Quantum Mechanics: Fall 2019
Final Exam: Brief Solutions

NOTE: Sentences in italic fonts are questions to be answered.

Possibly useful facts:

- 1D harmonic oscillator: $\hat{H} = \frac{\hat{p}^2}{2m} + \frac{m\omega^2}{2}\hat{x}^2 = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{m\omega^2}{2}x^2$.
  $[\hat{x}, \hat{p}] = \mathrm{i}\hbar$, and in position representation $\hat{p} = -\mathrm{i}\hbar\frac{\partial}{\partial x}$. Define $\hat{a}_\mp = \sqrt{\frac{m\omega}{2\hbar}}(\hat{x} \pm \mathrm{i}\frac{1}{m\omega}\hat{p}) = \sqrt{\frac{m\omega}{2\hbar}}(x \pm \frac{\hbar}{m\omega}\frac{\partial}{\partial x})$. Then $[\hat{a}_-, \hat{a}_+] = 1$ and $\hat{H} = \hbar\omega\,(\hat{a}_+\hat{a}_- + \frac{1}{2})$. It has a unique ground state $|\psi_0\rangle$ with $\hat{a}_-|\psi_0\rangle = 0$, and excited states $|\psi_n\rangle \equiv \frac{1}{\sqrt{n!}}(\hat{a}_+)^n|\psi_0\rangle$ with energy $E_n = (n+\frac{1}{2})\hbar\omega$. The ground state wavefunction is $\psi_0(x) = (\frac{m\omega}{\pi\hbar})^{1/4}\exp(-\frac{m\omega}{2\hbar}x^2)$.
- $\int_{-\infty}^{\infty} x^{2n} e^{-x^2/(2a)}\mathrm{d}x = (2n-1)!! \cdot a^n \cdot \sqrt{2\pi a}$, for $a > 0$ and non-negative integer n.
- Generic angular momentum: $[\hat{J}_x, \hat{J}_y] = \mathrm{i}\hbar\hat{J}_z$, $[\hat{J}_y, \hat{J}_z] = \mathrm{i}\hbar\hat{J}_x$, $[\hat{J}_z, \hat{J}_x] = \mathrm{i}\hbar\hat{J}_y$.
  For eigenstate $|j, m\rangle$ of $\hat{\boldsymbol{J}}^2$ and $\hat{J}_z$, $\hat{\boldsymbol{J}}^2|j, m\rangle = j(j+1)\hbar^2|j, m\rangle$, $\hat{J}_z|j, m\rangle = m\hbar|j, m\rangle$, and $(\hat{J}_x \pm \mathrm{i}\hat{J}_y)|j, m\rangle = \sqrt{(j \mp m)(j \pm m + 1)}\hbar|j, m \pm 1\rangle$.
  Here $2j$ is non-negative integer, $m = -j, -j+1, \ldots, j$.
  - Spin-1/2: basis states $|\uparrow\rangle$ and $|\downarrow\rangle$, namely $|S_z = +\frac{1}{2}\hbar\rangle$ and $|S_z = -\frac{1}{2}\hbar\rangle$.
    Under this basis, $\hat{S}_a = \frac{\hbar}{2}\sigma_a$ where $\sigma_{x,y,z}$ are Pauli matrices.
    $\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, $\sigma_y = \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}$, $\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$.
- (Degenerate) Time-independent perturbation theory: $\hat{H} = \hat{H}^{(0)} + \hat{H}^{(1)}$. Denote the (degenerate) orthonormal eigenstates of $\hat{H}^{(0)}$ by $|\psi_{n\alpha}^{(0)}\rangle$, $\hat{H}^{(0)}|\psi_{n\alpha}^{(0)}\rangle = E_n^{(0)}|\psi_{n\alpha}\rangle$.
  Suppose $\hat{H}|\psi_n\rangle = E_n|\psi_n\rangle$, with E_n close to $E_n^{(0)}$, then $(E_n - E_n^{(0)})$ is the eigenvalue of "secular equation", $\langle\psi_{n\beta}^{(0)}|\hat{H}^{(1)}|\psi_{n\alpha}^{(0)}\rangle + \sum_{m, m\neq n}\frac{1}{E_n^{(0)} - E_m^{(0)}}\langle\psi_{n\beta}^{(0)}|\hat{H}^{(1)}|\psi_m^{(0)}\rangle\langle\psi_m^{(0)}|\hat{H}^{(1)}|\psi_{n\alpha}^{(0)}\rangle$ up to second order. Here β & α are row/column index, the sum is over all eigenstates of $\hat{H}^{(0)}$ with energy different from $E_n^{(0)}$. In non-degenerate case, this is a 1×1 matrix.
- Some Taylor expansions: $\sqrt{1+x} = 1 + \frac{x}{2} - \frac{x^2}{8} + \ldots$; $\frac{1}{\sqrt{1+x}} = 1 - \frac{x}{2} + \frac{3x^2}{8} + \ldots$; $\frac{x}{\sin(x)} = 1 + \frac{x^2}{6} + \frac{7x^4}{360} + \ldots$; $\frac{1}{\cos(x)} = 1 + \frac{x^2}{2} + \frac{5x^4}{24} + \ldots$.
- Series inversion: from series $x = z + a_1 z^2 + a_2 z^3 + a_3 z^4 + O(z^5)$ for $|z| \ll 1$,
  solve z, then $z = x + (-a_1)x^2 + (2a_1^2 - a_2)x^3 + (-5a_1^3 + 5a_1 a_2 - a_3)x^4 + O(x^5)$.

