in which phase transition happens given some
       fixed tenperatures.\n

    Args:
        p_values: List of pressures in which the real isotherm is
        searched.\n
        T_values: List of tenperatures of the isotherms.\n


    Returns:
        pressures: List of pressures in which phase transition
        happens.\n
        v_range: Volume limits of phase transition zones.
    """

    eps = 1e-3

    pressures = []
    v_ranges = []

    for T in T_values:

        if T < 1.0:

            for p in p_values:

                roots = get_roots(p, T)

                if len(roots) == 3:

                    v_range = [roots[0], roots[2]]
                    area = definite_integral(p, v_range, T)

                    if abs(area) < eps:

                        pressures.append(p)
                        v_ranges.append(v_range)

                        break

        elif T == 1.0:

            pressures.append(1.0)
            v_ranges.append([1.0])

    return pressures, v_ranges
```

[13]:
```
def get_chemical_potential(p_values, v_values):
    """This function calculates chemical potential by integrating
    v(p) isotherms.\n

    Args:
        p_values: List of numpy arrays containing the pressures of
        the isotherms.\n
        v_values: List of numpy arrays containing the volumes of
```

(continues on next page)

(continued from previous page)

```
        the isotherms.\n


    Returns:
        mu: List of numpy arrays containing the chemical potentials of
        the isotherms.
    """

    mu = []


    for i in range(len(v_values)):

        v = v_values[i]
        p = p_values[i]

        pot = [10.0] #starting random value

        l = np.size(p)

        for j in range(1, l):
            pot.append(pot[j-1] + v[j]*(p[j] - p[j-1]))

        mu.append(pot)

    return mu
```

### 1.9.5 Functions related with the interaction

[14]:
```
def find_nearest_index(array, value):
    """This function find index of the element in an array which
    value is the nearest to the given one.

    Args:
        array: A list or numpy array containing the elements.\n
        value: Float number.\n

    Returns:
        idx: Index of the element in array which value is the nearest
        to value.
    """

    array = np.asarray(array)
    idx = (np.abs(array - value)).argmin()
    return idx
```

[15]:
```
def update_tracer(change):
    """This function updates the tracer marks tracer_117_003
    (fig_117_003) and tracer_117_004 (fig_117_004).\n
    """

    tracer_117_003.visible = True
    tracer_117_004.visible = True
```

(continues on next page)

(continued from previous page)

```
    if p_slider.value == p_slider.options[-1]:
        p_slider.disabled = True

    v = theo_v_values_inverted[T_slider.index][p_slider.index]
    p = theo_p_values_inverted[T_slider.index][p_slider.index]

    tracer_117_003.x, tracer_117_003.y = [p], [v]

    area_117_003.x = np.append(area_117_003.x, p)
    area_117_003.y = np.append(area_117_003.y, v)

    lines_117_004.x = np.append(lines_117_004.x, p)
    lines_117_004.y = np.append(lines_117_004.y, mu[T_slider.index][p_slider.index])

    tracer_117_004.x, tracer_117_004.y = [p], [mu[T_slider.index][p_slider.index]]
```

[16]:
```
def restart_chemical_potential(a):
    """This function clear fig_117_004 and restarts
    the tracers tracer_117_003 and tracer_117_004 and
    deletes the labels labels_117_003 and labels_117_004.\n
    """

    lines_117_004.x, lines_117_004.y = [], []
    area_117_003.x, area_117_003.y = [], []

    p_slider.index = 0
    p_slider.disabled = False

    axis_y_004.scale =  bqs.LinearScale(
        min = min(mu[T_slider.index]),
        max = max(mu[T_slider.index])
    )

    lines_117_004.scales = {'x': scale_x_004, 'y': axis_y_004.scale}

    fig_117_004.axis = [
        axis_x_004,
        axis_y_004
    ]

    labels_117_003.x, labels_117_003.y = [], []
    labels_117_003.names = []

    labels_117_004.x, labels_117_004.y = [], []
    labels_117_004.names = []
```

[17]:
```
def change_tenperature(change):
    """This function changes the visible isotherm
    in fig_117_001, fig_117_002 and fig_117_003.\n
    """

    p_slider.options = theo_v_values_inverted[T_slider.index]

    #restart chemical potential plot and tracer
    restart_chemical_potential(None)
    update_tracer(None)
```

(continues on next page)

(continued from previous page)

```
    obj = change.owner

    i = obj.index

    opacities = [0.0 for t in obj.options]
    opacities[i] = 1.0

    lines_117_001.opacities = opacities
    lines_117_002.opacities = opacities

    v = theo_v_values_inverted[T_slider.index][i]
    p = theo_p_values_inverted[T_slider.index][i]

    tracer_117_003.x, tracer_117_003.y = [p], [v]

    axis_y_004.scale =  bqs.LinearScale(
        min = min(mu[T_slider.index]),
        max = max(mu[T_slider.index])
    )

    lines_117_004.scales = {'x': scale_x_004, 'y': axis_y_004.scale}
    tracer_117_004.scales = {'x': scale_x_004, 'y': axis_y_004.scale}
    labels_117_004.scales = {'x': scale_x_004, 'y': axis_y_004.scale}

    fig_117_004.axis = [
        axis_x_004,
        axis_y_004
    ]
```

[18]:
```
def show_all_potentials(change):
    """This function show all mu(p,T) lines in
    fig_117_004.\n
    """

    max_limit = 0.0
    min_limit = 100.0

    for pot in mu:
        max_pot = max(pot)
        min_pot = min(pot)

        if max_pot > max_limit:
            max_limit = max_pot

        if min_pot < min_limit:
            min_limit = min_pot

    axis_y_004.scale =  bqs.LinearScale(min = min_limit, max = max_limit)

    lines_117_004.scales = {'x': scale_x_004, 'y': axis_y_004.scale}
    axis_y_004.tick_values = np.linspace(0.0, max_limit, 4)

    p_values = [p.tolist() for p in theo_p_values_inverted]
    mu_values = [m.tolist() for m in mu]
```

(continues on next page)

(continued from previous page)

```
    lines_117_004.x, lines_117_004.y = p_values, mu_values

    tracer_117_004.visible = False
```

[19]:
```
def update_text(change):
    """This function show all mu(p,T) lines in
    fig_117_004.\n
    """

    obj = change.owner
    i = obj.index

    p_text.value = '<p> {:.3f} </p>'.format(theo_p_values_inverted[T_slider.index][i])
```

[20]:
```
def add_label(mark, x, y, label):
    """This function adds a point and a name to the bqplot mark.\n

    Args:
        mark: A bqplot marks.\n
        x: x value of the new point.\n
        y: y value of the new point.\n
        label: String containing the new label.\n

    """

    x_labels = [elem for elem in mark.x]
    y_labels = [elem for elem in mark.y]

    x_labels.append(x)
    y_labels.append(y)

    mark.x, mark.y = x_labels, y_labels
    mark.names = np.append(mark.names, label)
```

[21]:
```
def get_new_label(labels):
    """This function returns an alphabetical label different
    from the ones given in the 'labels' list.

    Args:
        labels: A list consisted of the current labels.\n

    Returns:
        elem: A string with a new label which is not in 'labels'.\n
    """


    alpha = 'ABCDEFGHIJKLMNOPQRSTUVWXYZ'
    alpha2 = 'ABCDEFGHIJKLMNOPQRSTUVWXYZ'
    count = 0
    i = 0
    while i < len(alpha):

        elem = alpha[i]

        if not np.isin(elem,labels):
```

(continues on next page)

(continued from previous page)

```
            break

        if i == (len(alpha) - 1):
            alpha = [alpha2[count] + elem for elem in alpha2]
            i = 0
            count = count + 1

        i = i + 1

    return elem
```

[22]:
```
def add_label_button_clicked(a):
    """This function is called when 'add_label_button_117_003' or
    'add_label_button_117_004' are clicked and calls 'add_label'
    function.\n
    """

    if a is add_label_button_117_003:

        label = label_input_117_003.value

        if label == '':

            label = get_new_label(labels_117_003.names)

        add_label(
            labels_117_003,
            tracer_117_003.x[0],
            tracer_117_003.y[0],
            label
        )

        label_input_117_003.value = ''


    elif a is add_label_button_117_004:

        label = label_input_117_004.value

        if label == '':

            label = get_new_label(labels_117_004.names)

        add_label(
            labels_117_004,
            lines_117_004.x[-1],
            lines_117_004.y[-1],
            label
        )

        label_input_117_004.value = ''
```

[23]:
```
def undo_label_button_clicked(a):
    """This function is called when 'undo_label_button_117_003' or
    'undo_label_button_117_004' are clicked  and removes the last
    label added from the bqplot marks 'labels_117_003' or
```

(continues on next page)

(continued from previous page)

```
    'labels_117_004' of the bqplot figures 'fig_117_003'
    and 'fig_117_004'.\n
    """

    if a is undo_label_button_117_003 and len(labels_117_003.x) > 0:

        labels_117_003.x, labels_117_003.y = labels_117_003.x[:-1], labels_117_003.y[:
↪-1]
        labels_117_003.names = labels_117_003.names[:-1]

    elif a is undo_label_button_117_004 and len(labels_117_004.x) > 0:

        labels_117_004.x, labels_117_004.y = labels_117_004.x[:-1], labels_117_004.y[:
↪-1]
        labels_117_004.names = labels_117_004.names[:-1]
```

[24]:
```
def change_view(change):
    """This function changes the visualization of all the
    components of the application so they are suitable for
    a projection.\n
    """

    obj = change.owner

    if obj.value:

        obj.description = 'Presentation mode (ON)'

        display(HTML(
            "<style>" \
            ".widget-readout { font-size: 30px ; }" \
            ".widget-label-basic {font-size: 30px;}" \
            "option {font-size: 25px;}" \
            ".p-Widget.jupyter-widgets.widget-slider.widget-vslider.widget-inline-
↪vbox {width: auto}" \
            ".p-Widget .jupyter-widgets .widgets-label {width: auto; height: auto;␣
↪font-size: 30px;}" \
            ".widget-label {font-size: 30px ; height: auto !important;}" \
            ".p-Widget .bqplot .figure .jupyter-widgets {height: auto !important;}" \
            ".widget-text input[type='number'] {font-size: 30px;height: auto;}" \
            ".option { font-size: 30px ;}" \
            ".p-Widget .jupyter-widgets .jupyter-button.widget-button {font-size:␣
↪30px ; width: auto; height: auto;}" \
            ".p-Widget.jupyter-widgets.jupyter-button.widget-toggle-button{font-size:␣
↪30px ; width: auto; height: auto;}" \
            ".p-Widget.p-Panel.jupyter-widgets.widget-container.widget-box.widget-
↪vbox {padding-bottom: 30px}" \
            ".bqplot > svg .axis text.axislabel, .bqplot > svg .axis tspan.axislabel
↪{font-size: 30px;}"
            "</style>"
            )
        )

        for figure in figures:

            figure.legend_text = {'font-size': '30px'}
```

(continues on next page)

(continued from previous page)

```
            figure.title_style = {'font-size': '30px'}

            for axis in figure.axes:
                axis.tick_style = {'font-size': '30px'}
                axis.label_style = {'font-size': '30px'}

    else:

        obj.description = 'Presentation mode (OFF)'

        display(HTML(
            "<style>" \
            ".widget-readout { font-size: 14px ;}" \
            ".widget-label-basic {font-size: 14px;}" \
            "option {font-size: 12px;}" \
            ".p-Widget .jupyter-widgets .widgets-label {font-size: 14px;}" \
            ".widget-label {font-size: 14px ;}" \
            ".widget-text input[type='number'] {font-size: 14px;}" \
            ".option { font-size: 14px ;}" \
            ".p-Widget .jupyter-widgets .jupyter-button.widget-button {font-size:␣
↪14px;}" \
            ".p-Widget.jupyter-widgets.jupyter-button.widget-toggle-button {font-size:
↪ 14px;}" \
            ".bqplot > svg .axis text.axislabel, .bqplot > svg .axis tspan.axislabel
↪{font-size: 14px;}"
            "</style>"
            )
        )

        for figure in figures:

            figure.legend_text = {'font-size': '15px'}
            figure.title_style = {'font-size': '20px'}

            for axis in figure.axes:
                axis.tick_style = {'font-size': '15px'}
                axis.label_style = {'font-size': '15px'}
```

[25]:
```
def prepare_export(button):
    """This function sends the selected plot to the 'export_plot'
    function.
    """

    if button is prepare_export_fig_117_001_button:

        export_plot(fig_117_001)

    elif button is prepare_export_fig_117_002_button:

        export_plot(fig_117_002)

    elif button is prepare_export_fig_117_003_button:

        export_plot(fig_117_003)

    elif button is prepare_export_fig_117_004_button:
```

(continues on next page)

(continued from previous page)

```
        export_plot(fig_117_004)

    elif button is prepare_export_fig_117_005_button:

        export_plot(fig_117_005)

    elif button is prepare_export_fig_117_006_button:

        export_plot(fig_117_006)

    elif button is prepare_export_fig_117_007_button:

        export_plot(fig_117_007)

    elif button is prepare_export_fig_117_008_button:

        export_plot(fig_117_008)
```

[26]:
```
def export_plot(plot):
    """This function sends the selected plot to the export module.
    """

    global data

    text_lines = []

    np.set_printoptions(threshold=sys.maxsize)
    data =  repr((plot, text_lines))

    %store data

    rel_url = "../../../apps/modules/export_module.ipynb"
    abs_url = urllib.parse.urljoin(notebook_url, rel_url)

    if not webbrowser.open(abs_url):
        go_to_export_button.value = "<form action=" + abs_url + " target='_blank'>
↪<button type=''submit''>Open in export module</button></form>"
```

[ ]:
```
%%javascript

//Get the URL of the current notebook

var kernel = Jupyter.notebook.kernel;
var command = ["notebook_url = ",
               "'", window.location.href, "'" ].join('')

kernel.execute(command)
```

### 1.9.6 Functions related to visualization

[28]:
```
def hex_to_rgb(number_hex):
    """This function converts a hexadecimal color to its rgb
    equivalent.
```

(continues on next page)

(continued from previous page)

```
    Args:
        number_hex: String containing the hexadecimal representation
        of the color.\n

    Returns:
        number_rgb: Tuple consisted of the 3 numbers of the rgb
        representation of the color.\n
    """

    if '#' in number_hex:
        number_hex = number_hex[1:]

    number_rgb = (int(number_hex[0:2], 16), \
                  int(number_hex[2:4], 16), \
                  int(number_hex[4:], 16))

    return number_rgb
```

[29]:
```
def rgb_to_hex(number_rgb):
    """This function converts a rgb color to its hexadecimal
    equivalent.

    Args:
        number_rgb: Tuple consisted of the 3 numbers of the rgb
        representation of the color.\n

    Returns:
        number_hex: String containing the hexadecimal representation
        of the color.\n
    """

    number_rgb = '#' \
    + format(number_rgb[0], '02x') \
    + format(number_rgb[1], '02x') \
    + format(number_rgb[2], '02x')

    return number_rgb
```

[30]:
```
def generate_gradient(initial, final, length):
    """This function generates a color gradient consisted of N
    colors from the initial to the final.

    Args:
        initial: String of the hexadecimal representation of the
        initial color.\n
        final: String of the hexadecimal representation of the
        final color.\n
        length: Number of colors.\n

    Returns:
        colors: List consisted of strings of the hexadecimal
        colors.\n
    """

    i_r, i_g, i_b = hex_to_rgb(initial)
```

(continues on next page)

(continued from previous page)

```
    f_r, f_g, f_b = hex_to_rgb(final)

    r_step = (f_r - i_r)/length
    g_step = (f_g - i_g)/length
    b_step = (f_b - i_b)/length

    r, g, b = i_r, i_g, i_b
    colors = []

    for i in range(length):

        h = rgb_to_hex((int(round(r)),int(round(g)),int(round(b))))

        colors.append(h)

        r = r + r_step
        g = g + g_step
        b = b + b_step

    return colors
```

### 1.9.7 Main interface

[31]:
```
#v_values_1 = np.geomspace(0.48, 0.8, 1000)
#v_values_2 = np.geomspace(0.8, 5.2, 500)
#
#v_values = np.concatenate((v_values_1, v_values_2))
v_values = np.geomspace(0.48, 5.0, 1000)
T_values = np.round(np.linspace(0.85, 1.1, 15), 2)

if 1.0 not in T_values:
    T_values = np.sort(np.append(T_values, 1.0))

data = experimental_isotherms(
        p_range=[],
        v_range=v_values,
        T_range=T_values,
        fixed_T = True,
        fixed_p = False
)

expe_p_values = data[0]
theo_p_values = data[1]

p_limits = data[2]
v_limits = data[3]
T_limits = data[4]

colors = generate_gradient('#FF0000', '#FFfa00', len(T_limits))
opacities = [0.0 for t in T_values]
opacities[0] = 1.0

# change view button

change_view_button = widgets.ToggleButton(
```

(continues on next page)

(continued from previous page)

```
    value=False,
    description='Presentation mode (OFF)',
    disabled=False,
    button_style='',
    tooltip='',
    icon='desktop',
    layout=widgets.Layout(
        width='auto'
    )
)

change_view_button.observe(change_view, 'value')
```

[32]:
```
################################
######1ST BLOCK#################
################################

# This block shows the p(v,T) (fig_117_001) and
# v(p,T) (fig_117_002) figures.


block_1 = widgets.VBox(
    [],
    layout=widgets.Layout(
        align_items='center',
        align_self= 'center'
    )
)

scale_x = bqs.LinearScale(min = 0.4, max = 5.0)
scale_y = bqs.LinearScale(min = 0.0, max = 2.0)

axis_x_001 = bqa.Axis(
    scale=scale_x,
    tick_format='.2f',
    tick_style={'font-size': '15px'},
    tick_values = [1.0, 2.0, 3.0, 4.0, 5.0],
    grid_lines = 'none',
    grid_color = '#8e8e8e',
    label='v',
    label_location='middle',
    label_style={'stroke': 'black', 'default-size': 35},
    label_offset='50px'
)

axis_y_001 = bqa.Axis(
    scale=scale_y,
    tick_format='.1f',
    tick_style={'font-size': '15px'},
    tick_values = [0, 1.0, 2.0],
    grid_lines = 'none',
    grid_color = '#8e8e8e',
    orientation='vertical',
    label='p',
    label_location='middle',
    label_style={'stroke': 'red', 'default_size': 35},
```

(continues on next page)

(continued from previous page)

```
    label_offset='50px'
)

fig_117_001 = Figure(
    title='p vs v (fixed T, reduced variables)',
    marks=[],
    axes=[axis_x_001, axis_y_001],
    animation_duration=250,
    legend_location='top-right',
    background_style= {'fill': 'white',  'stroke': 'black'},
    min_aspect_ratio=1.0,
    max_aspect_ratio=1.0,
    fig_margin=dict(top=80, bottom=60, left=70, right=20),
    toolbar = True
)

lines_117_001 = bqm.Lines(
    x = v_values,
    y = np.array(theo_p_values),
    scales = {'x': scale_x, 'y': scale_y},
    opacities = opacities,
    visible = True,
    colors = colors,
)

fig_117_001.marks = [lines_117_001]

axis_x_002 = bqa.Axis(
    scale=scale_y,
    tick_format='.1f',
    tick_style={'font-size': '15px'},
    tick_values = [0, 1.0, 2.0],
    grid_lines = 'none',
    grid_color = '#8e8e8e',
    label='p',
    label_location='middle',
    label_style={'stroke': 'black', 'default-size': 35},
    label_offset='50px'
)

axis_y_002 = bqa.Axis(
    scale=scale_x,
    tick_format='.2f',
    tick_style={'font-size': '15px'},
    tick_values = [1.0, 2.0, 3.0, 4.0, 5.0],
    grid_lines = 'none',
    grid_color = '#8e8e8e',
    orientation='vertical',
    label='v',
    label_location='middle',
    label_style={'stroke': 'red', 'default_size': 35},
    label_offset='50px'
)

fig_117_002 = Figure(
    title='v vs p (fixed T, reduced variables)',
    marks=[],
```

(continues on next page)

(continued from previous page)

```
    axes=[axis_x_002, axis_y_002],
    animation_duration=250,
    legend_location='top-right',
    background_style= {'fill': 'white',  'stroke': 'black'},
    min_aspect_ratio=1.0,
    max_aspect_ratio=1.0,
    fig_margin=dict(top=80, bottom=60, left=70, right=20),
    toolbar = True,
)

lines_117_002 = bqm.Lines(
    x = np.array(theo_p_values),
    y = np.array([v_values for p in theo_p_values]),
    scales = {'x': scale_y, 'y': scale_x},
    opacities = opacities,
    visible = True,
    colors = colors
)

fig_117_002.marks = [lines_117_002]

# Export buttons

prepare_export_fig_117_001_button = widgets.Button(
    description='Export',
    disabled=False,
    button_style='',
    tooltip='',
)

prepare_export_fig_117_001_button.on_click(prepare_export)

prepare_export_fig_117_002_button = widgets.Button(
    description='Export',
    disabled=False,
    button_style='',
    tooltip='',
)

prepare_export_fig_117_002_button.on_click(prepare_export)


block_1.children = [
    widgets.HBox([
        widgets.VBox([
            fig_117_001,
            prepare_export_fig_117_001_button
        ],
        layout=widgets.Layout(
            align_items='center'
        )),
        widgets.VBox([
            fig_117_002,
            prepare_export_fig_117_002_button
        ],
        layout=widgets.Layout(
            align_items='center'
```

(continues on next page)

(continued from previous page)

```
        )),
    ],
        layout=widgets.Layout(
            width='100%',
            align_items='center'
        )
    )
]
```

[33]:
```
################################
######2ND BLOCK#################
################################

# This block shows the slider to control the tenperature
# (T_slider).

block_2 = widgets.VBox(
    [],
    layout=widgets.Layout(align_items='center')
)

T_slider = widgets.SelectionSlider(
    options= T_values,
    value=T_values[0],
    description=r'\( T \)',
    disabled=False,
    continuous_update=True,
    orientation='horizontal',
    readout=True,
    layout = widgets.Layout(
        width = '300px',
        height = 'auto',
        margin='0 0 0 50px'
    )
)

T_slider.observe(change_tenperature, 'value')

block_2.children = [T_slider]
```

[34]:
```
################################
######3RD BLOCK#################
################################

# This block shows the v(p,T) (fig_117_003) and
# mu(p,T) (fig_117_004) figures.

fig_117_003 = Figure(
    title='v vs p (fixed T, reduced variables)',
    marks=[],
    axes=[axis_x_002, axis_y_002],
    animation_duration=0, #500,
    legend_location='top-right',
    background_style= {'fill': 'white',  'stroke': 'black'},
    min_aspect_ratio=1.0,
    max_aspect_ratio=1.0,
```

(continues on next page)

(continued from previous page)

```
    fig_margin=dict(top=80, bottom=60, left=70, right=20),
    toolbar = True,
)

area_117_003 = bqm.Lines(
    x = [],
    y = [],
    scales = {'x': scale_y, 'y': scale_x},
    opacities = [1.0],
    visible = True,
    colors = ['#39362d'],
    fill = 'bottom',
    fill_colors = ['#ffd429'],
    fill_opacities = [0.4]
)

tracer_117_003 = bqm.Scatter(
    name = '',
    x = [0.0],
    y = [0.0],
    scales = {'x': scale_y, 'y': scale_x},
    opacity = [1.0, 0.0],
    visible = False,
    colors = ['#2807a3'],
)

tt_003 = bq.Tooltip(
    fields = ['x', 'y'],
    formats = ['.3f', '.3f'],
    labels = ['v', 'p']
)

labels_117_003 = bqm.Scatter(
    name = 'labels',
    x = [],
    y = [],
    scales = {'x': scale_y, 'y': scale_x},
    #opacities = [1.0],
    visible = True,
    colors = ['black'],
    names = [],
    labels=['labels'],
    tooltip = tt_003,
)

fig_117_003.marks = [
    lines_117_002,
    area_117_003,
    tracer_117_003,
    labels_117_003
]

theo_p_values_inverted = []
theo_v_values_inverted = []

for p_values in theo_p_values:
```

(continues on next page)

(continued from previous page)

