final

May 12, 2025

[1]:
```
from IPython.display import Image
import numpy as np
import sympy as sp
import matplotlib.pyplot as plt
import matplotlib.animation as animation
from matplotlib.collections import LineCollection
#from scipy.special import hermite, factorial, eval_hermite
from matplotlib.animation import FuncAnimation
import os
import glob
import shutil
import matplotlib.style as style
import pandas as pd
from scipy.integrate import quad
from scipy.linalg import eigh
import ipywidgets as widgets
from ipywidgets import interact

style.use('dark_background')
plt.rcParams['text.usetex'] = False



#display screenshots
for i in range(1, 3):
    display(Image(filename=f'p_statement/p{i}.jpg'))

#file moving for housekeeping
def move_plots():
    output_dir = 'graphs'
    if not os.path.exists(output_dir):
        os.makedirs(output_dir)

    #all gif and png
    files_to_move = glob.glob('*.png') + glob.glob('*.gif')

    for file in files_to_move:
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```
        destination = os.path.join(output_dir, file)

        #if exists, replace
        if os.path.exists(destination):
            os.remove(destination)

        #move it
        shutil.move(file, destination)
        print(f'Moved {file} to {output_dir}')
```

1. Suppose you could find a solution $\psi(r_1, r_2, \cdots, r_Z)$ to the Schroedinger equation $\hat{H}\psi = E\psi$ for the Hamiltonian of a neutral atom of atomic number Z. Describe how you would construct from it a completely symmetric function, and a completely antisymmetric function, which also satisfy the Schroedinger equation, with the same energy. What happens to the completely antisymmetric function if $\psi(r_1, r_2, \cdots, r_Z)$ is symmetric in (say) its first two arguments $(r_1 \leftrightarrow r_2)$?

2. [EXTRA CREDIT] The ground state energy of a system is estimated both by the Rayleigh-Ritz variational method and by a second order perturbation theory calculation. The Rayleigh-Ritz result is found to be -27.1eV and the perturbation theory result -26.0eV. Which lies closer to the true ground state energy? Suppose the numbers had been reversed. Would it still be possible to decide which estimate is better? Explain your reasoning.

[2]:
```
def problem_1():
    #when i use two particle wavefunc.
    x1, x2 = sp.symbols('x1 x2')
    phi1 = sp.Function('phi1')
    phi2 = sp.Function('phi2')

    #og product state (not symmetry)
    psi = phi1(x1)*phi2(x2)

    #symmetric combo
    psi_s = (phi1(x1)*phi2(x2) + phi1(x2)*phi2(x1))/sp.sqrt(2)

    #antisymmetric combo
    psi_a = (phi1(x1)*phi2(x2) - phi1(x2)*phi2(x1))/sp.sqrt(2)
```