Problem 1. (35 points) Consider a non-relativistic particle confined in a 1D infinite square potential well. $\hat{H}^{(0)} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V_0(x)$, with $V_0(x) = \begin{cases} +\infty, & |x| > L; \\ 0, & |x| < L. \end{cases}$ Here $L > 0$. Add a δ-function perturbation $\hat{H}^{(1)} = \alpha \cdot \delta(x)$. Here α is a "small" parameter, $\alpha > 0$, and δ denotes the Dirac-δ function hereafter. The full Hamiltonian is $\hat{H} = \hat{H}^{(0)} + \hat{H}^{(1)}$.

(a) (5pts) *Write down the eigenvalues* $E_n^{(0)}$ *and normalized eigenstates* $\psi_n^{(0)}(x)$ *of* $\hat{H}^{(0)}$.

(b) (5pts) *Compute the ground state energy of* $\hat{H}$ *up to 2nd order of perturbation.* [Note: leave the result as an infinite series, or use $\sum_{n=1}^{\infty} \frac{1}{x^2 - n^2} = \frac{\pi x \cos(\pi x) - \sin(\pi x)}{2x^2 \sin(\pi x)}$ (not required).]

(c) (5pts) *Draw qualitatively the ground state wavefunction of* $\hat{H}$*, and describe its properties.* [Hint: be careful about the "boundary conditions"]

(d) (5pts*) Denote the exact ground state energy of $\hat{H}$ by $\frac{\hbar^2 k^2}{2m}$. *Derive the equation for* k*. Solve this equation approximately to get the ground state energy of* $\hat{H}$ *to 2nd order of* α*.* [Hint: assume k deviates from unperturbed case by a small number δk, expand the appropriate form of this equation with respect to δk, solve δk to appropriate order of α; some facts on page 1 will be useful]

(e) (5pts) Suppose $\psi(x,t) = \sum_n c_n(t) \cdot e^{-\mathrm{i} E_n^{(0)} t/\hbar} \cdot \psi_n^{(0)}(x)$ satisfy the Schrödinger equation $\mathrm{i}\hbar \frac{\partial}{\partial t}\psi = \hat{H}\psi$. *Derive the differential equations for the coefficients* $c_n(t)$ *in terms of given quantities.*

(f) (10pts) Suppose the initial state $\psi(x, t = 0)$ is the ground state of $\hat{H}^{(0)}$. *Compute the transition probability* $|c_n(t)|^2$ *to second order of* α*, for all* n*.* [Hint: you need to compute $c_n(t)$ to appropriate order of α]

Solution:

(a) (2pts) $E_n^{(0)} = \frac{\hbar^2}{2m}(\frac{n\pi}{2L})^2$, (1pt) $n = 1, 2, \ldots$.

(2pts) One choice of the orthonormal basis is $\psi_n^{(0)} = \begin{cases} 0, & |x| > L; \\ \sqrt{\frac{1}{L}} \sin(\frac{n\pi}{2L}(x + L)), & |x| < L. \end{cases}$

Note that $\sin(\frac{n\pi}{2L}(x+L)) = \begin{cases} (-1)^{\frac{n-1}{2}}\cos(\frac{n\pi x}{2L}), & n \text{ is odd;} \\ (-1)^{\frac{n}{2}}\sin(\frac{n\pi x}{2L}), & n \text{ is even} \end{cases}$.

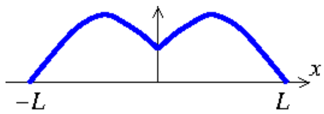
(b) (1pt) Ground state is $\psi_1^{(0)} = \sqrt{\frac{1}{L}}\sin(\frac{\pi}{2L}(x+L)) = \sqrt{\frac{1}{L}}\cos(\frac{\pi x}{2L})$, for $|x|<L$.

Use the non-degenerate time-independent perturbation theory result on page 1.

