PHYS 661 - Quantum Mechanics II

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Contents

Homework 1

Problem 1 - Pauli Matrices
Show that for Pauli matrices

$$\mathrm{e}^{\mathrm{i}\theta\mathbf{n}\cdot\boldsymbol{\sigma}} = \mathbb{I}\cos(\theta) + \mathrm{i}\mathbf{n}\cdot\boldsymbol{\sigma}\sin(\theta), \text{ where } \mathbf{n}^2 = 1$$

and

$$\mathrm{e}^{\mathrm{i}\frac{1}{2}\theta\sigma_y}\left(\sigma_x,\sigma_y,\sigma_z\right)\mathrm{e}^{-\mathrm{i}\frac{1}{2}\theta\sigma_y} = \left(\sigma_x,\sigma_y,\sigma_z\right)\cos(\theta) + \left(\sigma_z,0,-\sigma_x\right)\sin(\theta) + \left(0,\sigma_y,0\right)\left(1-\cos(\theta)\right)$$

Suppose we have a Hamiltonian $H = \begin{pmatrix} a & b \\ b & -a \end{pmatrix}$ with $a, b \in \mathbb{R}$. What are the eigenvalues $E_\pm$? Find the unitary transformation U that diagonalizes H, i.e.,

$$U^\dagger H U = \begin{pmatrix} E_+ & 0 \\ 0 & E_- \end{pmatrix}.$$

Solution. Let $\mathbf{S} = \frac{\hbar}{2}\boldsymbol{\sigma}$, where $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ is the vector of Pauli matrices. Rotations on spin states with respect to a unit vector $\mathbf{n}$ are given by

$$R_{\mathbf{n}}(\phi) = \mathrm{e}^{\mathrm{i}\frac{\phi}{\hbar}\mathbf{n}\cdot\mathbf{S}} = \mathrm{e}^{\mathrm{i}\frac{\phi}{2}\mathbf{n}\cdot\boldsymbol{\sigma}}.$$

We have the following property of the Pauli matrices

$$\sigma_j\sigma_k = \delta_{jk} + \mathrm{i}\sum_l \epsilon_{jkl}\sigma_l.$$

We will first show that, for any ordinary vectors in $\mathbb{R}^3$, we have

$$\left(\mathbf{a}\cdot\boldsymbol{\sigma}\right)\left(\mathbf{b}\cdot\boldsymbol{\sigma}\right) = \left(\mathbf{a}\cdot\mathbf{b}\right) + \mathrm{i}\boldsymbol{\sigma}\cdot\left(\mathbf{a}\times\mathbf{b}\right).$$

In fact

$$\begin{aligned}
\left(\mathbf{a}\cdot\boldsymbol{\sigma}\right)\left(\mathbf{b}\cdot\boldsymbol{\sigma}\right) &= \sum_j \sigma_j a_j \sum_k \sigma_k b_k \\
&= \sum_j\sum_k \sigma_j\sigma_k a_j b_k \\
&= \sum_j\sum_k \left(\delta_{jk} + \mathrm{i}\sum_l \epsilon_{jkl}\sigma_l\right) a_j b_k \\
&= \sum_j\sum_k \delta_{jk} a_j b_k + \mathrm{i}\sum_j\sum_k\sum_l \epsilon_{jkl}\sigma_l a_j b_k \\
&= \sum_j a_j b_j + \mathrm{i}\sum_l \sigma_l \left(\sum_j\sum_k \epsilon_{jkl} a_j b_k\right) \\
&= \left(\mathbf{a}\cdot\mathbf{b}\right) + \mathrm{i}\sum_l \sigma_l\left(\mathbf{a}\times\mathbf{b}\right) \\
&= \left(\mathbf{a}\cdot\mathbf{b}\right) + \mathrm{i}\boldsymbol{\sigma}\cdot\left(\mathbf{a}\times\mathbf{b}\right).
\end{aligned}$$

Note that, if we take $\mathbf{a} = \mathbf{b} = \mathbf{n}$, then

$$\left(\mathbf{n}\cdot\boldsymbol{\sigma}\right)^2 = \left(\mathbf{n}\cdot\boldsymbol{\sigma}\right)\left(\mathbf{n}\cdot\boldsymbol{\sigma}\right)^2 = \left(\mathbf{n}\cdot\mathbf{n}\right) + \mathrm{i}\boldsymbol{\sigma}\cdot\left(\mathbf{n}\times\mathbf{n}\right) = \mathbf{n}^2 + i\boldsymbol{\sigma}\cdot(0) = \mathbb{I}.$$

We have

$$\begin{aligned}
e^{i\theta \mathbf{n}\cdot\boldsymbol{\sigma}} &= \sum_{k=0}^{\infty} (i)^k \frac{\left[\theta\left(\mathbf{n}\cdot\boldsymbol{\sigma}\right)\right]^k}{k!} \\
&= \sum_{k=0}^{\infty} (i)^{2k} \frac{\left[\theta\left(\mathbf{n}\cdot\boldsymbol{\sigma}\right)\right]^{2k}}{(2k)!} + \sum_{k=0}^{\infty} (i)^{2k+1} \frac{\left[\theta\left(\mathbf{n}\cdot\boldsymbol{\sigma}\right)\right]^{2k+1}}{(2k+1)!} \\
&= \sum_{k=0}^{\infty} (-1)^k \frac{\left[\theta\left(\mathbf{n}\cdot\boldsymbol{\sigma}\right)\right]^{2k}}{(2k)!} + i\sum_{k=0}^{\infty} (-1)^k \frac{\left[\theta\left(\mathbf{n}\cdot\boldsymbol{\sigma}\right)\right]^{2k+1}}{(2k+1)!} \\
&= \sum_{k=0}^{\infty} (-1)^k \frac{\theta^{2k}\left(\mathbf{n}\cdot\boldsymbol{\sigma}\right)^{2k}}{(2k)!} + i\sum_{k=0}^{\infty} (-1)^k \frac{\theta^{2k+1}\left(\mathbf{n}\cdot\boldsymbol{\sigma}\right)^{2k+1}}{(2k+1)!} \\
&= \sum_{k=0}^{\infty} (-1)^k \frac{\theta^{2k}}{(2k)!}\mathbb{I} + i\sum_{k=0}^{\infty} (-1)^k \frac{\theta^{2k+1}}{(2k+1)!}\left(\mathbf{n}\cdot\boldsymbol{\sigma}\right) \\
&= \mathbb{I}\cos(\theta) + i\sin(\theta)\left(\mathbf{n}\cdot\boldsymbol{\sigma}\right)
\end{aligned}$$

Now that we calculated that, we can solve the following

$$\begin{aligned}
e^{i\frac{1}{2}\theta\sigma_y}\left(\sigma_x,\sigma_y,\sigma_z\right)e^{-i\frac{1}{2}\theta\sigma_y} &= \left[\mathbb{I}\cos\left(\frac{\theta}{2}\right) + i\sin\left(\frac{\theta}{2}\right)\sigma_y\right]\left(\sigma_x,\sigma_y,\sigma_z\right)\left[\mathbb{I}\cos\left(\frac{\theta}{2}\right) - i\sin\left(\frac{\theta}{2}\right)\sigma_y\right] \\
&= \cos^2\left(\frac{\theta}{2}\right)\left(\sigma_x,\sigma_y,\sigma_z\right) - i\cos\left(\frac{\theta}{2}\right)\sin\left(\frac{\theta}{2}\right)\left(\sigma_x,\sigma_y,\sigma_z\right)\sigma_y \\
&\quad + i\cos\left(\frac{\theta}{2}\right)\sin\left(\frac{\theta}{2}\right)\sigma_y\left(\sigma_x,\sigma_y,\sigma_z\right) + \sin^2\left(\frac{\theta}{2}\right)\sigma_y\left(\sigma_x,\sigma_y,\sigma_z\right)\sigma_y \\
&= \cos^2\left(\frac{\theta}{2}\right)\left(\sigma_x,\sigma_y,\sigma_z\right) - i\cos\left(\frac{\theta}{2}\right)\sin\left(\frac{\theta}{2}\right)\left(i\sigma_z, 1, -i\sigma_x\right) \\
&\quad + i\cos\left(\frac{\theta}{2}\right)\sin\left(\frac{\theta}{2}\right)\left(-i\sigma_z, 1, i\sigma_x\right) + \sin^2\left(\frac{\theta}{2}\right)\left(-\sigma_x,\sigma_y,-\sigma_z\right) \\
&= \cos^2\left(\frac{\theta}{2}\right)\left(\sigma_x,\sigma_y,\sigma_z\right) - \cos\left(\frac{\theta}{2}\right)\sin\left(\frac{\theta}{2}\right)\left(-\sigma_z, 1, \sigma_x\right) \\
&\quad + \cos\left(\frac{\theta}{2}\right)\sin\left(\frac{\theta}{2}\right)\left(\sigma_z, 1, -\sigma_x\right) + \sin^2\left(\frac{\theta}{2}\right)\left(-\sigma_x,\sigma_y,-\sigma_z\right) \\
&= \cos^2\left(\frac{\theta}{2}\right)\left(\sigma_x,\sigma_y,\sigma_z\right) + \sin^2\left(\frac{\theta}{2}\right)\left(-\sigma_x,\sigma_y,-\sigma_z\right) \\
&\quad + \cos\left(\frac{\theta}{2}\right)\sin\left(\frac{\theta}{2}\right)\left[\left(\sigma_z,-1,-\sigma_x\right) + \left(\sigma_z,1,-\sigma_x\right)\right] \\
&= \cos^2\left(\frac{\theta}{2}\right)\left(\sigma_x,\sigma_y,\sigma_z\right) - \sin^2\left(\frac{\theta}{2}\right)\left(\sigma_x,-\sigma_y,\sigma_z\right) \\
&\quad + 2\cos\left(\frac{\theta}{2}\right)\sin\left(\frac{\theta}{2}\right)\left(\sigma_z,0,-\sigma_x\right) \\
&= \cos^2\left(\frac{\theta}{2}\right)\left(\sigma_x,\sigma_y,\sigma_z\right) - \sin^2\left(\frac{\theta}{2}\right)\left(\sigma_x,\sigma_y,\sigma_z\right) \\
&\quad + 2\sin^2\left(\frac{\theta}{2}\right)\left(0,\sigma_y,0\right) + \sin(\theta)\left(\sigma_z,0,-\sigma_x\right) \\
&= \cos(\theta)\left(\sigma_x,\sigma_y,\sigma_z\right) + \left(1-\cos(\theta)\right)\left(0,\sigma_y,0\right) + \sin(\theta)\left(\sigma_z,0,-\sigma_x\right).
\end{aligned}$$

The eigenvalues of the Hamiltonian H are found by solving

$$\det(H - \lambda I) = 0.$$

We have

$$\begin{aligned}
\det(H-\lambda I) &= \begin{vmatrix} a-\lambda & b \\ b & -a-\lambda \end{vmatrix} \\
&= -(a-\lambda)(a+\lambda) - b^2 \\
&= \lambda^2 - (a^2+b^2) \\
&= 0 \\
\implies \lambda^2 &= a^2+b^2 \\
\implies \lambda_\pm \equiv E_\pm &= \pm\sqrt{a^2+b^2}.
\end{aligned}$$

The eigenvectors $e_\pm$ are given by solving the following set of equations

$$\begin{pmatrix} a-\lambda & b \\ b & -a-\lambda \end{pmatrix} \begin{pmatrix} e_1 \\ e_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

$$\implies \begin{cases} (a-\lambda)e_1 + be_2 &= 0 \\ be_1 + (-a-\lambda)e_2 &= 0 \end{cases}$$

$\boxed{\text{For } \lambda = E_+\text{:}}$

$$\begin{pmatrix} a-E_\pm & b \\ b & -a-E_\pm \end{pmatrix} \begin{pmatrix} e_{\pm,1} \\ e_{\pm,2} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

$$\begin{cases} (a-E_\pm)e_{\pm,1} + be_{\pm,2} &= 0 \\ be_{\pm,1} + (-a-E_\pm)e_{\pm,2} &= 0 \end{cases}$$

The two eigenvector equations are redundant, so considering the first, we have

$$\begin{aligned}
(a-E_\pm)e_{\pm,1} + be_{\pm,2} = 0 \\
be_{\pm,2} &= (E_\pm - a)e_{\pm,1} \\
e_{\pm,2} &= \frac{E_\pm - a}{b} e_{\pm,1}.
\end{aligned}$$

Since $e_{\pm,1}$ is arbitrary, we will set $e_{\pm,1} = 1$, then $e_{\pm,2} = \frac{E_\pm - a}{b}$. Thus, the two eigenvectors $e_\pm$ corresponding to $E_\pm$ are

$$e_\pm = \begin{pmatrix} e_{\pm,1} \\ e_{\pm,2} \end{pmatrix} = \begin{pmatrix} 1 \\ \frac{E_\pm - a}{b} \end{pmatrix} = \begin{pmatrix} 1 \\ \frac{\pm\sqrt{a^2+b^2}-a}{b} \end{pmatrix}.$$

Finally, we now normalize the eigenvectors

$$\begin{aligned}
e_\pm &= \frac{1}{\sqrt{\langle e_\pm | e_\pm \rangle}} \begin{pmatrix} 1 \\ \frac{\pm\sqrt{a^2+b^2}-a}{b} \end{pmatrix} \\
&= \frac{1}{\sqrt{1 + \frac{(\sqrt{a^2+b^2}\mp a)^2}{b^2}}} \begin{pmatrix} 1 \\ \frac{\pm\sqrt{a^2+b^2}-a}{b} \end{pmatrix} \\
&= \frac{1}{\sqrt{1 + \frac{(a^2+b^2\mp 2a\sqrt{a^2+b^2}+a^2)}{b^2}}} \begin{pmatrix} 1 \\ \frac{\pm\sqrt{a^2+b^2}-a}{b} \end{pmatrix} \\
&= \frac{1}{\sqrt{2 + \frac{2a(a\mp\sqrt{a^2+b^2})}{b^2}}} \begin{pmatrix} 1 \\ \frac{\pm\sqrt{a^2+b^2}-a}{b} \end{pmatrix}.
\end{aligned}$$

Let $c_\pm = \frac{1}{\sqrt{2+\frac{2a(a\mp\sqrt{a^2+b^2})}{b^2}}}$. The unitary transformation U that diagonalizes H is given by

$$U = (e_-, e_+) = \begin{pmatrix} c_- & c_+ \\ \frac{-\sqrt{a^2+b^2}-a}{b} c_- & \frac{\sqrt{a^2+b^2}-a}{b} c_+ \end{pmatrix}.$$

■

Problem 2 - 1D Harmonic Oscillator (Sakurai 5.1)
A simple harmonic oscillator in 1D is subjected to a perturbation

$$V = bx.$$

where $b \in \mathbb{R}$ is a constant.

(a) Calculate the energy shift of the ground state to the *lowest non-vanishing order*.

(b) Solve the problem *exactly* and compare your answer to (a).

Solution. (a) The energy shift in an unperturbed nth state can be calculated as

$$\Delta_n = \underset{\text{in energy}}{\text{first order correction}} + \underset{\text{in energy}}{\text{second order correction}} + \cdots + \underset{\text{in energy}}{n\text{th order correction}}.$$

The first-order correction to the energy is

$$\begin{aligned} E_n^{(1)} &= \langle n|V|n\rangle \\ &= b\,\langle n|\hat{x}|n\rangle \\ &= b\sqrt{\frac{\hbar}{2m\omega}}\,\langle n|\hat{a}+\hat{a}^\dagger|n\rangle \\ &= b\sqrt{\frac{\hbar}{2m\omega}}\left[\langle n|\hat{a}|n\rangle + \langle n|\hat{a}^\dagger|n\rangle\right] \\ &= b\sqrt{\frac{\hbar}{2m\omega}}\left[\sqrt{n}\,\langle n|n-1\rangle + \sqrt{n+1}\,\langle n|n+1\rangle\right] \\ &= b\sqrt{\frac{\hbar}{2m\omega}}\left[\sqrt{n}\delta_{n,n-1} + \sqrt{n+1}\delta_{n,n+1}\right]. \end{aligned}$$

For the ground state ($n = 0$), we have

$$E_n^{(1)} = b\sqrt{\frac{\hbar}{2m\omega}}\left[\sqrt{0}\delta_{0,-1} + \sqrt{1}\delta_{0,1}\right] = 0.$$

The second-order correction to the energy is

$$E_n^{(2)} = \sum_{m\neq n}\frac{|\langle m|V|n\rangle|^2}{E_n^{(0)} - E_m^{(0)}}.$$

We have that

$$\begin{aligned} \langle m|V|n\rangle &= b\,\langle m|\hat{x}|n\rangle \\ &= b\sqrt{\frac{\hbar}{2m\omega}}\,\langle m|\hat{a}+\hat{a}^\dagger|n\rangle \\ &= b\sqrt{\frac{\hbar}{2m\omega}}\left[\langle m|\hat{a}|n\rangle + \langle m|\hat{a}^\dagger|n\rangle\right]. \end{aligned}$$

If we replace in the sum, all the terms will be null, except for those where $m = n-1$ or $m = n+1$.

Then, we have

$$
\begin{aligned}
E_n^{(2)} &= \sum_{m\neq n} \frac{\left|\langle m|V|n\rangle\right|^2}{E_n^{(0)} - E_m^{(0)}} \\
&= \frac{\hbar b^2}{2m\omega}\left[\frac{\left|\langle n-1|\hat{a}|n\rangle + \langle n-1|\hat{a}^\dagger|n\rangle\right|^2}{E_n^{(0)} - E_{n-1}^{(0)}} + \frac{\left|\langle n+1|\hat{a}|n\rangle + \langle n+1|\hat{a}^\dagger|n\rangle\right|^2}{E_n^{(0)} - E_{n+1}^{(0)}}\right] \\
&= \frac{\hbar b^2}{2m\omega}\left[\frac{\left|\sqrt{n}\,\langle n-1|n-1\rangle + \sqrt{n+1}\,\langle n-1|n+1\rangle\right|^2}{\hbar\omega} + \frac{\left|\sqrt{n}\,\langle n+1|n-1\rangle + \sqrt{n+1}\,\langle n+1|n+1\rangle\right|^2}{-\hbar\omega}\right] \\
&= \frac{\hbar b^2}{2m\omega}\left[\frac{\left|\sqrt{n}\delta_{n-1,n-1} + \sqrt{n+1}\delta_{n-1,n+1}\right|^2}{\hbar\omega} - \frac{\left|\sqrt{n}\delta_{n-1,n+1} + \sqrt{n+1}\delta_{n+1,n+1}\right|^2}{\hbar\omega}\right] \\
&= \frac{\hbar b^2}{2m\omega}\left[\frac{\left|\sqrt{n}\right|^2}{\hbar\omega} - \frac{\left|\sqrt{n+1}\right|^2}{\hbar\omega}\right] \\
&= \frac{\hbar b^2}{2m\omega}\left[\frac{n}{\hbar\omega} - \frac{n+1}{\hbar\omega}\right] \\
&= -\frac{b^2}{2m\omega^2}.
\end{aligned}
$$

The energy correction to the lowest non-vanishing order is

$$
E = E_n^{(0)} + E_n^{(2)} = \hbar\omega\left(n + \frac{1}{2}\right) - \frac{b^2}{2m\omega^2}.
$$

The energy correction of the ground state ($n = 0$) is

$$
E = E_0^{(0)} + E_0^{(2)} = \frac{\hbar\omega}{2} - \frac{b^2}{2m\omega^2}.
$$

Thus, the energy shift of the ground state is $-\frac{b^2}{2m\omega^2}$.

(b) The Hamiltonian of the harmonic oscillator is given by

$$
\hat{\mathcal{H}}_0 = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2.
$$

The Hamiltonian of our perturbed system is

$$
\hat{\mathcal{H}} = \hat{\mathcal{H}}_0 + \hat{\mathcal{H}}_p = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2 + bx.
$$

To solve this problem exactly, we complete the square, getting

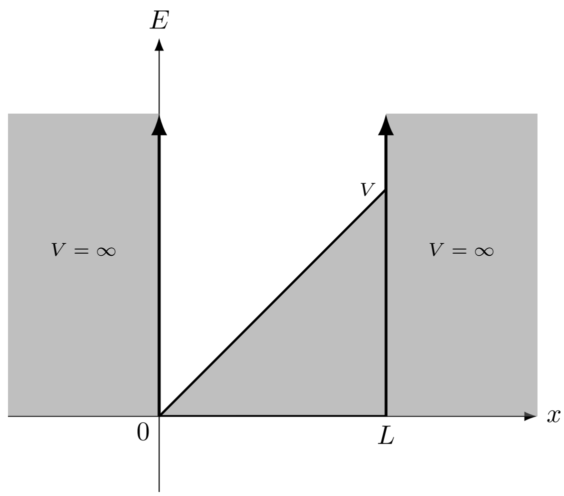
$$
\begin{aligned}
\hat{\mathcal{H}} &= \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2 + bx \\
&= \frac{p^2}{2m} + \frac{1}{2}m\omega^2\left(x^2 + \frac{2bx}{m\omega^2}\right) \\
&= \frac{p^2}{2m} + \frac{1}{2}m\omega^2\left(x^2 + 2x\frac{b}{m\omega^2} + \left(\frac{b}{m\omega^2}\right)^2 - \left(\frac{b}{m\omega^2}\right)^2\right) \\
&= \frac{p^2}{2m} + \frac{1}{2}m\omega^2\left(x + \frac{b}{m\omega^2}\right)^2 - \frac{1}{2}m\omega^2\left(\frac{b}{m\omega^2}\right)^2 \\
&= \frac{p^2}{2m} + \frac{1}{2}m\omega^2\left(x + \frac{b}{m\omega^2}\right)^2 - \frac{b^2}{2m\omega^2},
\end{aligned}
$$

Let $x' \equiv x + \frac{b}{m\omega^2}$, then we still obtain a simple harmonic oscillator, but with the equilibrium point shifted and with an overall energy shift of $-\frac{b^2}{2m\omega^2}$, which is the same energy shift calculated in (a). Thus, the second-order perturbation theory will give us the exact answer in this case.

■

Problem 3 - Potential Well (Sakurai 5.2)
Consider a 1D potential well with infinite walls at $x = 0,\ L$. The bottom is *not* flat, but increases linearly from 0 at $x = 0$ to V at $x = L$. Find the first-order shift in the energy levels as a function of principal quantum number n.

Solution. The 1D potential well with infinite walls looks like



For the unperturbed potential of the infinite potential well, the wave functions $\left|\psi_n^{(0)}\right\rangle$ and the energy eigenvalues $E_n^{(0)}$ are given by

$$\left|\psi_n^{(0)}\right\rangle = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right)$$
$$E_n^{(0)} = \frac{n^2\pi^2\hbar^2}{2mL^2}.$$

The Hamiltonian given by the perturbed potential is

$$\hat{\mathcal{H}}_p = \frac{V}{L}x.$$

The total Hamiltonian of the system is then given by

$$\hat{\mathcal{H}} = \hat{\mathcal{H}}_0 + \hat{\mathcal{H}}_p = -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \frac{V}{L}x.$$

We know how to exactly solve the first term of the Hamiltonian, but our perturbation theory kicks in with the second term, which is the potential term.