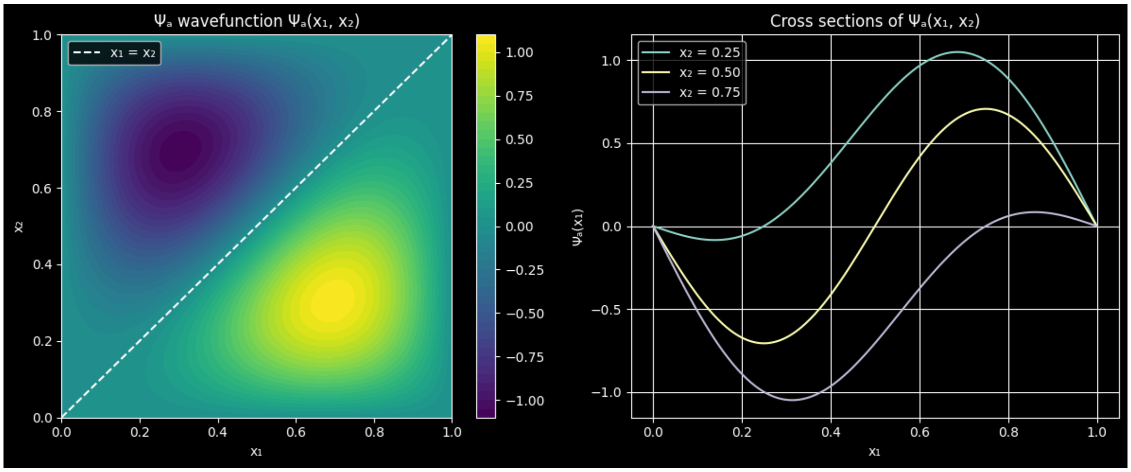
```python
#display symbolic results
display(sp.Eq(sp.Symbol('psi_s'), psi_s))
display(sp.Eq(sp.Symbol('psi_a'), psi_a))

#i can test antisymmetry when phi1 == phi2
psi_a_same = psi_a.subs(phi2(x2), phi1(x2)).subs(phi2(x1), phi1(x1))

#should simplify to zero
display(sp.Eq(sp.Symbol('psi_a_same'), sp.simplify(psi_a_same)))

#it does therefore psi_a vanishes if orbitals are same
#just a quick visual when psi1 not equal to phi2
def phi1_fn(x):
    return np.sin(np.pi * x)  #ex 1s

def phi2_fn(x):
    return np.sin(2 * np.pi * x)  #ex 2s

x = np.linspace(0, 1, 300)
X1, X2 = np.meshgrid(x, x)
psi_a_vals = (phi1_fn(X1) * phi2_fn(X2) - phi1_fn(X2) * phi2_fn(X1)) / np.sqrt(2)

fig, (ax1, ax2) = plt.subplots(1, 2, figsize=(12, 5))

#make subplot here, left will be contour
cs = ax1.contourf(X1, X2, psi_a_vals, levels=50)
fig.colorbar(cs, ax=ax1)
ax1.set_title('Ψ  wavefunction Ψ (x , x )')
ax1.set_xlabel('x ')
ax1.plot(x, x, 'w--', label='x  = x ')
ax1.legend()
ax1.set_ylabel('x ')

#right will now be cross section
for x2_fixed in [0.25, 0.5, 0.75]:
    psi_cross = (phi1_fn(x) * phi2_fn(x2_fixed) - phi1_fn(x2_fixed) * phi2_fn(x)) / np.sqrt(2)
    ax2.plot(x, psi_cross, label=f'x  = {x2_fixed:.2f}')

ax2.set_title('Cross sections of Ψ (x , x )')
ax2.set_xlabel('x ')
ax2.set_ylabel('Ψ (x )')
ax2.legend()
ax2.grid()
```

```
    plt.tight_layout()
    plt.savefig('problem_1.png', dpi=600)
    plt.show()


problem_1()
```

$$\psi_s = \frac{\sqrt{2}\left(\phi_1(x_1)\phi_2(x_2) + \phi_1(x_2)\phi_2(x_1)\right)}{2}$$

$$\psi_a = \frac{\sqrt{2}\left(\phi_1(x_1)\phi_2(x_2) - \phi_1(x_2)\phi_2(x_1)\right)}{2}$$