(2pts) The matrix element $\langle\psi_m^0|\hat{H}^{(1)}|\psi_1^{(0)}\rangle = \int_{-L}^{L}[\sqrt{\frac{1}{L}}\sin(\frac{m\pi}{2L}(x+L))]^*\cdot\alpha\delta(x)\cdot\sqrt{\frac{1}{L}}\sin(\frac{\pi}{2L}(x+L)) = \frac{\alpha}{L}\sin(\frac{m\pi}{2}) = \begin{cases} \frac{\alpha}{L}(-1)^k, & m=2k+1 \text{ is odd,} \\ 0, & m \text{ is even.} \end{cases}$

(2pts) $E_1 \approx E_1^{(0)} + \langle\psi_1^0|\hat{H}^{(1)}|\psi_1^{(0)}\rangle + \sum_{m,m\neq 1}\frac{|\langle\psi_m^0|\hat{H}^{(1)}|\psi_1^{(0)}\rangle|^2}{E_1^{(0)}-E_m^{(0)}}$
$= \frac{\hbar^2}{2m}(\frac{\pi}{2L})^2 + \frac{\alpha}{L} + \frac{8m\alpha^2}{\hbar^2\pi^2}\sum_{k=1}^{\infty}\frac{1}{1-(2k+1)^2}$.

(not required) $\sum_{k=0}^{\infty}\frac{1}{x^2-(2k+1)^2} = \sum_{n=1}^{\infty}\frac{1}{x^2-n^2} - \frac{1}{4}\sum_{n=1}^{\infty}\frac{1}{(x/2)^2-n^2} = -\frac{\pi\tan(\pi x/2)}{4x}$, then $\sum_{k=1}^{\infty}\frac{1}{1-(2k+1)^2} = \lim_{x\to 1}(-\frac{\pi\tan(\pi x/2)}{4x} - \frac{1}{x^2-1}) = -\frac{1}{4}$. So $E_1 \approx \frac{\hbar^2}{2m}(\frac{\pi}{2L})^2 + \frac{\alpha}{L} - \frac{2m\alpha^2}{\hbar^2\pi^2}$.

(c) Schematic picture of the ground state in $|x|<L$ region, .

(1pt) The wavefunction vanishes for $|x|\geq L$.

(1pt) The wavefunction has no node for $|x|<L$.

(1pt) The wavefunction is continuous.

(1pt) The wavefunction has discontinuous derivative at $x=0$, and $\frac{\partial\psi}{\partial x}|_{x=+0} - \frac{\partial\psi}{\partial x}|_{x=-0} > 0$.

(1pt) The wavefunction is an even function of x.

(d) (1pt) According to (c), the ground state wavefunction should be

$\psi(x) \propto \begin{cases} \sin(k(x+L)), & -L<x<0; \\ \sin(k(L-x)), & 0<x<L; \\ 0, & |x|>L \end{cases}$, for energy eigenvalue $E = \frac{\hbar^2k^2}{2m}$.

(2pts) The boundary condition at $x=0$ produces $-\frac{\hbar^2}{2m}(\frac{\partial\psi}{\partial x}|_{x=+0} - \frac{\partial\psi}{\partial x}|_{x=-0}) + \alpha\psi(x=0) = 0$, namely $\frac{\hbar^2 k}{m}\cos(kL) + \alpha\sin(kL) = 0$, or $(kL)\cot(kL) = -\frac{m\alpha L}{\hbar^2}$.

(1pt) Assume $k = \frac{\pi}{2L} + \delta k$, the above equation becomes $\frac{m\alpha L}{\hbar^2} = (\frac{\pi}{2} + \delta k\cdot L)\tan(\delta k\cdot L)$
$\approx \frac{\pi}{2}(\delta k\cdot L) + (\delta k\cdot L)^2 + \frac{\pi}{2}\frac{1}{3}(\delta k\cdot L)^3 + O((\delta k\cdot L)^4)$.

(1pt) Use the series inversion formula on page 1, $(\delta k\cdot L) \approx (\frac{2m\alpha L}{\hbar^2\pi}) - \frac{2}{\pi}(\frac{2m\alpha L}{\hbar^2\pi})^2 + O(\alpha^3)$.

Then $E = \frac{\hbar^2(\frac{\pi}{2L}+\delta k)^2}{2m} \approx \frac{\hbar^2}{2mL^2}\{\frac{\pi^2}{4} + \pi[(\frac{2m\alpha L}{\hbar^2\pi}) - \frac{2}{\pi}(\frac{2m\alpha L}{\hbar^2\pi})^2] + (\frac{2m\alpha L}{\hbar^2\pi})^2\} + O(\alpha^3)$
$= \frac{\hbar^2\pi^2}{8mL^2} + \frac{\alpha}{L} - \frac{2m\alpha^2}{\hbar^2\pi^2} + O(\alpha^3)$.