The expected value of the energy of the perturbed potential is

$$
\begin{aligned}
\left\langle \hat{\mathcal{H}}_p \right\rangle &= \left\langle \psi_n^{(0)} \middle| \hat{\mathcal{H}}_p \middle| \psi_n^{(0)} \right\rangle \\
&= \int_0^L \left(\psi_n^{(0)}\right)^* \hat{\mathcal{H}}_p \psi_n^{(0)} \, \mathrm{d}x \\
&= \int_0^L \left(\sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right)\right)^* \left(\frac{V}{L}x\right) \left(\sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right)\right) \mathrm{d}x \\
&= \frac{2V}{L^2} \int_0^L x \sin^2\left(\frac{n\pi x}{L}\right) \mathrm{d}x \\
&= \frac{2V}{L^2} \int_0^L x \left(\frac{1 - \cos\left(\frac{2n\pi x}{L}\right)}{2}\right) \mathrm{d}x \\
&= \frac{2V}{L^2} \int_0^L \left[\frac{x}{2} - \frac{x}{2}\cos\left(\frac{2n\pi x}{L}\right)\right] \mathrm{d}x \\
&= \frac{2V}{L^2} \left[\frac{x^2}{4} - \frac{x}{2}\frac{L}{2n\pi}\sin\left(\frac{2n\pi x}{L}\right) + \frac{1}{2}\frac{L^2}{4n^2\pi^2}\cos\left(\frac{2n\pi x}{L}\right)\right]_0^L \\
&= \frac{2V}{L^2} \left[\frac{x^2}{4} - \frac{xL}{4n\pi}\sin\left(\frac{2n\pi x}{L}\right) + \frac{L^2}{8n^2\pi^2}\cos\left(\frac{2n\pi x}{L}\right)\right]_0^L \\
&= \frac{2V}{L^2} \left[\frac{L^2}{4} - \frac{L^2}{4n\pi}\sin(2n\pi) + \frac{L^2}{8n^2\pi^2}\cos(2n\pi) - \frac{L^2}{8n^2\pi^2}\right] \\
&= \frac{2V}{L^2} \left[\frac{L^2}{8n^2\pi^2}\left(2n^2\pi^2 - 2n\pi\sin(2n\pi) + \cos(2n\pi) - 1\right)\right] \\
&= \frac{2V}{L^2} \left[\frac{L^2}{8n^2\pi^2}\left(2n^2\pi^2\right)\right] \\
&= \frac{V}{2}.
\end{aligned}
$$

Thus, the first-order energy shift is $\frac{V}{2}$. Notice that it does not depend on the principal quantum number n. ∎

Problem 4 - 2D Harmonic Oscillator (Sakurai 5.7)

Consider an isotropic harmonic oscillator in *two* dimensions. The Hamiltonian is

$$H = \frac{p_x^2}{2m} + \frac{p_y^2}{2m} + \frac{1}{2}m\omega^2\left(x^2 + y^2\right).$$

(a) Calculate the energies of the three lowest-lying states? Is there any degeneracy?

(b) We now apply a perturbation

$$V = \delta m\omega^2 xy,$$

where δ is a dimensionless real number much smaller than unity. Find the zeroth-order energy eigenstate and the corresponding energy to first order [that is, the unperturbed energy obtained in (a) plus the first-order energy shift] for each of the three lowest-lying states.

(c) Solve the $H + V$ problem *exactly*. Compare with the perturbation results obtained in (b).

Solution. (a) The energy for the state n of a harmonic oscillator with d degrees of freedom is given by

$$E = \left(\sum_{i=1}^{d} n_i + \frac{d}{2}\right)\hbar\omega.$$

In this case, we have two degrees of freedom. Hence, the energy for the state n of our isotropic harmonic oscillator will be

$$E = (n_x + n_y + 1)\hbar\omega.$$

We will now find the energy of the three lowest energy states.

- **Ground state**: We have $n_x = n_y = 0$, and the energy is

$$E = \hbar\omega.$$

- **First excited state**:
  - We have $n_x = 1$ and $n_y = 0$, and the energy is

$$E = 2\hbar\omega.$$

  - We have $n_x = 0$ and $n_y = 1$, and the energy is

$$E = 2\hbar\omega.$$

Thus, the two configurations of the first excited state both yield the same energy level and are therefore doubly degenerate.

(b) Given the perturbation

$$V = \delta m\omega^2 xy,$$

our total Hamiltonian becomes

$$\hat{\mathcal{H}} = \frac{p_x^2}{2m} + \frac{p_y^2}{2m} + \frac{1}{2}m\omega^2\left(x^2 + y^2\right) + \delta m\omega^2 xy$$

As we know, in time-independent perturbation theory, if we perturb an energy eigenvalue for the zeroth-order correction, then there will be no perturbation change in energy compared to the initial energy for the zeroth-order perturbation.

Finding the first-order energy correction, we have

$$\begin{aligned} E^{(1)}_{n_x,n_y} &= \langle n_x, n_y|V|n_x, n_y\rangle \\ &= \left\langle n_x, n_y\middle|\delta m\omega^2 xy\middle|n_x, n_y\right\rangle \\ &= \delta m\omega^2 \langle n_x, n_y|xy|n_x, n_y\rangle \\ &= \delta m\omega^2 \langle n_x|x|n_x\rangle \langle n_y|y|n_y\rangle, \end{aligned}$$

where the last step follows from the fact that x and y are independent.

The first-order energy shift is as follows

- For the ground state:

$$E^{(1)}_{0,0} = \langle 0,0|V|0,0\rangle = \delta m\omega^2 \langle 0|x|0\rangle \langle 0|y|0\rangle = 0.$$

- For the first excited state, this requires us to diagonalize the perturbation for the first order energy shift, but
  - For $(n_x, n_y) = (1, 0)$:

$$E^{(1)}_{1,0} = \langle 1,0|V|1,0\rangle = \delta m\omega^2 \langle 1|x|1\rangle \langle 0|y|0\rangle = 0.$$

  - For $(n_x, n_y) = (0, 1)$:

$$E^{(1)}_{1,0} = \langle 0,1|V|0,1\rangle = \delta m\omega^2 \langle 0|x|0\rangle \langle 1|y|1\rangle = 0.$$

The off-diagonal elements are

$$\begin{aligned}\langle 1,0|V|0,1\rangle &= \delta m\omega^2 \left\langle 1,0\middle|\sqrt{\frac{\hbar}{2m\omega}}\sqrt{1}\sqrt{\frac{\hbar}{2m\omega}}\sqrt{1}\middle|0,1\right\rangle \\ &= \frac{\delta\hbar\omega}{2} \\ &= \langle 0,1|V|1,0\rangle\,.\end{aligned}$$

The first-order energy shifts in the first excited state are the eigenvalues $\Delta_1^{(1)}$, where

$$\left(\Delta_1^{(1)}\right)^2 - \left(\frac{\delta\hbar\omega}{2}\right)^2 = 0 \implies \Delta_1^{(1)} = \pm\frac{\delta\hbar\omega}{2},$$

and

$$E = \left(2 \pm \frac{\delta}{2}\right)\hbar\omega$$

for the degenerate first excited state. The corresponding eigenstates are

$$\frac{|1,0\rangle + |0,1\rangle}{\sqrt{2}} \quad \text{and} \quad \frac{|1,0\rangle - |0,1\rangle}{\sqrt{2}}.$$

(c) To solve $H+V$ exactly, we can rewrite the potential energy as

$$\begin{aligned}V &= \frac{1}{2}m\omega^2(x^2+y^2+2\delta xy) \\ &= \frac{1}{2}m\omega^2\left[(1+\delta)\frac{(x+y)^2}{2} + (1-\delta)\frac{(x-y)^2}{2}\right].\end{aligned}$$

We can then rotate the xy-axes by $\frac{\pi}{4}$, and then the anharmonic oscillator has the normal coordinate $x' \equiv \frac{x+y}{\sqrt{2}}$ with frequency $\omega\sqrt{1+\delta}$, and $y' \equiv \frac{x-y}{\sqrt{2}}$ with frequency $\omega\sqrt{1-\delta}$.

Therefore, we have

- For $|0,0\rangle$:
$$\frac{1}{2}\hbar\omega\sqrt{1+\delta} + \frac{1}{2}\hbar\omega\sqrt{1-\delta} \approx \frac{1}{2}\hbar\omega\left(1+\frac{\delta}{2}+1-\frac{\delta}{2}\right) = \hbar\omega.$$
- For $|1,0\rangle$:
$$\frac{3}{2}\hbar\omega\sqrt{1+\delta} + \frac{1}{2}\hbar\omega\sqrt{1-\delta} \approx \frac{1}{2}\hbar\omega\left(3+\frac{3\delta}{2}+1-\frac{\delta}{2}\right) = \left(2+\frac{\delta}{2}\right)\hbar\omega.$$
- For $|0,1\rangle$:
$$\frac{1}{2}\hbar\omega\sqrt{1+\delta} + \frac{3}{2}\hbar\omega\sqrt{1-\delta} \approx \frac{1}{2}\hbar\omega\left(1+\frac{\delta}{2}+3-\frac{3\delta}{2}\right) = \left(2-\frac{\delta}{2}\right)\hbar\omega.$$

All three cases are in agreement with our lowest order results from perturbation theory in part (b). ■

Homework 2

Problem 1 - N-state All-to-All System
Consider an N-state system with a perturbation

$$V = \begin{pmatrix} v & v & \dots & v \\ v & v & & \\ \vdots & & \ddots & \\ v & & & v \end{pmatrix}, \quad v \in \mathbb{R}$$

where $\langle n^{(0)} | V | m^{(0)} \rangle = v$ for all n, m. Let us for simplicity assume that the unperturbed Hamiltonian is just zero, $H_0 = 0$, i.e. $E_n^{(0)} = 0$ for all $n = 1, 2, \dots, N$. In this case we can use Brillouin-Wigner (BW) perturbation theory.

(a) Before doing perturbation theory, find the eigenvalues of V and their degeneracies exactly.

(b) By using BW perturbation theory, evaluate the correction to the energy E of a state up to and including third-order corrections in v. You should get an equation for E of the form $E = a_0 + a_1 v + a_2 \frac{v^2}{E} + a_3 \frac{v^3}{E^2}$. (No need to try to solve that equation.)

(c) Going beyond 3rd order, the equation for the perturbed energy E will be of the form $E = a_0 + \sum_{k=0}^{\infty} a_{k+1} v \left(\frac{v}{E}\right)^k$. Find the general nth order coefficient a_n. Using your result, sum up the series $\sum_{k=0}^{\infty} a_{k+1} v \left(\frac{v}{E}\right)^k$. Solve the resulting equation for E.

Solution. (a) The perturbation V of the system can be written as

$$V = \begin{pmatrix} v & v & \dots & v \\ v & v & & \\ \vdots & & \ddots & \\ v & & & v \end{pmatrix} = v \begin{pmatrix} 1 & 1 & \dots & 1 \\ 1 & 1 & & \\ \vdots & & \ddots & \\ 1 & & & 1 \end{pmatrix},$$

where the matrix of ones on the right clearly has rank 1 since it has only 1 linearly independent column, making the eigenvalues N with multiplicity 1, and 0 with multiplicity $N-1$.

Similarly, the eigenvalues of V are $\lambda = 0$ that is $(N-1)$-fold degenerate and $\lambda = vN$ that is unique.

(b) The general correction to the energy E of a state using Brillouin-Wigner is given by

$$E_n = E_n^{(0)} + \lambda \sum_{p=0}^{\infty} \left\langle n^{(0)} \middle| V \left(\frac{\phi_n}{E_n - H_0} \lambda V \right)^p \middle| n^{(0)} \right\rangle.$$

We are asked to find the correction to the energy up to and including the third-order correction in v, which means we will stop evaluating the sum at $p = 2$. Recall the form of the projector

$$\phi_n = \sum_{k \neq n} \left| k^{(0)} \right\rangle \left\langle k^{(0)} \right|,$$

and that $\langle n^{(0)} | V | m^{(0)} \rangle = v$ for all n, m.

- **Ground State**: We are given that $H_0 = E_n^{(0)} = 0$.
- **First-Order**: For $p = 0$, we have that

$$\left\langle n^{(0)} \middle| V \middle| n^{(0)} \right\rangle = v.$$

- **Second-Order**: For $p = 1$, we have that

$$
\begin{aligned}
\left\langle n^{(0)} \middle| V \left(\frac{\phi_n}{E_n - H_0} \lambda V \right) \middle| n^{(0)} \right\rangle &= \frac{\lambda}{E_n} \left\langle n^{(0)} \middle| V \phi_n V \middle| n^{(0)} \right\rangle \\
&= \frac{\lambda}{E_n} \sum_{k \neq n} \left\langle n^{(0)} \middle| V \middle| k^{(0)} \right\rangle \left\langle k^{(0)} \middle| V \middle| n^{(0)} \right\rangle \\
&= \frac{\lambda}{E_n} \sum_{k \neq n} v^2 \\
&= \frac{\lambda}{E_n} (N-) v^2.
\end{aligned}
$$

- **Third-Order**: For $p = 2$, we have that

$$
\begin{aligned}
\left\langle n^{(0)} \middle| V \left(\frac{\phi_n}{E_n - H_0} \lambda V \right)^2 \middle| n^{(0)} \right\rangle &= \frac{\lambda^2}{E_n^2} \left\langle n^{(0)} \middle| V \phi_n V \phi_n V \middle| n^{(0)} \right\rangle \\
&= \frac{\lambda^2}{E_n^2} \sum_{k \neq n} \left\langle n^{(0)} \middle| V \middle| k^{(0)} \right\rangle \left\langle k^{(0)} \middle| V \phi_n V \middle| n^{(0)} \right\rangle \\
&= \frac{\lambda^2}{E_n^2} \sum_{k, k' \neq n} \left\langle n^{(0)} \middle| V \middle| k^{(0)} \right\rangle \left\langle k^{(0)} \middle| V \middle| k'^{(0)} \right\rangle \left\langle k'^{(0)} \middle| V \middle| n^{(0)} \right\rangle \\
&= \frac{\lambda^2}{E_n^2} \sum_{k, k' \neq n} v^3 \\
&= \frac{\lambda^2}{E_n^2} (N-1)^2 v^3.
\end{aligned}
$$

Thus, after replacing, we get

$$
\begin{aligned}
E_n &= E_n^{(0)} + \lambda \sum_{p=0}^{2} \left\langle n^{(0)} \middle| V \left(\frac{\phi_n}{E_n - H_0} \lambda V \right)^p \middle| n^{(0)} \right\rangle \\
&= E_n^{(0)} + \lambda \left\langle n^{(0)} \middle| V \middle| n^{(0)} \right\rangle + \lambda \left\langle n^{(0)} \middle| V \left(\frac{\phi_n}{E_n - H_0} \lambda V \right) \middle| n^{(0)} \right\rangle + \lambda \left\langle n^{(0)} \middle| V \left(\frac{\phi_n}{E_n - H_0} \lambda V \right)^2 \middle| n^{(0)} \right\rangle \\
&= 0 + \lambda v + \frac{\lambda}{E_n} (N-1) v^2 + \frac{\lambda^2}{E_n^2} (N-1)^2 v^3.
\end{aligned}
$$

(c) The nth-order correction to the energy is

$$
\begin{aligned}
E_n^{(n)} &= \lambda \left\langle n^{(0)} \middle| V \left(\frac{\phi_n}{E_n - H_0} \lambda V \right)^{n-1} \middle| n^{(0)} \right\rangle \\
&= \frac{\lambda^n}{E_n^{n-1}} \left\langle n^{(0)} \middle| V \left(\phi_n V \right)^{n-1} \middle| n^{(0)} \right\rangle \\
&= \frac{\lambda^n}{E_n^{n-1}} \sum_{k_1, k_2, \ldots, k_{n-1} \neq n} \left\langle n^{(0)} \middle| V \middle| k_1^{(0)} \right\rangle \left\langle k_1^{(0)} \middle| V \middle| k_2^{(0)} \right\rangle \cdots \left\langle k_{n-1}^{(0)} \middle| V \middle| n^{(0)} \right\rangle \\
&= \frac{\lambda^n}{E_n^{n-1}} \sum_{k_1, k_2, \ldots, k_{n-1} \neq n} v^n \\
&= \frac{\lambda^n}{E_n^{n-1}} (N-1)^{n-1} v^n,
\end{aligned}
$$

which means that the nth-order coefficient $a_n = (N-1)^{n-1} \lambda^n$.

The sum of the series is

$$\begin{aligned}
\sum_{k=0}^{\infty} a_{k+1} v \left(\frac{v}{E}\right)^k &= \sum_{k=0}^{\infty} (N-1)^k \lambda^{k+1} v \left(\frac{v}{E}\right)^k \\
&= \sum_{k=0}^{\infty} \lambda v \left(\frac{(N-1)\lambda v}{E}\right)^k \\
&= \frac{\lambda v}{1 - \frac{(N-1)\lambda v}{E}} \\
&= \frac{\lambda v E}{E - (N-1)\lambda v} \\
&= \frac{vE}{E - (N-1)v}.
\end{aligned}$$

where we set $\lambda = 1$ in the last line.

The series for the energy is then

$$\begin{aligned}
E &= a_0 + \sum_{k=0}^{\infty} a_{k+1} v \left(\frac{v}{E}\right)^k \\
&= 0 + \frac{vE}{E - (N-1)v} \\
&= 0 + \frac{vE}{E - (N-1)v} \\
\implies E(E - (N-1)v) &= vE \\
E &= (N-1)v + v \\
E &= Nv,
\end{aligned}$$

as expected from part (a).

■

Problem 2 - 1D δ-potential Well Under Electric Field
Consider a 1D potential well $U(x) = -\alpha\delta(x)$. The ground state of this system is a bound level with wave function $\psi_0(x) = \sqrt{\kappa}e^{-\kappa|x|}$ and energy $E_0^{(0)} = -\frac{\hbar^2\kappa^2}{2m}$, where $\kappa = \frac{m\alpha}{\hbar^2}$. The excited state wave functions are $\psi_{+,k}(x) = \frac{1}{\sqrt{\pi}}\cos\left(k|x| + \frac{\varphi_k}{2}\right)$ and $\psi_{-,k} = \frac{1}{\sqrt{\pi}}\sin(kx)$, both with energy $E_k^{(0)} = \frac{\hbar^2k^2}{2m}$. (The subscript $\pm$ denotes spatial parity eigenvalues.) Consider a perturbation $V = bx$ acting on the ground state. Calculate the first and second order energy shifts to the ground state energy. In the case of continuous spectrum the 2nd order correction to the ground state energy is

$$E^{(2)} = \sum_{\sigma=\pm}\int_0^\infty \frac{1}{E_0^{(0)} - E_k^{(0)}} \left|\langle\sigma, k|V|0\rangle\right|^2 \mathrm{d}k.$$

Hint: $\int_0^\infty xe^{-\kappa x}\sin(kx)\,\mathrm{d}x = \frac{2\kappa k}{(\kappa^2+k^2)^2}$.

Solution. The energy shift to the ground state is given by

$$\Delta_n = \lambda V_{nn} + \lambda^2 \sum_{k\neq n} \frac{|V_{nk}|^2}{E_n^{(0)} - E_k^{(0)}} + \cdots,$$

where

$$V_{nk} \equiv \left\langle n^{(0)}\middle|V\middle|k^{(0)}\right\rangle.$$

Consider $\lambda = 1$. We have

$$\begin{aligned}
\Delta_n &= E_n - E_n^{(0)} \\
&= E_0^{(0)} + E^{(1)} + E^{(2)} \\
&= -\frac{\hbar\kappa^2}{2m} + \lambda\left\langle n^{(0)}\middle|V\middle|n^{(0)}\right\rangle + \lambda^2\sum_{\sigma=\pm}\int_0^\infty \frac{\left|\langle\sigma|V|0\rangle\right|^2}{E_0^{(0)} - E_k^{(0)}}\,\mathrm{d}k.
\end{aligned}$$

The first-order energy shift of the ground state energy is given by

$$\begin{aligned}
\left\langle n^{(0)}\middle|V\middle|n^{(0)}\right\rangle &= \langle\psi_0|V|\psi_0\rangle \\
&= \int_{-\infty}^{\infty} \psi_0^*(x) V \psi_0(x)\,\mathrm{d}x \\
&= \int_{-\infty}^{\infty} \left(\sqrt{\kappa}e^{-\kappa|x|}\right)(bx)\left(\sqrt{\kappa}e^{-\kappa|x|}\right)\mathrm{d}x \\
&= \kappa b\int_{-\infty}^{\infty} xe^{-2\kappa|x|}\,\mathrm{d}x \\
&= 2\kappa b\int_0^\infty xe^{-2\kappa x}\,\mathrm{d}x \\
&= 2\kappa b\left(\frac{1}{4\kappa^2}\right) \\
&= \frac{b}{2\kappa}.
\end{aligned}$$

The second-order energy shift of the ground state energy is given by

$$\sum_{\sigma=\pm}\int_0^\infty \frac{\left|\langle\sigma|V|0\rangle\right|^2}{E_0^{(0)} - E_k^{(0)}}\,\mathrm{d}k = \int_0^\infty \frac{\left|\langle+|V|0\rangle\right|^2 + \left|\langle-|V|0\rangle\right|^2}{E_0^{(0)} - E_k^{(0)}}\,\mathrm{d}k.$$

- Solving for the first term, we have

$$\begin{aligned}
|\langle + | V | 0 \rangle|^2 &= \left| \int_{-\infty}^{\infty} \psi_{+,k}^*(x) V \psi_0(x)\, \mathrm{d}x \right|^2 \\
&= \left| \int_{-\infty}^{\infty} \left(\frac{1}{\sqrt{\pi}} \cos\left(k|x| + \frac{\varphi_k}{2} \right) \right) (bx) \left(\sqrt{\kappa} e^{-\kappa|x|} \right) \mathrm{d}x \right|^2 \\
&= \frac{b}{\pi\kappa} \left| \int_{-\infty}^{\infty} x \cos\left(k|x| + \frac{\varphi_k}{2} \right) e^{-\kappa|x|}\, \mathrm{d}x \right|^2 \\
&= 0,
\end{aligned}$$

  since the integrand is an odd function.