```
    indexes = np.where(p_values < 2.2)

    theo_p_values_inverted.append(
        np.flip(np.take(p_values, indexes[0]))
    )

    theo_v_values_inverted.append(
        np.flip(np.take(v_values, indexes[0]))
    )

mu = get_chemical_potential(
    theo_p_values_inverted,
    theo_v_values_inverted
)

for i in range(len(mu)):
    mu[i] = np.array(mu[i]) - 10.0*T_slider.options[i]

p_text = widgets.HTML(
    value='<p> {:.3f} </p>'.format(theo_p_values_inverted[T_slider.index][i]),
    layout = widgets.Layout(height='auto', margin='10px 0 0 10px')
)

p_slider = widgets.SelectionSlider(
    options= theo_v_values_inverted[0],
    value=theo_v_values_inverted[0][0],
    description=r'\( p \)',
    disabled=False,
    continuous_update=True,
    orientation='horizontal',
    readout=False,
    layout = widgets.Layout(
        width = '60%',
        height = 'auto',
        margin='0 0 0 50px'
    )
)

p_slider.observe(update_tracer, 'value')
p_slider.observe(update_text, 'value')


# Figure fig_117_004

scale_x_004 = bqs.LinearScale(min = 0.0, max = 2.0)
scale_y_004 = bqs.LinearScale(
    min = min(mu[T_slider.index]),
    max = max(mu[T_slider.index])
)

axis_x_004 = bqa.Axis(
    scale=scale_x_004,
    tick_format='.2f',
    tick_style={'font-size': '15px'},
    tick_values = [0.0, 1.0, 2.0],
    grid_lines = 'none',
    grid_color = '#8e8e8e',
```

(continues on next page)

(continued from previous page)

```
    label='p',
    label_location='middle',
    label_style={'stroke': 'black', 'default-size': 35},
    label_offset='50px'
)

axis_y_004 = bqa.Axis(
    scale=scale_y_004,
    tick_format='.2f',
    tick_style={'font-size': '15px'},
    num_ticks = 0,
    grid_lines = 'none',
    grid_color = '#8e8e8e',
    orientation='vertical',
    label='mu',
    label_location='middle',
    label_style={'stroke': 'red', 'default_size': 35},
    label_offset='50px'
)

fig_117_004 = Figure(
    title='mu vs p (fixed T)',
    marks=[],
    axes=[axis_x_004, axis_y_004],
    animation_duration=0,
    legend_location='top-right',
    background_style= {'fill': 'white',  'stroke': 'black'},
    min_aspect_ratio=1.0,
    max_aspect_ratio=1.0,
    fig_margin=dict(top=80, bottom=60, left=70, right=20),
    toolbar = True,
)

lines_117_004 = bqm.Lines(
    x = [],
    y = [],
    scales = {'x': scale_x_004, 'y': scale_y_004},
    opacities = [1.0],
    visible = True,
    colors = colors,
)

tracer_117_004 = bqm.Scatter(
    name = '',
    x = [0.0],
    y = [0.0],
    scales = {'x': scale_x_004, 'y': scale_y_004},
    opacity = [1.0, 0.0],
    visible = True,
    colors = ['#2807a3'],
)

labels_117_004 = bqm.Scatter(
    name = 'labels',
    x = [],
    y = [],
    scales = {'x': scale_x_004, 'y': scale_y_004},
```

(continues on next page)

(continued from previous page)

```
    #opacities = [1.0],
    visible = True,
    colors = ['black'],
    names = [],
    labels=['labels'],
)

fig_117_004.marks = [
    lines_117_004,
    tracer_117_004,
    labels_117_004,
]

restart_button = widgets.Button(
    description='Clean figure',
    disabled=False,
    button_style='',
    tooltip="",
    layout = widgets.Layout(height='auto')
)

restart_button.on_click(restart_chemical_potential)


show_all_button = widgets.Button(
    description='Show all potentials',
    disabled=False,
    button_style='',
    tooltip="",
    layout = widgets.Layout(height='auto')
)

show_all_button.on_click(show_all_potentials)


# Label buttons

label_input_117_003 = widgets.Text(
    value='',
    placeholder="Label:",
    disabled = False,
)

add_label_button_117_003 = widgets.Button(
    description='Add label',
    disabled=False,
    button_style='',
    tooltip="Add label in tracer's position",
)

add_label_button_117_003.on_click(add_label_button_clicked)

undo_label_button_117_003 = widgets.Button(
    description='Undo',
    disabled=False,
    button_style='',
    tooltip="Remove last added label",
```

(continues on next page)

(continued from previous page)

```
)

undo_label_button_117_003.on_click(undo_label_button_clicked)

label_input_117_004 = widgets.Text(
    value='',
    placeholder="Label:",
    disabled = False,
)

add_label_button_117_004 = widgets.Button(
    description='Add label',
    disabled=False,
    button_style='',
    tooltip="Add label in tracer's position",
)

add_label_button_117_004.on_click(add_label_button_clicked)

undo_label_button_117_004 = widgets.Button(
    description='Undo',
    disabled=False,
    button_style='',
    tooltip="Remove last added label",
)

undo_label_button_117_004.on_click(undo_label_button_clicked)

# Export buttons

prepare_export_fig_117_003_button = widgets.Button(
    description='Export',
    disabled=False,
    button_style='',
    tooltip='',
    layout=widgets.Layout(align_self='center')
)

prepare_export_fig_117_003_button.on_click(prepare_export)

prepare_export_fig_117_004_button = widgets.Button(
    description='Export',
    disabled=False,
    button_style='',
    tooltip='',
)

prepare_export_fig_117_004_button.on_click(prepare_export)


block_3 = widgets.VBox(
    [],
    layout=widgets.Layout(align_items='center')
)

block_3.children = [
    widgets.HBox([
```

(continues on next page)

(continued from previous page)

```
        widgets.VBox([
            fig_117_003,
            prepare_export_fig_117_003_button,
            widgets.HBox([p_slider, p_text])],
            layout=widgets.Layout(
                height='auto',
            )),
        widgets.VBox([
            fig_117_004,
            prepare_export_fig_117_004_button,
            widgets.HBox([restart_button, show_all_button]),
        ],
            layout=widgets.Layout(align_items='center')
        )
    ]),
    widgets.HBox([
        label_input_117_003,
        add_label_button_117_003,
        undo_label_button_117_003,
        widgets.HTML('<div style="width:10px"></div>'),
        label_input_117_004,
        add_label_button_117_004,
        undo_label_button_117_004
    ]),
]
```

[35]:
```
################################
######4TH BLOCK#################
################################

block_4 = widgets.HBox(
    [],
    layout=widgets.Layout(
        align_items='center'
    )
)

tt_005 = bq.Tooltip(
    fields = ['y', 'x'],
    formats = ['.3f', '.3f'],
    labels = ['p', 'v']
)

lines_117_005 = bqm.Lines(
    x = v_values,
    y = theo_p_values,
    scales = {'x': scale_x, 'y': scale_y},
    opacities = [1.0],
    visible = True,
    colors = colors,
)

scatter_117_005 = bqm.Scatter(
    name = '',
    x = v_limits,
    y = p_limits,
```

(continues on next page)

(continued from previous page)

```
    scales = {'x': scale_x, 'y': scale_y},
    visible = True,
    colors = ['black'],
    default_size = 15,
    tooltip = tt_005
)

fig_117_005 = Figure(
    title='v vs p (fixed T, reduced variables)',
    marks=[lines_117_005, scatter_117_005],
    axes=[axis_x_001, axis_y_001],
    animation_duration=0, #500,
    legend_location='top-right',
    background_style= {'fill': 'white',  'stroke': 'black'},
    min_aspect_ratio=1.0,
    max_aspect_ratio=1.0,
    fig_margin=dict(top=80, bottom=60, left=70, right=20),
    toolbar = True,
)

# fig_117_006

# Calculate the limits of the plot
max_limit = 0.0
min_limit = 100.0

for pot in mu:
    max_pot = max(pot)
    min_pot = min(pot)

    if max_pot > max_limit:
        max_limit = max_pot

    if min_pot < min_limit:
        min_limit = min_pot

# Calculate the phase transition points in the mu(p, T) plane
trans_mu = []

trans_p = np.unique(p_limits)

for i in range(len(trans_p)):

    p = trans_p[i]
    m = mu[i]

    j = find_nearest_index(theo_p_values_inverted[i], p)

    trans_mu.append(mu[i][j])

scale_x_006 = bqs.LinearScale(min = 0.0, max = 2.0)
scale_y_006 = bqs.LinearScale(min = min_limit, max = max_limit)

axis_x_006 = bqa.Axis(
    scale=scale_x_006,
    tick_format='.2f',
    tick_style={'font-size': '15px'},
```

(continues on next page)

(continued from previous page)

```
    tick_values = [0.0, 1.0, 2.0],
    grid_lines = 'none',
    grid_color = '#8e8e8e',
    label='p',
    label_location='middle',
    label_style={'stroke': 'black', 'default-size': 35},
    label_offset='50px'
)

axis_y_006 = bqa.Axis(
    scale=scale_y_006,
    tick_format='.2f',
    tick_style={'font-size': '15px'},
    num_ticks = 5,
    grid_lines = 'none',
    grid_color = '#8e8e8e',
    orientation='vertical',
    label='mu',
    label_location='middle',
    label_style={'stroke': 'red', 'default_size': 35},
    label_offset='50px'
)


lines_117_006 = bqm.Lines(
    x = [p.tolist() for p in theo_p_values_inverted],
    y = [m.tolist() for m in mu],
    scales = {'x': scale_x_006, 'y': scale_y_006},
    opacities = [1.0],
    visible = True,
    colors = colors,
)

scatter_117_006 = bqm.Scatter(
    name = '',
    x = trans_p,
    y = trans_mu,
    scales = {'x': scale_x_006, 'y': scale_y_006},
    visible = True,
    colors = ['black'],
    default_size = 15,
)

fig_117_006 = Figure(
    title='mu vs p (fixed T)',
    marks=[lines_117_006, scatter_117_006],
    axes=[axis_x_006, axis_y_006],
    animation_duration=0,
    legend_location='top-right',
    background_style= {'fill': 'white',  'stroke': 'black'},
    min_aspect_ratio=1.0,
    max_aspect_ratio=1.0,
    fig_margin=dict(top=80, bottom=60, left=70, right=20),
    toolbar = True,
)

# Export buttons
```

(continues on next page)

(continued from previous page)

```
prepare_export_fig_117_005_button = widgets.Button(
    description='Export',
    disabled=False,
    button_style='',
    tooltip='',
    layout=widgets.Layout(align_self='center')
)

prepare_export_fig_117_005_button.on_click(prepare_export)

prepare_export_fig_117_006_button = widgets.Button(
    description='Export',
    disabled=False,
    button_style='',
    tooltip='',
)

prepare_export_fig_117_006_button.on_click(prepare_export)


block_4.children = [
    widgets.HBox([
        widgets.VBox([
            fig_117_005,
            prepare_export_fig_117_005_button
        ],
        layout=widgets.Layout(
            align_items='center'
        )),
        widgets.VBox([
            fig_117_006,
            prepare_export_fig_117_006_button
        ],
        layout=widgets.Layout(
            align_items='center'
        )),
    ],
        layout=widgets.Layout(
            width='100%',
            align_items='center'
        )
    )
]
```

[36]:
```
################################
######5TH BLOCK#################
################################

# This block contains the p(T) and T(p) figures

block_5 = widgets.HBox(
    [],
    layout=widgets.Layout(align_items='center')
)
```

(continues on next page)

(continued from previous page)

```
scale_y_007 = bqs.LinearScale(
    min = min(T_values),
    max = max(T_values)
)

axis_y_007 = bqa.Axis(
    scale=scale_y_007,
    tick_format='.2f',
    tick_style={'font-size': '15px'},
    tick_values = [0.0, 1.0, 2.0],
    grid_lines = 'none',
    grid_color = '#8e8e8e',
    orientation='vertical',
    label='T',
    label_location='middle',
    label_style={'stroke': 'red', 'default_size': 35},
    label_offset='50px',
)

tt_007 = bq.Tooltip(
    fields = ['y', 'x'],
    formats = ['.3f', '.3f'],
    labels = ['T', 'p']
)

lines_117_007 = bqm.Lines(
    x = trans_p,
    y = T_values,
    scales = {'x': scale_x_006, 'y': scale_y_007},
    opacities = [1.0],
    visible = True,
    colors = ['red'],
)

scatter_117_007 = bqm.Scatter(
    name = '',
    x = trans_p,
    y = T_values,
    scales = {'x': scale_x_006, 'y': scale_y_007},
    visible = True,
    colors = ['black'],
    default_size = 15,
    tooltip = tt_007
)

fig_117_007 = Figure(
    title='T vs p (fixed v, reduced variables)',
    marks=[lines_117_007, scatter_117_007],
    axes=[axis_x_006, axis_y_007],
    animation_duration=0,
    legend_location='top-right',
    background_style= {'fill': 'white',  'stroke': 'black'},
    min_aspect_ratio=1.0,
    max_aspect_ratio=1.0,
    fig_margin=dict(top=80, bottom=60, left=70, right=20),
    toolbar = True,
)
```

(continues on next page)

(continued from previous page)

```
# fig_117_008

scale_y_008 = bqs.LinearScale(
    min = min(T_values),
    max = max(T_values),
    reverse = True
)

axis_x_008 = bqa.Axis(
    scale=scale_x_006,
    tick_format='.2f',
    tick_style={'font-size': '15px'},
    tick_values = [0.0, 1.0, 2.0],
    grid_lines = 'none',
    grid_color = '#8e8e8e',
    label='p',
    label_location='middle',
    label_style={'stroke': 'black', 'default-size': 35},
    label_offset='30px',
    side='top'
)

axis_y_008 = bqa.Axis(
    scale=scale_y_008,
    tick_format='.2f',
    tick_style={'font-size': '15px'},
    tick_values = [0.0, 1.0, 2.0],
    grid_lines = 'none',
    grid_color = '#8e8e8e',
    orientation='vertical',
    label='T',
    label_location='middle',
    label_style={'stroke': 'red', 'default_size': 35},
    label_offset='50px',
)

tt_008 = bq.Tooltip(
    fields = ['y', 'x'],
    formats = ['.3f', '.3f'],
    labels = ['T', 'p']
)

lines_117_008 = bqm.Lines(
    x = trans_p,
    y = T_values,
    scales = {'x': scale_x_006, 'y': scale_y_008},
    opacities = [1.0],
    visible = True,
    colors = ['red'],
)

scatter_117_008 = bqm.Scatter(
    name = '',
    x = trans_p,
    y = T_values,
    scales = {'x': scale_x_006, 'y': scale_y_008},
```

(continues on next page)

(continued from previous page)

```
    visible = True,
    colors = ['black'],
    default_size = 15,
    tooltip = tt_008
)

fig_117_008 = Figure(
    title='T vs p (fixed v, reduced variables)',
    marks=[lines_117_008, scatter_117_008],
    axes=[axis_x_008, axis_y_008],
    animation_duration=0,
    legend_location='top-right',
    background_style= {'fill': 'white',  'stroke': 'black'},
    min_aspect_ratio=1.0,
    max_aspect_ratio=1.0,
    fig_margin=dict(top=160, bottom=60, left=70, right=20),
    toolbar = True,
)

# Export buttons

prepare_export_fig_117_007_button = widgets.Button(
    description='Export',
    disabled=False,
    button_style='',
    tooltip='',
    layout=widgets.Layout(align_self='center')
)

prepare_export_fig_117_007_button.on_click(prepare_export)

prepare_export_fig_117_008_button = widgets.Button(
    description='Export',
    disabled=False,
    button_style='',
    tooltip='',
)

prepare_export_fig_117_008_button.on_click(prepare_export)

block_5.children = [
    widgets.HBox([
        widgets.VBox([
            fig_117_007,
            prepare_export_fig_117_007_button
        ],
        layout=widgets.Layout(
            align_items='center'
        )),
        widgets.VBox([
            fig_117_008,
            prepare_export_fig_117_008_button
        ],
        layout=widgets.Layout(
            align_items='center'
        )),
    ],
```

(continues on next page)

(continued from previous page)

```
        layout=widgets.Layout(
            width='100%',
            align_items='center'
        )
    )
]
```

[ ]:
```
###################################
#############MAIN BLOCK############
###################################

main_block_117_000 = widgets.VBox(
    [],
    layout=widgets.Layout(align_items='center')
)

main_block_117_000.children = [
    change_view_button,
    block_1,
    block_2,
    block_3,
    block_4,
    block_5
]

figures = [
    fig_117_001,
    fig_117_002,
    fig_117_003,
    fig_117_004,
    fig_117_005,
    fig_117_006,
    fig_117_007,
    fig_117_008,
]

main_block_117_000
```

## 1.10 Stability condition on van der Waals isotherms

**Code:** #11A-000

**File:** `apps/van_der_waals/stability.ipynb`

**Run it online:**

---

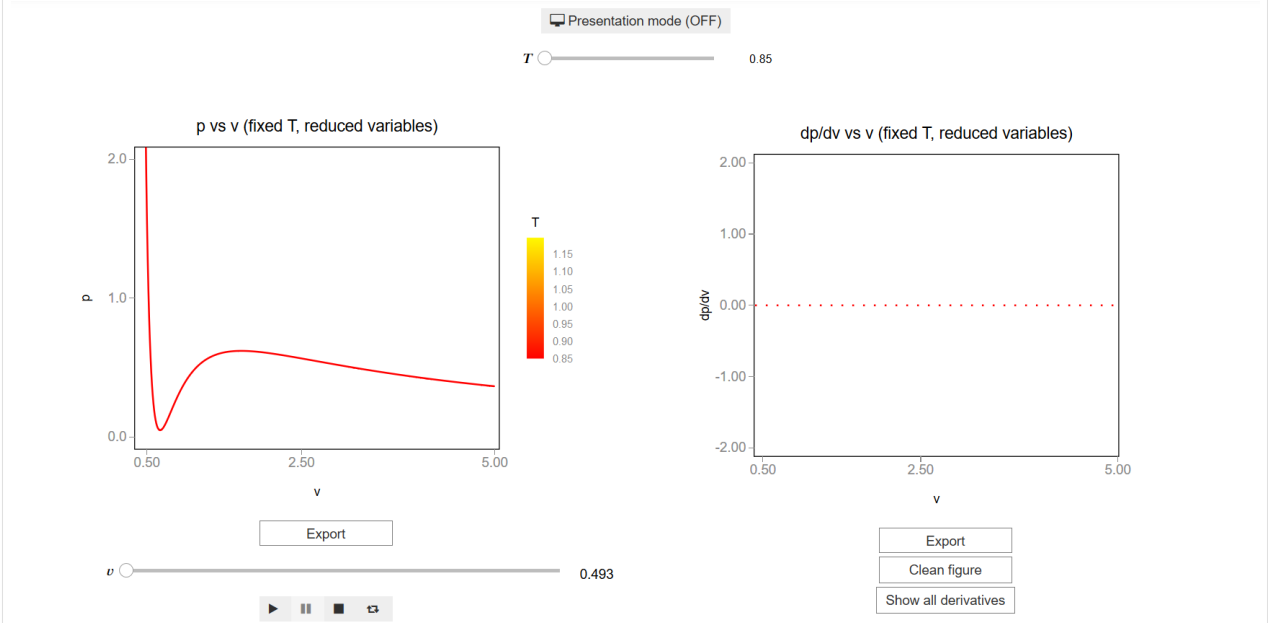
The aim of this notebook is to visualize the $\left(\frac{\partial p}{\partial v}\right)_{T,N} < 0$ stability condition on van der Waals isotherms.

### 1.10.1 Interface

The main interface (`main_block_11A_000`) is divided in two HBox: `top_block_11A_000` and `bottom_block_11A_000`. `bottom_block_11A_000` contains of 2 bqplot Figures: `fig_11A_001` and

fig_11A_002.

[1]:
```
from IPython.display import Image
Image(filename='../../static/images/apps/11A-000_1.png')
```

[1]:



The slider `T_slider` updates the values of $T$ which updates the lines of `fig_11A_001` and `fig_11A_002`.

[2]:
```
Image(filename='../../static/images/apps/11A-000_2.png')
```

[2]:



### 1.10.2 CSS

A custom `css` file is used to improve the interface of this application. It can be found here.

[3]:
```
from IPython.display import HTML
display(HTML("<head><link rel='stylesheet' type='text/css' href='./../../static/
↪custom.css'></head>"))
display(HTML("<style>.container { width:100% !important; }</style>"))
display(HTML("<style>.widget-label { display: contents !important; }</style>"))
display(HTML("<style>.slider-container { margin: 12px !important; }</style>"))
display(HTML("<style>.jupyter-widgets { overflow: auto !important; }</style>"))
```

```
<IPython.core.display.HTML object>
```

```
<IPython.core.display.HTML object>
```

```
<IPython.core.display.HTML object>
```

```
<IPython.core.display.HTML object>
```

```
<IPython.core.display.HTML object>
```

### 1.10.3 Packages

[4]:
```
from bqplot import *
import bqplot as bq
import bqplot.marks as bqm
import bqplot.scales as bqs
import bqplot.axes as bqa

import ipywidgets as widgets

import urllib.parse
import webbrowser

import sys
```

### 1.10.4 Physical functions

This are the functions that have a physical meaning:

- `get_relative_isotherms`
- `get_derivative_y_by_x`

[5]:
```
def get_relative_isotherms(v_range, T_range):
    """This function calculates the theoretical p(v, T) plane
        (in reduced coordinates) according to van der Waals
        equation of state from a given range of volumes
        and tenperatures.

    Args:
        v_range: An array containing the values of v
        (in reduced coordinates)for which the isotherms must be
        calculated.\n
        T_range: An array containing the values of T
        (in reduced coordinates)for which the isotherms must be
        calculated.\n


    Returns:
        isotherms: A list consisted of numpy arrays containing the
        pressures of each isotherm.
    """

    isotherms = []

    for T in T_range:
        p_R = []
        for v in v_range:
            val = (8.0/3.0*T/(v - 1.0/3.0) - 3.0/v**2)
            p_R = np.append(p_R, val)

        isotherms.append(p_R)

    return isotherms
```

[6]:
```
def get_derivative_y_by_x(y_values, x_values):
    """This function calculates the derivative an y array
    with respect to an x array calculated with the difference quotient.