(e) The Schrödinger equation for $|\psi(x,t)\rangle$ is $\mathrm{i}\hbar\sum_n[\frac{\partial c_n(t)}{\partial t}+c_n(t)(-\frac{\mathrm{i}}{\hbar}E_n^{(0)})]e^{-\mathrm{i}E_n^{(0)}t}|\psi_n^{(0)}\rangle$ $=\sum_n c_n(t)e^{-\mathrm{i}E_n^{(0)}t}E_n^{(0)}|\psi_n^{(0)}\rangle+\sum_{n,m}c_m(t)e^{-\mathrm{i}E_m^{(0)}t}|\psi_n^{(0)}\rangle\langle\psi_n^{(0)}|\hat{H}^{(1)}|\psi_m^{(0)}\rangle$. Namely,

(3pts) $\frac{\partial c_n(t)}{\partial t}=-\frac{\mathrm{i}}{\hbar}\sum_m\langle\psi_n^{(0)}|\hat{H}^{(1)}|\psi_m^{(0)}\rangle\, e^{\mathrm{i}(E_n^{(0)}-E_m^{(0)})t/\hbar}\,c_m(t)$. Here $n,m=1,2,\ldots$. $(E_n^{(0)}-E_m^{(0)})=\frac{\hbar^2\pi^2}{8mL^2}(n^2-m^2)$. (2pts) The matrix element $\langle\psi_n^{(0)}|\hat{H}^{(1)}|\psi_m^{(0)}\rangle$ $=\frac{\alpha}{L}\sin(\frac{n\pi}{2})\sin(\frac{m\pi}{2})=\begin{cases}\frac{\alpha}{L}(-1)^{\frac{n-1}{2}+\frac{m-1}{2}}, & n,m \text{ are both odd;}\\ 0, & \text{otherwise.}\end{cases}$

(f) (2pts) $\psi(x,t=0)=\psi_1^{(0)}(x)$, namely $c_1(t=0)=1$, $c_{n>1}(t=0)=0$.

(3pts) For $n>1$ cases, we just need to compute $c_n(t)$ to $O(\alpha)$ order,

$c_{n>1}(t)\approx-\frac{\mathrm{i}}{\hbar}\int_0^t\mathrm{d}t\,\langle\psi_n^{(0)}|\hat{H}^{(1)}|\psi_m^{(0)}\rangle\,e^{\mathrm{i}(E_n^{(0)}-E_1^{(0)})t/\hbar}$

$$=\begin{cases}-\frac{8\alpha mL}{\hbar^2\pi^2(n^2-1)}(-1)^{\frac{n-1}{2}}(e^{\mathrm{i}\frac{\hbar\pi^2}{8mL^2}(n^2-1)t}-1), & n \text{ is odd, and } n>1;\\ 0, & n \text{ is even.}\end{cases}$$

(3pts) Then for $n>1$, $|c_n(t)|^2\approx\begin{cases}\frac{256\alpha^2m^2L^2}{\hbar^4\pi^4(n^2-1)^2}\sin^2[\frac{\hbar\pi^2}{16mL^2}(n^2-1)t], & n \text{ is odd, and } n>1;\\ 0, & n \text{ is even.}\end{cases}$

(2pts) For $n=1$, use $\sum_{n=1}^{\infty}|c_n(t)|^2=1$,

$|c_1(t)|^2\approx1-\sum_{k=1}^{\infty}\frac{256\alpha^2m^2L^2}{\hbar^4\pi^4((2k+1)^2-1)^2}\sin^2[\frac{\hbar\pi^2}{16mL^2}((2k+1)^2-1)t]$.

Method #2 for $|c_1(t)|^2$:

to compute $c_1(t)$ directly, you need to keep α^2 order terms in $c_1(t)$, then you need to use 1st order results of $c_n(t)$ in the right-hand-side of $c_1(t)-c_1(t=0)$ $=-\frac{\mathrm{i}}{\hbar}\sum_n\int_0^t\mathrm{d}t\,\langle\psi_1^{(0)}|\hat{H}^{(1)}|\psi_n^{(0)}\rangle\,e^{\mathrm{i}(E_1^{(0)}-E_n^{(0)})t/\hbar}\,c_n(t)$.

For $n>1$ the first order result of $c_n(t)$ is given above, the first order result of $c_1(t)=1+(-\frac{\mathrm{i}}{\hbar})\int_0^t\mathrm{d}t\,\langle\psi_1^{(0)}|\hat{H}^{(1)}|\psi_1^{(0)}\rangle\cdot1+O(\alpha^2)=1-\mathrm{i}\frac{\alpha}{\hbar L}t+O(\alpha^2)$.

Then $c_1(t)=1+(-\frac{\mathrm{i}}{\hbar})\int_0^t\mathrm{d}t\,[\frac{\alpha}{L}\cdot(1-\mathrm{i}\frac{\alpha}{\hbar L}t)]+\sum_{k=1}^{\infty}(-\frac{\mathrm{i}}{\hbar})\int_0^t\mathrm{d}t\,[\frac{\alpha}{L}(-1)^k\,e^{\mathrm{i}\frac{\hbar\pi^2}{8mL^2}(1-(2k+1)^2)t}$ $\times(-\frac{8\alpha mL}{\hbar^2\pi^2((2k+1)^2-1)})(-1)^k(e^{\mathrm{i}\frac{\hbar\pi^2}{8mL^2}((2k+1)^2-1)t}-1)]+O(\alpha^3)$

$=1-\mathrm{i}\frac{\alpha}{\hbar L}t-\frac{\alpha^2}{2\hbar^2L^2}t^2+\sum_{k=1}^{\infty}[-\mathrm{i}\frac{8\alpha^2m}{\hbar^3\pi^2((2k+1)^2-1)}t+\frac{64\alpha^2m^2L^2}{\hbar^4\pi^4((2k+1)^2-1)^2}(e^{\mathrm{i}\frac{\hbar\pi^2}{8mL^2}(1-(2k+1)^2)t}-1)]+O(\alpha^3)$.