- Solving for the second term, we have

$$\begin{aligned}
|\langle - | V | 0 \rangle|^2 &= \left| \int_{-\infty}^{\infty} \psi_{-,k}^*(x) V \psi_0(x)\, \mathrm{d}x \right|^2 \\
&= \left| \int_{-\infty}^{\infty} \left(\frac{1}{\sqrt{\pi}} \sin(kx) \right) (bx) \left(\sqrt{\kappa} e^{-\kappa|x|} \right) \mathrm{d}x \right|^2 \\
&= \frac{b^2\kappa}{\pi} \left| \int_{-\infty}^{\infty} x \sin(kx)\, e^{-\kappa|x|}\, \mathrm{d}x \right|^2 \\
&= \frac{4b^2\kappa}{\pi} \left| \int_{0}^{\infty} x \sin(kx)\, e^{-\kappa x}\, \mathrm{d}x \right|^2 \\
&= \frac{4b^2\kappa}{\pi} \left| \frac{2\kappa k}{(\kappa^2 + k^2)^2} \right|^2 \\
&= \frac{16 b^2 \kappa^2 k^2}{\pi(\kappa^2 + k^2)^4}.
\end{aligned}$$

Replacing these values in the second-order energy shift, we get

$$\begin{aligned}
\sum_{\sigma=\pm} \int_0^\infty \frac{|\langle \sigma | V | 0 \rangle|^2}{E_0^{(0)} - E_k^{(0)}}\, \mathrm{d}k &= \int_0^\infty \frac{1}{E_0^{(0)} - E_k^{(0)}} \left(0 + \frac{16 b^2 \kappa^2 k^2}{\pi(\kappa^2 + k^2)^4} \right) \mathrm{d}k \\
&= \int_0^\infty \frac{1}{-\frac{\hbar^2\kappa^2}{2m} - \frac{\hbar^2 k^2}{2m}} \left(\frac{16 b^2 \kappa^2 k^2}{\pi(\kappa^2 + k^2)^4} \right) \mathrm{d}k \\
&= -\int_0^\infty \frac{2m}{\hbar^2(\kappa^2 + k^2)} \frac{16 b^2 \kappa^2 k^2}{\pi(\kappa^2 + k^2)^4}\, \mathrm{d}k \\
&= -\int_0^\infty \frac{32 b^2 m \kappa^2 k^2}{\hbar^2 \pi (\kappa^2 + k^2)^5}\, \mathrm{d}k \\
&= -\frac{32 b^2 m \kappa^2}{\hbar^2 \pi} \left(\frac{5\pi}{256 \kappa^7} \right) \\
&= -\frac{5 b^2 m}{8 \hbar^2 \kappa^5}.
\end{aligned}$$

Therefore,

$$\begin{aligned}
\Delta_n &= E_0^{(0)} + E^{(1)} + E^{(2)} \\
&= -\frac{\hbar\kappa^2}{2m} + \frac{b}{2\kappa} - \frac{5b^2 m}{8\hbar^2\kappa^5} \\
&= \frac{4\hbar^2\kappa^4(b - \hbar\kappa^3) - 5b^2 m}{8\hbar^2\kappa^5}.
\end{aligned}$$

■

Homework 3

Problem 1 - Variational Principle
In this problem you will learn the variational principle (see Sakurai Sec. 5.4 for more details) and apply it to the case of a double-well potential. The basic idea is that a guess $|\psi\rangle$ for the ground state of a Hamiltonian H satisfies $\langle\psi|H|\psi\rangle \geq E_0$, where E_0 is the exact ground state energy and $|\psi\rangle$ is assumed to be normalized. We can try to minimize $\langle\psi|H|\psi\rangle$ (and improve our bound on E_0) by taking derivative w.r.t. a parameter β in the guess state: $\partial_\beta \langle\psi(\beta)|H|\psi(\beta)\rangle = 0$.

1. Consider a 1D Harmonic oscillator Hamiltonian $H = \frac{p_x^2}{2m} + \frac{1}{2}m\omega_0^2 x^2$. Find the energy $E(\beta) = \langle\psi|H|\psi\rangle$ and its minimum value $E(\beta_*)$ for the following variational wave functions. Interpret your results.
   (a) $\psi_a(x,\beta) = \left(\frac{2\beta}{\pi}\right)^{\frac{1}{4}} \exp\left(-\beta x^2\right)$
   (b) $\psi_b(x,\beta) = \begin{cases} \left(\frac{15}{16}\right)^{\frac{1}{4}} \beta^{\frac{1}{4}} \left(1-\beta x^2\right), & |x| < \beta^{-\frac{1}{2}}, \\ 0, & |x| > \beta^{-\frac{1}{2}}. \end{cases}$
2. Let us consider the double well potential with Hamiltonian $H = \frac{p_x^2}{2m} + \frac{1}{2}m\frac{1}{4}\omega_0^2 a^2 \left(\frac{x^2}{a^2} - 1\right)^2$
   (a) Using $\psi_1 = \left(\frac{2\beta}{\pi}\right)^{1/4} \exp\left(-\beta(x-a)^2\right)$, find $E_1(\beta) = \langle\psi_1| H |\psi_1\rangle$. Minimizing $E_1(\beta)$ is in general cumbersome, but show that for large a, the minimum is given by $\beta_* = \frac{m\omega_0}{2\hbar}$. Find $E_1(\beta_*)$ and comment on your result.
   (b) Use now instead $\psi_2 = A\left[\exp\left(-\beta(x-a)^2\right) + \exp\left(-\beta(x+a)^2\right)\right]$. Find the normalization constant A. Evaluate $E_2(\beta) = \langle\psi_2| H |\psi_2\rangle$. Minimizing E_2 in this case is hopeless to do analytically. However, by using the above value $\beta_* = \frac{m\omega_0}{2\hbar}$, find the difference $E_2(\beta_*) - E_1(\beta_*)$ in the limit of large a and comment on your result.

Solution. 1. (a) Notice that

$$|\psi_a\rangle = \langle\psi_a| = \left(\frac{2\beta}{\pi}\right)^{\frac{1}{4}} \mathrm{e}^{-\beta x^2}.$$

Computing the energy, we have

$$\begin{aligned}
E(\beta) &= \langle\psi_a|H|\psi_a\rangle \\
&= \int_{-\infty}^{\infty} \psi_a^* H \psi_a \, \mathrm{d}x \\
&= \int_{-\infty}^{\infty} \left(\frac{2\beta}{\pi}\right)^{\frac{1}{4}} \mathrm{e}^{-\beta x^2} \left(\frac{p_x^2}{2m} + \frac{1}{2} m\omega_0^2 x^2\right) \left(\frac{2\beta}{\pi}\right)^{\frac{1}{4}} \mathrm{e}^{-\beta x^2} \, \mathrm{d}x \\
&= \frac{1}{2}\left(\frac{2\beta}{\pi}\right)^{\frac{1}{2}} \left[\frac{1}{m}\int_{-\infty}^{\infty} \mathrm{e}^{-\beta x^2} \left(p_x^2\right) \mathrm{e}^{-\beta x^2} \, \mathrm{d}x + m\omega_0^2 \int_{-\infty}^{\infty} \mathrm{e}^{-\beta x^2} \left(x^2\right) \mathrm{e}^{-\beta x^2} \, \mathrm{d}x\right] \\
&= \frac{1}{2}\left(\frac{2\beta}{\pi}\right)^{\frac{1}{2}} \left[-\frac{\hbar^2}{m}\int_{-\infty}^{\infty} \mathrm{e}^{-\beta x^2} \frac{\partial^2}{\partial x^2}\left(\mathrm{e}^{-\beta x^2}\right) \mathrm{d}x + m\omega_0^2 \int_{-\infty}^{\infty} x^2 \mathrm{e}^{-2\beta x^2} \, \mathrm{d}x\right] \\
&= \frac{1}{2}\left(\frac{2\beta}{\pi}\right)^{\frac{1}{2}} \left[-\frac{\hbar^2}{m}\int_{-\infty}^{\infty} \mathrm{e}^{-\beta x^2} \left(2\beta(2\beta x^2 - 1)\mathrm{e}^{-\beta x^2}\right) \mathrm{d}x + m\omega_0^2 \left(\frac{\sqrt{\pi}}{2^{\frac{5}{2}}\beta^{\frac{3}{2}}}\right)\right] \\
&= \frac{1}{2}\left(\frac{2\beta}{\pi}\right)^{\frac{1}{2}} \left[-\frac{2\beta\hbar^2}{m}\int_{-\infty}^{\infty} \left(2\beta x^2 - 1\right) \mathrm{e}^{-2\beta x^2} \, \mathrm{d}x + \frac{m\omega_0^2\sqrt{\pi}}{2^{\frac{5}{2}}\beta^{\frac{3}{2}}}\right] \\
&= \frac{1}{2}\left(\frac{2\beta}{\pi}\right)^{\frac{1}{2}} \left[-\frac{2\beta\hbar^2}{m}\left(-\frac{\sqrt{\pi}}{2^{\frac{3}{2}}\sqrt{\beta}}\right) + \frac{m\omega_0^2\sqrt{\pi}}{2^{\frac{5}{2}}\beta^{\frac{3}{2}}}\right] \\
&= \frac{1}{2}\left(\frac{2\beta}{\pi}\right)^{\frac{1}{2}} \left[\frac{\hbar^2\sqrt{\beta\pi}}{\sqrt{2}m} + \frac{m\omega_0^2\sqrt{\pi}}{2^{\frac{5}{2}}\beta^{\frac{3}{2}}}\right] \\
&= \frac{\hbar^2\beta}{2m} + \frac{m\omega_0^2}{8\beta}.
\end{aligned}$$

Now, we minimize the energy by setting its derivative with respect to β to 0. We have

$$\begin{aligned}
\frac{\partial E}{\partial \beta} &= 0 \\
\frac{\partial}{\partial \beta}\left(\frac{\hbar^2\beta}{2m} + \frac{m\omega_0^2}{8\beta}\right) &= 0 \\
\frac{\hbar^2}{2m} - \frac{m\omega_0^2}{8\beta^2} &= 0 \\
\beta^2 &= \frac{m^2\omega_0^2}{4\hbar^2} \\
\beta &= \pm\sqrt{\frac{m^2\omega_0^2}{4\hbar^2}} \quad (-\text{rejected}) \\
\beta &= \frac{m\omega_0}{2\hbar} \equiv \beta_*.
\end{aligned}$$

Then, β_* is the variational parameter that minimizes the energy. The minimum value of the energy is then

$$\begin{aligned}
E(\beta_*) &= \frac{\hbar^2\beta_*}{2m} + \frac{m\omega_0^2}{8\beta_*} \\
&= \frac{\hbar^2}{2m}\left(\frac{m\omega_0}{2\hbar}\right) + \frac{m\omega_0^2}{8}\left(\frac{2\hbar}{m\omega_0}\right) \\
&= \frac{\hbar\omega_0}{4} + \frac{\hbar\omega_0}{4} \\
&= \frac{\hbar\omega_0}{2}.
\end{aligned}$$

Therefore, for $\psi_a(x,\beta)$, the energy E and its minimum value are

$$E(\beta) = \frac{\hbar^2\beta}{2m} + \frac{m\omega_0^2}{8\beta}, \qquad E(\beta_*) = \frac{\hbar\omega_0}{2}.$$

(b) Computing the energy, we have

$$\begin{aligned}
E(\beta) &= \langle \psi_b | H | \psi_b \rangle \\
&= \int_{-\infty}^{\infty} \psi_b^* H \psi_b \,\mathrm{d}x \\
&= \int_{-\beta^{-\frac{1}{2}}}^{\beta^{-\frac{1}{2}}} \psi_b^* H \psi_b \,\mathrm{d}x \\
&= 2\int_{0}^{\beta^{-\frac{1}{2}}} \psi_b^* H \psi_b \,\mathrm{d}x \\
&= 2\int_{0}^{\beta^{-\frac{1}{2}}} \left(\frac{15}{16}\right)^{\frac{1}{2}} \beta^{\frac{1}{4}} \left(1-\beta x^2\right) \left(\frac{p_x^2}{2m} + \frac{1}{2}m\omega_0^2 x^2\right) \left(\frac{15}{16}\right)^{\frac{1}{2}} \beta^{\frac{1}{4}} \left(1-\beta x^2\right) \mathrm{d}x \\
&= \frac{15\sqrt{\beta}}{8}\left[\int_{0}^{\beta^{-\frac{1}{2}}} \left(1-\beta x^2\right)\left(\frac{p_x^2}{2m}\right)\left(1-\beta x^2\right)\mathrm{d}x + \int_{0}^{\beta^{-\frac{1}{2}}} \left(\frac{1}{2}m\omega_0^2 x^2\right)\left(1-\beta x^2\right)^2 \mathrm{d}x\right] \\
&= \frac{15\sqrt{\beta}}{8}\left[-\frac{\hbar^2}{2m}\int_{0}^{\beta^{-\frac{1}{2}}} \left(1-\beta x^2\right)\frac{\partial^2}{\partial x^2}\left(1-\beta x^2\right)\mathrm{d}x + \frac{1}{2}m\omega_0^2\int_{0}^{\beta^{-\frac{1}{2}}} x^2\left(1-\beta x^2\right)^2 \mathrm{d}x\right] \\
&= \frac{15\sqrt{\beta}}{8}\left[-\frac{\hbar^2}{2m}\int_{0}^{\beta^{-\frac{1}{2}}} \left(1-\beta x^2\right)\left(-2\beta\right)\mathrm{d}x + \frac{1}{2}m\omega_0^2\int_{0}^{\beta^{-\frac{1}{2}}} x^2\left(1-\beta x^2\right)^2 \mathrm{d}x\right] \\
&= \frac{15\sqrt{\beta}}{8}\left[-\frac{\hbar^2}{2m}\left(-\frac{4\sqrt{\beta}}{3}\right) + \frac{1}{2}m\omega_0^2\left(\frac{8}{105\beta^{\frac{3}{2}}}\right)\right] \\
&= \frac{15\sqrt{\beta}}{8}\left[\frac{2\sqrt{\beta}\hbar^2}{3m} + \frac{4m\omega_0^2}{105\beta^{\frac{3}{2}}}\right] \\
&= \frac{5\beta\hbar^2}{4m} + \frac{m\omega_0^2}{14\beta}.
\end{aligned}$$

Now, we minimize the energy by setting its derivative with respect to β to 0. We have

$$\begin{aligned}
\frac{\partial E}{\partial \beta} &= 0 \\
\frac{\partial}{\partial \beta}\left(\frac{5\beta\hbar^2}{4m} + \frac{1m\omega_0^2}{14\beta}\right) &= 0 \\
\frac{5\hbar^2}{4m} - \frac{m\omega_0^2}{14\beta^2} &= 0 \\
\beta^2 &= \frac{4m^2\omega_0^2}{70\hbar^2} \\
\beta &= \pm\sqrt{\frac{4m^2\omega_0^2}{70\hbar^2}} \quad (-\text{rejected}) \\
\beta &= \sqrt{\frac{2}{35}}\frac{m\omega_0}{\hbar} \equiv \beta_*.
\end{aligned}$$

Then, β_* is the variational parameter that minimizes the energy. The minimum value of the energy is then

$$\begin{aligned}
E(\beta_*) &= \frac{\hbar^2\beta_*}{2m} + \frac{m\omega_0^2}{8\beta_*} \\
&= \frac{\hbar^2}{2m}\left(\sqrt{\frac{2}{35}}\frac{m\omega_0}{\hbar}\right) + \frac{m\omega_0^2}{8}\left(\sqrt{\frac{35}{2}}\frac{\hbar}{m\omega_0}\right) \\
&= \left(\sqrt{\frac{1}{70}} + \sqrt{\frac{35}{128}}\right)\hbar\omega_0
\end{aligned}$$

Therefore, for $\psi_a(x,\beta)$, the energy E and its minimum value are

$$E(\beta) = \frac{5\beta\hbar^2}{4m} + \frac{m\omega_0^2}{14\beta}, \qquad E(\beta_*) = \left(\sqrt{\frac{1}{70}} + \sqrt{\frac{35}{128}}\right)\hbar\omega_0.$$

2. Considering the Hamiltonian

$$H = \frac{p_x^2}{2m} + \frac{1}{8}m\omega_0^2 a^2\left(\frac{x^2}{a^2} - 1\right)^2.$$

(a) Computing the energy, we have

$$\begin{aligned}
E(\beta) &= \langle\psi_1|H|\psi_1\rangle \\
&= \int_{-\infty}^{\infty}\psi_1^* H\psi_1\,\mathrm{d}x \\
&= \int_{-\infty}^{\infty}\left(\frac{2\beta}{\pi}\right)^{\frac{1}{4}}\mathrm{e}^{-\beta(x-a)^2}\left(\frac{p_x^2}{2m} + \frac{1}{8}m\omega_0^2a^2\left(\frac{x^2}{a^2}-1\right)^2\right)\left(\frac{2\beta}{\pi}\right)^{\frac{1}{4}}\mathrm{e}^{-\beta(x-a)^2}\,\mathrm{d}x \\
&= \left(\frac{2\beta}{\pi}\right)^{\frac{1}{2}}\left[\frac{1}{2m}\int_{-\infty}^{\infty}\mathrm{e}^{-\beta(x-a)^2}\left(p_x^2\right)\mathrm{e}^{-\beta(x-a)^2}\,\mathrm{d}x + \frac{1}{8}m\omega_0^2a^2\int_{-\infty}^{\infty}\mathrm{e}^{-\beta(x-a)^2}\left(\frac{x^2}{a^2}-1\right)^2\mathrm{e}^{-\beta(x-a)^2}\,\mathrm{d}x\right] \\
&= \left(\frac{2\beta}{\pi}\right)^{\frac{1}{2}}\left[-\frac{\hbar^2}{2m}\int_{-\infty}^{\infty}\mathrm{e}^{-\beta(x-a)^2}\frac{\partial^2}{\partial x^2}\left(\mathrm{e}^{-\beta(x-a)^2}\right)\mathrm{d}x + \frac{1}{8}m\omega_0^2a^2\int_{-\infty}^{\infty}\left(\frac{x^2}{a^2}-1\right)^2\mathrm{e}^{-2\beta(x-a)^2}\,\mathrm{d}x\right] \\
&= \left(\frac{2\beta}{\pi}\right)^{\frac{1}{2}}\left[-\frac{\hbar^2}{2m}\int_{-\infty}^{\infty}\left(4\beta^2\left(x-a\right)^2 - 2\beta\right)\mathrm{e}^{-2\beta(x-a)^2}\,\mathrm{d}x + \frac{1}{8}m\omega_0^2a^2\left(\frac{\sqrt{\pi}\left(16a^2\beta+3\right)}{2^{\frac{9}{2}}a^4\beta^{\frac{5}{2}}}\right)\right] \\
&= \left(\frac{2\beta}{\pi}\right)^{\frac{1}{2}}\left[-\frac{\hbar^2}{2m}\int_{-\infty}^{\infty}\left(2\beta x^2 - 1\right)\mathrm{e}^{-2\beta x^2}\,\mathrm{d}x + \frac{m\omega_0^2\sqrt{\pi}\left(16a^2\beta+3\right)}{2^{\frac{15}{2}}a^2\beta^{\frac{5}{2}}}\right] \\
&= \left(\frac{2\beta}{\pi}\right)^{\frac{1}{2}}\left[-\frac{\hbar^2}{2m}\left(-\frac{\sqrt{\pi\beta}}{\sqrt{2}}\right) + \frac{m\omega_0^2\sqrt{\pi}\left(16a^2\beta+3\right)}{2^{\frac{15}{2}}a^2\beta^{\frac{5}{2}}}\right] \\
&= \left(\frac{2\beta}{\pi}\right)^{\frac{1}{2}}\left[\frac{\hbar^2\sqrt{\beta\pi}}{2\sqrt{2}m} + \frac{m\omega_0^2\sqrt{\pi}\left(16a^2\beta+3\right)}{2^{\frac{15}{2}}a^2\beta^{\frac{5}{2}}}\right] \\
&= \left(\frac{2\beta}{\pi}\right)^{\frac{1}{2}}\left[\frac{\hbar^2\sqrt{\beta\pi}}{2\sqrt{2}m} + \frac{m\omega_0^2\sqrt{\pi}}{2^{\frac{7}{2}}\beta^{\frac{3}{2}}} + \frac{3m\omega_0^2\sqrt{\pi}}{2^{\frac{15}{2}}a^2\beta^{\frac{5}{2}}}\right] \\
&= \frac{\hbar^2\beta}{2m} + \frac{m\omega_0^2}{8\beta} + \frac{3m\omega_0^2}{2^7a^2\beta^2}.
\end{aligned}$$

For large a, the last term will tend to zero, and then

$$E(\beta) = \frac{\hbar^2\beta}{2m} + \frac{m\omega_0^2}{8\beta}.$$

Now, we minimize the energy by setting its derivative with respect to β to 0. We have

$$\begin{aligned}
\frac{\partial E}{\partial \beta} &= 0 \\
\frac{\partial}{\partial \beta}\left(\frac{\hbar^2 \beta}{2m} + \frac{m\omega_0^2}{8\beta}\right) &= 0 \\
\frac{\hbar^2}{2m} - \frac{m\omega_0^2}{8\beta^2} &= 0 \\
\beta^2 &= \frac{m^2\omega_0^2}{4\hbar^2} \\
\beta &= \pm\sqrt{\frac{m^2\omega_0^2}{4\hbar^2}} \quad (-\text{rejected}) \\
\beta &= \frac{m\omega_0}{2\hbar} \equiv \beta_*.
\end{aligned}$$

Then, β_* is the variational parameter that minimizes the energy. The minimum value of the energy is then

$$\begin{aligned}
E(\beta_*) &= \frac{\hbar^2\beta_*}{2m} + \frac{m\omega_0^2}{8\beta_*} + \frac{3m\omega_0^2}{2^7a^2\beta_*^2} \\
&= \frac{\hbar^2}{2m}\frac{m\omega_0}{2\hbar} + \frac{m\omega_0^2}{8}\frac{2\hbar}{m\omega_0} + \frac{3m\omega_0^2}{2^7a^2}\left(\frac{2\hbar}{m\omega_0}\right)^2 \\
&= \frac{\hbar\omega_0}{4} + \frac{\hbar\omega_0}{4} + \frac{3\hbar^2}{2^5m}\frac{1}{a^2} \\
&= \frac{\hbar\omega_0}{2} + \frac{3\hbar^2}{2^5m}\frac{1}{a^2}.
\end{aligned}$$

Therefore, for $\psi_a(x,\beta)$, the energy E and its minimum value are

$$E(\beta) = \frac{\hbar^2\beta}{2m} + \frac{m\omega_0^2}{8\beta} + \frac{3m\omega_0^2}{2^7a^2\beta^2}, \qquad E(\beta_*) = \frac{\hbar\omega_0}{2} + \frac{3\hbar^2}{2^5m}\frac{1}{a^2}.$$

(b) We have

$$\psi_2 = A\left(\mathrm{e}^{-\beta(x-a)^2} + \mathrm{e}^{-\beta(x+a)^2}\right).$$

Normalizing, we have

$$\begin{aligned}
\int_{-\infty}^{\infty} \left|\psi_2^2\right| \mathrm{d}x &= 1 \\
|A|^2 \int_{-\infty}^{\infty} \left(\mathrm{e}^{-\beta(x-a)^2} + \mathrm{e}^{-\beta(x+a)^2}\right)^2 \mathrm{d}x &= 1 \\
|A|^2 \int_{-\infty}^{\infty} \left(\mathrm{e}^{-2\beta(x-a)^2} + 2\mathrm{e}^{-2\beta(x^2+a^2)} + \mathrm{e}^{-2\beta(x+a)^2}\right) \mathrm{d}x &= 1 \\
|A|^2 \left(\frac{\sqrt{2\pi}\,\mathrm{e}^{-2a^2\beta}\left(\mathrm{e}^{2a^2\beta}+1\right)}{\sqrt{\beta}}\right) &= 1 \\
|A|^2 &= \sqrt{\frac{\beta}{2\pi}}\frac{1}{1+\mathrm{e}^{-2a^2\beta}} \\
A &= \left(\frac{\beta}{2\pi}\right)^{\frac{1}{4}} \frac{1}{\left(1+\mathrm{e}^{-2a^2\beta}\right)^{\frac{1}{2}}}.
\end{aligned}$$

