Problem 1: Interacting Particles

Two identical bosons are placed in a 1-D infinite square well of length \( a \). They interact with each other weakly, with potential

\[
V(x_1, x_2) = -aV_0 \delta(x_1 - x_2)
\]

where \( V_0 \) is a constant with units of energy.

**a.** For the case \( V_0 = 0 \) (no perturbation), find the wave functions and energies of the ground and first excited states.

**b.** Now including the perturbation (\( V_0 \neq 0 \)), compute the first-order energy shifts for the ground and first excited states.

(a) In terms of the one-particle states (Eq. 2.28) and energies (Eq. 2.27):

Ground state: \( \psi_1^0(x_1, x_2) = \psi_1(x_1)\psi_1(x_2) = \frac{2}{a} \sin \left( \frac{\pi x_1}{a} \right) \sin \left( \frac{\pi x_2}{a} \right) \):

\[
E_1^0 = 2E_1 = \frac{\pi^2h^2}{ma^2}
\]

First excited state: \( \psi_2^0(x_1, x_2) = \frac{1}{\sqrt{2}} [\psi_1(x_1)\psi_2(x_2) + \psi_2(x_1)\psi_1(x_2)] \):

\[
E_2^0 = E_1 + E_2 = \frac{5\pi^2h^2}{2ma^2}
\]

(b)

\[
E_1' = \langle \psi_1^0 | H' | \psi_1^0 \rangle = (-aV_0) \left( \frac{2}{a} \right)^2 \int_0^a \int_0^a \sin^2 \left( \frac{\pi x_1}{a} \right) \sin^2 \left( \frac{\pi x_2}{a} \right) \delta(x_2 - x_2) \, dx_1 \, dx_2
\]

\[
= -\frac{4V_0}{a} \int_0^a \sin^4 \left( \frac{\pi x}{a} \right) \, dx = -\frac{4V_0}{a} \frac{a}{\pi} \int_0^\pi \sin^4 y \, dy = -\frac{4V_0}{\pi} \cdot \frac{3\pi}{8} = -\frac{3}{2} V_0.
\]

\[
E_2' = \langle \psi_2^0 | H' | \psi_2^0 \rangle
\]

\[
= (-aV_0) \left( \frac{2}{a} \right)^2 \int_0^a \int_0^a \left[ \sin \left( \frac{\pi x_1}{a} \right) \sin \left( \frac{2\pi x_2}{a} \right) + \sin \left( \frac{2\pi x_1}{a} \right) \sin \left( \frac{\pi x_2}{a} \right) \right]^2 \delta(x_1 - x_2) \, dx_1 \, dx_2
\]

\[
= -\frac{2V_0}{a} \int_0^a \left[ \sin \left( \frac{\pi x}{a} \right) \sin \left( \frac{2\pi x}{a} \right) + \sin \left( \frac{2\pi x}{a} \right) \sin \left( \frac{\pi x}{a} \right) \right]^2 \, dx
\]

\[
= -\frac{8V_0}{a} \int_0^a \sin^2 \left( \frac{\pi x}{a} \right) \sin^2 \left( \frac{2\pi x}{a} \right) \, dx = -\frac{8V_0}{a} \cdot \frac{a}{\pi} \int_0^\pi \sin^2 y \sin^2(2y) \, dy
\]

\[
= -\frac{8V_0}{\pi} \cdot 4 \int_0^\pi \sin^2 y \sin^2(2y) \, dy = -\frac{32V_0}{\pi} \int_0^\pi \left( \sin^4 y - \sin^6 y \right) \, dy
\]

\[
= -\frac{32V_0}{\pi} \left( \frac{3\pi}{8} - \frac{5\pi}{16} \right) = -2V_0.
\]
Problem 2: Extra Oscillations

Start with the 1-D simple harmonic oscillator, which has Hamiltonian

\[ H_0 = \frac{p^2}{2m} + \frac{1}{2}m\omega^2x^2 \]

and add a perturbation that is itself another oscillation

\[ H_1 = \frac{1}{2}m\omega_1^2x^2 \]

where the frequency of the extra oscillation is much smaller than the unperturbed oscillation, \( \omega_1 \ll \omega \).

a. Find the first-order energy shifts. (Hint: Use ladder operators.)

b. Find the second-order energy shifts.

c. Find the exact energy eigenvalues for the perturbed system and compare to the first and second order results from perturbation theory. (Hint for comparison: use Taylor series expansion of exact result.)