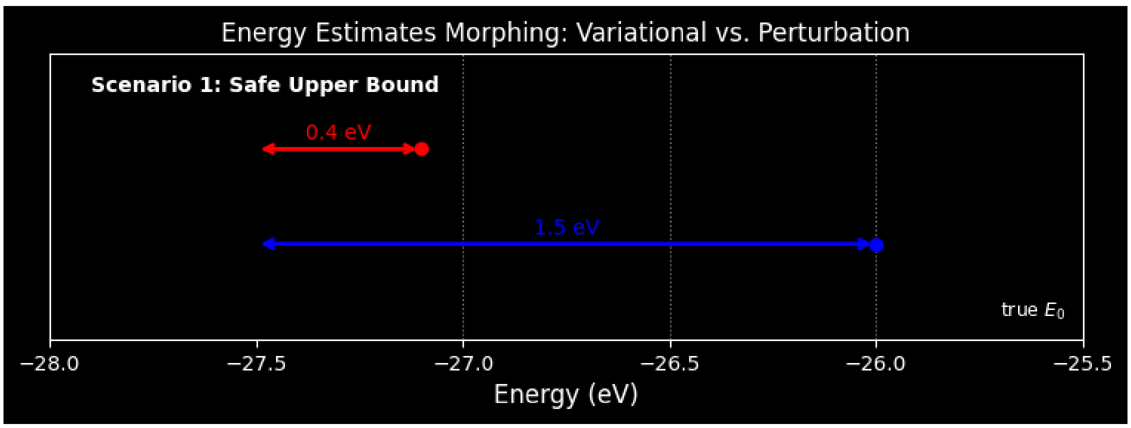
$$\psi_{asame} = 0$$



[3]:
```
#i wanna show the 'safe' regions that i state in math
#will try 'number line style'
#TODO: turn to gif if have time



#config
frames = 60  #param, total frames per
E0 = -27.5 #arbitrary but needed hard num
E_var_1, E_pert_1 = -27.1, -26.0 #scenario 1
E_var_2, E_pert_2 = -26.0, -27.1 #scenario 2

#fig ax call
fig, ax = plt.subplots(figsize=(9, 2.5))
ax.set_xlim(-28, -25.5)
ax.set_ylim(0, 1.5)
ax.set_yticks([])
ax.set_xlabel('Energy (eV)', fontsize=12)
ax.set_title('Energy Estimates Morphing: Variational vs. Perturbation')
```

```python
ax.grid(axis='x', linestyle=':', alpha=0.5)

#draw true static line for true energy E0
ax.axvline(E0, color='black', linewidth=2, label='true $E_0$')

#get this in for dynamic element, recalculate upon loop
dot_var, = ax.plot([], [], 'ro')
dot_pert, = ax.plot([], [], 'bo')
arrow_var = ax.annotate('', xy=(0, 0), xytext=(0, 0),
                        arrowprops=dict(arrowstyle='<->', color='red', lw=2))
arrow_pert = ax.annotate('', xy=(0, 0), xytext=(0, 0),
                         arrowprops=dict(arrowstyle='<->', color='blue', lw=2))
text_var = ax.text(0, 0, '', ha='center', color='red')
text_pert = ax.text(0, 0, '', ha='center', color='blue')
morph_label = ax.text(-27.9, 1.3, '', fontsize=10, weight='bold')

ax.legend(loc='lower right', fontsize=9, frameon=False)

#interpotlate this based on time
def interp(start, end, t):
    return (1 - t) * start + t * end

def update(frame):
    #bounce, forward 0 frame, backwards 2*count frame set abvoe
    if frame < frames:
        t = frame / (frames - 1)
    else:
        t = 1 - (frame - frames) / (frames - 1)

    #call interpolate funct
    E_var = interp(E_var_1, E_var_2, t)
    E_pert = interp(E_pert_1, E_pert_2, t)
    err_var = abs(E_var - E0)
    err_pert = abs(E_pert - E0)

    #update, wrap in list
    dot_var.set_data([E_var], [1])
    dot_pert.set_data([E_pert], [0.5])
    arrow_var.set_position((E_var, 1))
    arrow_var.xy = (E0, 1)
    arrow_pert.set_position((E_pert, 0.5))
    arrow_pert.xy = (E0, 0.5)
    text_var.set_position(((E_var + E0)/2, 1.05))
    text_pert.set_position(((E_pert + E0)/2, 0.55))
    text_var.set_text(f'{err_var:.1f} eV')
    text_pert.set_text(f'{err_pert:.1f} eV')
```

```python
    #morph condition and label morph label
    if t < 0.5:
        morph_label.set_text('Scenario 1: Safe Upper Bound')
    else:
        morph_label.set_text('Scenario 2: Perturbation Possibly Overshoots')

    return dot_var, dot_pert, arrow_var, arrow_pert, text_var, text_pert, morph_label

#call ani and save
ani = animation.FuncAnimation(fig, update, frames=2*frames, interval=60, blit=False)
ani.save('problem_2_ani.gif', writer='pillow')
```



[4]:
```python
move_plots()
```

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Moved problem_1.png to graphs
Moved problem_2_ani.gif to graphs
```