Replacing, we have

$$\psi_2 = \left(\frac{\beta}{2\pi}\right)^{\frac{1}{4}} \frac{1}{\left(1+\mathrm{e}^{-2a^2\beta}\right)^{\frac{1}{2}}} \left(\mathrm{e}^{-\beta(x-a)^2} + \mathrm{e}^{-\beta(x+a)^2}\right).$$

Computing the energy, we have

$$\begin{aligned}
E(\beta) &= \langle\psi_2|H|\psi_2\rangle \\
&= \int_{-\infty}^{\infty} \psi_2^* H \psi_2 \,\mathrm{d}x \\
&= \sqrt{\frac{\beta}{2\pi}} \frac{1}{1+\mathrm{e}^{-2a^2\beta}} \int_{-\infty}^{\infty} \left(\mathrm{e}^{-\beta(x-a)^2} + \mathrm{e}^{-\beta(x+a)^2}\right) \left(\frac{p_x^2}{2m} + \frac{1}{8} m\omega_0^2 a^2 \left(\frac{x^2}{a^2} - 1\right)\right)^2 \left(\mathrm{e}^{-\beta(x-a)^2} + \mathrm{e}^{-\beta(x+a)^2}\right) \mathrm{d}x \\
&= \sqrt{\frac{\beta}{2\pi}} \frac{1}{1+\mathrm{e}^{-2a^2\beta}} \left[\int_{-\infty}^{\infty} \left(\mathrm{e}^{-\beta(x-a)^2} + \mathrm{e}^{-\beta(x+a)^2}\right) \left(\frac{p_x^2}{2m}\right) \left(\mathrm{e}^{-\beta(x-a)^2} + \mathrm{e}^{-\beta(x+a)^2}\right) \mathrm{d}x\right. \\
&\quad \left. + \int_{-\infty}^{\infty} \left(\mathrm{e}^{-\beta(x-a)^2} + \mathrm{e}^{-\beta(x+a)^2}\right) \left(\frac{1}{8} m\omega_0^2 a^2 \left(\frac{x^2}{a^2} - 1\right)\right) \left(\mathrm{e}^{-\beta(x-a)^2} + \mathrm{e}^{-\beta(x+a)^2}\right) \mathrm{d}x\right] \\
&= \sqrt{\frac{\beta}{2\pi}} \frac{1}{1+\mathrm{e}^{-2a^2\beta}} \left[-\frac{\hbar^2}{2m} \int_{-\infty}^{\infty} \left(\mathrm{e}^{-\beta(x-a)^2} + \mathrm{e}^{-\beta(x+a)^2}\right) \frac{\partial^2}{\partial x^2} \left(\mathrm{e}^{-\beta(x-a)^2} + \mathrm{e}^{-\beta(x+a)^2}\right) \mathrm{d}x\right. \\
&\quad \left. + \frac{1}{8} m\omega_0^2 a^2 \int_{-\infty}^{\infty} \left(\mathrm{e}^{-\beta(x-a)^2} + \mathrm{e}^{-\beta(x+a)^2}\right) \left(\frac{x^2}{a^2} - 1\right) \left(\mathrm{e}^{-\beta(x-a)^2} + \mathrm{e}^{-\beta(x+a)^2}\right) \mathrm{d}x\right] \\
&= \sqrt{\frac{\beta}{2\pi}} \frac{1}{1+\mathrm{e}^{-2a^2\beta}} \\
&\quad \left[-\frac{\hbar^2}{2m} \int_{-\infty}^{\infty} \left(\mathrm{e}^{-\beta(x-a)^2} + \mathrm{e}^{-\beta(x+a)^2}\right) 2\beta \mathrm{e}^{-2\beta\left(x^2+a^2\right)} \left(2\beta (x-a)^2 - 1\right) \mathrm{e}^{\beta(x+a)^2} \,\mathrm{d}x\right. \\
&\quad - \frac{\hbar^2}{2m} \int_{-\infty}^{\infty} \left(\mathrm{e}^{-\beta(x-a)^2} + \mathrm{e}^{-\beta(x+a)^2}\right) 2\beta \mathrm{e}^{-2\beta\left(x^2+a^2\right)} \left(2\beta (x+a)^2 - 1\right) \mathrm{e}^{\beta(x-a)^2} \,\mathrm{d}x \\
&\quad \left. + \frac{1}{8} m\omega_0^2 a^2 \int_{-\infty}^{\infty} \left(\frac{x^2}{a^2} - 1\right) \left(\mathrm{e}^{-\beta(x-a)^2} + \mathrm{e}^{-\beta(x+a)^2}\right)^2 \mathrm{d}x\right] \\
&= \sqrt{\frac{\beta}{2\pi}} \frac{1}{1+\mathrm{e}^{-2a^2\beta}} \\
&\quad \left[-\frac{\hbar^2}{2m} \left(-\frac{\sqrt{\pi}\sqrt{\beta}}{\sqrt{2}} + \frac{\sqrt{\pi}\sqrt{\beta}\left(4a^2\beta - 1\right)\mathrm{e}^{-2a^2\beta}}{\sqrt{2}}\right)\right. \\
&\quad - \frac{\hbar^2}{2m} \left(\frac{\sqrt{\pi}\sqrt{\beta}\left(4a^2\beta - 1\right)\mathrm{e}^{-2a^2\beta}}{\sqrt{2}} - \frac{\sqrt{\pi}\sqrt{\beta}}{\sqrt{2}}\right) \\
&\quad \left. + \frac{1}{8} m\omega_0^2 a^2 \left[\frac{\sqrt{\pi}}{2^{\frac{5}{2}} a^2 \beta^{\frac{3}{2}}} + - \frac{\sqrt{\pi}\left(8a^2\beta - 1\right)\mathrm{e}^{-4a^2\beta}}{4a^2\beta^{\frac{3}{2}}} + \frac{\sqrt{\pi}}{2^{\frac{5}{2}} a^2 \beta^{\frac{3}{2}}}\right]\right] \\
&= \sqrt{\frac{\beta}{2\pi}} \frac{1}{1+\mathrm{e}^{-2a^2\beta}} \left[\left[-\frac{\hbar^2}{m} \sqrt{\frac{\pi\beta}{2}} \mathrm{e}^{-2a^2\beta} \left(\left(4a^2\beta - 1\right)\mathrm{e}^{-2a^2\beta} - 1\right)\right]\right. \\
&\quad \left. + m\omega_0^2 \left[\frac{\sqrt{\pi}}{2^{\frac{11}{2}} \beta^{\frac{3}{2}}} + - \frac{\sqrt{\pi}\left(8\beta - 1\right)\mathrm{e}^{-4a^2\beta}}{32\beta^{\frac{3}{2}}} + \frac{\sqrt{\pi}}{2^{\frac{11}{2}} \beta^{\frac{3}{2}}}\right]\right] \\
&= \frac{1}{1+\mathrm{e}^{-2a^2\beta}} \left[\left[-\frac{\hbar^2\beta}{m} \mathrm{e}^{-2a^2\beta} \left(\left(4a^2\beta - 1\right)\mathrm{e}^{-2a^2\beta} - 1\right)\right] + \frac{m\omega_0^2}{32\beta} \left[1 + - \frac{\left(8\beta - 1\right)\mathrm{e}^{-4a^2\beta}}{\sqrt{2}}\right]\right] \\
&= \frac{\hbar^2\beta}{m} \left(1 - 2a^2\beta\right) + \frac{m\omega_0^2}{8} \left(a^2 + \frac{1}{2\beta}\right),
\end{aligned}$$

where, for large a, we take $\frac{1}{a}, \mathrm{e}^{-a^2} \to 0$.
By using the value for $\beta_* = \frac{m\omega_0}{2\hbar}$ from part 1, we minimize E_2

$$\begin{aligned}
E_2(\beta_*) &= \frac{\hbar^2\beta_*}{m}\left(1 - 2a^2\beta_*\right) + \frac{m\omega_0^2}{8}\left(a^2 + \frac{1}{2\beta_*}\right)\\
&= \frac{\hbar^2}{m}\left(\frac{m\omega_0}{2\hbar}\right)\left(1 - 2a^2\frac{m\omega_0}{2\hbar}\right) + \frac{m\omega_0^2}{8}\left(a^2 + \frac{1}{2}\left(\frac{2\hbar}{m\omega_0}\right)\right)\\
&= \frac{\hbar\omega_0}{2} + \frac{m\omega_0^2 a^2}{2} + \frac{m\omega_0^2 a^2}{8} + \frac{\hbar\omega_0}{8}\\
&= \frac{5\hbar\omega_0}{8} + \frac{3m\omega_0^2 a^2}{8}.
\end{aligned}$$

In the limit of large a, the difference of the energies is then

$$\begin{aligned}
E_2(\beta_*) - E_1(\beta_*) &= \frac{5\hbar\omega_0}{8} + \frac{3m\omega_0^2 a^2}{8} - \frac{\hbar\omega_0}{2}\\
&= \frac{\hbar\omega_0}{8} + \frac{3m\omega_0^2 a^2}{8}\\
&= \frac{1}{8}\left(\hbar\omega_0 + \frac{3}{m}\omega_0^2 a^2\right).
\end{aligned}$$

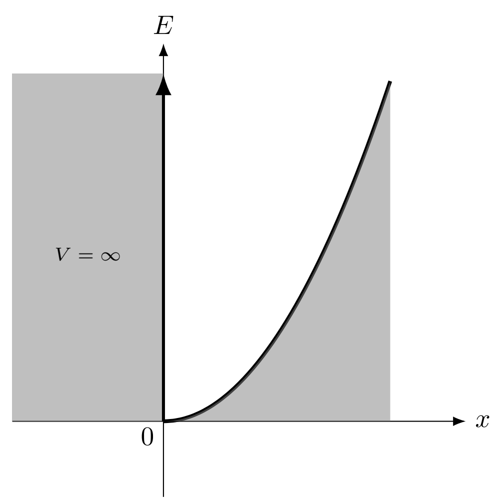
■

Problem 2 - WKB Approximation
Consider a 1D potential

$$V(x) = \begin{cases} \infty, & x < 0,\\ \frac{1}{2}m\omega_0^2 x^2, & x > 0, \end{cases}$$

i.e. a harmonic trap interrupted by a hard wall. By using the WKB approximation, find the bound state energies.

Solution. The 1D potential given is as follows



The momentum is given by $p(x) = \sqrt{2m(E - V(x))} = \sqrt{2m\left(E - \frac{1}{2}m\omega_0^2 x^2\right)}$.

We proceed by finding the turning points. In this case, we only need to find the right turning point. Additionally, the potential is equal to the energy at the turning point. Thus, we have

$$\begin{aligned} V(x) = \frac{1}{2}m\omega_0^2 x^2 &= E \\ \implies x^2 &= \frac{2E}{m\omega_0^2} \\ x &= \pm\sqrt{\frac{2E}{m\omega_0^2}}. \end{aligned}$$

Since $x > 0$, then we reject the negative solution, and we have that $x_1 = 0$ and $x_2 = \sqrt{\frac{2E}{m\omega_0^2}}$. The momentum can then be written as

$$\begin{aligned} p(x) &= \sqrt{2m\left(E - \frac{1}{2}m\omega_0^2 x^2\right)} \\ &= \sqrt{2m\left(\frac{1}{2}m\omega_0^2 x_{2,1}^2 - \frac{1}{2}m\omega_0^2 x^2\right)} \\ &= m\omega\sqrt{(x_2^2 - x^2)}. \end{aligned}$$

Integrating the momentum over the turning points, we get

$$\begin{aligned} \int_a^b p(x')\,\mathrm{d}x' &= m\omega_0 \int_{x_1}^{x_2} \sqrt{x_2^2 - x'^2}\,\mathrm{d}x' \\ &= m\omega_0 \int_0^{x_2} \sqrt{1 - \frac{x'^2}{x_2^2}}\,\mathrm{d}x' \\ &= \frac{\pi m\omega_0 x_2}{4}. \end{aligned}$$

Additionally, we know that

$$\frac{1}{\hbar}\int_b^a p(x')\,\mathrm{d}x = \left(n + \frac{3}{4}\right)\pi \leq 0,$$

then

$$\begin{aligned} \frac{1}{\hbar}\frac{\pi m\omega_0 x_2}{4} &= \left(n + \frac{3}{4}\right)\pi \\ \frac{1}{\hbar}\frac{\pi m\omega_0}{4}\left(\frac{2E}{m\omega_0^2}\right) &= \left(n + \frac{3}{4}\right)\pi \\ m\omega_0\left(\frac{2E}{m\omega_0^2}\right) &= (4n+3)\,\hbar \\ E &= \left(2n + \frac{3}{2}\right)\hbar\omega_0. \end{aligned}$$

■

Problem 3 - Wave Function Normalization in Perturbation Theory
In the lectures we chose the perturbed state $|n\rangle$ (with energy E_n) to be such that $\langle n^{(0)}|n\rangle = 1$. Let us define a normalized perturbed state $|n\rangle_N = Z_n^{\frac{1}{2}}|n\rangle$ (see lecture notes Sec. 2.1.1) which satisfies ${}_N\langle n|n\rangle_N = 1$. Show that

$$Z_n = \frac{\partial E_n}{\partial E_n^{(0)}}$$

where $E_n^{(0)}$ is the energy of the unperturbed state $|n^{(0)}\rangle$.

Solution. The Brillouin-Wigner expansion is given by

$$|n\rangle = \left|n^{(0)}\right\rangle + \sum_{p=0}^{\infty}\left(\frac{\phi_n}{E_n - H_0}\lambda V\right)^p \left|n^{(0)}\right\rangle,$$

where the energy E_n is

$$E_n = E_n^{(0)} + \lambda\sum_{p=0}^{\infty}\left\langle n^{(0)}\middle|V\left(\frac{\phi_n}{En - H_0}\lambda V\right)^p\middle|n^{(0)}\right\rangle.$$

Let $|n\rangle_N = \sqrt{Z_n}|n\rangle$ be the normalized perturbed state. By normalization, we have

$${}_N\langle n|n\rangle_N = Z_n\langle n|n\rangle = 1 \implies \langle n|n\rangle = \frac{1}{Z_n}.$$

Computing the inner product using Brillouin-Wigner up to the second-order, we have

$$\begin{aligned}
\langle n|n\rangle &= \left(\left\langle n^{(0)}\right| + \left\langle n^{(0)}\right|\frac{\phi_n}{E_n - H_0}\lambda V\right)\left(\left|n^{(0)}\right\rangle + \lambda V\frac{\phi_n}{E_n - H_0}\left|n^{(0)}\right\rangle\right) \\
&= \left\langle n^{(0)}\middle|n^{(0)}\right\rangle + \lambda\left\langle n^{(0)}\middle|\frac{\phi_n}{E_n - H_0}V\middle|n^{(0)}\right\rangle + \lambda\left\langle n^{(0)}\middle|V\frac{\phi_n}{E_n - H_0}\middle|n^{(0)}\right\rangle + \lambda^2\left\langle n^{(0)}\middle|V\frac{\phi_n^2}{E_n - H_0)^2}V\middle|n^{(0)}\right\rangle \\
&= 1 + \sum_{k\neq n}\frac{\lambda^2|V_{kn}|^2}{(E_n - E_n^{(0)})^2}.
\end{aligned}$$

Thus,

$$Z_n = \left(1 + \lambda^2\sum_{k\neq n}\frac{|V_{kn}|^2}{(E_n - E_n^{(0)})^2}\right)^{-1}$$

Using the sum of a geometric series formula, we can see that

$$Z_n = 1 - \lambda^2\sum_{k\neq n}\frac{|V_{kn}|^2}{(E_n - E_n^{(0)})^2}$$

Computing the energy up tot he second-order, we have

$$\begin{aligned}
E_n &= E_n^{(0)} + \lambda^2\left\langle n^{(0)}\middle|V\frac{\phi_n}{E_n - H - 0}V\middle|n^{(0)}\right\rangle \\
&= E_n^{(0)} + \lambda^2\sum_{k\neq n}\frac{|V_{nk}|^2}{E_n - E_n^{(0)}}.
\end{aligned}$$

Taking the derivative, we get

$$\frac{\partial E_n}{\partial E_n^{(0)}} = 1 - \lambda^2\sum_{k\neq n}\frac{|V_{kn}|^2}{(E_n - E_n^{(0)})^2} = Z_n.$$

■

Homework 4

Problem 1 - Harmonic Oscillator Wave Functions in the WKB Approximation
In the lecture we calculated the energy of the 1D harmonic oscillator [potential $V(x) = \frac{1}{2}m\omega_0^2 x^2$] in the WKB approximation. Compare numerically the WKB wave function $\psi_n^{(\mathrm{WKB})}(0)$ at the origin to the exact harmonic oscillator wave function for $n = 0, 1, 2, \ldots, 8$. Interpret your results. The WKB wave function is normalized as follows (no need to prove that this is the correct normalization): in the classically allowed region $\psi^{(\mathrm{WKB})}(x) = \frac{A}{\sqrt{p(x)}} \cos\left(\frac{1}{\hbar}\int_b^x \mathrm{d}x' p(x') - \frac{\pi}{4}\right)$ has $A^2 = \left[\int_b^a \frac{1}{2p(x)}\,\mathrm{d}x\right]^{-1}$ where a and b are the turning points.

Solution. The WKB wave function in the classically allowed region is given by

$$\psi^{(\mathrm{WKB})}(x) = \frac{A}{\sqrt{p(x)}} \cos\left(\frac{1}{\hbar}\int_b^x p(x')\,\mathrm{d}x' - \frac{\pi}{4}\right),$$

where

$$A = \left[\int_b^a \frac{1}{2p(x)}\,\mathrm{d}x\right]^{-\frac{1}{2}}$$

is the normalization constant.

For the harmonic oscillator, we have

$$p(x) = \sqrt{2m\left(E - \frac{1}{2}m\omega_0^2 x^2\right)}.$$

We need to find the turning points for the harmonic oscillator. We know that, at the turning points, the potential is equal to the energy. Then

$$V(x_0) = \frac{1}{2}m\omega_0^2 x_0^2 = E \implies x_0 = \pm\sqrt{\frac{2E}{m\omega_0^2}},$$

$$\implies a = \sqrt{\frac{2E}{m\omega_0^2}} = x_0 \qquad \text{and} \qquad b = -\sqrt{\frac{2E}{m\omega_0^2}} = -x_0.$$

Notice that $b = -a$. By replacing in the normalization constant A, we get

$$
\begin{aligned}
A &= \left[\int_b^a \frac{1}{2p(x)}\,\mathrm{d}x\right]^{-\frac{1}{2}} \\
&= \left[\int_{-x_0}^{x_0} \frac{1}{2\sqrt{2m\left(E - \frac{1}{2}m\omega_0^2x^2\right)}}\,\mathrm{d}x\right]^{-\frac{1}{2}} \\
&= \left[\frac{1}{2}\int_{-x_0}^{x_0} \frac{1}{\sqrt{2mE - m^2\omega_0^2x^2}}\,\mathrm{d}x\right]^{-\frac{1}{2}} \\
&= \left[\frac{1}{2\sqrt{2mE}}\int_{-x_0}^{x_0} \frac{1}{\sqrt{1 - \frac{m\omega_0^2}{2E}x^2}}\,\mathrm{d}x\right]^{-\frac{1}{2}} \\
&= \left[\frac{1}{2\sqrt{2mE}}\int_{-x_0}^{x_0} \frac{1}{\sqrt{1 - \frac{x^2}{x_0^2}}}\,\mathrm{d}x\right]^{-\frac{1}{2}} \\
&= \left[\frac{1}{2\sqrt{2mE}}\left(x_0 \arcsin\left(\frac{x}{x_0}\right)\right)_{-x_0}^{x_0}\right]^{-\frac{1}{2}} \\
&= \left[\frac{\pi x_0}{2\sqrt{2mE}}\right]^{-\frac{1}{2}} \\
&= \left[\frac{\pi}{2\sqrt{2mE}}\sqrt{\frac{2E}{m\omega_0^2}}\right]^{-\frac{1}{2}} \\
&= \left[\frac{\pi}{2m\omega_0}\right]^{-\frac{1}{2}} \\
&= \sqrt{\frac{2m\omega_0}{\pi}}.
\end{aligned}
$$

By replacing in the wave function, we get

$$
\begin{aligned}
\psi^{(\mathrm{WKB})}(x) &= \frac{A}{\sqrt{p(x)}} \cos\left(\frac{1}{\hbar}\int_b^x p\left(x'\right) \mathrm{d}x' - \frac{\pi}{4}\right) \\
&= \sqrt{\frac{2m\omega_0}{\pi p(x)}} \cos\left[\frac{1}{\hbar}\int_{-x_0}^{x} \sqrt{2m\left(E - \frac{1}{2}m\omega_0^2 x'^2\right)} \mathrm{d}x' - \frac{\pi}{4}\right] \\
&= \sqrt{\frac{2m\omega_0}{\pi}} \left(2m\left(E - \frac{1}{2}m\omega_0^2 x^2\right)\right) \cos\left[\frac{\sqrt{2mE}}{\hbar}\int_{-x_0}^{x} \sqrt{1 - \frac{m\omega_0^2}{2E}x'^2} \,\mathrm{d}x' - \frac{\pi}{4}\right] \\
&= \sqrt{\frac{\omega_0}{\pi}} \left(\frac{4m}{2E - m\omega_0^2 x^2}\right)^{\frac{1}{4}} \cos\left[\frac{\sqrt{2mE}}{\hbar} \left.\frac{x_0 \arcsin\left(\frac{x'}{x_0}\right) + x'\sqrt{1 - \frac{x'^2}{x_0^2}}}{2}\right|_{-x_0}^{x} - \frac{\pi}{4}\right] \\
&= \sqrt{\frac{\omega_0}{\pi}} \left(\frac{4m}{2E - m\omega_0^2 x^2}\right)^{\frac{1}{4}} \cos\left[\frac{\sqrt{2mE}}{\hbar} \left(\frac{x_0 \arcsin\left(\frac{x}{x_0}\right) + x\sqrt{1 - \frac{x^2}{x_0^2}}}{2} + \frac{\pi}{4}x_0\right) - \frac{\pi}{4}\right] \\
&= \sqrt{\frac{\omega_0}{\pi}} \left(\frac{4m}{2E - m\omega_0^2 x^2}\right)^{\frac{1}{4}} \cos\left[\frac{\sqrt{2mE}}{\hbar}x_0 \left(\frac{\arcsin\left(\frac{x}{x_0}\right) + \frac{x}{x_0}\sqrt{1 - \frac{x^2}{x_0^2}}}{2} + \frac{\pi}{4}\right) - \frac{\pi}{4}\right] \\
&= \sqrt{\frac{\omega_0}{\pi}} \left(\frac{4m}{2E - m\omega_0^2 x^2}\right)^{\frac{1}{4}} \cos\left[\frac{E}{\omega_0\hbar} \left(\arcsin\left(\frac{x}{x_0}\right) + \frac{x}{x_0}\sqrt{1 - \frac{x^2}{x_0^2}} + \frac{\pi}{2}\right) - \frac{\pi}{4}\right] \\
&= \sqrt{\frac{\omega_0}{\pi}} \left(\frac{4m}{2E - m\omega_0^2 x^2}\right)^{\frac{1}{4}} \cos\left[\left(n + \frac{1}{2}\right) \left(\arcsin\left(\frac{x}{x_0}\right) + \frac{x}{x_0}\sqrt{1 - \frac{x^2}{x_0^2}} + \frac{\pi}{2}\right) - \frac{\pi}{4}\right] \\
&= \sqrt{\frac{\omega_0}{\pi}} \left(\frac{4m}{2E - m\omega_0^2 x^2}\right)^{\frac{1}{4}} \cos\left[\left(n + \frac{1}{2}\right) \left(\arcsin\left(\frac{x}{x_0}\right) + \frac{x}{x_0}\sqrt{1 - \frac{x^2}{x_0^2}} + \frac{\pi}{2}\right) - \frac{\pi}{4}\right].
\end{aligned}
$$

Recall that the exact harmonic oscillator wave function is given by

$$
\psi_n(x) = \frac{1}{\sqrt{2^n n!}} H_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right) \mathrm{e}^{-\frac{m\omega}{2\hbar}x^2},
$$

where H_n are the n-th order Hermite polynomials.
To find the error, we take the absolute difference of the functions. In particular, we do so for the origin at $x = 0$ and only consider values up to $n = 8$.
The exact wave function at $x = 0$ is

$$
\psi_n(0) = \frac{1}{\sqrt{2^n n!}} H_n(0)\mathrm{e}^0 = \frac{H_n(0)}{\sqrt{2^n n!}}.
$$

The WKB approximation of the wave function at $x = 0$ is

$$
\psi^{(\mathrm{WKB})}(0) = \sqrt{\frac{\omega_0}{\pi}} \left(\frac{2}{E}\right)^{\frac{1}{4}} \cos\left[\frac{\pi}{2}\left(n + \frac{1}{2}\right) - \frac{\pi}{4}\right].
$$

The error at $x = 0$ for each n is given by

$$
\text{Error} = \left|\psi_n(0) - \psi^{(\mathrm{WKB})}(0)\right|.
$$

- **For $\mathbf{n = 0}$:** Error $= 1 - \sqrt{\frac{2}{\pi}}$.
- **For $\mathbf{n = 1}$:** Error $= 0$.