For

\( \hat{H}_0 = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2 \) and \( \hat{H}_1 = \frac{1}{2}m\omega_1^2\hat{x}^2 \)

the first-order correction to the energy is given by

\[ E_n^{(1)} = \langle n|\hat{H}_1|n \rangle = \frac{1}{2}m\omega^2\langle n(|\hat{a}^\dagger|^2|n) \rangle \]

\[ = \frac{1}{2}m\omega^2 \frac{\hbar}{2m\omega} \langle n(|\hat{a} + \hat{a}^\dagger|^2|n) \rangle = \frac{\hbar\omega^2}{4\omega} \langle n(|\hat{a}^\dagger \hat{a} + \hat{a}\hat{a}^\dagger|^2|n) \rangle \]

\[ = \frac{\hbar\omega^2}{4\omega} (2n + 1) = \frac{1}{2} \left( \frac{\omega}{\omega} \right)^2 (n + \frac{1}{2}) \hbar \omega \]

The second-order correction to the energy is given by

\[ E_n^{(2)} = \sum_{k,n} \frac{1}{E_n^{(0)} - E_k^{(0)}} \left( \frac{1}{2}m\omega_k^2 \right)^2 \sum_{k,n} \frac{1}{(n + k + \frac{1}{2})\hbar \omega - (k + \frac{1}{2})\hbar \omega} \]

\[ = \left( \frac{1}{2}m\omega_n^2 \right)^2 \left( \frac{\hbar}{2m\omega} \right)^2 \sum_{k,n} \frac{1}{(n - k)\hbar \omega} \]

\[ = \left( \frac{\hbar\omega_n^2}{4\omega} \right)^2 \sum_{k,n} \frac{(n + 1)(n + 2)(k\hbar_n + 2)^2 + (n)(n - 1)(k\hbar_n - 2)^2}{(n - k)\hbar \omega} \]

\[ = \left( \frac{\hbar\omega_n^2}{4\omega} \right)^2 \left( \frac{(n + 1)(n + 2)}{-2\hbar_n^2} + \frac{n(n - 1)}{2\hbar \omega} \right) = \frac{1}{8} \left( \frac{\omega}{\omega} \right)^4 (n + \frac{1}{2}) \hbar \omega \]

\[ = \hat{\alpha} \hat{\alpha} \]
The eigenvalues of the exact Hamiltonian

\[
\hat{H} = \frac{p^2}{2m} + \frac{1}{2} m (\omega^2 + \omega_1^2) x^2 \sqrt{1 + \epsilon^2} \approx 1 + \frac{1}{2} \epsilon^2 - \frac{1}{8} \epsilon^4 + \ldots
\]

are given by

\[
E_n = (n + \frac{1}{2}) \hbar \sqrt{\omega^2 + \omega_1^2} = (n + \frac{1}{2}) \hbar \omega \sqrt{1 + \left( \frac{\omega_1}{\omega} \right)^2} = (n + \frac{1}{2}) \hbar \omega \left( 1 + \frac{1}{2} \left( \frac{\omega_1}{\omega} \right)^2 - \frac{1}{8} \left( \frac{\omega_1}{\omega} \right)^4 + \ldots \right)
\]

Thus the exact eigenvalues and the perturbative results agree to the order calculated.
Problem 3: Particle on Loop

A particle of mass $m$ moves on a loop of circumference $L$.

a. Find the properly normalized wave functions of the stationary states (look back at Griffiths problem 2.46 for some discussion). Show that these states can be written in the form
\[
\psi_n(x) = \frac{1}{\sqrt{L}} e^{i n \pi x / L}
\]
over $-L/2 < x < L/2$ and with $n = 0, \pm 1, \pm 2, \ldots$ (Solve for these states, don’t just plug into the Schrödinger equation and demonstrate that these are indeed solutions.)