    Args:
        y_values: An array containing the values of y.\n
        x_values: An array containing the values of x.\n


    Returns:
        der: An array containing the values of the
        derivative of y_values with respect to x_values.
    """

    der = []


    for i in range(len(x_values)):

        x = x_values[i]
        y = y_values[i]

        d = []

        l = np.size(y)

        for j in range(1, l):
            d.append((y[j] - y[j-1])/(x[j] - x[j-1]))

        der.append(d)

    return der
```

### 1.10.5 Functions related to interaction

[7]:
```
def update_tracer(change):
    """This function updates the marks 'tracer_11A_001' and
    'lines_11A_002' from figures 'fig_11A_001' and
    'fig_11A_002'.
    """

    tracer_11A_001.visible = True

    i = change.get('owner').value
    v = dense_v_values_filtered[T_slider.index][i]
    p = dense_p_values_filtered[T_slider.index][i]

    tracer_11A_001.x, tracer_11A_001.y = [v], [p]

    x_values = np.append(lines_11A_002.x, v)
    y_values = np.append(lines_11A_002.y, der[T_slider.index][i])

    lines_11A_002.x, lines_11A_002.y = x_values, y_values
```

[8]:
```
def restart_derivative(a):
    """This function clears the mark 'lines_11A_002'
    from figure 'fig_11A_002' when 'restart_button' is pressed.
    """

    lines_11A_002.x, lines_11A_002.y = [], []
```

[9]:
```
def change_tenperature(change):
    """This function changes the tenperature of the
    marks 'lines_11A_002' and 'tracer_11A_001' from figures
    'fig_11A_002' and 'fig_11A_003'.
    """

    v_slider.max = len(dense_v_values_rounded[T_slider.index])-2
    restart_derivative(None)

    obj = change.owner

    opacities = [0.0 for t in T_values]
    opacities[T_slider.index] = 1.0
    lines_11A_001.opacities = opacities

    lines_11A_002.x, lines_11A_002.y = p_values[T_slider.index], v_values

    tracer_11A_001.x, tracer_11A_001.y = [lines_11A_002.x[0]], [lines_11A_002.y[0]]
```

[10]:
```
def show_all_derivatives(change):
    """This function shows all the calculated derivatives in
    'lines_11A_002'.
    """

    lines_11A_002.x, lines_11A_002.y = [v.tolist()[:-1] for v in dense_v_values_
↪filtered], der
```

[11]:
```
def update_text(change):
    """This function update the volume of the 'tracer_11A_001'
    shown in 'v_text' widget.
    """

    obj = change.owner
    i = obj.value

    v_text.value = '<p>' + str(dense_v_values_rounded[T_slider.index][i])+ '</p>'
```

[12]:
```
def change_view(change):
    """This function changes the visualization of all the
    components of the application so they are suitable for
    a projection.\n
    """

    obj = change.owner

    if obj.value:

        obj.description = 'Presentation mode (ON)'
```

(continues on next page)

(continued from previous page)

```
        display(HTML(
            "<style>" \
            ".widget-readout { font-size: 30px ; }" \
            ".widget-label-basic {font-size: 30px;}" \
            "option {font-size: 25px;}" \
            ".p-Widget.jupyter-widgets.widget-slider.widget-vslider.widget-inline-
↪vbox {width: auto}" \
            ".p-Widget .jupyter-widgets .widgets-label {width: auto; height: auto;␣
↪font-size: 30px;}" \
            ".widget-label {font-size: 30px ; height: auto !important;}" \
            ".p-Widget .bqplot .figure .jupyter-widgets {height: auto !important;}" \
            ".widget-text input[type='number'] {font-size: 30px;height: auto;}" \
            ".option { font-size: 30px ;}" \
            ".p-Widget .jupyter-widgets .jupyter-button.widget-button {font-size:␣
↪30px ; width: auto; height: auto;}" \
            ".p-Widget.jupyter-widgets.jupyter-button.widget-toggle-button{font-size:␣
↪30px ; width: auto; height: auto;}" \
            ".p-Widget.p-Panel.jupyter-widgets.widget-container.widget-box.widget-
↪vbox {padding-bottom: 30px}" \
            ".bqplot > svg .axis text.axislabel, .bqplot > svg .axis tspan.axislabel
↪{font-size: 30px;}" \
            ".q-grid .slick-cell {font-size: 30px;}" \
            ".slick-column-name {font-size: 30px;}" \
            ".widget-html-content {font-size: 30px;}"
            "</style>"
            )
        )

        for figure in figures:

            figure.legend_text = {'font-size': '30px'}
            figure.title_style = {'font-size': '30px'}

            for axis in figure.axes:
                axis.tick_style = {'font-size': '30px'}
                axis.label_style = {'font-size': '30px'}

    else:

        obj.description = 'Presentation mode (OFF)'

        display(HTML(
            "<style>" \
            ".widget-readout { font-size: 14px ;}" \
            ".widget-label-basic {font-size: 14px;}" \
            "option {font-size: 12px;}" \
            ".p-Widget .jupyter-widgets .widgets-label {font-size: 14px;}" \
            ".widget-label {font-size: 14px ;}" \
            ".widget-text input[type='number'] {font-size: 14px;}" \
            ".option { font-size: 14px ;}" \
            ".p-Widget .jupyter-widgets .jupyter-button.widget-button {font-size:␣
↪14px;}" \
            ".p-Widget.jupyter-widgets.jupyter-button.widget-toggle-button {font-size:
↪ 14px;}" \
            ".bqplot > svg .axis text.axislabel, .bqplot > svg .axis tspan.axislabel
↪{font-size: 14px;}" \
            ".q-grid .slick-cell {font-size: 14px;}" \
```

(continues on next page)

(continued from previous page)

```
            ".slick-column-name {font-size: 14px;}" \
            ".widget-html-content {font-size: 14px;}"
            "</style>"
            )
        )

        for figure in figures:

            figure.legend_text = {'font-size': '14px'}
            figure.title_style = {'font-size': '20px'}

            for axis in figure.axes:
                axis.tick_style = {'font-size': '14px'}
                axis.label_style = {'font-size': '14px'}
```

[13]:
```
def prepare_export(button):
    """This function sends the selected plot to the 'export_plot'
    function.
    """

    if button is prepare_export_fig_11A_001_button:

        export_plot(fig_11A_001)

    elif button is prepare_export_fig_11A_002_button:

        export_plot(fig_11A_002)
```

[14]:
```
def export_plot(plot):
    """This function sends the selected plot to the export module.
    """

    global data

    text_lines = []

    np.set_printoptions(threshold=sys.maxsize)

    tooltips = []

    for mark in plot.marks:
        tooltips.append(mark.tooltip)
        mark.tooltip = None

    data =  repr((plot, text_lines))

    %store data

    rel_url = "../../../apps/modules/export_module.ipynb"
    abs_url = urllib.parse.urljoin(notebook_url, rel_url)

    if not webbrowser.open(abs_url):
        go_to_export_button.value = "<form action=" + abs_url + " target='_blank'>
↪<button type=''submit''>Open in export module</button></form>"

    for i in range(len(plot.marks)):
```

(continues on next page)

(continued from previous page)

```
        mark = plot.marks[i]
        mark.tooltip = tooltips[i]
```

[ ]:
```
%%javascript

//Get the URL of the current notebook

var kernel = Jupyter.notebook.kernel;
var command = ["notebook_url = ",
               "'", window.location.href, "'" ].join('')

kernel.execute(command)
```

### 1.10.6 Main interface

[ ]:
```
v_values = np.linspace(0.4, 5.0, 500)
T_values = [0.85, 0.9, 0.95, 1.0, 1.05, 1.1, 1.15, 1.2]

p_values = get_relative_isotherms(v_values, T_values)

################################
######TOP BLOCK#################
################################

top_block = widgets.VBox(
    [],
    layout=widgets.Layout(align_items='center')
)

T_slider = widgets.SelectionSlider(
    options= T_values,
    value=T_values[0],
    description=r'\( T \)',
    disabled=False,
    continuous_update=True,
    orientation='horizontal',
    readout=True,
    layout = widgets.Layout(
        width = '300px',
        height = 'auto',
        margin='0 0 0 50px'
    )
)

T_slider.observe(change_tenperature, 'value')

change_view_button = widgets.ToggleButton(
    value=False,
    description='Presentation mode (OFF)',
    disabled=False,
    button_style='',
    tooltip='',
    icon='desktop',
    layout=widgets.Layout(
```

(continues on next page)

(continued from previous page)

```
        width='initial',
        align_self='center'
    )
)

change_view_button.observe(change_view, 'value')

top_block.children = [
    change_view_button,
    T_slider
]

################################
######BOTTOM BLOCK##############
################################

bottom_block = widgets.HBox(
    [],
    layout=widgets.Layout(
        width='100%',
        align_items='center'
    )
)

dense_v_values = np.linspace(min(v_values), max(v_values), 10000)
dense_p_values = get_relative_isotherms(dense_v_values, T_values)

dense_v_values_filtered = []
dense_p_values_filtered = []

dense_v_values_inverted = []
dense_p_values_inverted = []

dense_v_values_rounded = []

for i in range(len(T_values)):

    i_in_range, = np.where(dense_p_values[i] < 2.0)

    dense_v_values_filtered.append(np.take(dense_v_values, i_in_range))
    dense_p_values_filtered.append(np.take(dense_p_values[i], i_in_range))
    dense_v_values_rounded.append(np.round(dense_v_values_filtered[i], 3))

v_text = widgets.HTML(
    value="<p>" + str(dense_v_values_rounded[T_slider.index][i]) + "</p>",
    layout = widgets.Layout(
        height='auto',
        margin='8px 0 0 10px',
        width='initial'
    )
)

der = get_derivative_y_by_x(dense_p_values_filtered, dense_v_values_filtered)

v_slider = widgets.IntSlider(
    min=0,
    max=len(der[T_slider.index])-1,
```

(continues on next page)

(continued from previous page)

```
    value=0,
    description=r'\( v \)',
    disabled=False,
    continuous_update=True,
    orientation='horizontal',
    readout=False,
    layout = widgets.Layout(width = '75%', height='auto', margin='0 0 0 100px')
)

v_slider.observe(update_tracer, 'value')
v_slider.observe(update_text, 'value')

play = widgets.Play(
    interval=1,
    value=0,
    min=0,
    max=v_slider.max,
    step=1,
    description="Press play",
    disabled=False
)

widgets.jslink((play, 'value'), (v_slider, 'value'));

scale_x = bqs.LinearScale(min = min(v_values), max = max(v_values))
scale_y = bqs.LinearScale(min = 0.0, max = 2.0)

color_scale = bqs.ColorScale(
    colors = ['#FF0000', '#FFfa00'],
    min=min(T_values),
    max=max(T_values)
)

axis_x_001 = bqa.Axis(
    scale=scale_x,
    tick_format='.2f',
    tick_style={'font-size': '15px'},
    tick_values = [0.5, 2.5, 5.0],
    grid_lines = 'none',
    grid_color = '#8e8e8e',
    label='v',
    label_location='middle',
    label_style={'stroke': 'black', 'default-size': 35},
    label_offset='50px'
)

axis_y_001 = bqa.Axis(
    scale=scale_y,
    tick_format='.1f',
    tick_style={'font-size': '15px'},
    tick_values = [0.0, 1, 2],
    grid_lines = 'none',
    grid_color = '#8e8e8e',
    orientation='vertical',
    label='p',
    label_location='middle',
    label_style={'stroke': 'red', 'default_size': 35},
```

(continues on next page)

(continued from previous page)

```
    label_offset='50px'
)

axis_color = bqa.ColorAxis(
    label = 'T',
    scale=color_scale,
    tick_format='.2f',
    orientation='vertical',
    side='right'
)

fig_11A_001 = Figure(
    title='p vs v (fixed T, reduced variables)',
    marks=[],
    axes=[axis_x_001, axis_y_001, axis_color],
    animation_duration=0,
    legend_location='top-right',
    background_style= {'fill': 'white',  'stroke': 'black'},
    fig_margin=dict(top=70, bottom=75, left=80, right=100),
    toolbar = True,
    layout = widgets.Layout(width='85%')
)

lines_11A_001 = bqm.Lines(
    x = v_values,
    y = p_values,
    scales = {'x': scale_x, 'y': scale_y, 'color': color_scale},
    opacities = [1.0] + [0.0 for i in range(len(T_values)-1)],
    visible = True,
    color = T_values,
)

tracer_11A_001 = bqm.Scatter(
    name = '',
    x = [0.0],
    y = [0.0],
    scales = {'x': scale_x, 'y': scale_y},
    opacity = [1.0],
    visible = False,
    colors = ['#2807a3'],
)

fig_11A_001.marks = [
    lines_11A_001,
    tracer_11A_001
]

scale_x_002 = bqs.LinearScale(min = 0.0, max = 2.0)
scale_y_002 = bqs.LinearScale(min = -2.0, max = 2.0)

axis_y_002 = bqa.Axis(
    scale=scale_y_002,
    tick_format='.2f',#'0.2f',
    tick_style={'font-size': '15px'},
    tick_values = [-2, -1, 0, 1, 2],
    grid_lines = 'none',
    grid_color = '#8e8e8e',
```

(continues on next page)

(continued from previous page)

```
    orientation='vertical',
    label='dp/dv',
    label_location='middle',
    label_style={'stroke': 'red', 'default_size': 35},
    label_offset='50px'
)

fig_11A_002 = Figure(
    title='dp/dv vs v (fixed T, reduced variables)',
    marks=[],
    axes=[axis_x_001, axis_y_002],
    animation_duration=0,
    legend_location='top-right',
    background_style= {'fill': 'white',  'stroke': 'black'},
    fig_margin=dict(top=70, bottom=75, left=80, right=100),
    toolbar = True,
    layout = widgets.Layout(width='85%')
)

lines_11A_002 = bqm.Lines(
    x = [0.4],
    y = [1.0],
    scales = {'x': scale_x, 'y': scale_y_002, 'color':color_scale},
    opacities = [1.0],
    visible = True,
    color = T_values,
)

zero_11A_002 = bqm.Lines(
    x = v_values,
    y = [0.0 for v in v_values],
    scales = {'x': scale_x, 'y': scale_y_002},
    opacities = [1.0],
    visible = True,
    colors = ['#FF0000'],
    line_style = 'dotted'
)

fig_11A_002.marks = [
    zero_11A_002,
    lines_11A_002
]

restart_button = widgets.Button(
    description='Clean figure',
    disabled=False,
    button_style='',
    tooltip="",
    layout = widgets.Layout(height='auto')
)

restart_button.on_click(restart_derivative)

show_all_button = widgets.Button(
    description='Show all derivatives',
    disabled=False,
    button_style='',
```

(continues on next page)

(continued from previous page)

```
    tooltip="",
    layout = widgets.Layout(height='auto', width='initial')
)

show_all_button.on_click(show_all_derivatives)

prepare_export_fig_11A_001_button = widgets.Button(
    description='Export',
    disabled=False,
    button_style='',
    tooltip='',
)

prepare_export_fig_11A_001_button.on_click(prepare_export)

prepare_export_fig_11A_002_button = widgets.Button(
    description='Export',
    disabled=False,
    button_style='',
    tooltip='',
)

prepare_export_fig_11A_002_button.on_click(prepare_export)

slider_box = widgets.HBox([
    v_slider, v_text
    ],
    layout=widgets.Layout(
        height='auto',
        width='100%',
        align_items='center'
    )
)

bottom_block.children = [
    widgets.VBox([
        fig_11A_001,
        prepare_export_fig_11A_001_button,
        slider_box,
        play
    ],
    layout=widgets.Layout(
        height='auto',
        width='50%',
        align_items='center'
    )
    ),
    widgets.VBox([
        fig_11A_002,
        prepare_export_fig_11A_002_button,
        restart_button,
        show_all_button
    ],
    layout=widgets.Layout(
        height='auto',
        width='50%',
        align_items='center'
```

(continues on next page)

(continued from previous page)

```
    )
    )
]

main_block_11A_000 = widgets.VBox(
    [],
    layout=widgets.Layout(align_items='center')
)

main_block_11A_000.children = [
    top_block,
    bottom_block
]

figures = [
    fig_11A_001,
    fig_11A_002
]

main_block_11A_000
```

## 1.11 Visualization of molar volume during a liquid-gas phase transition

**Code:** #112-000

**File:** `apps/van_der_waals/phase_transition_volume.ipynb`

**Run it online:**

---

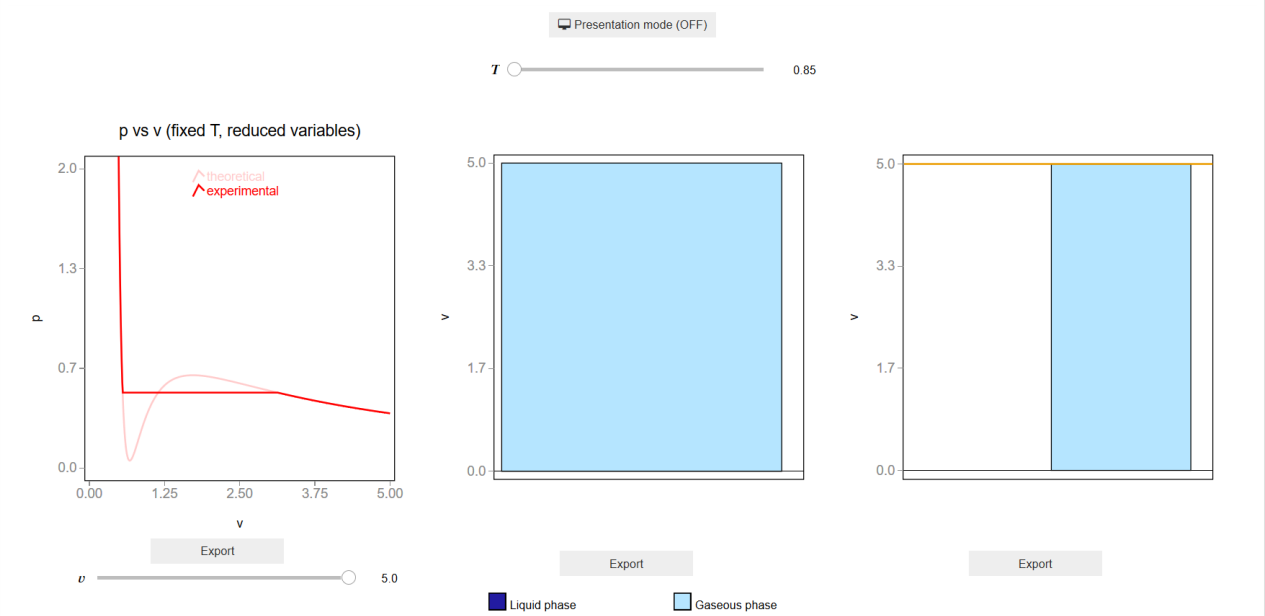
The aim of this notebook is to visualize the change in molar volume during a first-orden liquid-gas transition.

### 1.11.1 Interface

The main interface (`main_block_112_000`) is divided in two HBox: `top_block_112_000` and `bottom_block_112_000`. `bottom_block_112_000` contains of 3 bqplot Figures: `fig_112_001`, `fig_112_002` and `fig_112_003`.

[1]:
```
from IPython.display import Image
Image(filename='../../static/images/apps/112-000_1.png')
```

[1]:




The slider `T_slider` updates the values of $T$ which updates the bars and scatter points of `fig_112_001`, `fig_112_002` and `fig_112_003`.

[2]:
```
Image(filename='../../static/images/apps/112-000_2.png')
```

[2]:


### 1.11.2 CSS

A custom `css` file is used to improve the interface of this application. It can be found here.

[3]:
```
from IPython.display import HTML
display(HTML("<head><link rel='stylesheet' type='text/css' href='./../../static/
↪custom.css'></head>"))
display(HTML("<style>.container { width:100% !important; }</style>"))
```

```
<IPython.core.display.HTML object>
```

```
<IPython.core.display.HTML object>
```

### 1.11.3 Packages

[4]:
```
from bqplot import *
import bqplot as bq
import bqplot.marks as bqm
import bqplot.scales as bqs
import bqplot.axes as bqa

import ipywidgets as widgets
```

(continues on next page)

(continued from previous page)

```
import numpy as np

import urllib.parse
import webbrowser

import sys
```

### 1.11.4 Physical functions

This are the functions that have a physical meaning:

- get_relative_isotherms
- experimetal_isotherms
- get_roots
- p_indefinite_integral
- p_definite_integral
- find_real_fixed_T
- get_volumes_propotions

[5]:
```
def get_relative_isotherms(v_range, T_range):
    """This function calculates the theoretical p(v, T) plane
        (in reduced coordinates) according to Van der Waals
        equation of state from a given range of volumes
        and tenperatures.

    Args:
        v_range: An array containing the values of v
        (in reduced coordinates)for which the isotherms must be
        calculated.\n
        T_range: An array containing the values of v
        (in reduced coordinates)for which the isotherms must be
        calculated.\n


    Returns:
        isotherms: A list consisted consisted of numpy arrays containing the
        pressures of each isotherm.
    """

    isotherms = []

    for T in T_range:
        p_R = []
        for v in v_range:
            val = (8.0/3.0*T/(v - 1.0/3.0) - 3.0/v**2)
            p_R = np.append(p_R, val)

        isotherms.append(p_R)

    return isotherms
```

[6]:
```
def experimental_isotherms(p_range, v_range, T_range, fixed_p, fixed_T):
    """This function calculates the experimental p(v, T) plane
        (in reduced coordinates) according to van der Waals
        equation of state for a given range of volumes
        and tenperatures or for a given range of volumes
        and pressures.

    Args:
        p_range: An array containing the values of p
        (in reduced coordinates)for which the isotherms must be
        calculated. Only used if fixed_p == True.\n
        v_range: An array containing the values of v
        (in reduced coordinates)for which the isotherms must be
        calculated.\n
        T_range: An array containing the values of v
        (in reduced coordinates)for which the isotherms must be
        calculated. Only used if fixed_T == True.\n
        fixed_p: Boolean variable which represents if the isotherms
        must be calculated for a given pressures.\n
        fixed_T: Boolean variable which represents if the isotherms
        must be calculated for a given pressures.\n


    Returns:
        expe_data: A list consisted of numpy arrays containing the
        pressures of each theoretical isotherm.\n
        theo_data: A list consisted of numpy arrays containing the
        pressures of each theoretical isotherm.\n
        v_limits: A list consisted of arrays of the volume limits of
        the phase-transition of each subcritical isotherm.\n
        p_limits: A list consisted of arrays of the pressure limits of
        the phase-transition of each subcritical isotherm.\n
        tenperatures: A list consisted of the tenperatures of the
        isotherms.\n
    """

    if fixed_T:

        theo_data = get_relative_isotherms(v_range, T_range)
        expe_data = []

        v_limits = []
        p_limits = []

        p_range = np.linspace(0.001, 1.0, num=10000)
        pressures, v_isobaric_limits = find_real_fixed_T(p_range, T_range)

        for i in range(len(theo_data)):

            p_expe = []

            if i < len(v_isobaric_limits):

                    v_lim = v_isobaric_limits[i]

                    if len(v_lim) > 1: #check if there is only one point
                        for j in range(len(v_range)):
```

(continues on next page)

(continued from previous page)

```
                        if v_range[j] > v_lim[0] and v_range[j] < v_lim[1]:
                            p_expe.append(pressures[i])

                        else:
                            p_expe.append(theo_data[i][j])

                    v_limits = np.append(v_limits, [v_lim[0], v_lim[1]])
                    p_limits = np.append(p_limits, [pressures[i], pressures[i]])

                else:
                    p_expe = theo_data[i]
                    v_limits = np.append(v_limits, [1.0])
                    p_limits = np.append(p_limits, [1.0])

            else:

                p_expe = theo_data[i]

            expe_data.append(p_expe)

        tenperatures = T_range

        return expe_data, theo_data, p_limits, v_limits, tenperatures

    elif fixed_p:

        tenperatures, v_isobaric_limits = find_real_fixed_p(p_range, T_range)

        theo_data = get_relative_isotherms(v_range, tenperatures)
        expe_data = []

        v_limits = []
        p_limits = []

        for i in range(len(theo_data)):

            p_expe = []

            if i < len(v_isobaric_limits):

                    v_lim = v_isobaric_limits[i]

                    if len(v_lim) > 1: #check if there is only one point

                        for j in range(len(v_range)):

                            if v_range[j] > v_lim[0] and v_range[j] < v_lim[1]:
                                p_expe.append(p_range[i])

                            else:
                                p_expe.append(theo_data[i][j])

                        v_limits = np.append(v_limits, [v_lim[0], v_lim[1]])
                        p_limits = np.append(p_limits, [p_range[i], p_range[i]])

                    else:
```

(continues on next page)

(continued from previous page)

```
                        p_expe = theo_data[i]
                        v_limits = np.append(v_limits, [1.0])
                        p_limits = np.append(p_limits, [1.0])

            else:

                p_expe = theo_data[i]

            expe_data.append(p_expe)

        return expe_data, theo_data, p_limits, v_limits, tenperatures
```

[7]:
```
def get_roots(p, T):
    """This function finds the intersection between an isobaric curve
       and Van der Waals equation of state for a given T.\n
       Values of v with no physical meaning are dismissed
       (v < 0 or complex).