- **For n = 2:** Error $= \frac{1}{\sqrt{2}} - \frac{1}{5^{\frac{1}{4}}}\sqrt{\frac{2}{\pi}}$.
- **For n = 3:** Error $= 0$.
- **For n = 4:** Error $= \frac{1}{2}\sqrt{\frac{3}{2}} - \frac{1}{9^{\frac{1}{4}}}\sqrt{\frac{2}{\pi}}$.
- **For n = 5:** Error $= 0$.
- **For n = 6:** Error $= \frac{\sqrt{5}}{4} - \frac{1}{13^{\frac{1}{4}}}\sqrt{\frac{2}{\pi}}$.
- **For n = 7:** Error $= 0$.
- **For n = 8:** Error $= \frac{1}{8}\sqrt{\frac{35}{2}} - \frac{1}{17^{\frac{1}{4}}}\sqrt{\frac{2}{\pi}}$.

For large n, we can see that the error decreases, which means that the WKB approximation better matches the exact wave function. ■

Problem 2 - Number of Bound States of a Potential
Consider the 1D potential $V(x) = V_0 \operatorname{sech}^2(x/a)$ with $V_0 < 0$.

(a) Find the bound state energies in the WKB approximation. What is the number of bound states as a function of V_0?

(b) For a generic 1 D potential $U(x)$, by using the WKB approximation, estimate the number of bound states. Does your result agree with the estimate you get from part 1 above? How about in the case of the harmonic potential?

Solution. (a) In the WKB approximation, the quantization condition for bound states is given by

$$\frac{1}{2\pi\hbar}\oint p(x)\,\mathrm{d}x = \left(n + \frac{1}{2}\right),$$

where a and b are the turning points such that

$$\oint p(x)\,\mathrm{d}x = 2\int_b^a p(x)\,\mathrm{d}x \qquad \text{and} \qquad p(x) = \sqrt{2m(E - V(x))}.$$

Finding the classical turning points, we have

$$V(x_\pm) = V_0 \operatorname{sech}^2\left(\frac{x_\pm}{a}\right) = E \implies x_\pm = \pm a \operatorname{sech}^{-1}\left(\sqrt{\frac{E}{V_0}}\right).$$

By replacing in the integrand of the above condition, we have

$$\begin{aligned}
\int_b^a p(x)\,\mathrm{d}x &= \int_{x_-}^{x_+} \sqrt{2m(E - V(x))}\,\mathrm{d}x \\
&= \int_{x_-}^{x_+} \sqrt{2m\left(E - V_0 \operatorname{sech}^2\left(\frac{x}{a}\right)\right)}\,\mathrm{d}x \\
&= 2\sqrt{2mE}\int_0^{x_+} \sqrt{1 - \frac{V_0}{E}\operatorname{sech}^2\left(\frac{x}{a}\right)}\,\mathrm{d}x.
\end{aligned}$$

Let $u = \operatorname{sech}^2\left(\frac{x}{a}\right) \implies \mathrm{d}u = -\frac{2}{a}\operatorname{sech}^2\left(\frac{x}{a}\right)\tanh\left(\frac{x}{a}\right)\mathrm{d}x = -\frac{2}{a}u\sqrt{1-u}$. The limits of integration become from 1 to $\frac{E}{V_0}$. Replacing, we have

$$\begin{aligned}
\int_b^a p(x)\,\mathrm{d}x &= 2\sqrt{2mE}\int_0^{x_+}\sqrt{1-\frac{V_0}{E}\operatorname{sech}^2\left(\frac{x}{a}\right)}\,\mathrm{d}x \\
&= -2\sqrt{2mE}\int_1^{\frac{E}{V_0}}\sqrt{1-\frac{V_0}{E}u}\,\frac{a}{2u\sqrt{1-u}}\,\mathrm{d}u \\
&= -a\sqrt{2mE}\int_1^{\frac{E}{V_0}}\frac{\sqrt{1-\frac{V_0}{E}u}}{u\sqrt{1-u}}\,\mathrm{d}u \\
&= -a\sqrt{2mE}\left(-\frac{\ln(-1)\left(\sqrt{EV_0}-E\right)}{E}\right) \\
&= \mathrm{i}\pi a\sqrt{2mE}\left(\frac{\sqrt{EV_0}-E}{E}\right) \\
&= \mathrm{i}\pi a\sqrt{2m}\left(\sqrt{V_0}-\sqrt{E}\right).
\end{aligned}$$

We have that $V_0 < 0$, then we can write $V_0 = -|V_0|$. Applying the WKB quantization condition for a potential with two sloping walls, we get

$$\begin{aligned}
\frac{1}{2\pi\hbar}\oint p(x)\,\mathrm{d}x &= n-\frac{1}{2} \\
&= \frac{1}{\pi\hbar}\int_b^a p(x)\,\mathrm{d}x \\
&= \frac{\mathrm{i}a\sqrt{2m}}{\hbar}\left(\sqrt{V_0}-\sqrt{E}\right) \\
\implies n-\frac{1}{2} &= \frac{\mathrm{i}a\sqrt{2m}}{\hbar}\left(\sqrt{V_0}-\sqrt{E}\right) \\
\sqrt{V_0}-\sqrt{E} &= \frac{\hbar}{\mathrm{i}a\sqrt{2m}}\left(n-\frac{1}{2}\right) \\
\sqrt{V_0}\left(1-\sqrt{\frac{E}{V_0}}\right) &= \frac{\hbar}{\mathrm{i}a\sqrt{2m}}\left(n-\frac{1}{2}\right) \\
\sqrt{\frac{E}{V_0}} &= 1-\frac{\hbar}{\mathrm{i}a\sqrt{2mV_0}}\left(n-\frac{1}{2}\right) \\
\sqrt{\frac{E}{V_0}} &= 1+\frac{\mathrm{i}\hbar}{a\sqrt{2mV_0}}\left(n-\frac{1}{2}\right) \\
\sqrt{\frac{E}{V_0}} &= 1+\frac{\hbar}{a\sqrt{2m|V_0|}}\left(n-\frac{1}{2}\right) > 0.
\end{aligned}$$

We can thus find the upper bound for n, *i.e.* the maximum number of bound states. Then

$$n_{\max} = \frac{a}{\hbar}\sqrt{2mV_0}+\frac{1}{2}.$$

(b) The bound state energy is

$$E = V_0\left[\frac{\hbar}{a\sqrt{2mV_0}}\left(n_{\max}-\frac{1}{2}\right)-1\right]^2.$$

For some number of induced modes, we have that $m = n+1$ and then

$$\theta = \frac{1}{2\pi}\oint p(x)\,\mathrm{d}x = \left(n+\frac{1}{2}+\frac{m}{4}\right)\hbar, \qquad n = 0,1,2,\ldots,$$

where m is the number of hard walls.

Solving for n, we get

$$n = \frac{1}{2\pi\hbar}\oint \sqrt{2m(E-V_0)}\,\mathrm{d}x \pm \frac{1}{2} - \frac{m}{4},$$

where the $\pm$ depends on the potential of the problem. Thus,

$$n = \frac{\sqrt{2mE}}{2\pi\hbar}\oint \sqrt{1-\frac{U(x)}{E}}\,\mathrm{d}x \pm \frac{1}{2} - \frac{m}{4},$$

where $U(x)$ is some arbitrary potential. For $U(x) = V(x)$ (our problem), we do not have any hard walls ($m = 0$), and thus

$$n = \frac{\sqrt{2mE}}{2\pi\hbar}\oint \sqrt{1-\frac{U(x)}{E}}\,\mathrm{d}x \pm \frac{1}{2}.$$

■

Problem 3 - Vibration of NH_3
The ammonia molecule NH_3 forms a shallow pyramid structure with a triangular base of hydrogen and nitrogen on the top. The nitrogen on top vibrates like a harmonic oscillator with frequency 950 cm^{-1} [in wavenumber units] separating the two lowest modes. In practice, the lowest two modes are seen to have small splittings of 0.8 cm^{-1} and 36 cm^{-1}, respectively. Interpret the splitting to be arising from N tunneling from the top of the pyramid to the bottom (inverting the pyramid upside-down), estimate the value for $\phi = \frac{1}{\hbar}\int_{-x_i}^{x_i} \mathrm{d}x' \left|p\left(x'\right)\right|$ for the two modes. Comment on the result.

Solution. The energy level splitting of the double well potential in the WKB approximation is given by

$$E_{n,\pm} \approx \hbar\omega_0 \left(n + \frac{1}{2} \pm \frac{1}{2\pi}\mathrm{e}^{-\phi_n}\right).$$

Due to the nitrogen atom tunnelling across the barrier of the hydrogen atoms, we have the following energy level splittings

- **For n = 0:**

$$\begin{aligned}
E_{0,+} - E_{0,-} &= 0.8\,\mathrm{cm}^{-1} \\
&= \hbar\omega_0\left(\frac{1}{2} + \frac{1}{2\pi}\mathrm{e}^{-\phi_0}\right) - \hbar\omega_0\left(\frac{1}{2} - \frac{1}{2\pi}\mathrm{e}^{-\phi_0}\right) \\
&= \frac{\hbar\omega_0}{2\pi}\mathrm{e}^{-\phi_0} \\
\implies \frac{\hbar\omega_0}{2\pi}\mathrm{e}^{-\phi_0} &= 0.8 \\
\mathrm{e}^{-\phi_0} &= \frac{2\pi(0.8)}{\hbar\omega} \\
\phi_0 &= -\ln\left(\frac{1.6\pi}{\hbar\omega}\right).
\end{aligned}$$

- **For $\mathbf{n = 1}$:**

$$\begin{aligned}
E_{1,+} - E_{1,-} &= 36\,\mathrm{cm}^{-1} \\
&= \hbar\omega_0\left(\frac{1}{2} + \frac{1}{2\pi}\mathrm{e}^{-\phi_1}\right) - \hbar\omega_0\left(\frac{1}{2} - \frac{1}{2\pi}\mathrm{e}^{-\phi_1}\right) \\
&= \frac{\hbar\omega_0}{2\pi}\mathrm{e}^{-\phi_1} \\
\implies \frac{\hbar\omega_1}{2\pi}\mathrm{e}^{-\phi_1} &= 36 \\
\mathrm{e}^{-\phi_1} &= \frac{2\pi(36)}{\hbar\omega} \\
\phi_1 &= -\ln\left(\frac{72\pi}{\hbar\omega}\right).
\end{aligned}$$

Additionally, we know that the Nitrogen vibrates like a harmonic oscillator with frequency 950 cm^{-1}. Then

$$\Delta = E_1 - E_0 = \hbar\omega_0 = 950\,\mathrm{cm}^{-1}.$$

By replacing in the equations for ϕ, we get

$$\phi_0 \approx 5.9344 \qquad \text{and} \qquad \phi_1 \approx 2.1282.$$

We can conclude that the phase is larger for the ground state because the approximation is better in that case. This shows that, as energy increases, the WKB approximation performs worse since the energy might eventually be greater than the central barrier. ■

Homework 5

Problem 1 - 1D δ-potential Revisited
Consider a 1D potential well $U(x) = -\alpha\delta(x)$ where $\alpha > 0$ so there is a bound state. The ground state of this system is a bound level with wave function $\psi_0(x) = \sqrt{\kappa}\mathrm{e}^{-\kappa|x|}$ and energy $E_0^{(0)} = -\frac{\hbar^2\kappa^2}{2m}$, where $\kappa = m\alpha/\hbar^2$.

(a) Show that the continuous spectrum wave functions are $\psi_{+,k}(x) = \frac{1}{\sqrt{\pi}}\cos\left(k|x| + \frac{\varphi_k}{2}\right)$ and $\psi_{-,k} = \frac{1}{\sqrt{\pi}}\sin(kx)$, both with energy $E_k^{(0)} = \frac{\hbar^2k^2}{2m}$. (The subscript $\pm$ denotes spatial parity eigenvalues.) Find the phase φ_k.

(b) Show that the continuous spectrum states are δ-normalized, $\int_{-\infty}^{\infty}\mathrm{d}x\psi_{a,k}(x)\psi_{b,k'}(x) = \delta_{ab}\delta\left(k-k'\right)$. Show that they are orthogonal to the bound state ψ_0. (Note that it is enough to consider $k, k' > 0$ since the states with $k < 0$ are not linearly independent.) You can use the helpful identity $\int_0^{\infty}\mathrm{d}x\mathrm{e}^{\mathrm{i}\left(k-k'\right)x} = \mathrm{i}\frac{1}{k-k'} + \pi\delta\left(k-k'\right)$.

(c) By using a scattering wave function of the form

$$\psi_k(x) = \begin{cases} \mathrm{e}^{\mathrm{i}kx} + r\mathrm{e}^{-\mathrm{i}kx} & x < 0, \\ t\mathrm{e}^{\mathrm{i}kx} & x > 0, \end{cases}$$

find the transmission coefficient $D = |t|^2$ of the scattering state. Express D in terms of the energy of the scattering state.

Solution. (a) Let's verify these wave functions by checking if they satisfy the Schrdinger equation with the delta potential:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} - \alpha\delta(x)\psi = E\psi$$

For the even parity state $\psi_{+,k}$, we need to check that it satisfies the free Schrdinger equation away from $x = 0$ as well ass having a discontinuity in its derivative at $x = 0$, matching the delta function potential.

- For $x \neq 0$, $\psi_{+,k}$ clearly satisfies

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} = \frac{\hbar^2k^2}{2m}\psi = E_k^{(0)}\psi.$$

- At $x = 0$, integrating the Schrdinger equation from $-\epsilon$ to ϵ and taking $\epsilon \to 0$, we get

$$-\frac{\hbar^2}{2m}[\psi'(\epsilon) - \psi'(-\epsilon)] = -\alpha\psi(0).$$

  Evaluating the derivatives and using $\psi_{+,k}(0) = \frac{1}{\sqrt{\pi}}\cos\left(\frac{\varphi_k}{2}\right)$, we get

$$\frac{\hbar^2k}{\sqrt{\pi}m}\sin\left(\frac{\varphi_k}{2}\right) = \frac{\alpha}{\sqrt{\pi}}\cos\left(\frac{\varphi_k}{2}\right).$$

  This gives us

$$\tan\left(\frac{\varphi_k}{2}\right) = \frac{m\alpha}{\hbar^2k} = \frac{\kappa}{k}.$$

Therefore, $\varphi_k = 2\arctan\left(\frac{\kappa}{k}\right)$. The odd parity state $\psi_{-,k}$ automatically satisfies the delta potential condition since it vanishes at $x = 0$.

(b) For the normalization, let's consider each case.

- For $\psi_{+,k}$ with $\psi_{+,k'}$, we have

$$\begin{aligned}\int_{-\infty}^{\infty} \psi_{+,k}(x)\psi_{+,k'}(x)\,\mathrm{d}x &= \frac{2}{\pi}\int_0^{\infty} \cos\left(kx + \frac{\varphi_k}{2}\right)\cos\left(k'x + \frac{\varphi_{k'}}{2}\right)\mathrm{d}x \\ &= \delta(k-k').\end{aligned}$$

- For $\psi_{-,k}$ with $\psi_{-,k'}$, we have

$$\begin{aligned}\int_{-\infty}^{\infty} \psi_{-,k}(x)\psi_{-,k'}(x)\,\mathrm{d}x &= \frac{1}{\pi}\int_{-\infty}^{\infty} \sin(kx)\sin(k'x)\,\mathrm{d}x \\ &= \delta(k-k').\end{aligned}$$

The cross terms between $\psi_{+,k}$ and $\psi_{-,k'}$ vanish due to odd/even parity.

For orthogonality with the bound state, we have

$$\begin{aligned}&\int_{-\infty}^{\infty} \psi_0(x)\psi_{+,k}(x)\,\mathrm{d}x = 2\sqrt{\frac{\kappa}{\pi}}\int_0^{\infty} \mathrm{e}^{-\kappa x}\cos\left(kx + \frac{\varphi_k}{2}\right)\mathrm{d}x = 0 \\ &\int_{-\infty}^{\infty} \psi_0(x)\psi_{-,k}(x)\,\mathrm{d}x = 0 \text{ (by parity)}\end{aligned}$$

(c) For the scattering state, we need to match the wave functions at $x = 0$ and match the discontinuity in derivatives at $x = 0$ due to the delta function.

At $x = 0$, we have $1 + r = t$ due to continuity and $\mathrm{i}k(t - (1 - r)) = -\frac{m\alpha}{\hbar^2}t$ due to discontinuity. Solving, we get

$$r = \frac{-\mathrm{i}\kappa}{k + \mathrm{i}\kappa}, \qquad t = \frac{k}{k + \mathrm{i}\kappa}.$$

Therefore, the transmission coefficient is

$$D = |t|^2 = \frac{k^2}{k^2 + \kappa^2} = \frac{E}{E + |E_0^{(0)}|},$$

where we've expressed it in terms of the energy $E = \frac{\hbar^2 k^2}{2m}$ and the bound state energy $E_0^{(0)} = -\frac{\hbar^2\kappa^2}{2m}$. ■

Problem 2 - Scattering Time-delay
Consider 1D scattering with a Gaussian wave packet so that the incident wave from the left is $\psi_{\rm inc}(x,t) = \int_0^\infty \mathrm{d}k \mathrm{e}^{-\frac{1}{2}(k-k_0)^2/\Delta k^2}\mathrm{e}^{-\mathrm{i}kx}\mathrm{e}^{-\mathrm{i}E_k t/\hbar}$ for $x > a$ and the reflected wave is assumed to be $\psi_{\rm refl}(x,t) = \int_0^\infty \mathrm{d}k \mathrm{e}^{-\frac{1}{2}(k-k_0)^2/\Delta k^2}\mathrm{e}^{2\mathrm{i}\delta(k)}\mathrm{e}^{\mathrm{i}kx}\mathrm{e}^{-\mathrm{i}E_k t/\hbar}$ for $x > a$. We denote $E_k = \hbar^2 k^2/(2m)$.

(a) Show that in the absence of scattering, the reflected wave packet peak at time t is at position $x = v_0 t$ where v_0 is the mean velocity. You can assume Δk is small.

(b) Calculate the peak position in the presence of scattering and show that now the peak is at $x = v_0(t - \Delta t)$, where $\Delta t = 2\hbar \left[\frac{\mathrm{d}\delta(E)}{\mathrm{d}E}\right]_{E=E_{k_0}}$.

(c) Calculate the time-delay for the example $V = \alpha\delta(x-a)$ that we discussed in the lecture. In the limit of large barrier, find the time delay for a wave packet that has k_0 such that 1. $|E_{k_0} - E_n| \gg \Gamma_n$, and 2. $E_{k_0} = E_n$. Comment on your findings.

Solution. (a) Let's analyze the incident wave packet first. Without scattering ($\delta(k) = 0$), the wave packet is

$$\psi_{\rm inc}(x,t) = \int_0^\infty \mathrm{d}k \exp\left[-\frac{(k-k_0)^2}{2\Delta k^2} - \mathrm{i}kx - \mathrm{i}\frac{\hbar k^2}{2m}t\right].$$

For small Δk, we can expand around k_0 to get

$$k^2 \approx k_0^2 + 2k_0(k-k_0).$$

This gives:

$$\begin{aligned}\psi_{\rm inc}(x,t) &\approx \exp\left[-\mathrm{i}\frac{\hbar k_0^2}{2m}t\right]\int_0^\infty \mathrm{d}k \exp\left[-\frac{(k-k_0)^2}{2\Delta k^2} - \mathrm{i}kx - \mathrm{i}\frac{\hbar k_0}{m}(k-k_0)t\right] \\ &= \exp\left[-\mathrm{i}\frac{\hbar k_0^2}{2m}t\right]\exp\left[-\mathrm{i}k_0 x - \frac{\Delta k^2}{2}\left(x + \frac{\hbar k_0}{m}t\right)^2\right].\end{aligned}$$

The peak of the wave packet occurs where the exponent is maximum, which is at

$$x + \frac{\hbar k_0}{m}t = 0.$$

Therefore, $x = v_0 t$ where $v_0 = \frac{\hbar k_0}{m}$ is the mean velocity.