Then $(|c_1(t)|^2$ up to $O(\alpha^2))\approx(\mathrm{Re}[c_1(t)]$ up to $O(\alpha^2))^2$ $+(\mathrm{Im}[c_1(t)]$ up to $O(\alpha))^2$

$\approx[1-\frac{\alpha^2}{2\hbar^2L^2}t^2-\sum_k\frac{64\alpha^2m^2L^2}{\hbar^4\pi^4((2k+1)^2-1)^2}(1-\cos[\frac{\hbar\pi^2}{8mL^2}(1-(2k+1)^2)t])]^2+(-\frac{\alpha}{\hbar L}t)^2+O(\alpha^3)$

$\approx1-2\sum_k\frac{64\alpha^2m^2L^2}{\hbar^4\pi^4((2k+1)^2-1)^2}(1-\cos[\frac{\hbar\pi^2}{8mL^2}(1-(2k+1)^2)t])+O(\alpha^3)$

$=1-\sum_{k=1}^{\infty}\frac{256\alpha^2m^2L^2}{\hbar^4\pi^4((2k+1)^2-1)^2}\sin^2[\frac{\hbar\pi^2}{16mL^2}((2k+1)^2-1)t]$.

Problem 2. (15 points) Consider a 1D anharmonic oscillator $\hat{H}=\frac{\hat{p}^2}{2m}+\frac{m\omega^2}{2}\hat{x}^2-\frac{\alpha}{3}\hat{x}^3$, here m, ω, α are positive constants. α is a "small" parameter.

(a) (5pts) Consider $\hat{H}_f^{(0)} = \frac{\hat{p}^2}{2m} + \frac{m\omega^2}{2}\hat{x}^2 - f\hat{x}$, with normalized ground state $\psi_{0,f}(x)$, parametrized by a positive "variational" parameter f. It is easy to see that $\psi_{0,f}(x) = \psi_0(x - \frac{f}{m\omega^2})$. (see page 1 for harmonic oscillator ground state wavefunction ψ_0). *Compute* $E(f) \equiv \langle\psi_{0,f}|\hat{H}|\psi_{0,f}\rangle$.

(b) (5pts*) *Solve* f *from* $\frac{\partial}{\partial f}E(f) = 0$ *approximately up to 2nd order of* α*, and therefore obtain the minimal* $E(f)$ *to 2nd order of* α.

(c) (5pts*) Treat the $-\frac{\alpha}{3}\hat{x}^3$ term by perturbation theory. *Compute the ground state energy of* $\hat{H}$ *to 2nd order of* α. [Hint: use ladder operators, this may not match the result in (b)]

Solution:

Define $\hat{X} = \hat{x} - \frac{f}{m\omega^2}$, with conjugate momentum $\hat{P} = -\mathrm{i}\hbar\partial_X = \hat{p}$.

Then $\hat{H} = \frac{\hat{P}^2}{2m} + \frac{m\omega^2}{2}(\hat{X} + \frac{f}{m\omega^2})^2 - \frac{\alpha}{3}(\hat{X} + \frac{f}{m\omega^2})^3$

$= (\frac{\hat{P}^2}{2m} + \frac{m\omega^2}{2}\hat{X}^2) + (\frac{f^2}{2m\omega^2} - \alpha\frac{f^3}{3m^3\omega^6}) + (f - \alpha\frac{f^2}{m^2\omega^4})\hat{X} - \alpha\frac{f}{m\omega^2}\hat{X}^2 - \frac{\alpha}{3}\hat{X}^3.$

$\hat{H}_f^{(0)} = (\frac{\hat{P}^2}{2m} + \frac{m\omega^2}{2}\hat{X}^2) - \frac{f^2}{2m\omega^2}$, $\psi_{0,f}(x) = \psi_0(X) = (\frac{m\omega}{\pi\hbar})^{1/4}\exp(-\frac{m\omega}{2\hbar}X^2)$.