    Args:
        p: Pressure of the isobaric curve.\n
        T: Tenperature of the isotherm.\n


    Returns:
        roots_in_range: A sorted list of the volumes in which the
        isobaric curve intersects the isotherm.\n
    """

    roots = np.roots([1.0, - 1.0/3.0*(1.0 + 8.0*T/p), 3.0/p, -1.0/p])
    roots_in_range = []

    for root in roots:

        # A third degree polynomial has 3 complex roots,
        # but we are only interested in the ones which are
        # purely real.

        if np.isreal(root):

            root = np.real(root)

            if root > 0:

                roots_in_range.append(root)

    roots_in_range.sort()

    return roots_in_range
```

[8]:
```
def p_indefinite_integral(p_0, v_0, T):
    """This function calculates the indefinite integral between
    a van der Waals isotherm and a isobaric line.

    Args:
        p0: Isobaric line's pressure.\n
        v0: Value of the volume.\n
```

(continues on next page)

(continued from previous page)

```
        T: Value of the tenperature.\n

    Returns:
        integral: Value of the indefinite integral between a
        van der Waals isotherm at T and a isobaric line of p0 at a
        volume v0.\n
    """

    integral = 8.0/3.0 * T *np.log(v_0 - 1.0/3.0) + 3.0/v_0 - p_0*v_0

    return integral
```

[9]:
```
def definite_integral(p_0, v_range, T):
    """This function 'p_indefinite_integral' function to calculate
    the definite integral between a van der Waals isotherm and a
    isobaric line.

    Args:
        p0: Isobaric line's pressure.\n
        v_range: Tuple or list consisted of volume limits.\n
        T: Value of the tenperature.\n

    Returns:
        integral: Value of the definite integral between a
        van der Waals isotherm at T and a isobaric line of p0 in a
        volume range v_range.\n
    """

    v_0, v_1 = v_range[0], v_range[1]

    integral = p_indefinite_integral(p_0, v_1, T) - p_indefinite_integral(p_0, v_0, T)

    return integral
```

[10]:
```
def find_real_fixed_T(p_values, T_values):
    """This function uses Maxwell's construction to find the
       pressures in which phase transition happens given some
       fixed tenperatures.\n

    Args:
        p_values: List of pressures in which the real isotherm is
        searched.\n
        T_values: List of tenperatures of the isotherms.\n


    Returns:
        pressures: List of pressures in which phase transition
        happens.\n
        v_range: Volume limits of phase transition zones.
    """

    eps = 1e-3

    pressures = []
    v_ranges = []
```

(continues on next page)

(continued from previous page)

```
    for T in T_values:

        if T < 1.0:

            for p in p_values:

                roots = get_roots(p, T)

                if len(roots) == 3:

                    v_range = [roots[0], roots[2]]
                    area = definite_integral(p, v_range, T)

                    if abs(area) < eps:

                        pressures.append(p)
                        v_ranges.append(v_range)

                        break

        elif T == 1.0:

            pressures.append(1.0)
            v_ranges.append([1.0])

    return pressures, v_ranges
```

[11]:
```
def get_volumes_propotions(v_limits, v):
    """This function calculates the propotion of gas/liquid
       during a phase transistion at a volume v.\n

    Args:
        v_limits: Volume limits in which the phase transition
        happens.\n
        v: value of the volume.\n


    Returns:
        x_g: propotion of the gas phase.\n
        x_l: propotion of the liquid phase.
    """

    v_l = v_limits[0]
    v_g = v_limits[1]

    x_l = (v_g - v)/(v_g - v_l)
    x_g = (v - v_l)/(v_g - v_l)

    return x_g, x_l
```

### 1.11.5 Functions related to the interaction

[12]:
```
def update_tracer(change):
    """This function update the position of the tracer and the
```

(continues on next page)

(continued from previous page)

```
        values and colors of the bars.\n
    """

    tracer_112_001.visible = True

    i = change.get('owner').index
    v = v_values[i]
    p = expe_data[T_slider.index][i]

    tracer_112_001.x, tracer_112_001.y = [v], [p]

    lines_112_003.y = [v, v]

    if T_slider.value < 1.0:

        v_g = v_limits[2*T_slider.index + 1]
        v_l = v_limits[2*T_slider.index]

        if v > v_g:

            bar_112_002.colors = ['#b5e5ff', '#221ba1']
            bar_112_002.y = [[v],[0.0]]

            bar_112_003.colors = ['#221ba1', '#b5e5ff']
            bar_112_003.y = [[0.0], [v]]

        elif v > v_l and  v < v_g:
            x_g, x_l = get_volumes_propotions((v_l, v_g), v)

            bar_112_002.colors = ['#221ba1', '#b5e5ff']
            bar_112_002.y = [[v_l*x_l], [v_g*x_g]]

            bar_112_003.colors = ['#221ba1', '#b5e5ff']
            bar_112_003.y = [[v_l*x_l], [v_g*x_g]]

        elif v < v_l:

            bar_112_002.colors = ['#b5e5ff', '#221ba1']
            bar_112_002.y = [[0.0], [v]]

            bar_112_003.colors = ['#221ba1', '#b5e5ff']
            bar_112_003.y = [[v], [0.0]]

    else:

        bar_112_002.y = [[v],[0.0]]
        bar_112_002.colors = [gradient[i]]

        bar_112_003.y = [[v]]
        bar_112_003.colors = [gradient[i]]
```

[13]:
```
def change_tenperature(change):
    """This function changes the visible isotherm in the figure.\n
    """

    lines_112_001.y = [theo_data[T_slider.index], expe_data[T_slider.index]]
```

(continues on next page)

(continued from previous page)

```
    v_slider.value = v_slider.options[-1]

    i = v_slider.index

    v = v_values[i]
    p = expe_data[T_slider.index][i]

    tracer_112_001.x, tracer_112_001.y = [v], [p]
```

### 1.11.6 Functions related to visualization

[14]:
```
def hex_to_rgb(number_hex):
    """This function converts a color expressed in
       hexadecimal to rgb.\n

    Args:
        number_hex: A string expressing a color in hexadecimal format.\n

    Returns:
        A tuple containing the three integers of the rgb color.
    """

    if number_hex.startswith('#'):
        number_hex = number_hex[1:]

    return (int(number_hex[0:2], 16), int(number_hex[2:4], 16), int(number_hex[4:],␣
↪16))
```

[15]:
```
def rgb_to_hex(number_rgb):
    """This function converts a color expressed in
       rgb to hexadecimal.\n

    Args:
        number_rgb: A tuple containing the three integers of the rgb color.\n

    Returns:
        A string expressing a color in hexadecimal format.
    """

    return '#' + format(number_rgb[0], '02x') + format(number_rgb[1], '02x') +␣
↪format(number_rgb[2], '02x')
```

[16]:
```
def generate_gradient(initial, final, length):
    """This function generates a list of colors forming a gradient
       from initial color to final color.\n

    Args:
        initial: Initial color of the gradient in hexadecimal
        format.\n
        final: Final color of the gradient in hexadecimal
        format.\n
        lenght: An integer expressing the number of colors to
        calculate.\n
```

(continues on next page)

(continued from previous page)

```
    Returns:
        colors: A list consisted of the strings  of the colors
        colors of the gradient in hexadecimal format.
    """

    i_r, i_g, i_b = hex_to_rgb(initial)
    f_r, f_g, f_b = hex_to_rgb(final)

    r_step = (f_r - i_r)/length
    g_step = (f_g - i_g)/length
    b_step = (f_b - i_b)/length

    r, g, b = i_r, i_g, i_b
    colors = []

    for i in range(length):

        h = rgb_to_hex((int(round(r)),int(round(g)),int(round(b))))

        colors.append(h)

        r = r + r_step
        g = g + g_step
        b = b + b_step

    return colors
```

[17]:
```
def change_view(change):
    """This function changes the visualization of all the
    components of the application so they are suitable for
    a projection.\n
    """

    obj = change.owner

    if obj.value:

        obj.description = 'Presentation mode (ON)'

        display(HTML(
            "<style>" \
            ".widget-readout { font-size: 30px ; }" \
            ".widget-label-basic {font-size: 30px;}" \
            "option {font-size: 25px;}" \
            ".p-Widget.jupyter-widgets.widget-slider.widget-vslider.widget-inline-
↪vbox {width: auto}" \
            ".p-Widget .jupyter-widgets .widgets-label {width: auto; height: auto;␣
↪font-size: 30px;}" \
            ".widget-label {font-size: 30px ; height: auto !important;}" \
            ".p-Widget .bqplot .figure .jupyter-widgets {height: auto !important;}" \
            ".widget-text input[type='number'] {font-size: 30px;height: auto;}" \
            ".option { font-size: 30px ;}" \
            ".p-Widget .jupyter-widgets .jupyter-button.widget-button {font-size:␣
↪30px ; width: auto; height: auto;}" \
            ".p-Widget.jupyter-widgets.jupyter-button.widget-toggle-button{font-size:␣
↪30px ; width: auto; height: auto;}" \
```

(continues on next page)

(continued from previous page)

```
            ".p-Widget.p-Panel.jupyter-widgets.widget-container.widget-box.widget-
↪vbox {padding-bottom: 30px}" \
            ".bqplot > svg .axis text.axislabel, .bqplot > svg .axis tspan.axislabel
↪{font-size: 30px;}"
            "</style>"
            )
        )

        for figure in figures:

            figure.legend_text = {'font-size': '30px'}
            figure.title_style = {'font-size': '30px'}

            for axis in figure.axes:
                axis.tick_style = {'font-size': '30px'}
                axis.label_style = {'font-size': '30px'}

    else:

        obj.description = 'Presentation mode (OFF)'

        display(HTML(
            "<style>" \
            ".widget-readout { font-size: 14px ;}" \
            ".widget-label-basic {font-size: 14px;}" \
            "option {font-size: 12px;}" \
            ".p-Widget .jupyter-widgets .widgets-label {font-size: 14px;}" \
            ".widget-label {font-size: 14px ;}" \
            ".widget-text input[type='number'] {font-size: 14px;}" \
            ".option { font-size: 14px ;}" \
            ".p-Widget .jupyter-widgets .jupyter-button.widget-button {font-size:␣
↪14px;}" \
            ".p-Widget.jupyter-widgets.jupyter-button.widget-toggle-button {font-size:
↪ 14px;}" \
            ".bqplot > svg .axis text.axislabel, .bqplot > svg .axis tspan.axislabel
↪{font-size: 14px;}"
            "</style>"
            )
        )

        for figure in figures:

            figure.legend_text = {'font-size': '14px'}
            figure.title_style = {'font-size': '20px'}

            for axis in figure.axes:
                axis.tick_style = {'font-size': '14px'}
                axis.label_style = {'font-size': '14px'}
```

[18]:
```
def prepare_export(button):
    """This function sends the selected plot to the 'export_plot'
    function.
    """

    if button is prepare_export_fig_112_001_button:
```

(continues on next page)

(continued from previous page)

```
        export_plot(fig_112_001)

    elif button is prepare_export_fig_112_002_button:

        export_plot(fig_112_002)

    elif button is prepare_export_fig_112_003_button:

        export_plot(fig_112_003)
```

[19]:
```
def export_plot(plot):
    """This function sends the selected plot to the export module.
    """

    global data

    text_lines = []

    np.set_printoptions(threshold=sys.maxsize)
    data = repr((plot, text_lines))
    %store data

    rel_url = "../../../apps/modules/export_module.ipynb"
    abs_url = urllib.parse.urljoin(notebook_url, rel_url)

    webbrowser.open(abs_url)
```

[ ]:
```
%%javascript

//Get the URL of the current notebook

var kernel = Jupyter.notebook.kernel;
var command = ["notebook_url = ",
               "'", window.location.href, "'" ].join('')

kernel.execute(command)
```

### 1.11.7 Main interface

[ ]:
```
"""This module visualizes the change in molar volumen of both phases
during a liquid-gas phase transition.

"""

v_values = np.linspace(0.4, 5.0, 500)
T_values = np.round(np.linspace(0.85, 1.2, 10), 2)

colors = ['#221ba1','#b5e5ff'] #light blue, dark_blue
gradient = generate_gradient(colors[0], colors[1], 500)

expe_data, theo_data, p_limits, v_limits, tenperatures = experimental_isotherms(
    [],
    v_values,
    T_values,
```

(continues on next page)

(continued from previous page)

```
    fixed_p = False,
    fixed_T = True,
)

#######################
#######TOP BLOCK####
#######################

top_block = widgets.VBox([], layout=widgets.Layout(align_items='center', width='100%
↪'))

change_view_button = widgets.ToggleButton(
    value=False,
    description='Presentation mode (OFF)',
    disabled=False,
    button_style='',
    tooltip='',
    icon='desktop',
    layout=widgets.Layout(
        width='auto'
    )
)

change_view_button.observe(change_view, 'value')

T_slider = widgets.SelectionSlider(
    options= T_values,
    value=T_values[0],
    description=r'\( T \)',
    disabled=False,
    continuous_update=True,
    orientation='horizontal',
    readout=True,
    layout = widgets.Layout(
        width = '33%',
        align_self='center',
        margin='20px 0 0 0'
    )
)

T_slider.observe(change_tenperature, 'value')

top_block.children = [
    change_view_button,
    T_slider
]

#######################
#######MIDDLE BLOCK####
#######################

middle_block = widgets.HBox([], layout=widgets.Layout(align_items='center', width='100
↪%'))

scale_x = bqs.LinearScale(min = 0.0, max = max(v_values))
scale_y = bqs.LinearScale(min = 0, max = 2.0)
```

(continues on next page)

(continued from previous page)

```
axis_x = bqa.Axis(
    scale=scale_x,
    tick_format='.2f',
    tick_style={'font-size': '15px'},
    tick_values = np.linspace(0, max(v_values), 5),
    grid_lines = 'none',
    grid_color = '#8e8e8e',
    label='v',
    label_location='middle',
    label_style={'stroke': 'black', 'default-size': 35},
    label_offset='50px'
)

axis_y = bqa.Axis(
    scale=scale_y,
    tick_format='.1f',
    tick_style={'font-size': '15px'},
    tick_values = np.linspace(0, 2.0, 4),
    grid_lines = 'none',
    grid_color = '#8e8e8e',
    orientation='vertical',
    label='p',
    label_location='middle',
    label_style={'stroke': 'red', 'default_size': 35},
    label_offset='50px'
)

fig_112_001 = bq.Figure(
    title='p vs v (fixed T, reduced variables)',
    marks=[],
    axes=[axis_x, axis_y],
    animation_duration=0, #500,
    legend_location='top-right',
    legend_text =  {'font-size': '14px'},
    background_style= {'fill': 'white',  'stroke': 'black'},
    fig_margin=dict(top=80, bottom=60, left=80, right=30),
    toolbar = True,
    layout = widgets.Layout(width='100%', height='500px'),
)

lines_112_001 = bqm.Lines(
    x = v_values,
    y = [theo_data[T_slider.index], expe_data[T_slider.index]],
    scales = {'x': scale_x, 'y': scale_y},
    opacities = [0.2, 1.0],
    visible = True,
    colors = ['red'],
    labels = ['theoretical', 'experimental'],
    display_legend = True
)

tracer_112_001 = bqm.Scatter(
    name = '',
    x = [0.0],
    y = [0.0],
    scales = {'x': scale_x, 'y': scale_y},
    opacity = [1.0, 0.0],
```

(continues on next page)

(continued from previous page)

```
    visible = False,
    colors = ['#2807a3'],
)

fig_112_001.marks = [lines_112_001, tracer_112_001]

v_values_rounded = np.round(v_values, 3)

v_slider = widgets.SelectionSlider(
    options=v_values_rounded,
    value=v_values_rounded[-1],
    description=r'\( v \)',
    disabled=False,
    continuous_update=True,
    orientation='horizontal',
    readout=True,
    layout = widgets.Layout(width = '100%', margin='0 50px 0 50px')
)

v_slider.observe(update_tracer, 'value')


new_x_scale = bqs.LinearScale(min=0.5, max=1.5)

bar_112_002 = bqm.Bars(
    x=[1.0],
    y=[max(v_values)],
    scales={'x': bqs.OrdinalScale(), 'y': scale_x},
    colors=['#b5e5ff', '#221ba1'],
)

original_112_002 = bqm.Bars(
    x=[1.0],
    y=[max(v_values)],
    scales={'x': bqs.OrdinalScale(), 'y': scale_x},
    colors=['#d9d9d9'],
    opacities = [0.2]
)

axis_x_002 = bqa.Axis(
    scale=new_x_scale,
    tick_format='.2f',
    tick_style={'font-size': '15px'},
    num_ticks=0,
    grid_lines = 'none',
    grid_color = '#8e8e8e',
    label='',
    label_location='middle',
    label_style={'stroke': 'black', 'default-size': 35},
    label_offset='50px'
)

axis_y_002 = bqa.Axis(
    scale=scale_x,
    tick_format='.1f',
    tick_style={'font-size': '15px'},
    tick_values = np.linspace(0, max(v_values), 4),
```

(continues on next page)

(continued from previous page)

```
    grid_lines = 'none',
    grid_color = '#8e8e8e',
    orientation='vertical',
    label='v',
    label_location='middle',
    label_style={'stroke': 'red', 'default_size': 35},
    label_offset='50px'
)

fig_112_002 = bq.Figure(
    title='',
    marks=[],
    axes=[axis_x_002, axis_y_002],
    animation_duration=0,
    legend_location='top-right',
    background_style= {'fill': 'white',  'stroke': 'black'},
    fig_margin=dict(top=65, bottom=75, left=80, right=30),
    toolbar = True,
    layout = widgets.Layout(width='100%', height='500px')
)

fig_112_002.marks = [original_112_002, bar_112_002, ]

bar_112_003 = bqm.Bars(
    x=[[1.0],[1.0]],
    y=[[0.0], [max(v_values)]],
    scales={'x': bqs.OrdinalScale(), 'y': scale_x},
    colors=['#221ba1', '#b5e5ff'],
    type='grouped'
)

lines_112_003 = bqm.Lines(
    x = [0.0, 5.0],
    y = [max(v_values), max(v_values)],
    scales = {
        'x': bqs.LinearScale(min=0, max=1.0),
        'y': scale_x
    },
    visible = True,
    colors = ['#eb9c00'],
)

axis_x_003 = bqa.Axis(
    scale=new_x_scale,
    tick_format='.2f',
    tick_style={'font-size': '15px'},
    num_ticks=0,
    grid_lines = 'none',
    grid_color = '#8e8e8e',
    label='',
    label_location='middle',
    label_style={'stroke': 'black', 'default-size': 35},
    label_offset='50px'
)

axis_y_003 = bqa.Axis(
    scale=scale_x,
```

(continues on next page)

(continued from previous page)

```
    tick_format='.1f',
    tick_style={'font-size': '15px'},
    tick_values = np.linspace(0, max(v_values), 4),
    grid_lines = 'none',
    grid_color = '#8e8e8e',
    orientation='vertical',
    label='v',
    label_location='middle',
    label_style={'stroke': 'red', 'default_size': 35},
    label_offset='50px'
)

fig_112_003 = bq.Figure(title='',
    marks=[],
    axes=[axis_x_003, axis_y_003],
    animation_duration=0,
    legend_location='top-right',
    background_style= {'fill': 'white',  'stroke': 'black'},
    fig_margin=dict(top=65, bottom=75, left=80, right=30),
    toolbar = True,
    layout = widgets.Layout(width='100%', height='500px')
)

fig_112_003.marks = [bar_112_003, lines_112_003]

prepare_export_fig_112_001_button = widgets.Button(
    description='Export',
    disabled=False,
    button_style='',
    tooltip='',
)

prepare_export_fig_112_001_button.on_click(prepare_export)

prepare_export_fig_112_002_button = widgets.Button(
    description='Export',
    disabled=False,
    button_style='',
    tooltip='',
)

prepare_export_fig_112_002_button.on_click(prepare_export)

prepare_export_fig_112_003_button = widgets.Button(
    description='Export',
    disabled=False,
    button_style='',
    tooltip='',
)

prepare_export_fig_112_003_button.on_click(prepare_export)

export_button = widgets.HTML(
    value = ""
)

middle_block.children = [
```

(continues on next page)

(continued from previous page)

```
    widgets.VBox([
         fig_112_001,
         prepare_export_fig_112_001_button,
         v_slider
    ],
        layout = widgets.Layout(
            align_items='center',
            width='33%'
        )
    ),
    widgets.VBox([
        fig_112_002,
        prepare_export_fig_112_002_button,
    ],
        layout = widgets.Layout(
            align_items='center',
            width='33%'
        )
    ),
    widgets.VBox([
        fig_112_003,
        prepare_export_fig_112_003_button
    ],
        layout = widgets.Layout(
            align_items='center',
            width='33%'
        )
    ),
]

#######################
#######BOTTOM BLOCK######
#######################

bottom_block_112_000 = widgets.VBox([
    widgets.HBox([
        widgets.HTML(
            '<svg width="20" height="20">' \
            '<rect width="20" height="20"' \
            'style="fill:#221ba1;stroke-width:3;' \
            'stroke:rgb(0,0,0)"/></svg>' \
        ),
        widgets.Label("Liquid phase",),
        widgets.HTML('<span style="display:inline-block; width: 100px;"></span>'),
        widgets.HTML(
                '<svg width="20" height="20">' \
                '<rect width="20" height="20"' \
                'style="fill:#b5e5ff;stroke-width:3;' \
                'stroke:rgb(0,0,0)"/></svg>' \
            ),
        widgets.Label("Gaseous phase"),
    ])],
    layout=widgets.Layout(
        align_items='center',
        width='100%'
    )
)
```

(continues on next page)

(continued from previous page)

```
#######################
#######MAIN BLOCK######
#######################

main_block_112_000 = widgets.VBox(
    [],
    layout=widgets.Layout(
        align_items='center',
        width='100%'
    )
)

main_block_112_000.children = [
    top_block,
    middle_block,
    bottom_block_112_000
]


figures = [
    fig_112_001,
    fig_112_002,
    fig_112_003
]

main_block_112_000
```

## 1.12 Change in molar entropy during a first-order phase transition

**Code:** #11D-000

**File:** `apps/van_der_waals/entropy.ipynb`

**Run it online:**

---

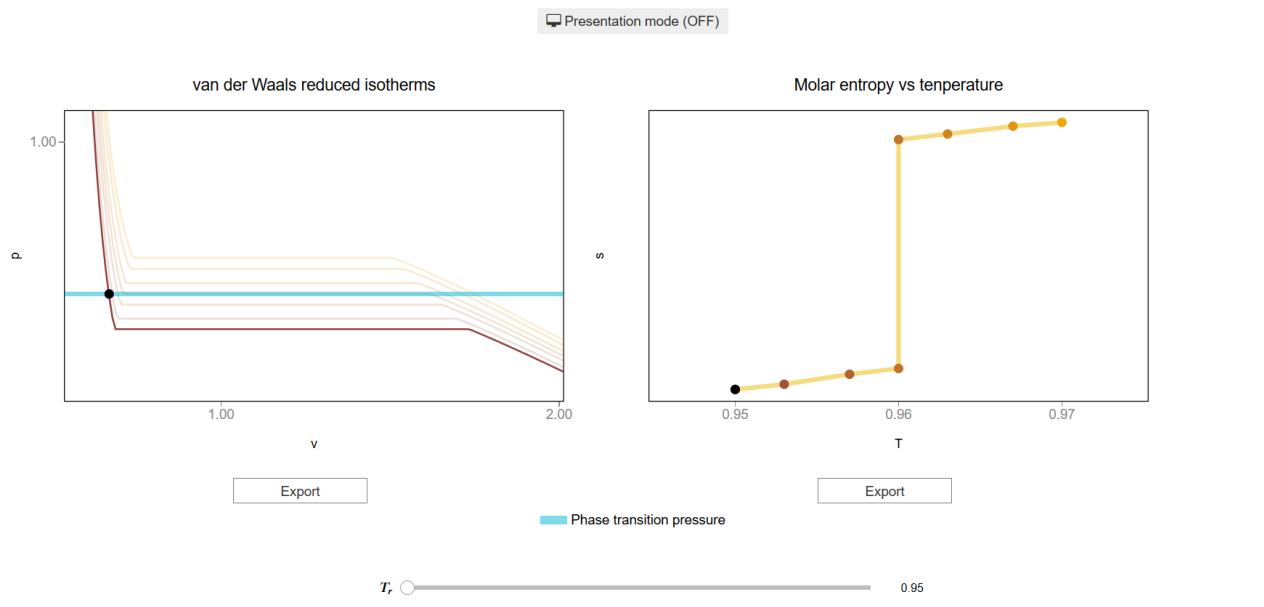
The aim of this notebook is to visualize the change in molar entropy during a first-orden liquid-gas transition.

### 1.12.1 Interface

The main interface (`main_block_11D_000`) is divided in two HBox: `top_block_11D_000` and `bottom_block_11D_000`. `bottom_block_11D_000` contains of 2 bqplot Figures: `fig_11D_001` and `fig_11D_002`.

[1]:
```
from IPython.display import Image
Image(filename='../../static/images/apps/11D-000_1.png')
```

[1]:




The slider `T_slider` updates the values of $T$ which updates the lines and scatter points of `fig_11D_001` and `fig_11D_002`.

[2]:
```
Image(filename='../../static/images/11D-000_2.png')
```

[2]:


### 1.12.2 CSS

A custom `css` file is used to improve the interface of this application. It can be found here.

[3]:
```
from IPython.display import HTML
display(HTML("<head><link rel='stylesheet' type='text/css' href='./../../static/
↪custom.css'></head>"))
display(HTML("<style>.container { width:100% !important; } .jupyter-button {white-
↪space: normal !important;}</style>"))
```

```
<IPython.core.display.HTML object>
```

```
<IPython.core.display.HTML object>
```

### 1.12.3 Packages

[4]:
```
from bqplot import *
import bqplot as bq
import bqplot.marks as bqm
import bqplot.scales as bqs
import bqplot.axes as bqa

import ipywidgets as widgets

from scipy.signal import argrelextrema
```

(continues on next page)

(continued from previous page)

```
import urllib.parse
import webbrowser

import sys
```

### 1.12.4 Physical functions

This are the functions that have a physical meaning:

- get_relative_isotherms
- experimetal_isotherms
- get_roots
- p_indefinite_integral
- p_definite_integral
- find_real_fixed_p
- find_real_fixed_T

[5]:
```
def get_relative_isotherms(v_range, T_range):
    """This function calculates the theoretical p(v, T) plane
        (in reduced coordinates) according to van der Waals
        equation of state from a given range of volumes
        and tenperatures.