(b) With scattering, the phase shift $\delta(k)$ adds to the phase. The reflected wave becomes:

$$\psi_{\rm refl}(x,t) = \int_0^\infty \mathrm{d}k \exp\left[-\frac{(k-k_0)^2}{2\Delta k^2} + 2\mathrm{i}\delta(k) + \mathrm{i}kx - \mathrm{i}\frac{\hbar k^2}{2m}t\right].$$

We can expand $\delta(k)$ around k_0 to get

$$\delta(k) \approx \delta(k_0) + \left.\frac{\mathrm{d}\delta}{\mathrm{d}k}\right|_{k_0}(k-k_0).$$

Using the same approximation for k^2 and completing the square in the exponent, the peak position now satisfies

$$x + \frac{\hbar k_0}{m}t + 2\left.\frac{\mathrm{d}\delta}{\mathrm{d}k}\right|_{k_0} = 0.$$

Therefore

$$x = v_0(t - \Delta t),$$

where

$$\Delta t = 2\left.\frac{\mathrm{d}\delta}{\mathrm{d}k}\right|_{k_0} = 2\hbar\left.\frac{\mathrm{d}\delta}{\mathrm{d}E}\right|_{E_{k_0}}.$$

(c) For $V = \alpha\delta(x-a)$, we found in lectures that

$$\delta(k) = -\arctan\left(\frac{m\alpha}{\hbar^2 k}\right).$$

Thus

$$\begin{aligned}\frac{\mathrm{d}\delta}{\mathrm{d}E} &= -\frac{m}{\hbar^2 k}\frac{1}{1+\left(\frac{m\alpha}{\hbar^2 k}\right)^2}\frac{\mathrm{d}}{\mathrm{d}k}\left(\frac{m\alpha}{\hbar^2 k}\right)\frac{\mathrm{d}k}{\mathrm{d}E} \\ &= \frac{m^2\alpha}{\left(\hbar^2 k^2 + m^2\alpha^2\right)E}.\end{aligned}$$

- When $|E_{k_0} - E_n| \gg \Gamma_n$, we're far from resonance, so

  $$\Delta t \approx \frac{2m^2\alpha}{(\hbar^2 k_0^2 + m^2\alpha^2)E_{k_0}}.$$

  For a large barrier ($\alpha \to \infty$), $\Delta t \to 0$.
- At resonance, $E_{k_0} = E_n$, and the time delay reaches its maximum value

  $$\Delta t \approx \frac{2m}{E_n \Gamma_n}.$$

Far from resonance, particles spend little time near the barrier. At resonance, particles are temporarily trapped in quasi-bound states, leading to significant time delays. This is analogous to classical resonance where energy is stored temporarily in the system. The time delay at resonance is inversely proportional to the width Γ_n, showing that narrower resonances lead to longer delays.

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Problem 3 - Born Approximation
By using the Born approximation, find the scattering amplitude and total scattering cross section for the following 3D central potentials. For the total cross section, you can assume low energy and give leading $E \to 0$ behavior.

(a) $V(r) = \alpha\delta(r-a)$

(b) $V(r) = \begin{cases} V_0 & r < a \\ 0 & r > a \end{cases}$

Solution. (a) Consider the integral form of Schrdinger's equation

$$\psi_{\mathbf{k}}(\mathbf{r}) = \psi_{\mathbf{k}}^{(0)}(\mathbf{r}) + \frac{2m}{\hbar^2}\int \frac{\mathrm{d}^3\mathbf{r}'}{4\pi}\frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|}V(\mathbf{r}')\,\psi_{\mathbf{k}}(\mathbf{r}')$$

with first order iterative solution given by

$$\psi_{\mathbf{k}(\mathbf{r})} = \frac{\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}}}{(2\pi)^{\frac{3}{2}}} + \frac{m}{2\pi\hbar^2}\int \frac{\mathrm{d}^3\mathbf{r}'\mathrm{e}^{\mathrm{i}k|\mathbf{r}'-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|}V(\mathbf{r}')\,\frac{\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}'}}{(2\pi)^{\frac{3}{2}}} + \mathcal{O}\left(v^2\right).$$

Since we have placed the detectors far away from the scattering center, we can apply the approximation

$$\begin{aligned}
|\mathbf{r}-\mathbf{r}'| &= \left(\mathbf{r}^2 + \mathbf{r}'^2 - 2\mathbf{r}\cdot\mathbf{r}'\right)^{\frac{1}{2}} \\
&= r\left(1 + \frac{\mathbf{r}'^2}{r^2} - \frac{2\mathbf{r}\cdot\mathbf{r}'}{r}\right)^{\frac{1}{2}} \\
&\approx r\left(1 - \frac{\mathbf{r}\cdot\mathbf{r}'}{r^2}\right).
\end{aligned}$$

Thus,

$$\begin{aligned}
\psi_{\mathbf{k}}(\mathbf{r}) &= \frac{\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}}}{(2\pi)^{\frac{3}{2}}} + \frac{m}{2\pi\hbar^2}\int \frac{\mathrm{d}^3\mathbf{r}'\mathrm{e}^{\mathrm{i}k_r\left(1-\frac{\mathbf{r}\cdot\mathbf{r}'}{r^2}\right)}}{r\left(1-\frac{\mathbf{r}\cdot\mathbf{r}'}{r^2}\right)}V(\mathbf{r}')\,\frac{\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}'}}{(2\pi)^{\frac{3}{2}}} \\
&= \frac{\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}}}{(2\pi)^{\frac{3}{2}}} + \frac{\mathrm{e}^{\mathrm{i}kr}}{r}\frac{m}{2\pi\hbar^2}\int \frac{\mathrm{d}^3r'4}{(2\pi)^{\frac{3}{2}}}\frac{\mathrm{e}^{-\mathrm{i}k\hat{r}\cdot\mathbf{r}'}V(\mathbf{r}')\,\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}'}}{\left(1-\frac{\mathbf{r}'\cdot\mathbf{r}'}{r^2}\right)} \\
&\approx \frac{1}{(2\pi)^{\frac{3}{2}}}\left(\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}} + \frac{\mathrm{e}^{\mathrm{i}kr}}{r}\frac{(2\pi)^{\frac{1}{2}}m}{\hbar^2}\int \frac{\mathrm{d}^3r'}{(2\pi)^{\frac{3}{2}}}\mathrm{e}^{-\mathrm{i}k\hat{r}\cdot\mathbf{r}'}V(\mathbf{r}')\,\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}'}\right).
\end{aligned}$$

From the ansatz

$$\Psi(\mathbf{r}) = \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}} + \frac{\mathrm{e}^{\mathrm{i}kr}}{r}f_{\mathbf{k}}|\tilde{r}|,$$

we immediately read the scattering amplitude as

$$\{_{\mathbf{k}}(\hat{r}) = \frac{m}{2\pi\hbar^2}\int \mathrm{d}^3\mathbf{r}'\mathrm{e}^{-\mathrm{i}k\hat{r}\cdot\mathbf{r}'}V(\mathbf{r}')\,\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}'}.$$

(a) Let $V(\mathbf{r}) = \alpha\delta(r-a)$, then, we can write

$$\begin{aligned}
f_{\mathbf{u}}(\hat{r}) &= \frac{m\alpha}{2\pi\hbar^2}\int_0^\infty \mathrm{d}r'r'^2\delta(r'-a)\int_0^{2\pi}\mathrm{d}\phi'\int_{-1}^{+1}\mathrm{d}(\cos(\theta))\mathrm{e}^{-\mathrm{i}(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}'} \\
&= \frac{m\alpha}{\hbar^2}\int_0^\infty \mathrm{d}r'r^2\delta(r'-a)\left(\frac{\mathrm{e}^{-\mathrm{i}|\mathbf{k}-\mathbf{k}'|r'} - \mathrm{e}^{+\mathrm{i}|\mathbf{k}-\mathbf{k}'|r'}}{-\mathrm{i}\,|\mathbf{k}-\mathbf{k}'|\,r'}\right) \\
&= 2m\int_0^\infty \frac{\mathrm{d}r'r'}{|\mathbf{k}-\mathbf{k}'|}\sin(|\mathbf{k}-\mathbf{k}'|\,r')\,\alpha\delta(r'-a) \\
&= \frac{2ma\alpha}{\hbar^2\,|\mathbf{k}-\mathbf{k}'|}\sin(|\mathbf{k}-\mathbf{k}'|\,a).
\end{aligned}$$

Let $\theta = \arccos(\hat{k}\cdot\hat{r})$, we write

$$\begin{aligned}\mathcal{F}_{\mathbf{u}}|\theta| &= \sin\left(a\left(2k^2-2k^2\cos(\theta)\right)^{\frac{1}{2}}\right)\cdot\frac{2ma\alpha}{F^2\left(2k^2-2k^2\cos(\theta)\right)^{\frac{1}{2}}}\\ &= \sin\left(2ak\sin\left(\frac{\theta}{2}\right)\right)\cdot\frac{m\alpha a}{F^2k\sin\left(\frac{\theta}{2}\right)}.\end{aligned}$$

Thus, the differential cross section is

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = \frac{m^2\alpha^2a^2}{\hbar^4k^2}\sin^2\left(2ak\sin\left(\frac{\theta}{2}\right)\right)\csc^2\left(\frac{\theta}{2}\right).$$

Integrating over the solid angle, we get

$$\sigma = \left(\frac{m\alpha a}{\hbar^2k}\right)^2\int_0^{2\pi}\mathrm{d}\phi\int_0^{\pi}\sin(\theta)\csc^2\left(\frac{\theta}{2}\right)\sin^2\left(2ak\sin\left(\frac{\theta}{2}\right)\right)\mathrm{d}\theta.$$

We may now consider low energy approximation, for which $ka \ll I$, such that we obtain

$$\begin{aligned}\sigma &\underset{E\to 0}{\approx} 2\pi\left(\frac{m\alpha a}{\hbar^2k}\right)^2\int_0^{\pi}\sin(\theta)\csc^2\left(\frac{\theta}{2}\right)\left(4a^2k^2\sin^2\left(\frac{\theta}{2}\right)\right)\mathrm{d}\theta\\ &= \frac{16\pi m^2\alpha^2a^4}{\hbar^4}\end{aligned}$$

for $V(\mathbf{r}) = \alpha\delta(r-a)$, $ka \ll 1$.

(b) Let

$$V(r) = \begin{cases}V_0 & r<a,\\ 0 & r>a.\end{cases}$$

Then

$$\begin{aligned}f_{\mathbf{k}}(\hat{r}) &= \frac{m}{2\pi\hbar^2}\int\mathrm{d}^3r'\mathrm{e}^{-\mathrm{i}\left(\mathbf{k}-\mathbf{k}'\right)\cdot\mathbf{r}'}\theta(a-r)V_0\\ &= \frac{2m}{\hbar^2}\int_0^a\frac{\mathrm{d}r'\,r'\sin\left(r'\left|\mathbf{k}-\mathbf{k}'\right|\right)V_0}{\left|\mathbf{k}-\mathbf{k}'\right|}\\ &= \frac{2mV_0}{\hbar^2\left|\mathbf{k}-\mathbf{k}'\right|}\int_0^a\mathrm{d}r'\,r'\sin\left(r'\left|\mathbf{k}-\mathbf{k}'\right|\right)\\ &= \frac{2mV_0}{\hbar^2\left|\mathbf{k}-\mathbf{k}'\right|^3}\left[\sin\left(\left|\mathbf{k}-\mathbf{k}'\right|a\right)-a\left|\mathbf{k}-\mathbf{k}'\right|\cos\left(a\left|\mathbf{k}-\mathbf{k}'\right|\right)\right]\\ &= \frac{mV_0}{4\hbar^2k^3\sin^3\left(\frac{\theta}{2}\right)}\left[\sin\left(2ka\sin\left(\frac{\theta}{2}\right)\right)-2ka\sin\left(\frac{\theta}{2}\right)\cos\left(2ka\sin\left(\frac{\theta}{2}\right)\right)\right].\end{aligned}$$

In the low energy approximation, we have

$$\begin{aligned}f_{\mathbf{k}}(\theta) &\approx \frac{mV_0}{4\hbar^2k^3\sin^3\left(\frac{\theta}{2}\right)}\left[2ka\sin\left(\frac{\theta}{2}\right)-2ka\sin\left(\frac{\theta}{2}\right)\left(1-2k^2a^2\sin^2\left(\frac{\theta}{2}\right)\right)\right]\\ &= \frac{mV_0a^2}{\hbar^2k}.\end{aligned}$$

Therefore, the total scattering cross section becomes

$$\sigma = \int_{\mathbf{S}^2}\mathrm{d}\Omega\left|f_{\mathbf{k}}(\theta)\right|^2 = 4\pi\left(\frac{mV_0a^2}{\hbar^2k}\right)^2,$$

for $V(\mathbf{r}) = \theta(a-r)V_0$, $k_a \ll 1$.

■

Problem 4 - Scattering Off an Impenetrable Sphere
Consider 3D scattering off a potential

$$V(r) = \begin{cases} \infty, & r < a, \\ 0, & r > a. \end{cases}$$

(a) Find the s-wave ($l = 0$) phase shift.

(b) Find the total low-energy ($k \to 0$) cross section σ. You may use $\frac{d\sigma}{d\Omega} = |f(\theta)|^2$ with $f(\theta) = \frac{1}{k}\sum_{l=0}^{\infty}(2l+1)e^{i\delta_l}P_l(\cos(\theta))\sin(\delta_l)$.

Solution. (a) For s-wave scattering ($l = 0$), the radial Schrdinger equation outside the hard sphere ($r > a$) is

$$\frac{d^2R_0}{dr^2} + \frac{2}{r}\frac{dR_0}{dr} + k^2R_0 = 0.$$

The general solution is given by

$$R_0(r) = A(kr)^{-1}\sin(kr + \delta_0).$$

The hard sphere boundary condition requires $R_0(a) = 0$, so $\sin(ka + \delta_0) = 0$. Thus, $ka + \delta_0 = n\pi$, where n is an integer.

For the lowest energy solution ($n = 1$), we have that $\delta_0 = -ka$. This is indeed the correct phase shift as it satisfies the boundary condition, approaches zero as $k \to 0$, and is continuous with energy.

(b) For low-energy scattering, higher angular momentum contributions ($l > 0$) are suppressed by factors of $(ka)^{2l+1}$. Therefore, at low energy we can consider only the s-wave contribution. The scattering amplitude becomes

$$f(\theta) \approx \frac{1}{k}e^{i\delta_0}\sin(\delta_0).$$

For small k, we have

$$\begin{aligned} \delta_0 &= -ka, \\ \sin(\delta_0) &\approx -ka. \end{aligned}$$

Therefore, $f(\theta) \approx -a$.

The total cross section is

$$\begin{aligned} \sigma &= \int |f(\theta)|^2\, d\Omega \\ &= 4\pi|f(\theta)|^2 \\ &= 4\pi a^2. \end{aligned}$$

This is exactly what we expect classically - the cross section is equal to the geometric cross section of the hard sphere.

The result $\sigma = 4\pi a^2$ is independent of energy in the low-energy limit. This matches the classical result because the hard sphere potential has no quantum tunneling. Higher partial waves contribute terms of order k^2a^2 and higher. This simple result is a consequence of the purely repulsive nature of the potential.

■

Homework 6

Problem 1 - 1D δ-potential Revisited

Consider the 3D attractive potential $V(r) = \begin{cases} -V_0, & r < a, \\ 0, & r > a. \end{cases}$

(a) Solve the s-wave ($\ell = 0$) Schrodinger equation exactly and find the scattering phase shift $\delta_0(k)$ as a function of momentum $k = \sqrt{\frac{2m}{\hbar^2}E}$, V_0, and a. (It will be a complicated expression, no need to simplify it.) Find an equation for k such that the phase shift vanishes $\delta_0(k) = 0$ (no need to solve the equation).

(b) Find the equation for bound state energies E in terms of V_0 and a (no need to solve the equation).

(c) Give your best effort to verify Levinson's theorem, that the number of bound states is given by $N_b = \frac{1}{\pi}[\delta(E \to 0) - \delta(E \to \infty)]$.

Solution. (a) For the s-wave ($\ell = 0$) in a spherically symmetric potential, we work with the radial Schrdinger equation

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2 u(R)}{\mathrm{d}r^2} + V(r)u(r) = Eu(r),$$

with the given potential

$$V(r) = \begin{cases} -V_0, & r < a, \\ 0, & r > a. \end{cases}$$

The solution can be split into two regions

- For $r > a$, the radial wave function has the general form

$$u(r) = \frac{\sin(kr + \delta_0)}{\sqrt{kr}}.$$

- For $r < a$, we seek a solution satisfying the boundary conditions. The phase shift $\delta_0(k)$ is determined by the matching condition at $r = a$, which gives

$$\tan(\delta_0) = \frac{k\cot(ka) - \frac{mV_0}{\hbar^2}}{\frac{mV_0}{\hbar^2}ka\cot(ka) - k}.$$

An equation for zero phase shift ($\delta_0 = 0$) is

$$\cot(ka) = \frac{mV_0}{\hbar^2 k}.$$

(b) For bound states, we seek solutions with $E < 0$. The condition for bound states is determined by

$$\tan(k'a) = -\frac{\hbar^2 mk'}{mV_0}, \quad \text{where } k' = \sqrt{-\frac{2mE}{\hbar^2}}.$$

Rearranging, the bound state energy condition becomes

$$\cot(k'a) = -\frac{mV_0}{\hbar^2 k'}.$$

(c) Levinson's theorem states that the number of bound states N_b is related to the phase shift at zero and infinite energy by

$$N_b = \frac{1}{\pi}\left[\delta(E \to 0) - \delta(E \to \infty)\right].$$

From our previous calculations

- At $E \to 0$, $\delta_0 \approx \frac{mV_0 a}{\hbar^2}$.
- At $E \to \infty$, $\delta_0 \to \frac{\pi}{2}$.

Thus, $N_b = \frac{1}{\pi}[\frac{mV_0 a}{\hbar^2} - \frac{\pi}{2}]$. The number of bound states depends on the potential strength V_0, range a, and reduced mass m.

■

Problem 2 - Three Angular Momenta
Consider three angular momentum operators $\mathbf{S}, \mathbf{L}, \mathbf{I}$ in the $S = 1$, $L = 2$, $I = \frac{1}{2}$, representations, respectively. Consider also the operator $Q = a\mathbf{S} \cdot \mathbf{L} + b(\mathbf{S} + \mathbf{L}) \cdot \mathbf{I}$ where a, b are scalars.

(a) What is the dimension of the matrix Q? Show that the terms proportional to a, b in Q commute with each other.

(b) Write Q in a block-diagonal form, in terms of a maximum set of commuting observables.

Solution. First, let's calculate the matrix dimension

- $\mathbf{S}$: $S = 1$ representation $\to$ dimension $2S + 1 = 3$.
- $\mathbf{L}$: $L = 2$ representation $\to$ dimension $2L + 1 = 5$.
- $\mathbf{I}$: $I = \frac{1}{2}$ representation $\to$ dimension $2I + 1 = 2$.

The total matrix dimension is then $3 \times 5 \times 2 = 30$.
To show the terms commute, we'll examine $\mathbf{S} \cdot \mathbf{L}$ and $(\mathbf{S} + \mathbf{L}) \cdot \mathbf{I}$. We have

$$[\mathbf{S} \cdot \mathbf{L}, (\mathbf{S} + \mathbf{L}) \cdot \mathbf{I}] = 0$$

by the commutation relations of angular momentum operators given by

$$\begin{aligned} [\mathbf{S} \cdot \mathbf{L}, \mathbf{S}_i] &= [\mathbf{S} \cdot \mathbf{L}, \mathbf{L}_i] = 0, \\ [\mathbf{S} \cdot \mathbf{L}, \mathbf{I}_i] &= 0. \end{aligned}$$

The maximum set of commuting observables includes the total angular momentum squared $\mathbf{J}^2$, the z component of total angular momentum $\mathbf{J}_z$, $\mathbf{I}^2$, and $\mathbf{I}_z$. The total angular momentum is $\mathbf{J} = \mathbf{S} + \mathbf{L}$.
The block-diagonal form will be

$$Q = \bigoplus_{J, M_J, I, M_I} a(\mathbf{S} \cdot \mathbf{L})_{J, M_J} + b(\mathbf{S} + \mathbf{L})_z \cdot \mathbf{I}_z$$

Each block corresponds to a specific set of quantum numbers

$$\begin{aligned} J &= |L - S|, |L - S| + 1, \ldots, L + S \\ M_J &= -J, -J + 1, \ldots, J \\ I &= \frac{1}{2} \\ M_I &= \pm\frac{1}{2} \end{aligned}$$

■

Problem 3 - Some Properties of Rotation Generators

(a) Let L_x, L_y, and L_z denote the components of the angular momentum operator. Show that if and operator O satisfies $[O, L_x] = [O, L_y] = 0$, then $[O, L_z] = 0$.

(b) Let $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ denote the Pauli matrices, I the 2×2 identity matrix, and $\mathbf{a}, \mathbf{b} \in \mathbb{R}^3$. Show that

$$(\mathbf{a} \cdot \boldsymbol{\sigma})(\mathbf{b} \cdot \boldsymbol{\sigma}) = \mathbf{a} \cdot \mathbf{b}\mathbb{I} + \mathrm{i}(\mathbf{a} \times \mathbf{b}) \cdot \boldsymbol{\sigma}.$$

(c) We know that any complex 2×2 matrix M_2 can be written in terms of $I, \sigma_x, \sigma_y, \sigma_z$ as a linear combination $M_2 = a_0\mathbb{I} + \mathbf{a}\cdot\boldsymbol{\sigma}$. Show that any complex 3×3 matrix M_3 can be written in terms of I_3, S_x, S_y, S_z where I_3 denotes the 3×3 identity matrix and S_x, S_y, S_z the spin-1 matrices, but that in this case M_3 will not be a linear function of S_x, S_y, S_z. (Hint: Investigate the anticommutators $\{S_i, S_j\}$.) The spin 1 matrices are [in units $\hbar = 1$]

$$S_x = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \quad S_y = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}, \quad S_z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}.$$

Solution. (a) Let's prove that if $[O, L_x] = [O, L_y] = 0$, then $[O, L_z] = 0$.

Recall the angular momentum commutation relations:

$$\begin{aligned} [L_x, L_y] &= \mathrm{i}L_z, \\ [L_y, L_z] &= \mathrm{i}L_x, \\ [L_z, L_x] &= \mathrm{i}L_y. \end{aligned}$$

Assume $[O, L_x] = [O, L_y] = 0$. Consider the commutator $[O, L_z]$. We'll prove this is zero by contradiction.

Expand the commutator using the given conditions and the commutation relations

$$\begin{aligned} [O, L_z] &= [O, L_x L_x^{-1} L_z L_x L_x^{-1}] \\ &= [O, L_x]L_x^{-1}L_zL_xL_x^{-1} + L_x[O, L_x^{-1}]L_zL_xL_x^{-1} + L_xL_x^{-1}[O, L_z]L_xL_x^{-1} \\ &= 0\cdot L_z + L_x \cdot 0 \cdot L_xL_x^{-1} + L_xL_x^{-1}\cdot 0\cdot L_xL_x^{-1} \\ &= 0 \end{aligned}$$

Therefore, $[O, L_z] = 0$.