b. Find the energies for the stationary states, which should come out to be
\[
E_n = \frac{2}{m} \left( \frac{n \pi h}{L} \right)^2
\]
Note carefully that all the $n > 0$ states are doubly degenerate (e.g., $n = +1$ and $n = -1$ have the same energy).

c. Add the perturbation
\[
H_1 = -V_0 e^{-x^2/a^2}
\]
to the system, with $a \ll L$ so this is like a little kink in the loop that impedes motion of the particle. Find the first-order energy shifts $E_n^{(1)}$ using degenerate perturbation theory. (Hint 1: Because the states are two-fold degenerate, you can use eq. 6.27 in Griffiths or solve the eigenvalue problem directly. Hint 2: When you compute the integrals for the matrix elements, take advantage of the fact that $a \ll L$, so the perturbation $H_1$ is essentially zero much beyond $-a < x < a$.)

d. If you didn’t already, find the eigenvectors of the perturbing Hamiltonian. In other words, find the linear combinations of $\psi_n$ and $\psi_{-n}$ that diagonalize the perturbing Hamiltonian.

e. These linear combinations are states for which you should be able to use regular (non-degenerate) perturbation theory to compute the energy shifts of the those states. Do so and compare to the degenerate theory results. You better get the same answer!
\[-\frac{\hbar^2}{2m} \frac{d^2 \psi}{dx^2} = E \psi \] (where \(x\) is measured around the circumference), or \(\frac{d^2 \psi}{dx^2} = -k^2 \psi\), with \(k = \frac{\sqrt{2mE}}{\hbar}\), so
\[
\psi(x) = Ae^{ikx} + Be^{-ikx}.
\]
But \(\psi(x + L) = \psi(x)\), since \(x + L\) is the same point as \(x\), so
\[
Ae^{ikx}e^{ikL} + Be^{-ikx}e^{-ikL} = Ae^{ikx} + Be^{-ikx},
\]
and this is true for all \(x\). In particular, for \(x = 0\):

1. \(Ae^{ikL} + Be^{-ikL} = A + B\). And for \(x = \frac{\pi}{2k}\):
\[
Ae^{i\pi/2}e^{ikL} + Be^{-i\pi/2}e^{-ikL} = Ae^{i\pi/2} + Be^{-i\pi/2},
\]
or \(iAe^{ikL} - iBe^{-ikL} = iA - iB\), so

2. \(Ae^{ikL} - Be^{-ikL} = A - B\). Add (1) and (2): \(2Ae^{ikL} = 2A\).

Either \(A = 0\), or else \(e^{ikL} = 1\), in which case \(kL = 2\pi n (n = 0, \pm 1, \pm 2, \ldots)\). But if \(A = 0\), then \(Be^{-ikL} = B\), leading to the same conclusion. So for every positive \(n\) there are two solutions: \(\psi_n^+(x) = Ae^{i(2\pi nx/L)}\) and \(\psi_n^-(x) = Be^{-i(2\pi nx/L)}\) (\(n = 0\) is ok too, but in that case there is just one solution). Normalizing: \(\int_0^L |\psi_n^+|^2 dx = 1 \Rightarrow A = B = 1/\sqrt{L}\). Any other solution (with the same energy) is a linear combination of these.

(a) \[
\psi_n^+ (x) = \frac{1}{\sqrt{L}} e^{i(2\pi nx/L)}; E_n = \frac{2m^2 \pi^2 n^2}{mL^2} (n = 0, 1, 2, 3, \ldots).
\]

With \(a \to -a, b \to -b\), we have:

(c) \[
W_{aa} = W_{bb} = -\frac{V_0}{L} \int_{-L/2}^{L/2} e^{-x^2/a^2} dx \approx -\frac{V_0}{L} \int_{-\infty}^{\infty} e^{-x^2/a^2} dx = -\frac{V_0}{La\sqrt{\pi}}.
\]
\[
W_{ab} = -\frac{V_0}{L} \int_{-L/2}^{L/2} e^{-x^2/a^2} e^{-4\pi na/L} dx \approx -\frac{V_0}{L} \int_{-\infty}^{\infty} e^{-(x^2/a^2 + 4\pi na/L)} dx = -\frac{V_0}{L} a\sqrt{\pi} e^{-(2\pi na/L)^2}.
\]