    Args:
        v_range: An array containing the values of v
        (in reduced coordinates)for which the isotherms must be
        calculated.\n
        T_range: An array containing the values of T
        (in reduced coordinates)for which the isotherms must be
        calculated.\n


    Returns:
        isotherms: A list consisted of numpy arrays containing the
        pressures of each isotherm.
    """

    isotherms = []

    for T in T_range:
        p_R = []
        for v in v_range:
            val = (8.0/3.0*T/(v - 1.0/3.0) - 3.0/v**2)
            p_R = np.append(p_R, val)

        isotherms.append(p_R)

    return isotherms
```

[6]:
```
def experimental_isotherms(p_range, v_range, T_range, fixed_p, fixed_T):
    """This function calculates the experimental p(v, T) plane
        (in reduced coordinates) according to van der Waals
        equation of state for a given range of volumes
        and tenperatures or for a given range of volumes
        and pressures.

    Args:
        p_range: An array containing the values of p
        (in reduced coordinates)for which the isotherms must be
        calculated. Only used if fixed_p == True.\n
        v_range: An array containing the values of v
        (in reduced coordinates)for which the isotherms must be
        calculated.\n
        T_range: An array containing the values of v
        (in reduced coordinates)for which the isotherms must be
        calculated. Only used if fixed_T == True.\n
        fixed_p: Boolean variable which represents if the isotherms
        must be calculated for a given pressures.\n
        fixed_T: Boolean variable which represents if the isotherms
        must be calculated for a given pressures.\n


    Returns:
        expe_data: A list consisted of numpy arrays containing the
        pressures of each theoretical isotherm.\n
        theo_data: A list consisted of numpy arrays containing the
        pressures of each theoretical isotherm.\n
        v_limits: A list consisted of arrays of the volume limits of
        the phase-transition of each subcritical isotherm.\n
        p_limits: A list consisted of arrays of the pressure limits of
        the phase-transition of each subcritical isotherm.\n
        tenperatures: A list consisted of the tenperatures of the
        isotherms.\n
    """

    if fixed_T:

        theo_data = get_relative_isotherms(v_range, T_range)
        expe_data = []

        v_limits = []
        p_limits = []

        p_range = np.linspace(0.001, 1.0, num=10000)
        pressures, v_isobaric_limits = find_real_fixed_T(p_range, T_range)

        for i in range(len(theo_data)):

            p_expe = []

            if i < len(v_isobaric_limits):

                    v_lim = v_isobaric_limits[i]

                    if len(v_lim) > 1: #check if there is only one point
                        for j in range(len(v_range)):
```

(continues on next page)

(continued from previous page)

```
                        if v_range[j] > v_lim[0] and v_range[j] < v_lim[1]:
                            p_expe.append(pressures[i])

                        else:
                            p_expe.append(theo_data[i][j])

                    v_limits = np.append(v_limits, [v_lim[0], v_lim[1]])
                    p_limits = np.append(p_limits, [pressures[i], pressures[i]])

                else:
                    p_expe = theo_data[i]
                    v_limits = np.append(v_limits, [1.0])
                    p_limits = np.append(p_limits, [1.0])

            else:

                p_expe = theo_data[i]

            expe_data.append(p_expe)

        tenperatures = T_range

        return expe_data, theo_data, p_limits, v_limits, tenperatures

    elif fixed_p:

        tenperatures, v_isobaric_limits = find_real_fixed_p(p_range, T_range)

        theo_data = get_relative_isotherms(v_range, tenperatures)
        expe_data = []

        v_limits = []
        p_limits = []

        for i in range(len(theo_data)):

            p_expe = []

            if i < len(v_isobaric_limits):

                    v_lim = v_isobaric_limits[i]

                    if len(v_lim) > 1: #check if there is only one point

                        for j in range(len(v_range)):

                            if v_range[j] > v_lim[0] and v_range[j] < v_lim[1]:
                                p_expe.append(p_range[i])

                            else:
                                p_expe.append(theo_data[i][j])

                        v_limits = np.append(
                            v_limits,
                            [v_lim[0],
                             v_lim[1]]
```

(continues on next page)

(continued from previous page)

```
                        )
                        p_limits = np.append(
                            p_limits,
                            [p_range[i],
                             p_range[i]]
                        )

                    else:
                        p_expe = theo_data[i]
                        v_limits = np.append(v_limits, [1.0])
                        p_limits = np.append(p_limits, [1.0])

            else:

                p_expe = theo_data[i]

            expe_data.append(p_expe)

        return expe_data, theo_data, p_limits, v_limits, tenperatures
```

[7]:
```
def get_roots(p, T):
    """This function calculates the roots of a van der Waals
    isotherm of a given T and set of pressures.

    Args:
        p: Numpy array consisted of the pressures of the isotherm.\n
        T: Value of the tenperature.\n

    Returns:
        roots_in_range: A list consisted of the real roots.\n
    """


    roots = np.roots([1.0, - 1.0/3.0*(1.0 + 8.0*T/p), 3.0/p, -1.0/p])
    roots_in_range = []

    for root in roots:
        if np.isreal(root):
            root = np.real(root)
            if root > 0:
                roots_in_range.append(root)
    roots_in_range.sort()

    return roots_in_range
```

[8]:
```
def p_indefinite_integral(p_0, v_0, T):
    """This function calculates the indefinite integral between
    a van der Waals isotherm and a isobaric line.

    Args:
        p0: Isobaric line's pressure.\n
        v0: Value of the volume.\n
        T: Value of the tenperature.\n

    Returns:
        integral: Value of the indefinite integral between a
```

(continues on next page)

(continued from previous page)

```
        van der Waals isotherm at T and a isobaric line of p0 at a
        volume v0.\n
    """

    integral = 8.0/3.0 * T *np.log(v_0 - 1.0/3.0) + 3.0/v_0 - p_0*v_0

    return integral
```

[9]:
```
def definite_integral(p_0, v_range, T):
    """This function 'p_indefinite_integral' function to calculate
    the definite integral between a van der Waals isotherm and a
    isobaric line.

    Args:
        p0: Isobaric line's pressure.\n
        v_range: Tuple or list consisted of volume limits.\n
        T: Value of the tenperature.\n

    Returns:
        integral: Value of the definite integral between a
        van der Waals isotherm at T and a isobaric line of p0 in a
        volume range v_range.\n
    """

    v_0, v_1 = v_range[0], v_range[1]

    integral = p_indefinite_integral(p_0, v_1, T) - p_indefinite_integral(p_0, v_0, T)

    return integral
```

[10]:
```
def find_real_fixed_T(p_values, T_values):
    """This function uses Maxwell's construction to find the
       pressures in which phase transition happens given some
       fixed tenperatures.\n

    Args:
        p_values: List of pressures in which the real isotherm is
        searched.\n
        T_values: List of tenperatures of the isotherms.\n


    Returns:
        pressures: List of pressures in which phase transition
        happens.\n
        v_range: Volume limits of phase transition zones.
    """

    eps = 1e-3

    pressures = []
    v_ranges = []

    for T in T_values:

        if T < 1.0:
```

(continues on next page)

(continued from previous page)

```
            for p in p_values:

                roots = get_roots(p, T)

                if len(roots) == 3:

                    v_range = [roots[0], roots[2]]
                    area = definite_integral(p, v_range, T)

                    if abs(area) < eps:

                        pressures.append(p)
                        v_ranges.append(v_range)

                        break

        elif T == 1.0:

            pressures.append(1.0)
            v_ranges.append([1.0])

    return pressures, v_ranges
```

[11]:
```
def find_real_fixed_p(p_values, T_values):
    """This function uses Maxwell's construction to find the
       tenperatures in which phase transition happens given some
       fixed pressures.\n

    Args:
        p_values: List of pressures of the isotherms.\n
        T_values: List of tenperatures in which the real isotherm is
        searched.\n


    Returns:
        tenperatures: List of tenperatures in which phase transition
        happens.\n
        v_range: Volume limits of phase transition zones.
    """

    eps = 1e-3

    tenperatures = []
    v_ranges = []

    for p in p_values:

        if p < 1.0:

            for T in T_values:

                roots = get_roots(p, T)

                if len(roots) == 3:

                    v_range = [roots[0], roots[2]]
```

(continues on next page)

(continued from previous page)

```
                    area = definite_integral(p, v_range, T)

                    if abs(area) < eps:

                        tenperatures.append(T)
                        v_ranges.append(v_range)

                        break

        elif p == 1.0:

            tenperatures.append(1.0)
            v_ranges.append([1.0])

    return tenperatures, v_ranges
```

[12]:
```
def get_entropy(v_values):
    """This function calculates the entropy for a given
    array of molar volumes.

    Args:
        v_values: Array consisted of the values of molar volume.

    Returns:
        s: Array containing the values of the entropy.
    """
    v_values = np.asarray(v_values)
    s = 8.0/3.0*np.log(3.0*v_values - 1.0)

    return s
```

### 1.12.5 Functions related to the interaction

[13]:
```
def find_nearest_index(array, value):
    """This function find index of the element in an array which
    value is the nearest to the given one.

    Args:
        array: A list or numpy array containing the elements.\n
        value: Float number.\n

    Returns:
        idx: Index of the element in array which value is the nearest
        to value.
    """

    array = np.asarray(array)
    idx = (np.abs(array - value)).argmin()
    return idx
```

[14]:
```
def change_tenperature(change):

    index = change.owner.index
```

(continues on next page)

(continued from previous page)

```
    opacities = [def_op for T in T_values]
    opacities[index] = 1.0

    isotherms.opacities = opacities

    if index == selected:

        state.x, state.y = state_v[index], [p_0, p_0]
        state_s.x, state_s.y = [T_values[index], T_values[index]], s_values[index]

    else:

        state.x, state.y = [state_v[index]], [p_0]
        state_s.x, state_s.y = [T_values[index]],[s_values[index]]
```

[16]:
```
def change_view(change):
    """This function changes the visualization of all the
    components of the application so they are suitable for
    a projection.\n
    """

    obj = change.owner

    if obj.value:

        obj.description = 'Presentation mode (ON)'

        display(HTML(
            "<style>" \
            ".widget-readout { font-size: 30px ; }" \
            ".widget-label-basic {font-size: 30px;}" \
            "option {font-size: 25px;}" \
            ".p-Widget.jupyter-widgets.widget-slider.widget-vslider.widget-inline-
↪vbox {width: auto}" \
            ".p-Widget .jupyter-widgets .widgets-label {width: auto; height: auto;
↪font-size: 30px;}" \
            ".widget-label {font-size: 30px ; height: auto !important;}" \
            ".p-Widget .bqplot .figure .jupyter-widgets {height: auto !important;}" \
            ".widget-text input[type='number'] {font-size: 30px;height: auto;}" \
            ".option { font-size: 30px ;}" \
            ".p-Widget .jupyter-widgets .jupyter-button.widget-button {font-size:
↪30px ; width: auto; height: auto;}" \
            ".p-Widget.jupyter-widgets.jupyter-button.widget-toggle-button{font-size:
↪30px ; width: auto; height: auto;}" \
            ".p-Widget.p-Panel.jupyter-widgets.widget-container.widget-box.widget-
↪vbox {padding-bottom: 30px}" \
            ".bqplot > svg .axis text.axislabel, .bqplot > svg .axis tspan.axislabel
↪{font-size: 30px;}" \
            ".q-grid .slick-cell {font-size: 30px;}" \
            ".slick-column-name {font-size: 30px;}" \
            ".widget-html-content {font-size: 30px;}"
            "</style>"
            )
        )

        for figure in figures:
```

(continues on next page)

(continued from previous page)

```
            figure.legend_text = {'font-size': '30px'}
            figure.title_style = {'font-size': '30px'}

            for axis in figure.axes:
                axis.tick_style = {'font-size': '30px'}
                axis.label_style = {'font-size': '30px'}

    else:

        obj.description = 'Presentation mode (OFF)'

        display(HTML(
            "<style>" \
            ".widget-readout { font-size: 14px ;}" \
            ".widget-label-basic {font-size: 14px;}" \
            "option {font-size: 12px;}" \
            ".p-Widget .jupyter-widgets .widgets-label {font-size: 14px;}" \
            ".widget-label {font-size: 14px ;}" \
            ".widget-text input[type='number'] {font-size: 14px;}" \
            ".option { font-size: 14px ;}" \
            ".p-Widget .jupyter-widgets .jupyter-button.widget-button {font-size:
↪14px;}" \
            ".p-Widget.jupyter-widgets.jupyter-button.widget-toggle-button {font-size:
↪ 14px;}" \
            ".bqplot > svg .axis text.axislabel, .bqplot > svg .axis tspan.axislabel
↪{font-size: 14px;}" \
            ".q-grid .slick-cell {font-size: 14px;}" \
            ".slick-column-name {font-size: 14px;}" \
            ".widget-html-content {font-size: 14px;}"
            "</style>"
            )
        )

        for figure in figures:

            figure.legend_text = {'font-size': '14px'}
            figure.title_style = {'font-size': '20px'}

            for axis in figure.axes:
                axis.tick_style = {'font-size': '14px'}
                axis.label_style = {'font-size': '14px'}
```

[17]:
```
def prepare_export(button):
    """This function sends the selected plot to the 'export_plot'
    function.
    """

    if button is prepare_export_fig_11D_001_button:

        export_plot(fig_11D_001)

    elif button is prepare_export_fig_11D_002_button:

        export_plot(fig_11D_002)
```

[18]:
```
def export_plot(plot):
    """This function sends the selected plot to the export module.
    """

    global data

    text_lines = []

    np.set_printoptions(threshold=sys.maxsize)
    data =  repr((plot, text_lines))

    %store data

    rel_url = "../../../apps/modules/export_module.ipynb"
    abs_url = urllib.parse.urljoin(notebook_url, rel_url)

    if not webbrowser.open(abs_url):
        go_to_export_button.value = "<form action=" + abs_url + " target='_blank'>
↪<button type=''submit''>Open in export module</button></form>"
```

[19]:
```
%%javascript

//Get the URL of the current notebook

var kernel = Jupyter.notebook.kernel;
var command = ["notebook_url = ",
               "'", window.location.href, "'" ].join('')

kernel.execute(command)
```

```
<IPython.core.display.Javascript object>
```

### 1.12.6 Functions related to visualization

[20]:
```
def hex_to_rgb(number_hex):
    """This function converts a hexadecimal color to its rgb
    equivalent.

    Args:
        number_hex: String containing the hexadecimal representation
        of the color.\n

    Returns:
        number_rgb: Tuple consisted of the 3 numbers of the rgb
        representation of the color.\n
    """

    if '#' in number_hex:
        number_hex = number_hex[1:]

    number_rgb = (int(number_hex[0:2], 16), \
                  int(number_hex[2:4], 16), \
                  int(number_hex[4:], 16))

    return number_rgb
```

[21]:
```
def rgb_to_hex(number_rgb):
    """This function converts a rgb color to its hexadecimal
    equivalent.

    Args:
        number_rgb: Tuple consisted of the 3 numbers of the rgb
        representation of the color.\n

    Returns:
        number_hex: String containing the hexadecimal representation
        of the color.\n
    """

    number_rgb = '#' \
    + format(number_rgb[0], '02x') \
    + format(number_rgb[1], '02x') \
    + format(number_rgb[2], '02x')

    return number_rgb
```

[22]:
```
def generate_gradient(initial, final, length):
    """This function generates a color gradient consisted of N
    colors from the initial to the final.

    Args:
        initial: String of the hexadecimal representation of the
        initial color.\n
        final: String of the hexadecimal representation of the
        final color.\n
        length: Number of colors.\n

    Returns:
        colors: List consisted of strings of the hexadecimal
        colors.\n
    """

    i_r, i_g, i_b = hex_to_rgb(initial)
    f_r, f_g, f_b = hex_to_rgb(final)

    r_step = (f_r - i_r)/length
    g_step = (f_g - i_g)/length
    b_step = (f_b - i_b)/length

    r, g, b = i_r, i_g, i_b
    colors = []

    for i in range(length):

        h = rgb_to_hex((int(round(r)),int(round(g)),int(round(b))))

        colors.append(h)

        r = r + r_step
        g = g + g_step
        b = b + b_step

    return colors
```

### 1.12.7 Main interface

```
[ ]: T_values = np.round(np.linspace(0.95, 0.97, 7), 3)
v_values = np.linspace(0.45, 5.2, 500)

colors = generate_gradient('#914040', '#feb901', len(T_values))

def_op = 0.2
opacities = [def_op for T in T_values]
opacities[0] = 1.0

data = experimental_isotherms(
    p_range=[],
    v_range=v_values,
    T_range=T_values,
    fixed_T = True,
    fixed_p = False
)

expe_p_values = data[0]
theo_p_values = data[1]

p_limits = data[2]
v_limits = data[3]
T_limits = data[4]

# The index of the pressure of the selected isotherm
selected = 3

p_0 = np.unique(p_limits)[selected]

state_v = []
T_values_repeated = []
colors_repeated = []

for i in range(len(T_values)):

    if i == selected:

        state_v.append(
            np.array([v_limits[2*i],v_limits[2*i+1]])
        )

        T_values_repeated.append(
            T_values[i]
        )

        colors_repeated.append(colors[i])

    else:

        idx = find_nearest_index(expe_p_values[i], p_0)
        state_v.append(v_values[idx])

    T_values_repeated.append(
        T_values[i]
    )
```

(continues on next page)

(continued from previous page)

```
    colors_repeated.append(colors[i])

s_values = []

for v in state_v:
    s_values.append(get_entropy(v))

s_values_plain = np.hstack(s_values)

##########################
########TOP BLOCK#########
##########################

top_block_11D_000 = widgets.HBox(
    [],
    layout=widgets.Layout(
        align_items='center',
        width='100%'
    )
)

# fig_11D_001

scale_x_11D_001 = bqs.LinearScale(min = 0.55, max = 2.0)
scale_y_11D_001 = bqs.LinearScale(min = 0.75, max = 1.02)

axis_x_11D_001 = bqa.Axis(
    scale=scale_x_11D_001,
    tick_format='0.2f',
    tick_style={'font-size': '15px'},
    tick_values=[1.0, 2.0, 3.0, 4.0, 5.0],
    grid_lines = 'none',
    grid_color = '#8e8e8e',
    label='v',
    label_location='middle',
    label_style={'stroke': 'black', 'default-size': 35},
    label_offset='50px'
)

axis_y_11D_001 = bqa.Axis(
    scale=scale_y_11D_001,
    tick_format='0.2f',
    tick_style={'font-size': '15px'},
    tick_values=[0.0, 1.0],
    grid_lines = 'none',
    grid_color = '#8e8e8e',
    orientation='vertical',
    label='p',
    label_location='middle',
    label_style={'stroke': 'red', 'default_size': 35},
    label_offset='50px'
)

isotherms = bqm.Lines(
    x = np.array([v_values]),
    y = np.array([expe_p_values]),
```

(continues on next page)

(continued from previous page)

```
    scales = {'x': scale_x_11D_001, 'y': scale_y_11D_001},
    opacities = opacities,
    visible = True,
    colors = colors,
    labels = [str(t) for t in T_limits],
)

isobaric = bqm.Lines(
    x = [v_values[0], v_values[-1]],
    y = np.array([p_0, p_0]),
    scales = {'x': scale_x_11D_001, 'y': scale_y_11D_001},
    opacities = [0.5],
    visible = True,
    colors = ['#01b6cf'],
    stroke_width = 5,
)

state = bqm.Scatter(
    x = [state_v[0]],
    y = [p_0],
    scales = {'x': scale_x_11D_001, 'y': scale_y_11D_001},
    visible = True,
    colors = ['black'],
    names = [],
    #tooltip = tt
)

fig_11D_001 = bq.Figure(
    title='van der Waals reduced isotherms',
    marks=[],
    axes=[axis_x_11D_001, axis_y_11D_001],
    animation_duration=0,
    layout = widgets.Layout(
        align_self='center',
    ),
    legend_location='top-right',
    background_style= {'fill': 'white','stroke': 'black'},
    fig_margin=dict(top=80,bottom=80,left=60,right=30),
    toolbar = True
)

fig_11D_001.marks = [
    isotherms,
    isobaric,
    state
]

# fig_11D_002

scale_x_11D_002 = bqs.LinearScale(min=0.945, max=0.975)
scale_y_11D_002 = bqs.LinearScale()

axis_x_11D_002 = bqa.Axis(
    scale=scale_x_11D_002,
    tick_format='0.2f',
    tick_style={'font-size': '15px'},
    tick_values=[0.95, 0.96, 0.97],
```

(continues on next page)

(continued from previous page)