(a) (5pts)

$E(f) \equiv \langle\psi_{0,f}|\hat{H}|\psi_{0,f}\rangle = \frac{\hbar\omega}{2} + (\frac{f^2}{2m\omega^2} - \alpha\frac{f^3}{3m^3\omega^6}) + (f - \alpha\frac{f^2}{m^2\omega^4})\langle\hat{X}\rangle - \alpha\frac{f}{m\omega^2}\langle\hat{X}^2\rangle - \frac{\alpha}{3}\langle\hat{X}^3\rangle$

$= \frac{\hbar\omega}{2} + (\frac{f^2}{2m\omega^2} - \alpha\frac{f^3}{3m^3\omega^6}) + 0 - \alpha\frac{f}{m\omega^2}\cdot\frac{\hbar}{2m\omega} - 0 = \frac{\hbar\omega}{2} - \frac{\alpha\hbar}{2m^2\omega^3}f + \frac{1}{2m\omega^2}f^2 - \frac{\alpha}{3m^3\omega^6}f^3.$

Here we have used the results $\langle\hat{X}\rangle = 0$, $\langle\hat{X}^2\rangle = \frac{\hbar}{2m\omega}$, $\langle\hat{X}^3\rangle = 0$, under the ground state of harmonic oscillator for X.

(b) (1pt) $\frac{\partial}{\partial f}E(f) = -\frac{\alpha\hbar}{2m^2\omega^3} + \frac{1}{m\omega^2}f - \frac{\alpha}{m^3\omega^6}f^2 = -\frac{\alpha}{m^3\omega^6}(f^2 - \frac{m^2\omega^4}{\alpha}f + \frac{\hbar m\omega^3}{2}) = 0.$

(2pts) Then $f = \frac{m^2\omega^4}{2\alpha} - \sqrt{(\frac{m^2\omega^4}{2\alpha}) - \frac{\hbar m\omega^3}{2}} \approx \frac{\hbar}{2m\omega}\alpha + O(\alpha^3)$.

(2pts) Minimal of $E(f)$ is approximately $\frac{\hbar\omega}{2} - \frac{\hbar^2}{8m^3\omega^4}\alpha^2 + O(\alpha^3)$.

(c) (1pts) The unperturbed Hamiltonian is just the harmonic oscillator for x, with unperturbed ground state $\psi_0^{(0)}(x) = \psi_0(x)$, and $E_0^{(0)} = \frac{\hbar\omega}{2}$.

(2pts) Rewrite the perturbation term by ladder operators, $-\frac{\alpha}{3}\hat{x}^3 = -\frac{\alpha}{3}(\frac{\hbar}{2m\omega})^{3/2}(\hat{a}_- + \hat{a}_+)^3$.

Then $-\frac{\alpha}{3}\hat{x}^3|\psi_0\rangle = -\frac{\alpha}{3}(\frac{\hbar}{2m\omega})^{3/2}(\hat{a}_- + \hat{a}_+)^2|\psi_1\rangle = -\frac{\alpha}{3}(\frac{\hbar}{2m\omega})^{3/2}(\hat{a}_- + \hat{a}_+)(|\psi_0\rangle + \sqrt{2}|\psi_2\rangle)$
$= -\frac{\alpha}{3}(\frac{\hbar}{2m\omega})^{3/2}(3|\psi_1\rangle + \sqrt{6}|\psi_3\rangle)$.

(2pts) Directly use the non-degenerate time-independent perturbation theory result on page 1, the energy to second order is $E_0 \approx \frac{\hbar\omega}{2} + 0 + (\frac{\alpha}{3}(\frac{\hbar}{2m\omega})^{3/2})^2(\frac{3^2}{-\hbar\omega} + \frac{(\sqrt{6})^2}{-3\hbar\omega}) = \frac{\hbar\omega}{2} - \frac{11\hbar^2}{72m^3\omega^4}\alpha^2$.

Note that this is lower than the variational method result in (b).

Problem 3. (10 points) Consider two spin-1/2 moments, labeled by subscripts $_1$ and $_2$ respectively. One set of complete orthonormal basis of the entire Hilbert space is the tensor products of S_z-eigenbasis $|S_{1,z}\rangle|S_{2,z}\rangle$, namely $|\uparrow\rangle|\uparrow\rangle$, $|\uparrow\rangle|\downarrow\rangle$, $|\downarrow\rangle|\uparrow\rangle$, and $|\downarrow\rangle|\downarrow\rangle$.

(a) (5pts) *Write down the eigenvalues and normalized eigenstates of* $\hat{H} = J\hat{\boldsymbol{S}}_1 \cdot \hat{\boldsymbol{S}}_2 = J\cdot(\hat{S}_{1,x}\hat{S}_{2,x} + \hat{S}_{1,y}\hat{S}_{2,y} + \hat{S}_{1,z}\hat{S}_{2,z})$. J is a positive constant. [Hint: $\hat{H}$ is related to $(\hat{\boldsymbol{S}}_1 + \hat{\boldsymbol{S}}_2)^2$.]