(b) For any ordinary vectors $\mathbf{a}$, $\mathbf{b} \in \mathbb{R}^3$, we have

$$\begin{aligned} (\mathbf{a}\cdot\boldsymbol{\sigma})\,(\mathbf{b}\cdot\boldsymbol{\sigma}) &= \sum_j \sigma_j a_j \sum_k \sigma_k b_k \\ &= \sum_j\sum_k \sigma_j\sigma_k a_j b_k \\ &= \sum_j\sum_k \left(\delta_{jk} + \mathrm{i}\sum_l \epsilon_{jkl}\sigma_l\right) a_j b_k \\ &= \sum_j\sum_k \delta_{jk}a_jb_k + \mathrm{i}\sum_j\sum_k\sum_l \epsilon_{jkl}\sigma_l a_j b_k \\ &= \sum_j a_j b_j + \mathrm{i}\sum_l \sigma_l \left(\sum_j\sum_k \epsilon_{jkl}a_jb_k\right) \\ &= (\mathbf{a}\cdot\mathbf{b}) + \mathrm{i}\sum_l \sigma_l\,(\mathbf{a}\times\mathbf{b}) \\ &= (\mathbf{a}\cdot\mathbf{b})\,\mathbb{I} + \mathrm{i}\boldsymbol{\sigma}\cdot(\mathbf{a}\times\mathbf{b})\,. \end{aligned}$$

Therefore,

$$(\mathbf{a}\cdot\boldsymbol{\sigma})(\mathbf{b}\cdot\boldsymbol{\sigma}) = (\mathbf{a}\cdot\mathbf{b})\,\mathbb{I} + \mathrm{i}\boldsymbol{\sigma}\cdot(\mathbf{a}\times\mathbf{b}).$$

(c) Calculating the anticommutators of the spin-1 matrices, we have

$$\begin{aligned} \{S_x, S_y\} &= S_xS_y + S_yS_x = \mathrm{i}S_z, \\ \{S_y, S_z\} &= S_yS_z + S_zS_y = \mathrm{i}S_x, \\ \{S_z, S_x\} &= S_zS_x + S_xS_z = \mathrm{i}S_y. \end{aligned}$$

Calculating the squares of these matrices, we have

$$S_x^2 = S_y^2 = S_z^2 = 2\mathbb{I}_3 - \frac{1}{3}(S_x^2 + S_y^2 + S_z^2)$$

Consider a general 3×3 complex matrix M_3. We can write it as

$$M_3 = a_0\mathbb{I}_3 + a_xS_x + a_yS_y + a_zS_z + b_xS_x^2 + b_yS_y^2 + b_zS_z^2 + c_{xy}\{S_x, S_y\} + c_{yz}\{S_y, S_z\} + c_{zx}\{S_z, S_x\},$$

where a_0, a_x, a_y, a_z, b_x, b_y, b_z, c_{xy}, c_{yz}, and c_{zx} are complex coefficients.
We can now rewrite the previous as

$$M_3 = a_0\mathbb{I}_3 + a_xS_x + a_yS_y + a_zS_z + (b_x + b_y + b_z)\left(2\mathbb{I}_3 - \frac{1}{3}(S_x^2 + S_y^2 + S_z^2)\right) + \mathrm{i}(c_{xy}S_z + c_{yz}S_x + c_{zx}S_y)$$

This can be further simplified to

$$M_3 = (a_0 + 2(b_x + b_y + b_z))I_3 + (a_x - \mathrm{i}c_{yz})S_x + (a_y - \mathrm{i}c_{zx})S_y + (a_z - \mathrm{i}c_{xy})S_z - \frac{1}{3}(b_x + b_y + b_z)(S_x^2 + S_y^2 + S_z^2)$$

This expression shows that any 3×3 complex matrix can indeed be written in terms of $\mathbb{I}_3$, S_x, S_y, and S_z. However, it's not a linear function of S_x, S_y, and S_z because of the presence of the squared terms S_x^2, S_y^2, and S_z^2.

■

Final Exam

Problem 1 - Scattering in Born Approximation and Beyond
In the lectures, we derived the elastic scattering amplitude from $\mathbf{k}$ to $\mathbf{k}' = k\hat{\mathbf{r}}$ in Born approximation,

$$f_{\mathbf{k}}^{(1)}(\hat{\mathbf{r}}) = -\frac{m}{2\pi\hbar^2}\int_{\mathbb{R}^3} \mathrm{d}^3\mathbf{r}' \mathrm{e}^{-\mathrm{i}\mathbf{q}\cdot\mathbf{r}'} V(\mathbf{r}') = -\frac{m}{2\pi\hbar^2} V(\mathbf{q}),$$

where $\mathbf{q} = \mathbf{k}' - \mathbf{k}$ is the momentum transfer. (Superscript 1 reminds us that this is first order in V.)

1. Express the momentum transfer wave number $q = |\mathbf{q}|$ in terms of the scattering angle θ.
2. Derive an expression for the scattering amplitude in the Born approximation for the special case of an arbitrary spherically symmetric potential V. Your final formula should be an integral only over r.
3. By using the previous expression (from part 2) for the scattering amplitude, what does optical theorem yield for the total cross section σ? Interpret/explain your finding.
4. One may go beyond the Born approximation by expanding the scattering amplitude in higher orders of the potential V,

$$f_{\mathrm{k}} = f_{\mathrm{k}}^{(1)} + f_{\mathrm{k}}^{(2)} + \ldots$$

The 2nd order scattering amplitude is (no need to prove this)

$$f_{\mathbf{k}}^{(2)}(\hat{\mathbf{r}}) = \left(-\frac{m}{2\pi\hbar^2}\right)^2 \int_{\mathbb{R}^3} \mathrm{d}^3\mathbf{p} \frac{V(\mathbf{k}' - \mathbf{p})\, V(\mathbf{p} - \mathbf{k})}{2\pi^2(\mathbf{p}^2 - \mathbf{k}^2 - \mathrm{i}\eta)},$$

where η denotes a positive infinitesimal. Evaluate the total cross section σ to second order in V and show that the following two methods agree: (i) use the optical theorem, (ii) use $\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = |f_{\mathbf{k}}(\hat{\mathbf{r}})|^2$ and integrate over angles. You do not need to assume that V is spherically symmetric. Hint:

$$\frac{1}{x - \mathrm{i}\eta} = P\frac{1}{x} + \mathrm{i}\pi\delta(x).$$

Solution. 1. For the momentum transfer magnitude, we have

$$\begin{aligned}
|\mathbf{q}|^2 &= |\mathbf{k}' - \mathbf{k}|^2 \\
&= \mathbf{k}'^2 + \mathbf{k}^2 - 2\mathbf{k}' \cdot \mathbf{k} \\
&= k^2 + k^2 - 2k^2\cos(\theta) \\
&= 2k^2(1 - \cos(\theta)) \\
&= 4k^2 \sin^2\left(\frac{\theta}{2}\right).
\end{aligned}$$

Therefore,

$$q = 2k\sin\left(\frac{\theta}{2}\right).$$

2. For a spherically symmetric potential $V(r)$, the scattering amplitude is

$$f_k(\theta) = -\frac{m}{2\pi\hbar^2}\int \mathrm{e}^{-\mathrm{i}\mathbf{q}\cdot\mathbf{r}'} V(r')\, \mathrm{d}^3\mathbf{r}'.$$

In spherical coordinates, with $\mathbf{q}$ along the z-axis (due to rotational symmetry), we have

$$\begin{aligned} f_k(\theta) &= -\frac{m}{2\pi\hbar^2}\int_0^\infty r'^2 V(r')\,\mathrm{d}r' \int_0^\pi \sin(\theta')\,\mathrm{d}\theta' \int_0^{2\pi} \mathrm{e}^{-\mathrm{i}qr'\cos(\theta')}\,\mathrm{d}\phi' \\ &= -\frac{m}{2\pi\hbar^2}(2\pi)\int_0^\infty r'^2 V(r')\,\mathrm{d}r' \int_0^\pi \sin(\theta')\mathrm{e}^{-\mathrm{i}qr'\cos(\theta')}\,\mathrm{d}\theta' \\ &= -\frac{m}{\hbar^2}\int_0^\infty rV(r)\left(\frac{2\sin(qr)}{qr}\right)\mathrm{d}r \\ &= -\frac{2m}{\hbar^2}\int_0^\infty \frac{\sin(qr)}{qr} rV(r)\,\mathrm{d}r. \end{aligned}$$

3. The optical theorem (Eq. 273) states that

$$\sigma = \frac{4\pi}{k}\Im(f_k(\theta=0)).$$

When $\theta = 0$, then $q = 0$, and $\frac{\sin(qr)}{qr} \to 1$. Therefore $\Im(f_k(0)) = 0$ for real $V(r)$, implying $\sigma = 0$.

4. For the second-order cross section, we solve this with the two proposed methods.

   (i) **Using optical theorem:** The scattering amplitude to second-order in the potential V is given by

$$f_k = f_k^{(1)} + f_k^{(2)},$$

where

$$\begin{aligned} f_k^{(1)}(\mathbf{r}) &= -\frac{m}{2\pi\hbar^2}V(q), \\ f_k^{(2)}(\mathbf{r}) &= \left(-\frac{m}{2\pi\hbar^2}\right)^2 \int_{\mathbb{R}^3} \frac{V(\mathbf{k'}-\mathbf{p})V(\mathbf{p}-\mathbf{k})}{2\pi^2(\mathbf{p}^2-\mathbf{k}^2-\mathrm{i}\eta)}\,\mathrm{d}\mathbf{p}^3. \end{aligned}$$

Using the hint

$$\frac{1}{x-\mathrm{i}\eta} = P\frac{1}{x} + \mathrm{i}\pi\delta(x),$$

and by letting $x = \mathbf{p}^2 - \mathbf{k}^2$, we get that

$$f_k^{(2)}(\mathbf{r}) = \frac{m^2}{8\pi^4\hbar^4}\int_{\mathbb{R}^3} V(\mathbf{k'}-\mathbf{p})V(\mathbf{p}-\mathbf{k})\left(P\frac{1}{\mathbf{p}^2-\mathbf{k}^2} + i\pi\delta(\mathbf{p}^2-\mathbf{k}^2)\right)\mathrm{d}\mathbf{p}^3.$$

Taking the imaginary parts of both equations, we get

$$\begin{aligned} \Im\left(f_k^{(1)}(0)\right) &= 0, \\ \Im\left(f_k^{(2)}(0)\right) &= \frac{m^2}{8\pi^3\hbar^4}\int_{\mathbb{R}^3} V(\mathbf{k'}-\mathbf{p})V(\mathbf{p}-\mathbf{k})\,\delta(\mathbf{p}^2-\mathbf{k}^2)\,\mathrm{d}\mathbf{p}^3. \end{aligned}$$

Thus, the total cross section by the optical theorem is

$$\begin{aligned}
\sigma &= \frac{4\pi}{k}\left[\Im\left(f_k^{(1)}(0)\right) + \Im\left(f_k^{(2)}(0)\right)\right] \\
&= \frac{m^2}{2k\pi^2\hbar^4}\int_{\mathbb{R}^3} V(\mathbf{k}'-\mathbf{p})V(\mathbf{p}-\mathbf{k})\,\delta(\mathbf{p}^2-\mathbf{k}^2)\ \mathrm{d}\mathbf{p}^3 \\
&= \frac{m^2}{2k\pi^2\hbar^4}\int_S\int_{-\infty}^{\infty} V(\mathbf{k}'-\mathbf{p})V(\mathbf{p}-\mathbf{k})\,\delta(\mathbf{p}^2-\mathbf{k}^2)\,\mathbf{p}^2\,\mathrm{d}\mathbf{p}\,\mathrm{d}\Omega \\
&= \frac{m^2}{2k\pi^2\hbar^4}\int_S\int_{-\infty}^{\infty} V(\mathbf{k}'-\mathbf{p})V(\mathbf{p}-\mathbf{k})\,\left(\frac{1}{2|\mathbf{k}|}\left(\delta(\mathbf{p}-|\mathbf{k}|)+\delta(\mathbf{p}+|\mathbf{k}|)\right)\right)\,\mathbf{p}^2\,\mathrm{d}\mathbf{p}\,\mathrm{d}\Omega \\
&= \frac{m^2}{2k\pi^2\hbar^4}\frac{1}{2|\mathbf{k}|}\left[\int_S\int_{-\infty}^{\infty} V(\mathbf{k}'-\mathbf{p})V(\mathbf{p}-\mathbf{k})\,\delta(\mathbf{p}-|\mathbf{k}|)\,\mathbf{p}^2\,\mathrm{d}\mathbf{p}\,\mathrm{d}\Omega\right. \\
&\qquad\qquad\left.+\int_S\int_{-\infty}^{\infty} V(\mathbf{k}'-\mathbf{p})V(\mathbf{p}-\mathbf{k})\,\delta(\mathbf{p}+|\mathbf{k}|)\,\mathbf{p}^2\,\mathrm{d}\mathbf{p}\,\mathrm{d}\Omega\right] \\
&= \frac{m^2}{2k\pi^2\hbar^4}\frac{1}{2|\mathbf{k}|}\left[\int_S V(\mathbf{k}'-|\mathbf{k}|)V(0)\,\mathbf{k}^2\,\mathrm{d}\Omega + \int_S V(\mathbf{k}'+|\mathbf{k}|)V(-|\mathbf{k}|-\mathbf{k})\,\mathbf{k}^2\,\mathrm{d}\Omega\right] \\
&= \frac{m^2}{4\pi^2\hbar^4}\left[\int_S V(\mathbf{q})V(0)\ \mathrm{d}\Omega + \int_S V(\mathbf{k}'+|\mathbf{k}|)V(-|\mathbf{k}|-\mathbf{k})\ \mathrm{d}\Omega\right],
\end{aligned}$$

where $S \subset \mathbb{S}^1$ is the surface integral over the appropriate portion of the unit sphere. Note that in the fourth equality, the following property was used

$$\int_{-\infty}^{\infty} f(x)\delta(x^2-a^2)\,\mathrm{d}x = \int_{-\infty}^{\infty} f(x)\left[\frac{1}{2|a|}\Big(\delta(x+|a|)+\delta(x-|a|)\Big)\right]\mathrm{d}x.$$

The second integral over Ω will evaluate to zero since $V(\mathbf{k}'+|\mathbf{k}|)$ is unphysical. Due to the optical theorem being a forward elastic scattering, we have that $\mathbf{k}'=\mathbf{k}$, so that $\mathbf{p}=0$. Thus, we have

$$\sigma = \frac{m^2}{4\pi^2\hbar^4}\int_S \left(V(\mathbf{q})\right)^2\ \mathrm{d}\Omega.$$

(ii) **Direct integration:** Consider

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = |f_k(\hat{\mathbf{r}})|^2.$$

Integrating, we get

$$\begin{aligned}
\sigma &= \int_S \left|f_k^{(1)} + f_k^{(2)}\right|^2 \mathrm{d}\Omega \\
&= \int_S \left[\left|f_k^{(1)}\right|^2 + 2\Re\left(f_k^{(1)*}f_k^{(2)}\right) + \left|f_k^{(2)}\right|^2\right]\mathrm{d}\Omega.
\end{aligned}$$

The cross term $f_k^{(1)*}f_k^{(2)}$ will be of order V^3 and $\left|f_k^{(2)}\right|^2$ will be of order V^4, so we will neglect them. Thus, we have

$$\begin{aligned}
\sigma &= \int_S \left|f_k^{(1)}\right|^2 \mathrm{d}\Omega \\
&= \int_S \left|-\frac{m}{2\pi\hbar^2}V(q)\right|^2 \mathrm{d}\Omega \\
&= \frac{m^2}{4\pi^2\hbar^4}\int_S |V(q)|^2\,\mathrm{d}\Omega,
\end{aligned}$$

which matches what we found in method (i).

■

Problem 2 - Angular Momenta and the Wigner-Eckart Theorem

1. Consider a rank-k tensor operator $T_q^{(k)}$. Show that a state with angular momentum $j \leq k/2$ cannot have a non-zero average of $T_q^{(k)}$.
2. Consider an electron (spin-1/2) in a state with an orbital angular momentum $l = 1$. A spin-orbit interaction Hamiltonian can be described by a term $H_{\text{SOC}} = \alpha \mathbf{S} \cdot \mathbf{L}$, where $\mathbf{S}, \mathbf{L}$ are the respective spin and orbital angular momentum operators. Find a suitable complete set of commuting observables and use it to find the energies of H_{SOC} and their degeneracies.
3. Consider a perturbation $H_{\text{Z}} = \beta S_z$ in the above Hamiltonian H_{SOC}. Evaluate the first order corrections to the energies of H_{SOC}.
4. Between which eigenstates of H_{SOC} does S_z have non-zero off-diagonal elements?
5. Consider a spin-1 system with Hamiltonian $H = aS_z + bS_x$. Find its eigenvalues and eigenvectors.

Solution. 1. From the Wigner-Eckart theorem (Eq. 321), we know that matrix elements of a rank-k tensor operator are given by

$$\left\langle \alpha' j' m' \middle| T_q^{(k)} \middle| \alpha j m \right\rangle = \left\langle \alpha' j' \middle\| T^{(k)} \middle\| \alpha j \right\rangle \langle j' m' | kq, jm \rangle .$$

For diagonal elements ($j' = j$, $m' = m$), the Clebsch-Gordan coefficient $\langle j'm'|kq, jm\rangle$ must be non-zero for $T_q^{(k)}$ to have a non-zero expectation value. For the Clebsch-Gordan coefficient to be non-zero, we must have $|k - j| \leq j$. Thus, we have

$$k - j \leq j \implies k \leq 2j.$$

Thus, if $j \leq \frac{k}{2}$, the expectation value must vanish.

2. The total angular momentum $\mathbf{J} = \mathbf{S} + \mathbf{L}$ can be used to derive an expression for $\mathbf{S} \cdot \mathbf{L}$. We have

$$\begin{aligned} \mathbf{J}^2 &= (\mathbf{S} + \mathbf{L})^2 \\ &= \mathbf{S}^2 + 2\mathbf{S} \cdot \mathbf{L} + \mathbf{L}^2 \\ \implies \mathbf{S} \cdot \mathbf{L} &= \frac{1}{2}\left(J^2 - S^2 - L^2\right). \end{aligned}$$

The total angular momentum $\mathbf{J}$ commutes with H_{SOC}, *i.e.* $[\mathbf{J}, H_{\text{SOC}}] = 0$, since

$$\begin{aligned} H_{\text{SOC}} &= \alpha \mathbf{S} \cdot \mathbf{L} \\ &= \frac{\alpha}{2}\left(J^2 - L^2 - S^2\right). \end{aligned}$$

A complete set of commuting observables is $\left\{J^2, J_z, L^2, S^2\right\}$. We have $\ell = 1$ and $s = \frac{1}{2}$, thus

$$\begin{aligned} L^2 |\ell, m_\ell\rangle &= 2\hbar^2 |\ell, m_\ell\rangle , \\ S^2 |s, m_s\rangle &= \frac{3\hbar^2}{4} |s, m_s\rangle . \end{aligned}$$

The possible values of total angular momentum j are $|\ell - s| \leq j \leq \ell + s$, giving us $j = \frac{3}{2}$ or $j = \frac{1}{2}$.

- **For $j = \frac{3}{2}$:** We have

$$J^2 = \frac{15\hbar^2}{4} \implies H_{\text{SOC}} = \frac{\alpha}{2}\left(\frac{15}{4} - 2 - \frac{3}{4}\right)\hbar^2 = \frac{\alpha\hbar^2}{2}.$$

  The $j = \frac{3}{2}$ states are 4-fold degenerate $\left(m_j = \pm\frac{3}{2}, \pm\frac{1}{2}\right)$ with energy $\frac{\alpha\hbar^2}{2}$.

- **For $j = \frac{1}{2}$:** We have

$$J^2 = \frac{3\hbar^2}{4} \implies H_{\text{SOC}} = \frac{\alpha}{2}\left(\frac{3}{4} - 2 - \frac{3}{4}\right)\hbar^2 = -\alpha\hbar^2.$$

  The $j = \frac{1}{2}$ states are 2-fold degenerate $\left(m_j = \pm\frac{1}{2}\right)$ with energy $-\alpha\hbar^2$.

3. The first-order correction to the energy due to the perturbation is given by

$$\Delta E^{(1)} = \langle j, m_j | H_Z | j, m_j \rangle = \beta \langle j, m_j | S_z | j, m_j \rangle .$$

Using the Wigner-Eckart theorem (Eq. 321), we have

$$\langle j, m_j | S_z | j, m_j \rangle = \frac{\langle j || S || j \rangle}{2j+1} m_j.$$

- For $j = \frac{3}{2}$ states, we have $\left\langle \frac{3}{2} \middle| |S| \middle| \frac{3}{2} \right\rangle = \hbar\sqrt{3}$, giving first-order corrections

$$\Delta E^{(1)}_{j=\frac{3}{2}} = \beta\hbar\frac{m_j}{2},$$

  which gives energy corrections of $\pm\frac{\hbar\beta}{2}$ for $m_j = \pm\frac{3}{2}$ and $\pm\frac{\hbar\beta}{6}$ for $m_j = \pm\frac{1}{2}$.
- For $j = \frac{1}{2}$ states, we have $\left\langle \frac{1}{2} \middle| |S| \middle| \frac{1}{2} \right\rangle = -\hbar\sqrt{3}$, giving first-order corrections

$$\Delta E^{(1)}_{j=\frac{1}{2}} = -\beta\hbar\frac{m_j}{2},$$

  which gives energy corrections of $\mp\frac{\hbar\beta}{6}$ for $m_j = \pm\frac{1}{2}$.

An alternative way is to use the Clebsch-Gordon coefficients from the following table.