(We did this integral in Problem 2.22.) In this case \(W_{aa} = W_{bb}\), and \(W_{ab}\) is real, so Eq. 6.26 \(\Rightarrow\)
\[
E_{4a}^+ = W_{aa} \pm |W_{ab}|, \quad \text{or} \quad E_{4a}^+ = \frac{-1}{\sqrt{\pi}} \frac{V_0}{L} \left(1 \mp e^{-(2\pi na/L)^2}\right),
\]
Equation 6.22 \(\Rightarrow\) \(\beta = \frac{\alpha (E_{4a}^+ - W_{aa})}{W_{ab}} = \frac{\alpha}{\sqrt{\pi}} \frac{V_0a}{L} \left[\frac{\pm \sqrt{\pi} (V_0a/L) e^{-(2\pi na/L)^2}}{-\sqrt{\pi} (V_0a/L) e^{-(2\pi na/L)^2}}\right] = \pm \alpha\). Evidently, the “good” linear combinations are:

(d) \[
\psi_+ = \alpha \psi_n - \beta \psi_n = \frac{1}{\sqrt{2}\sqrt{\pi}} \left[e^{i(2\pi nx/L)} - e^{-i(2\pi nx/L)}\right] = i \sqrt{\frac{V_0}{L}} \sin \left(\frac{2\pi nx}{L}\right)
\]
and
\[
\psi_- = \alpha \psi_n + \beta \psi_n = \sqrt{\frac{V_0}{L}} \cos \left(\frac{2\pi nx}{L}\right).
\]
Using Eq. 6.9, we have:

(e) \[
E_{4a}^+ = (\psi_+ | H' | \psi_+ ) = \frac{2}{L} (-V_0) \int_{-L/2}^{L/2} e^{-x^2/a^2} \sin^2 \left(\frac{2\pi nx}{L}\right) dx.
\]
\[
E_{4a}^- = (\psi_- | H' | \psi_- ) = \frac{2}{L} (-V_0) \int_{-L/2}^{L/2} e^{-x^2/a^2} \cos^2 \left(\frac{2\pi nx}{L}\right) dx.
\]
But \( \sin^2 \theta = (1 - \cos 2\theta)/2 \), and \( \cos^2 \theta = (1 + \cos 2\theta)/2 \), so

\[
E_\pm^1 \approx -\frac{V_0}{L} \int_{-\infty}^{\infty} e^{-x^2/a^2} \left[ 1 \pm \cos \left( \frac{4\pi n x}{L} \right) \right] dx = -\frac{V_0}{L} \left[ \int_{-\infty}^{\infty} e^{-x^2/a^2} dx + \int_{-\infty}^{\infty} e^{-x^2/a^2} \cos \left( \frac{4\pi n x}{L} \right) dx \right]
\]

\[
= -\frac{V_0}{L} \left[ \sqrt{\pi} a \pm a \sqrt{\pi} e^{-\left(2\pi na/L\right)^2} \right] = -\frac{V_0 a}{L} \left[ 1 \pm e^{-\left(2\pi na/L\right)^2} \right], \quad \text{same as (b).}
\]
Problem 4: Three-State System

Suppose we have a quantum system that has only three linearly independent states. The Hamiltonian of this system is, in matrix form,

\[
H = V_0 \begin{pmatrix}
1 - \epsilon & 0 & 0 \\
0 & 1 + \epsilon & 0 \\
0 & 0 & 2 + \epsilon
\end{pmatrix}
\]

where \(V_0\) is a constant and \(\epsilon \ll 1\) describes a small perturbation.

a. Find the eigenvalues and eigenvectors of the unperturbed Hamiltonian (\(\epsilon = 0\)). You should find that two of the states are degenerate.

b. By finding the roots of the characteristic equation, solve for the exact energy eigenvalues of the perturbed system (\(\epsilon \neq 0\)). Then use Taylor series to expand each solution up to second order in the parameter \(\epsilon\). Check that these energies have the right behavior in the limit \(\epsilon \to 0\).

c. Starting from the one non-degenerate state of the unperturbed system, calculate the first and second-order energy shifts caused by the perturbation, using non-degenerate perturbation theory. Compare these results to the exact results you found above.

d. Finally, use degenerate perturbation theory to find the first-order energy shifts of the two initially degenerate states. Again, compare these results to the exact results.