(b) (5pts*) Denote the ground state of $\hat{H}$ in (a) by $|\psi_0\rangle$. *Measure* $\hat{S}_{1,x}$ *under* $|\psi_0\rangle$. *What are the possible measurement results* $S_{1,x}$ *and their corresponding probabilities* $P(S_{1,x})$*? After measuring* $\hat{S}_{1,x}$*, measure* $\hat{S}_{2,z}$*, what are the possible measurement results* $S_{2,z}$ *and the corresponding conditional probability* $P(S_{2,z}|S_{1,x})$*?* [Note: conditional probability $P(S_{2,z}|S_{1,x})$ means that after getting result $S_{1,x}$ by measuring $\hat{S}_{1,x}$, the probability of getting result $S_{2,z}$ by measuring $\hat{S}_{2,z}$] [Hint: it may help to first rewrite $|\psi_0\rangle$ using $\hat{S}_{1,x}$ and $\hat{S}_{2,z}$ eigenstates]

Solution:

(a) $\hat{H} = \frac{J}{2}(\hat{\boldsymbol{S}}_1 + \hat{\boldsymbol{S}}_2)^2 - \frac{J}{2}(\hat{\boldsymbol{S}}_1^2 + \hat{\boldsymbol{S}}_2^2) = \frac{J}{2}(\hat{\boldsymbol{S}}_1 + \hat{\boldsymbol{S}}_2)^2 - \frac{3J\hbar^2}{4}$.

$E_{S=0} = \frac{J}{2}\cdot\hbar^2\cdot 0\cdot(0+1) - \frac{3J\hbar^2}{4} = -\frac{3J\hbar^2}{4}$,
spin singlet state $|\psi_0\rangle \equiv |S=0, S_z=0\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle|\downarrow\rangle - |\downarrow\rangle|\uparrow\rangle)$.

$E_{S=1} = \frac{J}{2}\cdot\hbar^2\cdot 1\cdot(1+1) - \frac{3J\hbar^2}{4} = \frac{J\hbar^2}{4}$,
spin triplet states $|S=1, S_z=1\rangle = |\uparrow\rangle|\uparrow\rangle$, $|S=1, S_z=0\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle|\downarrow\rangle + |\downarrow\rangle|\uparrow\rangle)$, $|S=1, S_z=-1\rangle = |\downarrow\rangle|\downarrow\rangle$.

(b) (1pts) $\hat{S}_{1,x}$ has eigenvalue $+\frac{\hbar}{2}$ for $|\rightarrow\rangle \equiv \frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle)$, and eigenvalue $-\frac{\hbar}{2}$ for $|\leftarrow\rangle \equiv \frac{1}{\sqrt{2}}(|\uparrow\rangle - |\downarrow\rangle)$. $\hat{S}_{1,x}$ and $\hat{S}_{2,z}$ commute, so we can have simultaneous eigenbasis of them.

Rewrite $|\psi_0\rangle$ in terms of $|S_{1,x}\rangle|S_{2,z}\rangle$ basis, $|\psi_0\rangle = \frac{1}{2}(|\rightarrow\rangle|\downarrow\rangle + |\leftarrow\rangle|\downarrow\rangle - |\rightarrow\rangle|\uparrow\rangle + |\leftarrow\rangle|\downarrow\rangle)$

Therefore the probability for any combination of $(S_{1,x}, S_{2,z})$, with $S_{1,x} = \pm\frac{\hbar}{2}$ and $S_{2,z} = \pm\frac{\hbar}{2}$, is $P(S_{1,x}, S_{2,z}) = |\pm\frac{1}{2}|^2 = \frac{1}{4}$.

$P(S_{1,x}) = \sum_{S_{2,z}} P(S_{1,x}, S_{2,z})$, $P(S_{2,z}|S_{1,x}) = \frac{P(S_{1,x},S_{2,z})}{\sum_{S_{2,z}} P(S_{1,x},S_{2,z})}$

(2pts) Measurement result $S_{1,x}$ can be $\pm\frac{\hbar}{2}$, and $P(S_{1,x}) = \frac{1}{2}$, independent of $S_{1,x}$.

(2pts) Measurement result $S_{2,z}$ can be $\pm\frac{\hbar}{2}$, and $P(S_{2,z}|S_{1,x}) = \frac{1}{2}$, independent of $S_{2,z}$ and $S_{1,x}$.

Problem 4. (40 points) Consider two identical particles in the 1D infinite potential well defined in Problem 1. The unperturbed Hamiltonian is $\hat{H}^{(0)} = -\frac{\hbar^2}{2m}(\frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2}) + V_0(x_1) + V_0(x_2)$. Subscripts $_1$ and $_2$ label the two particles. If they are distinguishable, the orthonormal eigenstates of $\hat{H}^{(0)}$ can be chosen as $\psi^{(0)}_{n_1,n_2}(x_1; x_2) = \psi^{(0)}_{n_1}(x_1) \cdot \psi^{(0)}_{n_2}(x_2)$, with energy eigenvalue $E^{(0)}_{n_1,n_2} = E^{(0)}_{n_1} + E^{(0)}_{n_2}$. Here $E^{(0)}_n$ and $\psi^{(0)}_n(x)$ are defined in Problem 1(a). For identical particles, $\psi(x_1; x_2)$ must satisfy certain permutation symmetry. The normalization is $\int \mathrm{d}x_1 \int \mathrm{d}x_2\, |\psi(x_1; x_2)|^2 = 1$.