- **For $j = \frac{3}{2}$:** In Clebsch-Gordon coefficients, we have the $\left| j = \frac{3}{2}, m_j \right\rangle$ states composed of $|\ell, m_\ell; s, m_s\rangle$. For all m_j values, we have
  - $m_j = \frac{3}{2}$**:** The state is

$$\left| j = \frac{3}{2}, m_j = \frac{3}{2} \right\rangle = \left| 1, 1; \frac{1}{2}, \frac{1}{2} \right\rangle,$$

    which gives

$$\beta \langle S_z \rangle = \frac{\hbar}{2}\beta.$$

  - $m_j = \frac{1}{2}$**:** The state is

$$\left| j = \frac{3}{2}, m_j = \frac{1}{2} \right\rangle = \sqrt{\frac{2}{3}} \left| 1, 0; \frac{1}{2}, \frac{1}{2} \right\rangle + \sqrt{\frac{1}{3}} \left| 1, 1; \frac{1}{2}, -\frac{1}{2} \right\rangle,$$

    which gives

$$\beta \langle S_z \rangle = \frac{\hbar}{6}\beta.$$

  - $m_j = -\frac{1}{2}$**:** The state is

$$\left| j = \frac{3}{2}, m_j = -\frac{1}{2} \right\rangle = \sqrt{\frac{2}{3}} \left| 1, 0; \frac{1}{2}, -\frac{1}{2} \right\rangle + \sqrt{\frac{1}{3}} \left| 1, -1; \frac{1}{2}, \frac{1}{2} \right\rangle,$$

    which gives

$$\beta \langle S_z \rangle = -\frac{\hbar}{6}\beta.$$

– $m_j = -\frac{3}{2}$**:** The state is

$$\left|j = \frac{3}{2}, m_j = -\frac{3}{2}\right\rangle = \left|1, -1; \frac{1}{2}, -\frac{1}{2}\right\rangle,$$

which gives

$$\beta \langle S_z \rangle = -\frac{\hbar}{2}\beta.$$

- **For** $j = \frac{1}{2}$**:** In Clebsch-Gordon coefficients, we have the $\left|j = \frac{1}{2}, m_j\right\rangle$ states composed of $|\ell, m_\ell; s, m_s\rangle$. For all m_j values, we have
  – $m_j = \frac{1}{2}$**:** The state is

$$\left|j = \frac{1}{2}, m_j = \frac{1}{2}\right\rangle = \sqrt{\frac{1}{3}}\left|1, 0; \frac{1}{2}, \frac{1}{2}\right\rangle - \sqrt{\frac{2}{3}}\left|1, 1; \frac{1}{2}, -\frac{1}{2}\right\rangle,$$

which gives

$$\beta \langle S_z \rangle = \frac{\hbar}{3}\beta.$$

  – $m_j = -\frac{1}{2}$**:** The state is

$$\left|j = \frac{1}{2}, m_j = -\frac{1}{2}\right\rangle = \sqrt{\frac{1}{3}}\left|1, 0; \frac{1}{2}, -\frac{1}{2}\right\rangle - \sqrt{\frac{2}{3}}\left|1, -1; \frac{1}{2}, \frac{1}{2}\right\rangle,$$

which gives

$$\beta \langle S_z \rangle = -\frac{\hbar}{3}\beta.$$

Therefore, the first-order corrections to the energies are

- **For** $j = \frac{3}{2}$**:**

$$\Delta E^{(1)}_{\frac{3}{2}} = \frac{\hbar\beta}{2}, \qquad \Delta E^{(1)}_{\frac{1}{2}} = \frac{\hbar\beta}{6},$$
$$\Delta E^{(1)}_{-\frac{1}{2}} = -\frac{\hbar\beta}{6}, \qquad \Delta E^{(1)}_{-\frac{3}{2}} = -\frac{\hbar\beta}{2}.$$

- **For** $j = \frac{1}{2}$**:**

$$\Delta E^{(1)}_{\frac{1}{2}} = \frac{\hbar\beta}{3}, \qquad \Delta E^{(1)}_{-\frac{1}{2}} = -\frac{\hbar\beta}{3}.$$

4. Since S_z is a vector (rank-1) operator, it follows from angular momentum addition rules that it can only connect states with $|j - j'| \leq 1$ and $\Delta m_j = 0$. Therefore, S_z has non-zero matrix elements between:

   - States with the same j ($\Delta j = 0$) and the same m_j (diagonal elements)
   - States with $j = \frac{3}{2}$ and $j = \frac{1}{2}$ ($\Delta j = \pm 1$), but only for states with $m_j = \pm\frac{1}{2}$
   - Note that the $m_j = \pm\frac{3}{2}$ states of $j = \frac{3}{2}$ cannot connect to any $j = \frac{1}{2}$ states due to angular momentum conservation

   These selection rules come directly from the properties of the Clebsch-Gordan coefficients in the Wigner-Eckart theorem for a vector operator.

5. For spin-1, the matrices for S_z and S_x in the standard basis are given by

$$S_z = \hbar \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \qquad \text{and} \qquad S_x = \frac{\hbar}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}.$$

From those, we have

$$\begin{aligned}
\frac{H}{\hbar} &= a\frac{S_z}{\hbar} + b\frac{S_x}{\hbar} \\
&= a\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} + b\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \\
&= \begin{pmatrix} a & \frac{b}{\sqrt{2}} & 0 \\ \frac{b}{\sqrt{2}} & 0 & \frac{b}{\sqrt{2}} \\ 0 & \frac{b}{\sqrt{2}} & -a \end{pmatrix}.
\end{aligned}$$

The characteristic equation is

$$\det(H - \lambda\mathbb{I}) = \begin{vmatrix} a-\lambda & \frac{b}{\sqrt{2}} & 0 \\ \frac{b}{\sqrt{2}} & 0-\lambda & \frac{b}{\sqrt{2}} \\ 0 & \frac{b}{\sqrt{2}} & -a-\lambda \end{vmatrix} = 0 \implies \lambda^3 - (a^2+b^2)\lambda = 0$$

giving eigenvalues

$$\lambda_1 = -\sqrt{a^2+b^2}, \qquad \lambda_2 = 0, \qquad \lambda_3 = \sqrt{a^2+b^2}.$$

- **For** $\lambda_1 = -\sqrt{a^2+b^2}$**:** We have

$$\begin{aligned}
\begin{pmatrix} a-\lambda_1 & \dfrac{b}{\sqrt{2}} & 0 \\ \dfrac{b}{\sqrt{2}} & 0-\lambda_1 & \dfrac{b}{\sqrt{2}} \\ 0 & \dfrac{b}{\sqrt{2}} & -a-\lambda_1 \end{pmatrix} |\lambda_1\rangle &= \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} \\
\begin{pmatrix} a+\sqrt{a^2+b^2} & \dfrac{b}{\sqrt{2}} & 0 \\ \dfrac{b}{\sqrt{2}} & \sqrt{a^2+b^2} & \dfrac{b}{\sqrt{2}} \\ 0 & \dfrac{b}{\sqrt{2}} & -a+\sqrt{a^2+b^2} \end{pmatrix} \begin{pmatrix} \lambda_{11} \\ \lambda_{12} \\ \lambda_{13} \end{pmatrix} &= \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} \\
\implies &\begin{cases} \left(a+\sqrt{a^2+b^2}\right)\lambda_{11} + \dfrac{b}{\sqrt{2}}\lambda_{12} = 0 \\ \dfrac{b}{\sqrt{2}}\lambda_{11} + \sqrt{a^2+b^2}\lambda_{12} + \dfrac{b}{\sqrt{2}}\lambda_{13} = 0 \\ \dfrac{b}{\sqrt{2}}\lambda_{12} + \left(-a+\sqrt{a^2+b^2}\right)\lambda_{13} = 0 \end{cases} \\
\implies |\lambda_1\rangle &= \begin{pmatrix} \dfrac{2a^2+b^2-2a\sqrt{a^2+b^2}}{b^2} \\ \dfrac{a\sqrt{2}-\sqrt{2}\sqrt{a^2+b^2}}{b} \\ 1 \end{pmatrix}.
\end{aligned}$$

- **For** $\lambda_2 = 0$**:** We have

$$\begin{pmatrix} a-\lambda_2 & \frac{b}{\sqrt{2}} & 0 \\ \frac{b}{\sqrt{2}} & 0-\lambda_2 & \frac{b}{\sqrt{2}} \\ 0 & \frac{b}{\sqrt{2}} & -a-\lambda_2 \end{pmatrix} |\lambda_2\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

$$\begin{pmatrix} a & \frac{b}{\sqrt{2}} & 0 \\ \frac{b}{\sqrt{2}} & 0 & \frac{b}{\sqrt{2}} \\ 0 & \frac{b}{\sqrt{2}} & -a \end{pmatrix} \begin{pmatrix} \lambda_{21} \\ \lambda_{22} \\ \lambda_{23} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

$$\implies \begin{cases} a\lambda_{21} + \frac{b}{\sqrt{2}}\lambda_{22} = 0 \\ \frac{b}{\sqrt{2}}\lambda_{21} + \frac{b}{\sqrt{2}}\lambda_{23} = 0 \\ \frac{b}{\sqrt{2}}\lambda_{22} - a\lambda_{23} = 0 \end{cases}$$

$$\implies |\lambda_1\rangle = \begin{pmatrix} -1 \\ \frac{a\sqrt{2}}{b} \\ 1 \end{pmatrix}.$$

- **For** $\lambda_3 = \sqrt{a^2+b^2}$**:** We have

$$\begin{pmatrix} a-\lambda_3 & \frac{b}{\sqrt{2}} & 0 \\ \frac{b}{\sqrt{2}} & 0-\lambda_3 & \frac{b}{\sqrt{2}} \\ 0 & \frac{b}{\sqrt{2}} & -a-\lambda_3 \end{pmatrix} |\lambda_2\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

$$\begin{pmatrix} a-\sqrt{a^2+b^2} & \frac{b}{\sqrt{2}} & 0 \\ \frac{b}{\sqrt{2}} & \sqrt{a^2+b^2} & \frac{b}{\sqrt{2}} \\ 0 & \frac{b}{\sqrt{2}} & -a-\sqrt{a^2+b^2} \end{pmatrix} \begin{pmatrix} \lambda_{31} \\ \lambda_{32} \\ \lambda_{33} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

$$\implies \begin{cases} \left(a-\sqrt{a^2+b^2}\right)\lambda_{31} + \frac{b}{\sqrt{2}}\lambda_{32} = 0 \\ \frac{b}{\sqrt{2}}\lambda_{31} - \sqrt{a^2+b^2}\lambda_{32} + \frac{b}{\sqrt{2}}\lambda_{13} = 0 \\ \frac{b}{\sqrt{2}}\lambda_{32} + \left(-a-\sqrt{a^2+b^2}\right)\lambda_{33} = 0 \end{cases}$$

$$\implies |\lambda_1\rangle = \begin{pmatrix} \frac{2a^2+b^2+2a\sqrt{a^2+b^2}}{b^2} \\ \frac{a\sqrt{2}+\sqrt{2}\sqrt{a^2+b^2}}{b} \\ 1 \end{pmatrix}.$$

Thus, the normalized eigenvectors are

$$\left|\lambda = -\sqrt{a^2+b^2}\right\rangle = \begin{pmatrix} \dfrac{2a^2+b^2-2a\sqrt{a^2+b^2}}{b^2} \\ \dfrac{a\sqrt{2}-\sqrt{2}\sqrt{a^2+b^2}}{b} \\ 1 \end{pmatrix},$$

$$|\lambda = 0\rangle = \begin{pmatrix} -1 \\ \dfrac{a\sqrt{2}}{b} \\ 1 \end{pmatrix},$$

$$\left|\lambda = \sqrt{a^2+b^2}\right\rangle = \begin{pmatrix} \dfrac{2a^2+b^2+2a\sqrt{a^2+b^2}}{b^2} \\ \dfrac{a\sqrt{2}+\sqrt{2}\sqrt{a^2+b^2}}{b} \\ 1 \end{pmatrix}.$$

■

Problem 3 - Semiclassical Approximations

1. Consider a 1D potential $V = \alpha|x|^q$ where $q > 0, \alpha > 0$. Find the bound state energies in terms of $\alpha, m, \hbar, q$ in the semiclassical approximation. Present some kind of limiting case of your choosing to check whether your result makes sense. You may denote simply by letter c_q the number

$$\int_0^1 \mathrm{d}z\sqrt{1-z^q} = \frac{\sqrt{\pi}\,\Gamma\left(1+\frac{1}{q}\right)}{2\Gamma\left(\frac{3}{2}+\frac{1}{q}\right)} \equiv c_q.$$

2. Show that for a rotationally symmetric potential $V(r)$, the radial $l = 0$ (s-wave) Schrodinger equation is equivalent to a one-dimensional one with a boundary condition that the wave function vanishes at $r = 0$.

3. Consider a rotationally symmetric scattering potential

$$V(r) = \begin{cases} 0, & r > a, \\ \left(\frac{r^2}{a^2} - 1\right) V_0, & 0 \leq r \leq a, \end{cases}$$

where $V_0 > 0$. Find the bound state energies of s orbitals ($l = 0$ orbital angular momentum) in the semiclassical approximation. In the same approximation, estimate the number of bound s-wave orbitals in terms of a, V_0, $\hbar$, and m. Interpret your findings. Hint: The Bohr-Sommerfeld quantization condition is now $\frac{1}{\hbar}\int_0^{r_0} \mathrm{d}r p(r) = \left(n + \frac{3}{4}\right)\pi$ because of the boundary condition from part 2.

Solution. 1. In the semi-classical approximation, we use the WKB approximation, where the quantization condition (Eq. 112) is given by

$$\int_b^a p(x)\,\mathrm{d}x = \pi\hbar\left(n + \frac{1}{2}\right),$$

where $p(x) = \sqrt{2m(E - V(x))}$ is the classical momentum and a and b are the classical turning points.

At the turning points, the potential is equal to the energy. Since our potential is symmetric around

$x = 0$, then we have that $a = -b \equiv x_0$. For our potential $V(x) = \alpha|x|^q$, we have

$$\begin{aligned}
V(x_0) &= E \\
\alpha|x_0|^q &= E \\
|x_0| &= \left(\frac{E}{\alpha}\right)^{\frac{1}{q}} \\
x_0 &= \pm\left(\frac{E}{\alpha}\right)^{\frac{1}{q}}.
\end{aligned}$$

Let the positive value of x_0 equal a and the negative value equal b. Recall the the energy E is the bound state energy. Thus,

$$\begin{aligned}
\int_{-x_0}^{x_0} \sqrt{2m(E-\alpha|x|^q)}\,\mathrm{d}x &= 2\int_0^{x_0} \sqrt{2m(E-\alpha|x|^q)}\,\mathrm{d}x \\
&= 2\sqrt{2mE}\int_0^{x_0} \sqrt{1-\frac{\alpha|x|^q}{E})}\,\mathrm{d}x \\
&= 4\sqrt{2mE}\int_0^{x_0} \sqrt{1-\frac{\alpha x^q}{E}}\,\mathrm{d}x \\
&= 4\sqrt{2mE}x_0\int_0^{1} \sqrt{1-z^q}\,\mathrm{d}z \\
&= 4\sqrt{2mE}\left(\frac{E}{\alpha}\right)^{\frac{1}{q}} c_q,
\end{aligned}$$

where we substituted $z = \frac{x}{x_0} \implies \mathrm{d}x = x_0\,\mathrm{d}z$ and used $x_0 = \left(\frac{E}{\alpha}\right)^{\frac{1}{q}}$.
Setting this equal to $2\pi\hbar\left(n+\frac{1}{2}\right)$, we get

$$\begin{aligned}
4\sqrt{2mE}\left(\frac{E}{\alpha}\right)^{\frac{1}{q}} c_q &= 2\pi\hbar\left(n+\frac{1}{2}\right) \\
\sqrt{E}\left(\frac{E}{\alpha}\right)^{\frac{1}{q}} &= \frac{\pi\hbar\left(n+\frac{1}{2}\right)}{2c_q\sqrt{2m}} \\
E^{\frac{q+2}{2q}} &= \frac{\pi\hbar\left(n+\frac{1}{2}\right)}{2c_q\sqrt{2m}}\alpha^{\frac{1}{q}} \\
E_n &= \left[\frac{\pi\hbar\left(n+\frac{1}{2}\right)}{2c_q\sqrt{2m}}\right]^{\frac{2q}{q+2}}\alpha^{\frac{2}{q+2}}.
\end{aligned}$$

We can check $q = 1$, but we suggest using $q = 2$ instead since the exponent, given by $\frac{2q}{q+2}$, will evaluate to unity. Solving c_q for $q = 2$ gives

$$\begin{aligned}
c_2 &= \frac{\sqrt{\pi}\Gamma\left(1+\frac{1}{2}\right)}{2\Gamma\left(\frac{3}{2}+\frac{1}{2}\right)} \\
&= \frac{\sqrt{\pi}}{2}\frac{\Gamma\left(\frac{3}{2}\right)}{\Gamma\left(2\right)} \\
&= \frac{\sqrt{\pi}}{2}\frac{\frac{\sqrt{\pi}}{2}}{1} \\
&= \frac{\pi}{4}.
\end{aligned}$$

Plugging this into the equation for E_n, we get

$$\begin{aligned}
E_n &= \left[\frac{\pi\hbar\left(n+\frac{1}{2}\right)}{2c_2\sqrt{2m}}\right]\alpha^{\frac{1}{2}} \\
&= \left[\frac{\pi\hbar\left(n+\frac{1}{2}\right)}{2\left(\frac{\pi}{4}\right)}\right]\sqrt{\frac{\alpha}{2m}} \\
&= 2\hbar\left(n+\frac{1}{2}\right)\sqrt{\frac{\alpha}{2m}} \\
&= \hbar\sqrt{\frac{2\alpha}{m}}\left(n+\frac{1}{2}\right),
\end{aligned}$$

which matches the exact quantum harmonic oscillator result, where $\omega = \sqrt{\frac{2\alpha}{m}}$.

2. The radial Schrodinger equation for $\ell = 0$ (s-wave) is

$$-\frac{\hbar^2}{2m}\frac{1}{r^2}\frac{\mathrm{d}}{\mathrm{d}r}\left(r^2\frac{\mathrm{d}R(r)}{\mathrm{d}r}\right) + V(r)R(r) = ER(r).$$

Define $u(r) = rR(r)$, then

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}r}\left(r^2\frac{\mathrm{d}R}{\mathrm{d}r}\right) &= \frac{\mathrm{d}}{\mathrm{d}r}\left(r^2\frac{\mathrm{d}}{\mathrm{d}r}\left(\frac{u}{r}\right)\right) \\
&= \frac{\mathrm{d}}{\mathrm{d}r}\left(r\frac{\mathrm{d}u}{\mathrm{d}r} - u\right) \\
&= \frac{\mathrm{d}r}{\mathrm{d}r}\frac{\mathrm{d}u}{\mathrm{d}r} + r\frac{\mathrm{d}^2u}{\mathrm{d}r^2} - \frac{\mathrm{d}u}{\mathrm{d}r} \\
&= r\frac{\mathrm{d}^2u}{\mathrm{d}r^2}.
\end{aligned}$$

Replacing in the radial Schrodinger equation, we have

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2u(r)}{\mathrm{d}r^2} + V(r)u(r) = Eu(r)$$

This is a one-dimensional Schrdinger equation. Since $R(r)$ must be finite at $r = 0$, we must have $u(0) = 0$; hence, a boundary condition that the wave-function vanishes at $r = 0$.

3. For the rotationally symmetric scattering potential given by

$$V(r) = \begin{cases} 0, & r > a, \\ \left(\frac{r^2}{a^2} - 1\right)V_0, & 0 \le r \le a, \end{cases}$$

we use the semi-classical approximation with the Bohr-Sommerfeld quantization condition. We know that the classical turning points are when the potential is equal to the energy. Thus,

$$\begin{aligned}
E &= V(r) \\
E &= \left(\frac{r^2}{a^2} - 1\right)V_0 \\
\frac{E+V_0}{V_0} &= \frac{r^2}{a^2} \\
r_{1,2} &= \pm a\sqrt{\frac{E+V_0}{V_0}}.
\end{aligned}$$

From the given potential, we can see that $r < 0$ is not physical, so the classical turning points are

$$r_1 = 0 \quad \text{and} \quad r_2 = a\sqrt{\frac{E+V_0}{V_0}}.$$

In that case, the Bohr-Sommerfeld quantization condition, as mentioned in the hint, will be

$$\frac{1}{\hbar}\int_0^{a\sqrt{\frac{E+V_0}{V_0}}} p(r)\,\mathrm{d}r = \left(n+\frac{3}{4}\right)\pi,$$

where $p(r) = \sqrt{2m(E - V(r))}$ is the classical momentum. Solving the integral in the quantization condition, we have

$$\begin{aligned}\int_0^a p(r)\,\mathrm{d}r &= \int_0^{a\sqrt{\frac{E+V_0}{V_0}}} \sqrt{2m(E-V(r))}\,\mathrm{d}r \\ &= \int_0^{a\sqrt{\frac{E+V_0}{V_0}}} \sqrt{2m\left(E-\left(\frac{r^2}{a^2}-1\right)V_0\right)}\,\mathrm{d}r.\end{aligned}$$

Let $z = \frac{r}{a} \implies \mathrm{d}r = a\,\mathrm{d}z$, then

$$\begin{aligned}\int_0^{a\sqrt{\frac{E+V_0}{V_0}}} p(r)\,\mathrm{d}r &= a\int_0^{\sqrt{\frac{E+V_0}{V_0}}} \sqrt{2m\left(E-(z^2-1)\,V_0\right)}\,\mathrm{d}z \\ &= a\sqrt{2m}\int_0^{\sqrt{\frac{E+V_0}{V_0}}} \sqrt{E-(z^2-1)\,V_0}\,\mathrm{d}z \\ &= a\sqrt{2m}\int_0^{\sqrt{\frac{E+V_0}{V_0}}} \sqrt{E+V_0-V_0z^2}\,\mathrm{d}z \\ &= a\sqrt{2m(E+V_0)}\int_0^{\sqrt{\frac{E+V_0}{V_0}}} \sqrt{1-\frac{V_0z^2}{E+V_0}}\,\mathrm{d}z \\ &= a\sqrt{2m(E+V_0)}\left(\frac{\pi}{4}\sqrt{\frac{E+V_0}{V_0}}\right),\end{aligned}$$

where the last equality was reached by computing the integral using an online integral calculator. Thus, we have

$$\int_0^{a\sqrt{\frac{E+V_0}{V_0}}} p(r)\,\mathrm{d}r = \sqrt{\frac{2m}{V_0}}\frac{a\pi}{4}(E+V_0).$$

Plugging the value of the integral into the Bohr-Sommerfeld quantization condition, we get

$$\begin{aligned}\frac{1}{\hbar}\int_0^a p(r)\,\mathrm{d}r &= \left(n+\frac{3}{4}\right)\pi \\ \int_0^a p(r)\,\mathrm{d}r &= \pi\hbar\left(n+\frac{3}{4}\right) \\ \sqrt{\frac{2m}{V_0}}\frac{a\pi}{4}(E+V_0) &= \pi\hbar\left(n+\frac{3}{4}\right) \\ E_n &= \sqrt{\frac{V_0}{2m}}\frac{4\hbar}{a}\left(n+\frac{3}{4}\right) - V_0.\end{aligned}$$

For E_n to correspond to a bound state, we must have $E_n < 0$. Solving for n with that condition, we have

$$\begin{aligned} E_n = \sqrt{\frac{V_0}{2m}}\frac{4\hbar}{a}\left(n+\frac{3}{4}\right) - V_0 &< 0 \\ \left(n+\frac{3}{4}\right) &< \sqrt{\frac{2m}{V_0}}\frac{a}{4\hbar}V_0 \\ n &< \frac{a\sqrt{2mV_0}}{4\hbar} - \frac{3}{4}. \end{aligned}$$

Thus, the maximum quantum number $n_{\max}$ is

$$n_{\max} \approx \frac{a\sqrt{2mV_0}}{4\hbar} - \frac{3}{4}.$$

Since $n_{\max}$ must be an integer, we take the largest value less than or equal to the above, *i.e.* take the floor function, getting

$$n_{\max} = \left\lfloor \frac{a\sqrt{2mV_0}}{4\hbar} - \frac{3}{4} \right\rfloor.$$

The total number of bound s-orbitals is then

$$N = n_{\max} + 1 = \left\lfloor \frac{a\sqrt{2mV_0}}{4\hbar} + \frac{1}{4} \right\rfloor.$$

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