```
    grid_lines = 'none',
    grid_color = '#8e8e8e',
    label='T',
    label_location='middle',
    label_style={'stroke': 'black', 'default-size': 35},
    label_offset='50px'
)

axis_y_11D_002 = bqa.Axis(
    scale=scale_y_11D_002,
    tick_format='0.2f',
    tick_style={'font-size': '15px'},
    num_ticks=0,
    grid_lines = 'none',
    grid_color = '#8e8e8e',
    orientation='vertical',
    label='s',
    label_location='middle',
    label_style={'stroke': 'red', 'default_size': 35},
    label_offset='50px'
)

entropy_line = bqm.Lines(
    x = T_values_repeated,
    y = s_values_plain,
    scales = {'x': scale_x_11D_002, 'y': scale_y_11D_002},
    opacities = [0.5],
    visible = True,
    colors = ['#edba00'],
    labels = [str(t) for t in T_limits],
    stroke_width = 5,
)

entropy_scatter = bqm.Scatter(
    x = T_values_repeated,
    y = s_values_plain,
    scales = {'x': scale_x_11D_002, 'y': scale_y_11D_002},
    opacities = opacities,
    visible = True,
    colors = colors_repeated,
    labels = [str(t) for t in T_limits],
)

state_s = bqm.Scatter(
    x = [T_values[0]],
    y = [s_values_plain[0]],
    scales = {'x': scale_x_11D_002, 'y': scale_y_11D_002},
    visible = True,
    colors = ['black'],
    names = [],
)

fig_11D_002 = bq.Figure(
    title='Molar entropy vs tenperature',
    marks=[],
    axes=[axis_x_11D_002, axis_y_11D_002],
    animation_duration=0,
```

(continues on next page)

(continued from previous page)

```
    layout = widgets.Layout(
        align_self='center',
    ),
    legend_location='top-right',
    background_style= {'fill': 'white','stroke': 'black'},
    fig_margin=dict(top=80,bottom=80,left=60,right=30),
    toolbar = True
)

fig_11D_002.marks = [
    entropy_line,
    entropy_scatter,
    state_s
]

prepare_export_fig_11D_001_button = widgets.Button(
    description='Export',
    disabled=False,
    button_style='',
    tooltip='',
    layout = widgets.Layout(
        align_self='center'
    )
)

prepare_export_fig_11D_001_button.on_click(prepare_export)

prepare_export_fig_11D_002_button = widgets.Button(
    description='Export',
    disabled=False,
    button_style='',
    tooltip='',
    layout = widgets.Layout(
        align_self='center'
    )
)

prepare_export_fig_11D_002_button.on_click(prepare_export)

top_block_11D_000.children = [
    widgets.VBox([
        fig_11D_001,
        prepare_export_fig_11D_001_button
    ]),
    widgets.VBox([
        fig_11D_002,
        prepare_export_fig_11D_002_button
    ])
]

bottom_block_11D_000 = widgets.VBox(
    [],
    layout=widgets.Layout(
        align_items='center',
        width='100%'
    )
)
```

(continues on next page)

(continued from previous page)

```
isobaric_line =  widgets.HTML(
    value="<div style='width:30px;text-align:left;display:inline-block;" \
          + "border: 5px solid #01b6cf;opacity: 0.5'> </div>" \
          + "  Phase transition pressure"
)

T_slider = widgets.SelectionSlider(
    options=T_values,
    value=T_values[0],
    description=r'\( T_r \)',
    disabled=False,
    continuous_update=True,
    orientation='horizontal',
    readout=True,
    layout = widgets.Layout(
        width = '50%',
        margin = '45px 0 0 0'
    )
)

T_slider.observe(change_tenperature, 'value')

bottom_block_11D_000.children = [
    isobaric_line,
    T_slider
]

change_view_button = widgets.ToggleButton(
    value=False,
    description='Presentation mode (OFF)',
    disabled=False,
    button_style='',
    tooltip='',
    icon='desktop',
    layout=widgets.Layout(
        width='initial',
        align_self='center'
    )
)

change_view_button.observe(change_view, 'value')

main_block_11D_000 = widgets.VBox(
    [],
    layout=widgets.Layout(
        align_items='center',
        width='100%'
    )
)

main_block_11D_000.children = [
    change_view_button,
    top_block_11D_000,
    bottom_block_11D_000,
]
```

(continues on next page)

(continued from previous page)

```
figures = [
    fig_11D_001,
    fig_11D_002
]

main_block_11D_000
```

## 1.13 Van der Waals isotherms in 3D

**Code:** #116-000

**File:** `apps/van_der_waals/p_v_T_3D.ipynb`

**Run it online:**

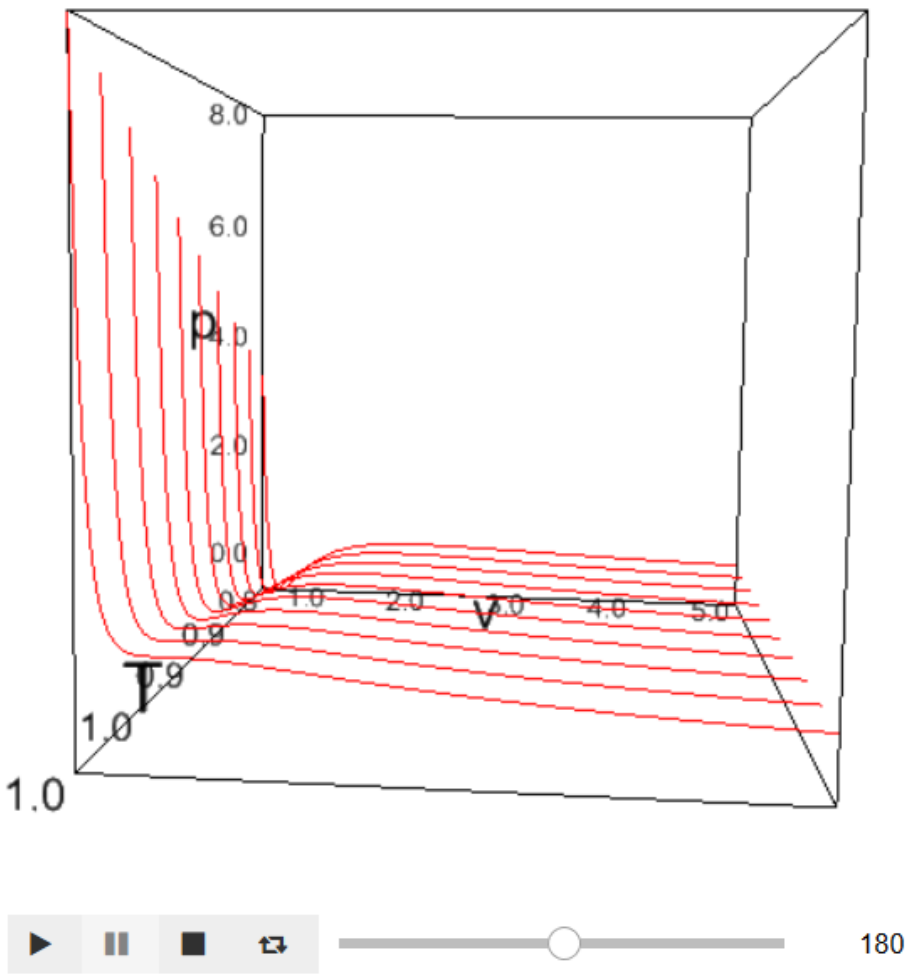
---

### 1.13.1 Interface

The main interface (`main_block_116_000`) contains the 3D ipyvolume figure `fig3d` and the `play` and `degrees_slider` widgets. Those widgets update the angle of the camera of the figure.

[1]:
```
from IPython.display import Image
Image(filename='../../static/images/apps/116-000_1.png')
```

[1]:




### 1.13.2 Packages

[2]:
```
import ipywidgets as widgets
import ipyvolume as ipv

import numpy as np
```

### 1.13.3 Physical functions

This are the functions that have a physical meaning:

- `get_relative_isotherms`

[3]:
```
def get_relative_isotherms(v_range, T_range):
    """This function calculates the theoretical p(v, T) plane
        (in reduced coordinates) according to van der Waals
        equation of state from a given range of volumes
        and tenperatures.

    Args:
        v_range: An array containing the values of v
        (in reduced coordinates)for which the isotherms must be
        calculated.\n
        T_range: An array containing the values of T
        (in reduced coordinates)for which the isotherms must be
        calculated.\n


    Returns:
        isotherms: A list consisted of numpy arrays containing the
        pressures of each isotherm.
    """

    isotherms = []

    for T in T_range:
        p_R = []
        for v in v_range:
            val = (8.0/3.0*T/(v - 1.0/3.0) - 3.0/v**2)
            p_R = np.append(p_R, val)

        isotherms.append(p_R)

    return isotherms
```

### 1.13.4 Functions related to interaction

[4]:
```
def update_camera_angle(change):
    """This function updates the camera angle taking
    the values from dregees_slider widget.
    """

    ipv.pylab.view(azimuth=degrees_slider.value)
```

### 1.13.5 Main interface

[ ]:
```
T_values = np.linspace(0.8, 1.0, 10)
v_values = np.linspace(0.45, 5.0, 500)

p_values = get_relative_isotherms(v_values, T_values)

fig3d = ipv.pylab.figure(
    key=None,
    width=600,
    height=500,
    lighting=True,
```

(continues on next page)

(continued from previous page)

```
    controls=True,
    controls_vr=False,
    controls_light=False,
    debug=False
)

ipv.pylab.xlim(min(v_values), max(v_values))
ipv.pylab.ylim(0.0, 2.0)
ipv.pylab.zlim(min(T_values), max(T_values))

ipv.pylab.xlabel('v')
ipv.pylab.ylabel('p')
ipv.pylab.zlabel('T')

ipv.pylab.view(azimuth=180, elevation=None, distance=None)

for i in range(len(T_values)):

    x_values = np.asarray(v_values)
    y_values = np.asarray(p_values[i])
    z_values = np.asarray(
        [T_values[i] for elem in v_values]
    )

    ipv.pylab.plot(
        x_values,
        y_values,
        z_values
    )

degrees_slider = widgets.IntSlider(
    value=180,
    min=0,
    max=360,
    step=1,
    description='',
    disabled=False,
    continuous_update=True,
    orientation='horizontal',
    readout=True,
    readout_format='d'
)

degrees_slider.observe(update_camera_angle, 'value')

play = widgets.Play(
    value=180,
    min=0,
    max=360,
    step=1,
    description="Press play",
    disabled=False
)

widgets.jslink((play, 'value'), (degrees_slider, 'value'));

main_block_116_000 = widgets.VBox([
```

(continues on next page)

(continued from previous page)

```
    fig3d,
    widgets.HBox([
        play,
        degrees_slider
    ])
    ],
    layout=widgets.Layout(
        align_items='center'
    )
)