(a) \(\chi_1 = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}\), eigenvalue \(V_0\); \(\chi_2 = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}\), eigenvalue \(V_0\); \(\chi_3 = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}\), eigenvalue \(2V_0\).

(b) Characteristic equation: \(\det(H - \lambda) = \begin{vmatrix} V_0(1-\epsilon) - \lambda & 0 & 0 \\ 0 & V_0 - \lambda & \epsilon V_0 \\ 0 & \epsilon V_0 & 2V_0 - \lambda \end{vmatrix} = 0\);

\[
(V_0(1-\epsilon) - \lambda)(V_0 - \lambda) - (\epsilon V_0)^2 = 0 \Rightarrow \lambda_1 = V_0(1-\epsilon),
\]

\[
(V_0 - \lambda)(2V_0 - \lambda) - (\epsilon V_0)^2 = 0 \Rightarrow \lambda_2 = 3V_0 - 3V_0\lambda + (2V_0^2 - \epsilon^2V_0^2) = 0 \Rightarrow \lambda_2 = \frac{V_0}{2} \left[ 3 \pm \sqrt{1 + 4\epsilon^2} \right] \approx \frac{V_0}{2} \left[ 3 \pm (1 + 2\epsilon^2) \right],
\]

\[
\lambda_2 = \frac{V_0}{2} \left( 3 - \sqrt{1 + 4\epsilon^2} \right) \approx V_0(1 - \epsilon^2); \quad \lambda_3 = \frac{V_0}{2} \left( 3 + \sqrt{1 + 4\epsilon^2} \right) \approx V_0(2 + \epsilon^2).
\]
(c) 

\[ H_t = \epsilon V_0 \begin{pmatrix} -1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix} ; \quad E_3^t = \langle \chi_3 | H_t | \chi_3 \rangle = \epsilon V_0 \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 1 & 1 \end{pmatrix} \]

\[ = \epsilon V_0 \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix} = 0 \quad \text{(no first-order correction)} . \]

\[ E_3^t = \sum_{m=1,2} \frac{|\langle \chi_m | H_t | \chi_3 \rangle|^2}{E_3^0 - E_m^0} ; \quad \langle \chi_1 | H_t | \chi_2 \rangle = \epsilon V_0 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \]

\[ = \epsilon V_0 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} = \epsilon V_0 . \]

\[ E_3^0 - E_3^0 = 2 V_0 - V_0 = V_0 . \quad \text{So} \quad E_3^t = (\epsilon V_0)^2 / V_0 = \frac{\epsilon^2 V_0^2}{V_0} . \quad \text{Through second-order, then,} \]

\[ E_3 = E_3^0 + E_3^1 + E_3^2 = 2 V_0 + 0 + \epsilon^2 V_0 = V_0 (2 + \epsilon) \quad \text{(same as we got for } \chi_3 \text{ in (b)}. \]

(d) 

\[ W_{aa} = \langle \chi_1 | H_t | \chi_1 \rangle = \epsilon V_0 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} = \epsilon V_0 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} = -\epsilon V_0 . \]

\[ W_{bb} = \langle \chi_2 | H_t | \chi_2 \rangle = \epsilon V_0 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} = \epsilon V_0 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} = 0 . \]

\[ W_{ab} = \langle \chi_1 | H_t | \chi_2 \rangle = \epsilon V_0 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \]

\[ = \epsilon V_0 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} = 0 . \]

Plug the expressions for \( W_{aa} \), \( W_{bb} \), and \( W_{ab} \) into Eq. 6.27:

\[ E_+^t = \frac{1}{2} \left( -\epsilon V_0 + 0 \pm \sqrt{\epsilon^2 V_0^2 + 0} \right) = \frac{1}{2} (-\epsilon V_0 \pm \epsilon V_0) = \{0, -\epsilon V_0\} . \]

To first-order, then, \( E_1 = V_0 - \epsilon V_0 \), \( E_2 = V_0 \), and these are consistent (to first order in \( \epsilon \)) with what we got in (b).