main_block_116_000
```

CHAPTER 2

# Azalpen teorikoak

## 2.1 Fase-trantsizioak

Azalpen guztiak Josu M. Igartua irakasleak gainbegiratu ditu.

Fase-trantsizio bat sistema batek bere ezaugarrietan jasaten duen aldaketa da, sistemaren potentzial termodinamikoen deribaturen batek ez-jarraitasun bat azaltzen duenean gertatzen dena [1].

Potentzial termodinamikoak sistemaren egoera-funtzioak konbinatzean lortzen diren magnitude eskalarrak dira, energiaren dimentsioak dituztenak [2]. Egoera-funtzio horien balioak sistemak konfigurazio-espazioan duen kokapenaren menpekoak baino ez dira. Ondorioz, konfigurazio-espazioko puntu batetik beste batera mugitzean, egoera-funtzioak jasandako aldaketa hasierako eta amaierako puntuen araberakoa da eta ez batetik bestera joateko jarraitutako bidearena.

Aipaturiko egoera-funtzioen artean $U$ sistemaren barne-energia dago. Barne-energia $p$, $V$, $T$ eta $S$ egoera-funtzioekin konbinatzean lortzen dira potentzial termodinamikoak. Konbinazio posible guztietatik hiru bereziki erabilgarriak dira eta izen bereziak jasotzen dituzte: $H = U + pV$ (entalpia), $F = U - TS$ (Helmholtz-en energia) eta $G = U + pV - TS$ (Gibbs-en energia).

Sistema baten egonkortasun-baldintzak potentzial termodinamikoen menpe idatzi daitezke: sistema bat egonkorra izan dadin potentzial horiek beraien aldagai intentsiboekiko ganbilak izan behar dira eta estentsiboekiko, aldiz, ahurrak (ikus 2.1, 2.2 eta 2.3. ekuazioak) [3].

$$\left(\frac{\partial^2 F}{\partial T^2}\right)_{V,N} \leq 0 \qquad \left(\frac{\partial^2 F}{\partial V^2}\right)_{T,N} \geq 0 \tag{2.1}$$

$$\left(\frac{\partial^2 H}{\partial S^2}\right)_{P,N} \geq 0 \qquad \left(\frac{\partial^2 F}{\partial V^2}\right)_{S,N} \leq 0 \tag{2.2}$$

$$\left(\frac{\partial^2 G}{\partial T^2}\right)_{P,N} \leq 0 \qquad \left(\frac{\partial^2 G}{\partial P^2}\right)_{T,N} \leq 0 \tag{2.3}$$

Orokortasunik galdu gabe Gibbs-en energiaren (edota potentzial kimikoaren) kasua bakarrik azter daiteke. Sarritan potentzial hori erabiltzen da bere aldagai naturalak ($p$ eta $T$) laborategian erraz manipulagarriak direlako. Jarraian egingo diren hausnarketa eta azalpenak beste potentzial bat oinarritzat hartuta emango liratekeenen analogoak dira.

Paul Ehrenfest-ek proposatutako sailkapenaren arabera [1], fase-trantsizio baten ordena ez-jarraitasuna agertzen duen $G$-ren (edota $\mu$-ren) ordena txikieneko deribatuaren ordena da. Gaur egun, aldiz, lehen ordenako trantsizioak eta trantsizio ''jarraituak'' (lehen ordenatik goragoko trantsizioak) ezberdintzen dira. Izan ere, lehen eta bigarren ordenako trantsizioen arteko ezberdintasunak gainontzeko trantsizioen artekoak baino esanguratsuagoak dira.

Lehen ordenako fase-trantsizio bat lehen aipatutako egonkortasun-baldintzen hutsegitea bezala uler daiteke. Egonkortasun-baldintzak betetzen ez direnean, sistema bi fase ezberdin eta bereizgarrietan (edo gehiagotan) banatzen da. Bi fase horiek ezberdinak eta bereizgarriak izateak konfigurazio-espazioko bi puntu ezberdin eta urrunetan kokatuta daudela esan nahi du eta bien arteko trantsizioa berehala gertatzen dela. Kasu honetan, ''bat-batekotasun'' honek ez dauka prozesuak denboran iraun dezakeenarekin zerikusirik: ''berehala'' gertatzeak sistema egonkorrak diren tarteko egoera guztietatik kuasiestatikoki pasatu beharrean hasierako egoeratik zuzenean amaierakora igarotzen dela adierazi nahi du.

Gibbs-en energiaren ikuspuntutik, lehen ordenako trantsizioen bidez lotutako $N$ fasetan aurki daitekeen sistema baten Gibbs-en energiak $N$ minimo izango ditu. Azpimarragarria da minimo bakoitzak fase bati dagokiola eta minimo ugari egoteak ezinbestean egonkortasun baldintzen haustura suposatzen duela, bi minimoen artean aurkako kurbadura duen eremua baitago derrigor. Sistema beti agertuko da minimorik sakonenean eta konfigurazio-espaziotik mugitzean minimoen arteko sakonera erlatiboak aldatuz joango dira. Ondoz-ondoko bi minimoen arteko sakonera berdina denean, hau da, bi faseen Gibbs-en energiaren balioa berdina denean, sistema fase batetik bestera alda daiteke lehen ordenako trantsizio baten bidez.

Ehrenfest-en sailkapenean oinarrituta, trantsizio horretan kontserbatuko ez diren aldagaiak identifika daitezke. Lehen ordenako fase-trantsizio batean Gibbs-en energiaren lehenengo deribatua ez-jarraitua izango da. Partikula kopurua konstante mantentzen dela onartuz, ondorengo garapenak egin daitezke:

$$\left(\frac{\partial G}{\partial p}\right)_{T,N} = \left(\frac{\partial(\mu N)}{\partial p}\right)_{T,N} = N\left(\frac{\partial \mu}{\partial p}\right)_{T,N} \tag{2.4}$$

$$\left(\frac{\partial G}{\partial T}\right)_{p,N} = \left(\frac{\partial(\mu N)}{\partial T}\right)_{p,N} = N\left(\frac{\partial \mu}{\partial T}\right)_{p,N} \tag{2.5}$$

Potenzial kimikoaren adierazpen diferentziala erabiliz:

$$d\mu = v\ dp - s\ dT \tag{2.6}$$

$$\left(\frac{\partial \mu}{\partial p}\right)_{T,N} = v \qquad \left(\frac{\partial \mu}{\partial T}\right)_{p,N} = -s \tag{2.7}$$

Bolumen eta entropia molarrak (eta potentzial kimikoaren ordena altuagoko deribatuak) izango dira, beraz, lehen ordenako trantsizio batean bi faseen artean jarraituak izango ez diren ezaugarriak. Aipatu behar da hemengo garapena sistema hidrostatiko baten kasurako egin dela baina prozedura hau guztiz analogoa izango litzatekeela beste izaera bateko sistema baten kasuan (sistema magnetiko batean, esaterako [4]).

Sistema hidrostatikoaren egonkortasun-baldintzak sistemaren egoera-aldagaien menpe idatz daitezke, 2.3 eta 2.7. adierazpenak erabilita:

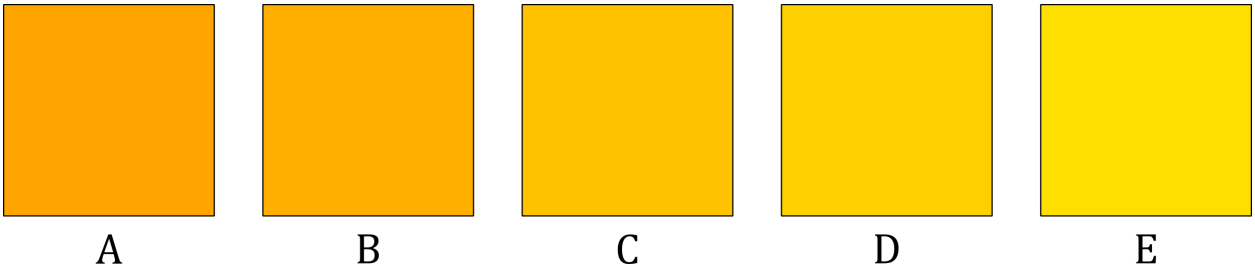
$$\left(\frac{\partial^2 \mu}{\partial p^2}\right)_{T,N} = \left(\frac{\partial v}{\partial p}\right)_{T,N} \leq 0 \tag{2.8}$$

$$\left(\frac{\partial^2 \mu}{\partial T^2}\right)_{p,N} = \left(\frac{\partial s}{\partial T}\right)_{p,N} \leq 0 \tag{2.9}$$

Bigarren ordenako fase-trantsizioei dagokionez, ez dira egonkortasun-balditzak hausten eta, ondorioz, sistema fase batetik bestera egonkorrak diren egoeretatik pasatzen da, kuasiestatikoki. Bigarren ordenako (eta ordena altuagoko) fase-trantsizio baten bidez lotutako bi egoera konfigurazio-espazioan bata bestearen alboan kokatuta daude, bien arteko ezberdintasunak nahi bezain txikiak izanik.

Nahiz eta aurrerago kontzeptu horietan sakondu, aipagarria da kasu batzuetan posible dela sistema hasierako egoera batetik amaierakora lehen zein bigarren ordenako fase-trantsizioen bidez eramatea. Lehenengo kasuan, sistema ezegonkortu egin beharko da eta, ondorioz, fase-trantsizioa gertatzen den bitartean hasierako eta amaierako faseak

aldi berean existituko dira. Bigarrenean aldiz, sistema guztia modu jarraituan aldatuz joango da, elkarren artean ia bereiztezinak diren egoeretatik pasatuz amaierako egoerara iritsi arte.




1. irudia: Bigarren ordenako fase-trantsizioak azaltzeko sortutako irudia. Karratu bakoitzak koloreaz ezaugarritutako sistemaren egoera bati dagokio.

Bigarren ordenako fase-trantsizioen izaera argitzeko **??**. irudiko adibidea prestatu da. Kutxa bakoitzak sistema beraren egoera ezberdin bat adierazten du, fase-aldagai bakarrez ezaugarritua: kolorea. Muturretako karratuek (A eta E) hasierako eta amaierako egoerak adierazten dituzte. A eta B-ren artean bigarren ordenako trantsizio bat gertatzen da, nahiz eta bi sistemak ia berdinak izan. Antzera gertatzen da B-C, C-D eta D-E trantsizioekin: konfigurazio-espazioan ondoan egonik, ezaugarri gehienak komunean dituzte. Hala ere, A eta E-ren arteko ezberdintasunak nabarmenak dira, sistemaren egoera oso gutxi (nahi bezain gutxi) aldatzen duten bigarren ordenako fase-trantsizioak etengabe jasatean sistema konfigurazio-espazioan aldenduta egon daitezkeen puntu batetik bestera mugi baitaiteke. Aipatzekoa da ere adibide honetan A-tik E-rako aldaketa zuzenean egiten duen fase-trantsizioa lehen ordenakoa izango litzatekeela, sistema elkarren artean bereizgarriak diren egoera batetik bestera joango bailitzake.

Lehen egindakoaren antzera, bigarren ordenako trantsizioetan ez-jarraitasunak agertuko dituzten aldagaiak identifika daitezke:

$$\left(\frac{\partial^2 \mu}{\partial p^2}\right)_{T,N} = \left(\frac{\partial v}{\partial p}\right)_{T,N} = -v\ \kappa_T \tag{2.10}$$

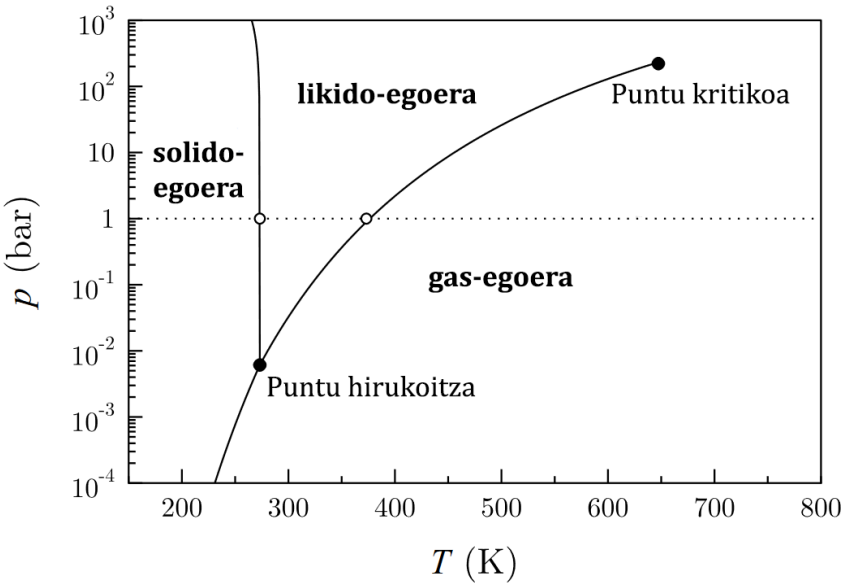
$$\left(\frac{\partial^2 \mu}{\partial T^2}\right)_{p,N} = \left(\frac{\partial s}{\partial T}\right)_{p,N} = c_p/T \tag{2.11}$$

$$\left(\frac{\partial^2 \mu}{\partial p \partial T}\right)_{N} = \left(\frac{\partial v}{\partial T}\right)_{p,N} = v\ \alpha \tag{2.12}$$

Bigarren ordenako fase-trantsizio bat denez, bolumen molarra jarraitua izango da eta $\kappa_T$ (konprimagarritasun isotermoa), $c_p$ (presio konstantepeko bero kapazitatea) eta $\alpha$ (zabalkuntza termikoaren koefizientea) ez-jarraituak izango dira [1].

Zenbait kasutan, badago lehen eta bigarren ordenako trantsizioak erlazionatzen dituen konfigurazio-espazioko puntu bat: puntu kritikoa. Bertan, Gibbs-en energia minimo ugari izatetik bakar bat izatera pasatzen da: lehen eta bigarren ordenako trantsizioen arteko muga adierazten du puntu horrek.

Une honetan interesgarria izan daiteke sistema baten fase-diagramari erreparatzea. Adibidez, 2. irudian ageri dena sistema hidrostatiko bati dagokio. Bertan, fase bakoitza egonkorra den guneak lerro batzuen bidez bereizita azaltzen dira. Lerro horiek *koexistentzia kurba* izenaz ezagutzen dira: bertan bi faseen potentzial kimikoak berdinak direnez, sistemaren bi faseak koexistitu egiten dira eta sistema kurba horiek zeharkatzean fase batetik bestera lehen ordenako trantsizio baten bidez pasatzen da.




2. irudia: Solido, likido eta gas-faseak erakusten dituen uraren fase-diagrama. Lerro horizontalak presio atmosferikoa adierazten du eta puntu txurien bidez uraren irakite eta izozte-puntuak adierazi dira. Iturria: "Concepts in Thermal Physics" [1].

Diagraman bi puntu berezi azpimarratu behar dira: lehena, puntu hirukoitza, zeinetan koexistentzia kurba guztiak elkartzen diren eta, ondorioz, hiru faseak potentzial kimiko berdina agertzen duten. Bigarrena, aldiz, lehen aipatutako puntu kritikoa da, likido-gas kurbaren amaiera markatzen duena. Sistema bat kurba horretan zehar puntu hirukoitzetik puntu kritikora eramatean, fase bien entropia eta bolumen molarrak berdinduz joango dira. Puntu kritikora iristean, ezaugarri horiek guztiz identikoak izango dira bi faseetan eta, ondorioz, sistema osoa fase bakarrean agertuko da.

Antzeko zerbait gertatzen da Gibbs-en energiaren kasuan: puntu hirukoitzean sakonera berdineko hiru minimo ikusten diren bitartean, sistema likido-gas koexistentzia kurbatik gora mugitzen den heinean bi minimoen artean topa daitekeen maximoaren altuera txikituz joango da. Maximo hori guztiz desagertuko da sistema puntu kritikora iristean. Koexistentzia kurba puntu hortatik harago jarraituz gero, bertan gertatuko liratekeen fase-trantsizio guztiak bigarren ordenakoak izango lirateke.

Likido-gas koexistentzia kurbaren malda Clausius-Clapeyron-en ekuazioak ematen du (ikus 2.13. ekuazioa), kurban zehar bi faseen potentzial kimikoak berdinak izatetik ondorioztatzen dena [1].

$$\frac{dp}{dT} = \frac{s_2 - s_1}{v_2 - v_1} \tag{2.13}$$

Amaitzeko, aipagarria da solido-likido koexistentzia kurbak ez duela puntu kritikorik azaltzen eta, ondorioz, bi fase horien arteko trantsizioa lehen ordenakoa izango dela beti.

### 2.1.1 Bibliografia

[1] Stephen J. Blundell eta Katherine M. Blundell. Phase transition. In *Concepts in Thermal Physics*, 305-323 or. Oxford University Press, 2009.

[2] Stephen J. Blundell eta Katherine M. Blundell. Thermodynamic potentials. In *Concepts in Thermal Physics*, 164-167 or. Oxford University Press, 2009.

[3] Herbert B. Callen. Stability of thermodynamic system. In *Thermodynamics and an Introduction to Thermostatistics*, 207-208 or. Wiley, 2. edizioa, 1985.

[4] Yevgen Melikhov, R. L. Hadimani, eta Arun Raghunathan. Phenomenological modelling of first order phase transitions in magnetic systems. *Journal of Applied Physics*,115(18), 2014.

## 2.2 van der Waals-en egoera-ekuazioa

Azalpen guztiak Josu M. Igartua irakasleak gainbegiratu ditu.

---

Nahiz eta fase-trantsizioen atzean dagoen oinarri fisikoa potentzial kimikoaren topologia izan, sarritan sistema termodinakoen azterketa lerro isotermoen forman oinarritzen da. Jariakin baten kasuan, oso interesgarria da van der Waals-en egoera-ekuazio mekanikoa (ikus 2.14. ekuazioa)betetzen duen jariakin errealaren kasua aztergaitzat hartzea.

$$\left(p + \frac{a}{v^2}\right)(v - b) = RT \tag{2.14}$$

non $a$ eta $b$ van der Waals-en parametroak, $v$ jariakinaren bolumen molarra, $p$ presioa, $T$ tenperatura eta $R$ gas idealen konstantea diren.

Gas idealen egoera-ekuazio mekanikoaren moldaketa bat bezala uler daiteke J.D. van der Waals herbeheretar fisikariak bere tesian proposatutako ekuazioa [1].

$$pv = RT \tag{2.15}$$

Gas idealen egoera-ekuazioa (ikus 2.15. ekuazioa) gas partikulak puntualak eta elkarren artean elkarrekintzarik gabekoak izatetik ondorioztatzen da. Van der Waals-en egoera ekuazioak, aldiz, bi faktore horiek kontuan hartzen ditu gas idealaren ekuazioari bi atal gehituz: $a$ parametroarekiko proportzionala denak partikulen arteko elkarrekintza integratzen du eta $b$ parametroak, aldiz, partikulek espazioan betetzen duten bolumena adierazten du [3]. Konposatu bakoitzerako bi parametro horien balioa esperimentalki lor daiteke.

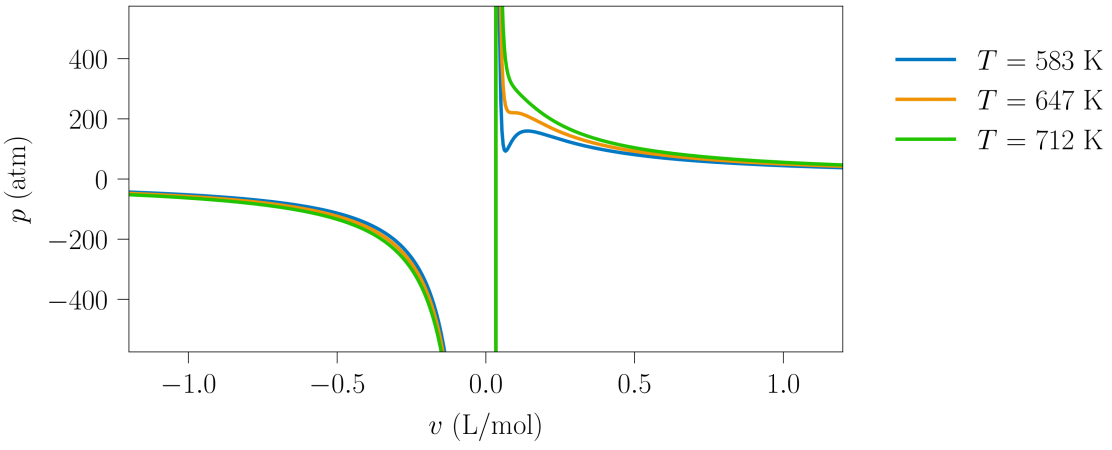
Van der Waals-en arabera, jariakina osatzen duten partikulen bolumena zein haien arteko elkarrekintza berdina da sistemaren likido eta gas faseetan eta bi faseetako portaera bere egoera-ekuazioaren bidez deskriba daiteke, ondorioz. Are gehiago, ekuazioa bi faseetan baliagarria denez, bien arteko trantsizioak deskribatzeko ere baliagarria izango da.

Aipatu beharra dago egoera-ekuazio horrek ez duela jariakin errealen portaera modu kuantitatibo batean azaltzen, baina bai erabilgarria dela azalpen kualitatibo edota erdi-kuantitatiboak emateko.

Funtzioaren analisi-matematikoa lerro isotermoetan oinarritutako azterketaren abiapuntua izan daiteke, proposatutako funtzioak ez baitauka esangura fisikorik bere izate-eremu guztian. Lerro isotermoen adierazpena 2.14. ekuaziotik ondoriozta daiteke.

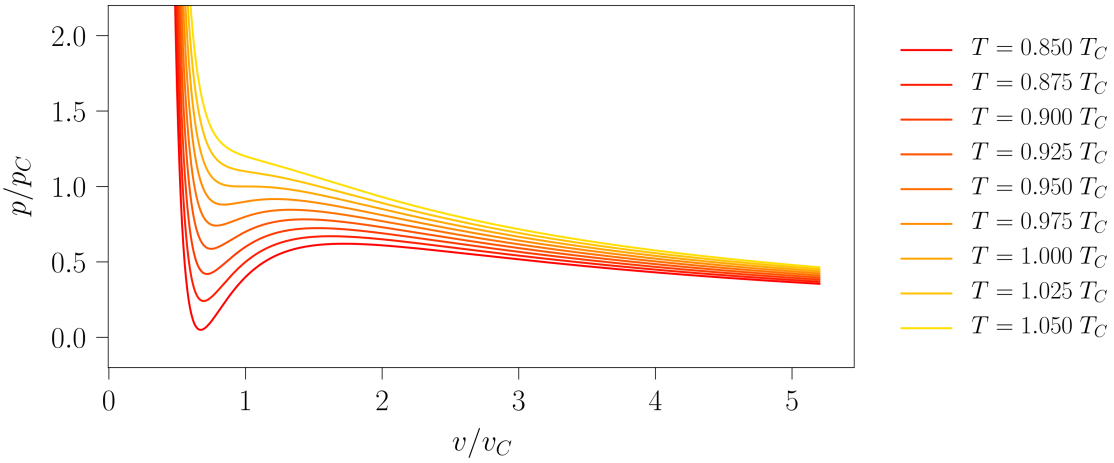
$$p(v;T) = \frac{RT}{v - b} - \frac{a}{v^2} \tag{2.16}$$

Begi-bistakoa denez, lerro isotermoen funtzioak polo bana du $v = 0$ eta $v = b$ puntuetan, 2.16. adierazpenak erakusten duen moduan. Edozein elementurentzat $T$ tenperaturako lerro isotermoa $v > 0$ eremuan irudikatuz (ikus **??**. irudia) aipagarria da $v \in (0, b)$ tartean $(\partial p/\partial v)_T > 0$ dela. Sistema ezengonkorra da tarte horretan, egonkortasun-baldintzen arabera. Zonalde ezegonkor hori bi poloen artean mugatuta dagoenez, ez da posible sistema fisikoa eremu horretan egotea. Ondorioz, van der Waals-en egoera ekuazioak esangura fisikoa duen eremua $v \in (b, \infty)$ da eta hori izango da hemendik aurrera aztertuko dena.



1. irudia: van der Waals-en egoera-ekuaziotik lortutako lerro isotermoen itxura. Irudia 118-000 programarekin sortu da.

Eremu horren barruan lerro isotermo ezberdinak irudikatzean, nabarmena da bi zonalde ezberdintzen direla (ikus 2. irudia). Tenperatuta baxuetan agertzen den zonaldean lehen aipatutako egonkortasun-baldintzak huts egiten duen eremuak identifika daitezke eta, beraz, tenperatura horietan sistemak lehen ordenako fase-trantsizio bat jasaten duela ondoriozta daiteke. Tenperatura altuetan aldiz, sistema egonkorra da eremu guztian.




2. irudia: van der Waals-en egoera-ekuaziotik lortutako lerro isotermoen itxura. Irudia 111-000 programarekin sortu da.

### 2.2.1 Puntu kritikoa

Van der Waals-en egoera-ekuazioak lehen ordenako fase-trantsizioak aurreikusten dituenez, onargarria da puntu kritikoaren existentzia ere aurreikusi dezakeela pentsatzea. Kasu honetan, nahikoa da hurrengo baldintzak aplikatzea puntu kritikoa kalkulatzeko (baldintza orokorra potentzial kimikoaren ordena guztietako deribatuak nuluak izatea da):

$$\left(\frac{\partial^2\mu}{\partial p^2}\right)_T = 0 \quad \text{eta} \quad v \equiv \left(\frac{\partial\mu}{\partial p}\right)_T \rightarrow \quad \left(\frac{\partial^2\mu}{\partial p^2}\right)_T \equiv \left(\frac{\partial v}{\partial p}\right)_T = 0 \tag{2.17}$$

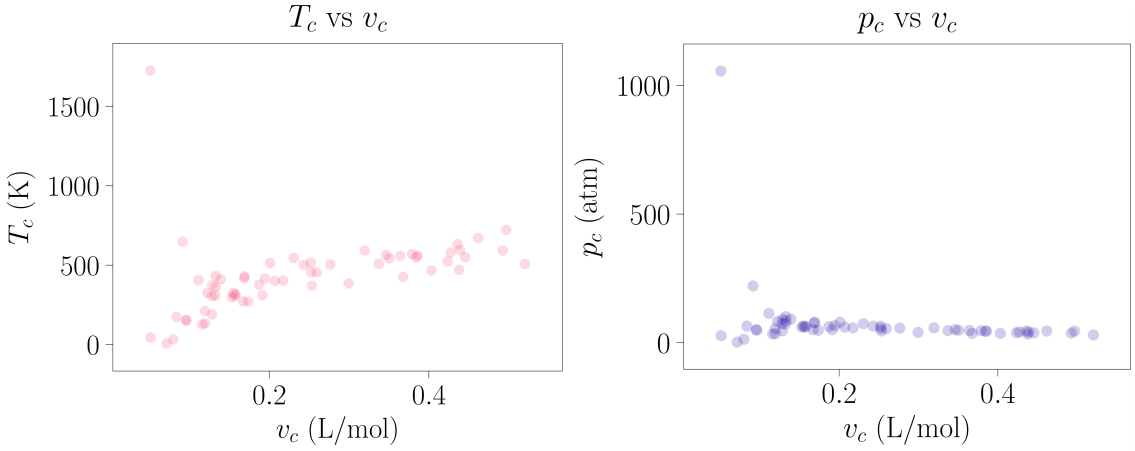
$$\left(\frac{\partial^3\mu}{\partial p^3}\right)_T = 0 \quad \rightarrow \quad \left(\frac{\partial^3\mu}{\partial p^3}\right)_T \equiv \left(\frac{\partial^2 v}{\partial p^2}\right)_T = 0 \tag{2.18}$$

Puntu kritikoaren adierazpena 2.17 eta 2.18 adierazpenetako baldintzak 2.16. ekuazioko lerro isotermoari aplikatzean lortzen da:

$$p_C = \frac{a}{27b^2} \qquad v_C = 3b \qquad T_C = \frac{8a}{27b} \tag{2.19}$$

Tenperatura kritikoko lerro isotermoa *lerro isotermo kritikoa* izango da eta horrek bananduko ditu 2. irudian ageri diren bi zonaldeak [3].

Van der Waals-en egoera-ekuazioko $a$ eta $b$ parametroak deskribatutako jariakinaren partikulen bolumenarekin eta haien arteko elkarrekintzarekin erlazionatuta daudenez, jariakin bakoitzarentzat bakarrak eta bereizgarriak dira. Puntu kritikoaren kokapena bi parametro horien menpekoa baino ez denez, jariakin bakoitzaren puntu kritikoa konfigurazio-espazioko puntu ezberdin batean egongo da kokatuta. Hori bistaratzeko 113-000 programa garatu da: ohiko elementu eta konposatuen parametroen balioak jasotzeaz gain haien puntu kritikoak grafika ezberdinetan erakusten ditu (ikus 3. irudiko grafikak).




3. irudia: Elementu eta konposatu batzuen puntu kritikoak. Parametroen balioak "CRC Handbook of Chemistry and Physics" liburutik atera dira [4]. Irudia 113-000 programarekin sortu da.

Puntu kritikoaren kokapena aztertutako jariakinaren menpekoa izateak, tenperatura berdinerako elementu bakoitzaren lerro isotermoek forma ezberdina azaltzea eragiten du (hori 113-000 programan ere behatu daiteke). Hala ere, behin puntu kritikoaren adierazpena ezagututa, posible da egoera-ekuazioa puntu kritikoaren menpe adieraztea:

$$\left(p_R + \frac{3}{v_R^2}\right)(3v_R - 1) = 8T_R \qquad \text{non} \qquad p_R = \frac{p}{p_C} \quad v_R = \frac{v}{v_C} \quad T_R = \frac{T}{T_C} \tag{2.20}$$

Ekuazio horri *egoera-ekuazio laburtua* deritzo eta jariakin guztietarako komuna da, ez baitu $a$ eta $b$ parametroekiko menpekotasun espliziturik [2]. Forma laburtua oso erabilgarria da adierazpen-grafikoak eta garapenak egiterako orduan, orokortasunik galdu gabe manipulatu beharreko parametroen kopurua murrizten baita eta, gainera, sistema guztiak aldi berean azaltzen baitira. Horregatik, hemendik aurrera adierazpen horretatik lortutako lerro isotermoak aztertuko dira (ikus 2.21. ekuazioa).

$$p_R\left(v_R, T_R\right) = \frac{8T_R}{(3v_R - 1)} - \frac{3}{v_R^2} \tag{2.21}$$

### 2.2.2 Potentzial kimikoaren azterketa

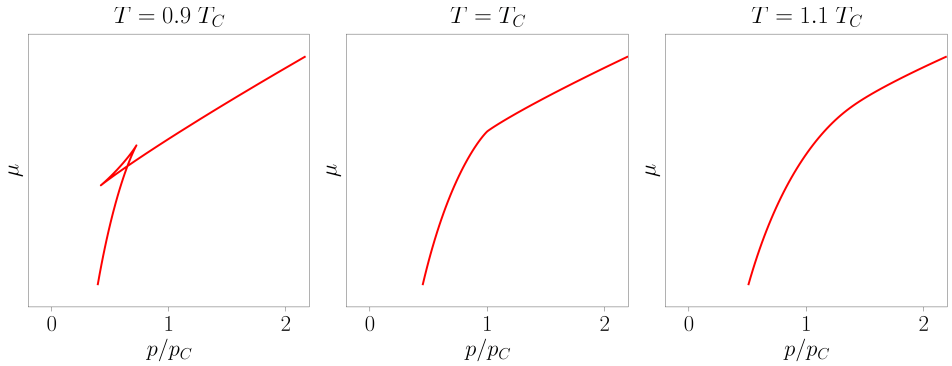
Fase-trantsizioen inguruko teoria orokorrak van der Waals-en egoera-ekuazioan duen eragina aztertzeko, $\mu$ potentzial kimikoaren adierazpena lortu behar da. Horretarako, 2.22. adierazpeneko Gibbs-Duhem-en erlaziotik abiatuz lerro isotermoan zehar tenperatura konstantea dela aplika daiteke integrala ebazteko:

$$d\mu = -s\ dT + v\ dp \xrightarrow{T=\text{kte}} (d\mu)_T = v\ (dp)_T \tag{2.22}$$

$$\mu = \int v\ dp + \phi(T) \tag{2.23}$$

non 2.23. adierazpeneko $\phi(T)$ gaia integrazio-konstantea den, tenperaturaren menpekoa. Gai horren ondorioz, metodo horren bidez lortutako $\mu = \mu(p, T)$ planoa ez da kuantitatiboki baliagarria izango, beti faltako baitu konstante horren ekarpena [2].

Zenbait tenperaturatan kokatutako sistementzat integral horren balioa kalkulatuz gero (117-000 programan lantzen den moduan), honelako $\mu$-ren adierazpenak lortzen dira:




4. irudia: Tenperatura ezberdinetarako lortutako potentzial kimikoak. Irudiak 117-000 programarekin sortu dira.

Hiru adar bereiz daitezke 4. irudiko lehenengo grafikan: irudiko lehenengo grafikan: lehena, puntu baxuenetik hasita kurbadura negatiboarekin igotzen dena, gas egoerari dagokion potentzial kimikoa da. Bigarrena presio handietan bakarrik topa daitekeen kurba da, hau ere kurbadura negatiboduna eta likido egoeraren potentzial kimikoa adierazten duena.

Bi kurba horiek eskuragarri dauden presioetan kontuan izan behar da sistema beti bi kurbetatik $\mu$ txikiena duenean egongo dela, aurreko atalean azaldu denez. Ondorioz, $p$ txikietan sistema gas egoeran egongo da. Bi kurbak elkartzen diren puntuan bien potentzial kimikoak berdinak direnez, sistemak lehen ordenako fase-trantsizioa jasango du. Hortik aurrera sistema likido egoeran egongo da, horri dagokiona izango baita balio baxueneko potentzial kimikoak dituen kurba.

Bi adar horien artekoari dagokionez, azpimarragarria da bere kurbadurak besteek azaltzen dutenaren aurkako zeinua duela. Aurreko atalean aipatutako egonkortasun-baldintzei erreparatuz (ikus 2.3. adierazpenak), argi gelditzen da gune horretan sistema ez dela egonkorra eta, ondorioz, sistemak ez duela inoiz hirugarren adar hori jarraituko. Ohartu, 4. irudian potentzial kimikoa aldagai intentsibo baten menpe adierazten dela eta, beraz, sistema egonkorra izan dadin bere bigarren deribatua negatiboa izan behar dela.

Beste bi grafiketan ageri denez, $T \geq T_C$ kasuetan ez da hirugarren adar hori azaltzen. Ondorioz, sistema egonkorra da eremu guztian eta lehen ordenako fase-trantsizioak jasan beharrean, bigarren ordenakoak jasaten ditu.

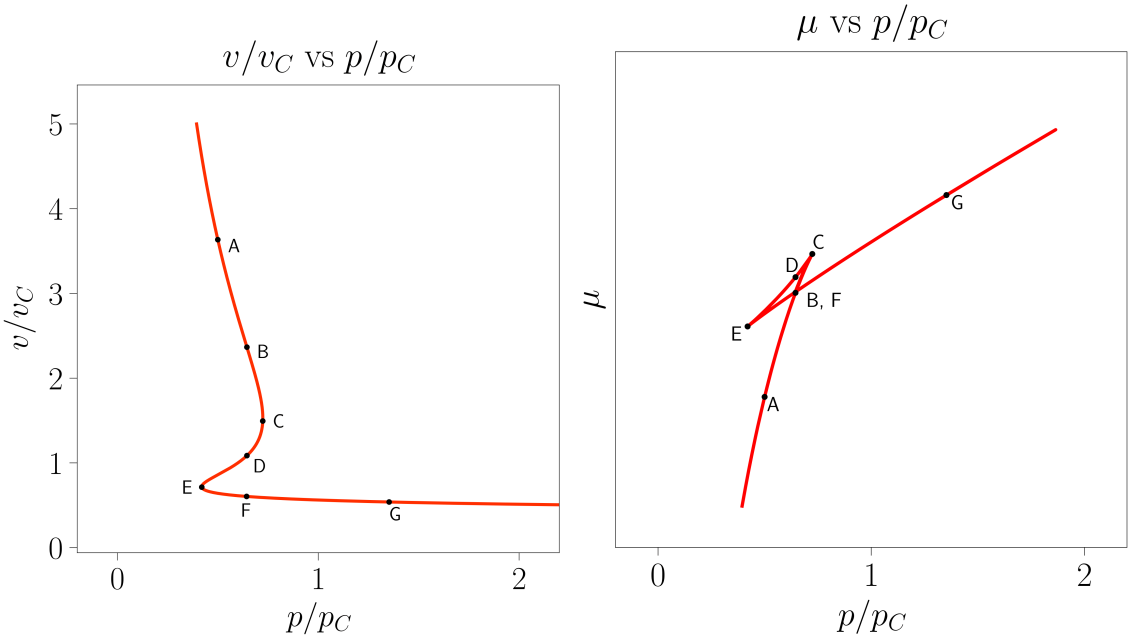
### 2.2.3 Lerro isotermo errealak

Egonkortasun-baldintzak betetzen diren edozein puntutan topatu daiteke sistema; hau da: posiblea da sistema 5. irudiko C edo E puntuetan topatzea, nahiz eta potentzial kimikoa minimizatzen duten egoerak ez izan. Egoera *metaegonkorrak* dira horiek: ertan kokatutako sistema batek perturbazio txiki bat jasanez gero, bi fase bereizgarrietan banatuko da.

Sistema C puntuan dagoenean *likido gain berotua* egoeran dagoela esaten da eta E puntuan aldiz *gas azpi hoztua* egoeran [3].

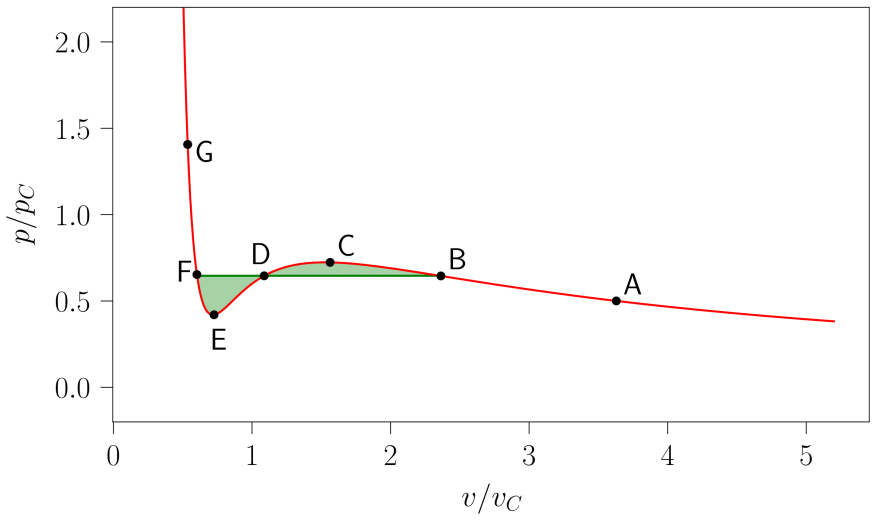
Sistema ezin denez egoera ezegonkor batean egon, argi dago ez dela C puntutik E puntura 2.23. irudiko lerro isotermoan zehar joaten eta behin fase-trantsizioa hasita sistema beste lerro isotermo bati jarraitzen diola.

Ideia horretan sakontzeko,117-000 programan $v = v(p,T)$ grafikako puntuak $\mu = \mu(p,T)$ grafikako puntuekin zuzenenan erlazionatu daitezke, 7. irudian erakusten denez. Ezkerreko grafikako lerro isotermoan zehar 6. ekuazioko integrala kalkulatuz eskuineko irudiko potentzial kimikoa lor daiteke. Markatutako puntuek esangura berezia dute: lehen azaldutako C eta E puntuez gain, A eta G puntuek sistema fase bakarrean ageri deneko egoerak adierazten dituzte, B eta F puntuek lehen ordenado fase-trantsizioaren muga azaltzen dute eta D puntuak sistema ezegonkorra den egoera adierazten du.




5. irudia: Potentzial kimikoaren eraikuntza erakusteko sortutako irudiak. Aukeratutako lerro isotermoa $T = 0.9\ T_C$ tenperaturari dagokio. Irudiak 117-000 programarekin sortu dira.

Azaldutako puntu berezi horiek ohiko lerro isotermoaren gainean proiektatu daitezke fase-trantsizioa hasten denean lerro isotermoan gertatzen dena aztertzeko.




6. irudia: Tenperatura azpikritikodun lerro isotermoa, 5. irudiko grafikak sortzeko erabilitakoa. Koloreztatutako azalerak Maxwell-en eraikuntzari dagokio: sistema tenperatura batean finkatu ostean bi azalera horien balioak berdintzen presioan gertatuko da lehen ordenako fase trantsizioa. Irudia 111-000 programarekin sortu da.

Lehen aipatu denez, bi faseen potentzial kimikoak berdinak direnean gertatuko da lehen ordenako fase-trantsizioa. Ondorioz, B eta F puntuetan $\mu_1 = \mu_2$ baldintza bete behar da, $\mu_i$ fase bakoitzari dagokion potentzial kimikoa izanik.

$$\mu_1 = \mu_2 \ \rightarrow \ \int_F^B v(p)dp = 0 \tag{2.24}$$

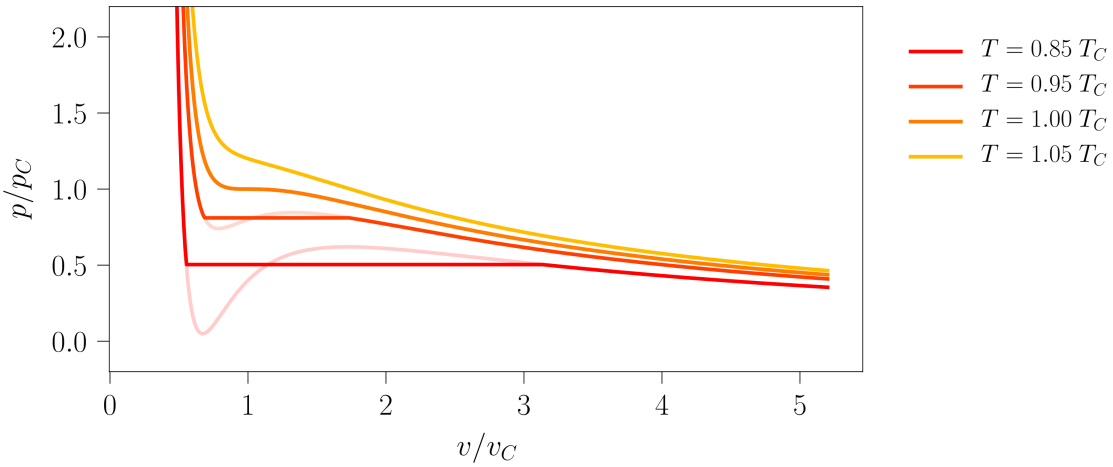
Integral hori bi zatitan bana daiteke:

$$\int_F^D v(p)dp + \int_D^B v(p)dp = 0 \tag{2.25}$$

Hau da, 6. irudian koloreztatutako bi azalerak balioz berdinak izan behar dira. Arau horri *Maxwell-en eraikuntza* deritzo: sistemaren isoterma erreala trunkatutako isoterma ideala izango da [2].

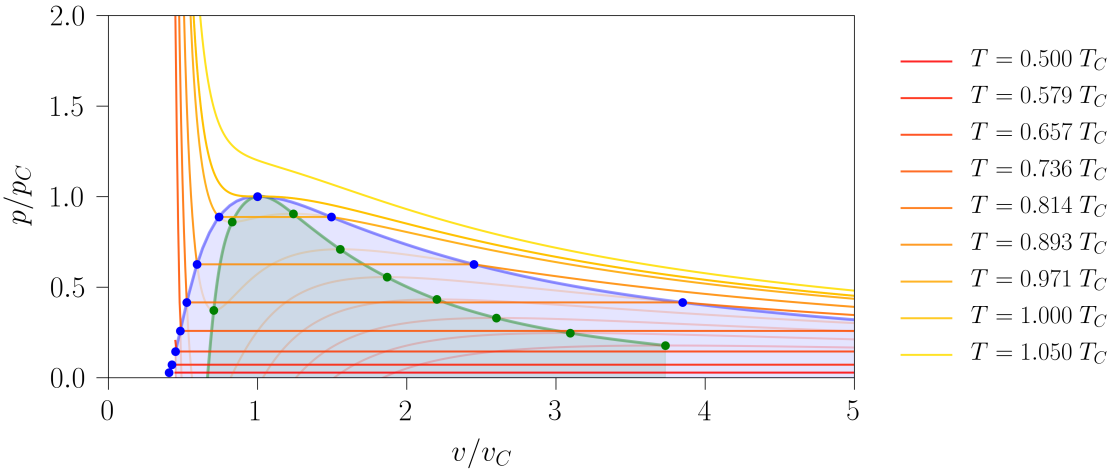
Sistemaren tenperatura tenperatura kritikoa baino baxuagoa den kasuetan (6. irudikoa, esaterako), sistema G puntutik B puntura van der Waals-ek proposatutako lerro isotermoari jarraituz garatuko da, F-B tartea lerro isobarikoan zehar egingo du eta B puntutik A punturako bidea berriro ere hasierako lerrotik egingo du, trantsizio guztian egonkortasun-baldintza hautsi gabe. Sistema tenperatura kritikoaren gainetik finkatzean, bigarren ordenako fase-trantsizioa van der Waals-en isotermei jarraituz gertatuko da.

Hori hobeto azaltzeko, 111-000 programaren bidez 7. irudia sortu da. Bertan, zenbait tenperatura ezberdinetan kokatutako sistemek errealitatean izango luketen garapena azaltzen da, Maxwell-en eraikuntzaren bidez kalkulatutakoa. Gainera, $T < T_C$ kasuetan van der Waals-en lerro isotermo idealak ere adierazten dira, opakutasun txikiagoko lerroen bitartez.




7. irudia: Zenbait tenperaturatan kokatutako sistema hidrostatiko baten lerro isotermo errealak. Koloreztatutako azalerak Maxwell-en eraikuntzari dagokio: sistema tenperatura batean finkatu ostean bi azalera horien balioak berdintzen presioan gertatuko da lehen ordenako fase trantsizioa. Irudia 111-000 programarekin sortu da.

Azterketa hori sakontzeko, tenperatura gehiagotan ipin daiteke sistema, 8. irudian azaltzen den grafika lortuz. Lerro urdinak mugatutako guneari *koexistentzia-gunea* deritzo: bi fasetan banatuta agertu ohi da bertan kokatutako sistema [2]. Lerro berdeak, aldiz, egonkortasun-baldintzak betetzen ez diren gunea inguratzen du: ezinezkoa da, beraz, berdez koloreztatutako gunean sistema fase bakarrean topatzea. Zonalde urdinean egonkortasun-baldintzak betetzen direnez, baldintza egokiak betez gero, sistema osoa egoera metaegonkor batean ager daiteke [5]. Bi muga horien eta irudikatutako lerro isotermoen arteko ebakidurak puntuek adierazten dituzte.



8. irudia: Zenbait tenperaturatan kokatutako sistema hidrostatiko baten lerro isotermo errealak. Koexistentzia-gunea urdinez koloreztatu da eta existentziarik gabeko gunea berdez. Koloretako puntuek bi muga horien eta lerro isotermoen arteko ebakidurak adierazten dituzte. Irudia 111-000 programarekin sortu da.

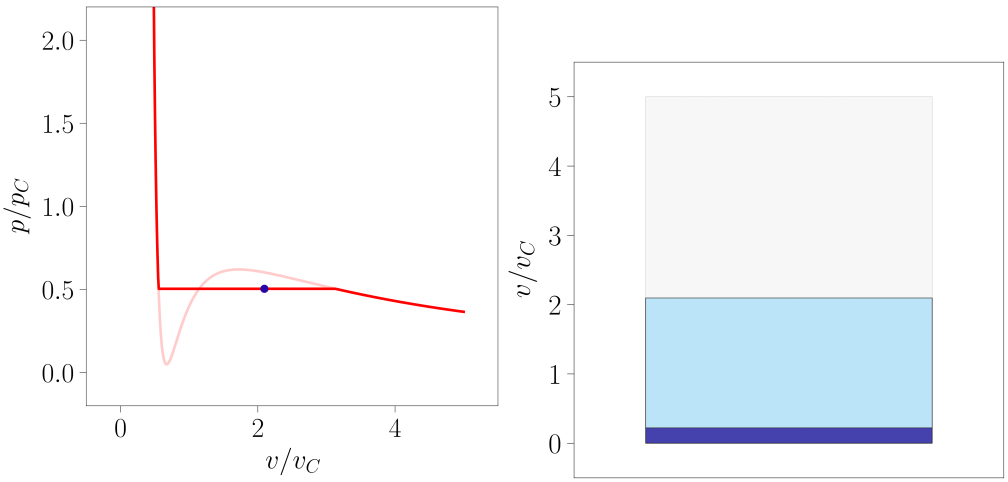
### 2.2.4 Bolumen molarraren aldaketa

Aurreko atalean azaldutako koexistentzia-gunearen mugak sistemaren fase bakoitzeko bolumen molarrak jakiteko erabil daitezke. Lehen aipatu denez, sistema lerro isotermoko eremu isobarikoan zehar garatuko da lehen ordenako fase-trantsizioa jasatean. Trantsizio hori gertatzen den bitartean, fase banatan agertzen den bolumenaren proportzioa *palankaren erregela*-ren bitartez kalkula daiteke (ikus 2.27. adierazpena) [2]. Sistemaren bolumen molar osoa $v$ izanik eta $v_g$ eta $v_l$, hurrenez hurren, gas eta likido faseen bolumen molarrak badira, honakoa ondorizta daiteke:

$$v = \frac{V}{N} \quad \rightarrow \quad V = vN = N(x_l v_l + x_g v_g) \tag{2.26}$$

$$x_l = \frac{v_g - v}{v_g - v_l} \qquad x_g = \frac{v - v_l}{v_g - v_l} \tag{2.27}$$

Bi adierazpen horiek oso erabilgarriak izan daitezke likido/gas fase-trantsizioa irudikatzeko, 112-000 programan egin den moduan. Aipaturiko programaz baliatuz 9. irudiko bi diagramak sortu dira. Ezkerrekoan $T = 0.85\ T_C$ tenperaturari dagokion sistemaren lerro isotermo esperimental eta teorikoa azaltzen dira (azken hau opakutasun gutxiagorekin). Bertako puntu urdinak sistemaren egoera adierazten du, jatorrizko programan lerro isotermo guztian zehar mugi daitekeena. Eskuinean, aldiz, laborategian behatuko litzatekeenaren diagrama sinplifikatu bat ageri da, puntu urdinak finkatutako egoerari dagokiona hain zuzen ere. Diagramako blokeen koloreak faseen bolumen molarrarekin erlazionatuta daude: urdin argiak gas-faseak betetzen duen bolumen molarra adierazten duen bitartean, ilunak likido-fasearena adierazten du.



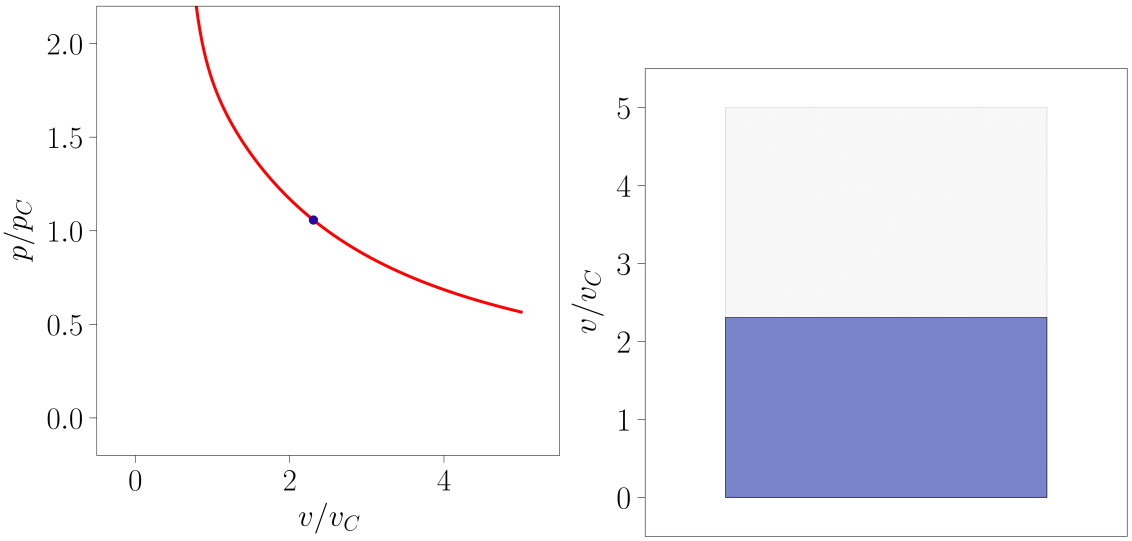

9. irudia: Laborategian sistema hidrostatiko baten fase-trantsizioa lantzean behatuko litzatekeena azaltzeko sortutako irudiak. Kasu honetan $T = 0.85\ T_C$ tenperaturan kokatu da sistema. Irudiak 112-000 programarekin sortu dira.

Bigarren grafika horrek jariakinaren portaera esperimentala aurreikusteko aukera ematen du. Presio txikietan sistema gas egoera egongo litzateke (urdin argia) eta presioa handitu ahala gasaren bolumen molarra txikituz joango litzateke fase-trantsizioa hasi arte. Une horretan likido tantak agertuko lirateke (urdin iluna) eta fase-trantsizioak iraun bitartean bi egoeren bolumenen arteko proportzioa palankaren erregelak emandakoa izango litzateke. Sistema osoa fasez aldatzean argi gelditzen da likidoaren konprimagarritasun isotermoa askoz txikiagoa dela, presio aldaketa berdinerako bolumenean eragindako aldaketa lehen baino txikiagoa baita.

Programa beraz baliatuz, sistema $T > T_C$ tenperatura batean finkatu eta bigarren ordenako fase-trantsizioen ezaugarriak behatzea ere interesgarria izan daiteke. Kasu horretan, 10. irudian aurkeztutako diagramak lortzeko $T = 1.2\ T_C$

tenperaturan finkatu da sistema. Baldintza horren pean sistemak bigarren ordenako fase-trantsizioa jasaten duenez, ez dira aldi berean bi fase bereizi inoiz behatzen: presio baxuko egoera batetik hasi eta presioa pixkanaka handituz, diagramako sistema urdin argiz margotuta egotetik urdin ilunez margotuta egotera pasa da.

Horrek fase-trantsizioen inguruko mezu garrantzitsu bat ematen du, fase-trantsizioen inguruko atalean aipatutakoa: sistema hidrostatikoaren kasuan, lehen ordenako trantsizio batean bolumen molarrak jauzi bat aurkezten du eta bigarren ordenekoetan, aldiz, aipaturiko ezaugarria modu jarraituan garatzen da.




10. irudia: Laborategian sistema hidrostatiko baten fase-trantsizioa lantzean behatuko litzatekeena azaltzeko sortutako irudiak. Kasu honetan $T = 1.20\ T_C$ tenperaturan kokatu da sistema. Irudiak 112-000 programarekin sortu dira.

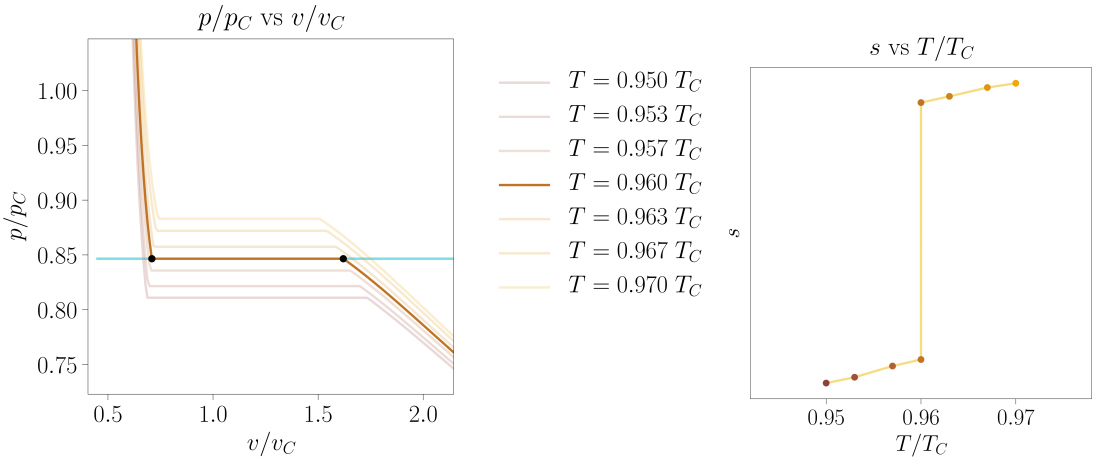
### 2.2.5 Entropia molarraren aldaketa

Bolumen molarraz gain, entropia molarrak ere ez-jarraitasuna azaltzen du lehen ordenako fase-trantsizioetan. Entropiaren adierazpena bere definizioa eta 2.21. ekuazioan aurkeztutako lerro isotermoen adierazpena erabiliz kalkula daiteke.

$$ds = \left(\frac{\partial p}{\partial T}\right)_v dv \quad \text{eta} \quad p_R\left(v_R, T_R\right) = \frac{8T_R}{(3v_R - 1)} - \frac{3}{v_R^2} \;\rightarrow\; ds = \frac{8}{3v - 1} \tag{2.28}$$

$$s = \int \frac{8}{3v - 1} dv = \frac{8}{3} \ln|3v - 1| + \text{kte} \tag{2.29}$$

Lortutako adierazpen horrek ez du entropiaren balio absolutua kalkulatzeko balio, baina bere itxura irudikatzeko erabil daiteke (ikus 11. irudia). Oraingoan, sistema tenperatura jakin batean finkatu beharrean presio konstateko baldintzetan mantendu da. Horrela, tenperatura aldatzean, presio eta tenperatura horri dagozkion bolumena hartuko du sistemak. Lehen ordenako fase-trantsizioari dagozkion presio eta tenperaturara iristean, bi bolumen izango ditu eskuragarri, bi faseei dagozkienak, hain zuzen ere. Entropia molarraren bi balio bereizgarri ere izan ahalko ditu, ondorioz. Trantsizioa gertatzen deneko tenperatura gainditua, sistemak berriro ere entropia bakar bat izango du eskuragarri. Prozesu hau erakusteko 11D-000 programa sortu da, 11. irudiko grafikak egiteko aukera ematen duena.




11. irudia: Presio konstantean mantendutako sistema baten entropiak tenperaturarekiko duen menpekotasuna azaltzeko sortutako irudiak. Kasu honetan $T = 1.20\ T_C$ tenperaturan kokatu da sistema. 11D-000 programarekin sortu dira.

Sistema presio konstantean mantentzen denez, urdinez markatutako lerro isobarikoaren eta bere tenperaturari dagokion lerro isotermoaren arteko ebakiduran egongo da. Ezkerreko grafikan ikusten denez, tenperatura eta presio jakinetan sistemak lehen ordenako fase-trantsizioa jasaten badu, ebakidura horretako puntuen kopurua infinitoa izango da eta sistema ezkerreko grafikan beltzez adierazitako bi egoeren nahasketa bezala agertuko da. Tenperatuta gehiago handituz gero, fase-trantsizioa amaituko da eta sistema osoa fase bakar batean agertuko da (kasu honetan gas egoeran).

Amaitzeko, aipagarria da orain arte azaldutako programa ezberdinak erabiliz fase-trantsizioan gertatutako bero sorra kalkula daitekeela (ikus 2.30. garapena) [2].

$$\delta Q = \left(\frac{\partial s}{\partial T}\right) \xrightarrow{T=\text{kte}} \Delta Q = \frac{1}{T}\,\Delta s = \frac{8}{3T}\ln\left|\frac{3v_l - 1}{3v_g - 1}\right| \tag{2.30}$$

### 2.2.6 Bibliografia

[1] J. D. van der Waals. *On the Continuity of the Gaseous and Liquid States.* Elsevier Science Publisher B.V., 2004.

[2] Herbert B. Callen. First-order phase transitions in single component systems. In *Thermodynamics and an Introduction to Thermostatistics*, 215-241 or. Wiley, 2. edizioa, 1985.

[3] Stephen J. Blundell eta Katherine M. Blundell. Real gases. In *Concepts in Thermal Physics*, 280–288 or. Oxford University Press, 2009.

[4] David R. Lide. Fluid properties. In *CRC Handbook of Chemistry and Physics*, 43 or. CRC Press, 84. edizioa, 2003.

[5] Pablo G. Debenedetti. Thermodynamics. In *Metastable liquids: concepts and principles*, Physical chemistry (Princeton, N.J.), 84–88 or. Princeton University Press,1996.

CHAPTER 3

# Indices and tables

- genindex
- modindex
- search