(a) (5pts) *Write down the energies and ORTHONORMAL eigenstate wavefunctions for two BOSONS for the lowest THREE energy levels of $\hat{H}^{(0)}$.*

(b) (5pts) *Write down the energies and ORTHONORMAL eigenstate wavefunctions for two FERMIONS for the lowest THREE energy levels of $\hat{H}^{(0)}$.*

(c) (5pts) *Compute the probability that the two particles are both in the left half of the potential well, namely the probability of "$x_1 < 0$ and $x_2 < 0$", for the ground state of two BOSONS in (a), and for the ground state of two FERMIONS in (b).*

(d) (10pts) Suppose the particles have spin-1/2 internal degrees of freedom, the wavefunction should be $\psi(x_1, s_1; x_2, s_2)$ where $s_i =\uparrow, \downarrow$ label the eigenvalues $\pm\frac{\hbar}{2}$ of $\hat{S}_{i,z}$ for particle $i = 1, 2$. The normalization becomes $\sum_{s_1,s_2} \int \mathrm{d}x_1 \int \mathrm{d}x_2\, |\psi(x_1, s_1; x_2, s_2)|^2 = 1$. *For the case of two BOSONS, write down the energies and ORTHONORMAL eigenstate wavefunctions $\psi(x_1, s_1; x_2, s_2)$ for the lowest THREE energy levels of $\hat{H}^{(0)}$.* [Note: may have degeneracy, represent $\psi(x_1, s_1; x_2, s_2)$ as a 4-component vector function $\begin{pmatrix} \psi(x_1,\uparrow;x_2,\uparrow) \\ \psi(x_1,\uparrow;x_2,\downarrow) \\ \psi(x_1,\downarrow;x_2,\uparrow) \\ \psi(x_1,\downarrow;x_2,\downarrow) \end{pmatrix}$ of $x_{1,2}$; be careful about the permutation symmetry $\psi(x_2, s_2; x_1, s_1) = \psi(x_1, s_1; x_2, s_2)$ for bosons]

(e) (10pts**) For the two spin-1/2 BOSONS in (d), add a perturbation $\hat{H}^{(1)} = \lambda \cdot [\cos(kx_1)\hat{S}_{1,x} + \sin(kx_1)\hat{S}_{1,y} + \cos(kx_2)\hat{S}_{2,x} + \sin(kx_2)\hat{S}_{2,y}]$, which is a Zeeman field whose direction depends on position. Here λ is a "small" real parameter. $k > 0$ is a positive parameter. Note that the spin operators' action on the wavefunction is $(\hat{S}_{1,x}\psi)(x_1, s_1; x_2, s_2) = \sum_{s'_1=\uparrow,\downarrow}(\hat{S}_{1,x})_{s_1,s'_1} \cdot \psi(x_1, s'_1; x_2, s_2)$, where $(\hat{S}_{1,x})_{s_1,s'_1}$ is the matrix element of $\hat{S}_{1,x}$ between $S_{1,z} = s_1$ and s'_1 states (see page 1), other spin operators' actions are similar and omitted here. *Compute the ground state(s) energy of $\hat{H} = \hat{H}^{(0)} + \hat{H}^{(1)}$ for two BOSONS under 1st order perturbation.* [Hint: you need degenerate perturbation theory, it may help to rewrite $\hat{H}^{(1)}$ in terms of ladder operators]

(f) (5pts***) *Compute the ground state(s) energy of $\hat{H}$ for two BOSONS in (e) to second order of λ.* [Hint: see page 1, 2nd order secular equation may be avoided by changing basis]

Solution:

If $|x_1| > L$ or $|x_2| > L$, $\psi(x_1, x_2) = 0$. So we will only write down $\psi(x_1, x_2)$ for $|x_{1,2}| < L$. Use superscript $^{(B)}$ and $^{(F)}$ to denote boson and fermion states respectively, they must satisfy $\psi^{(B)}(x_1, x_2) = \psi^{(B)}(x_2, x_1)$, $\psi^{(F)}(x_1, x_2) = -\psi^{(F)}(x_2, x_1)$.

(a)

$E^{(0)}_{1,1} = E^{(0)}_1 + E^{(0)}_1 = \frac{\hbar^2\pi^2}{8mL^2} \cdot 2$,

$\psi^{(B,0)}_{1,1}(x_1, x_2) = \psi^{(0)}_1(x_1)\psi^{(0)}_1(x_2) = \frac{1}{L}\cos(\frac{\pi x_1}{2L})\cos(\frac{\pi x_2}{2L})$.

$E^{(0)}_{1,2} = E^{(0)}_1 + E^{(0)}_2 = \frac{\hbar^2\pi^2}{8mL^2} \cdot 5$,

$\psi^{(B,0)}_{1,2}(x_1, x_2) = \frac{1}{\sqrt{2}}[\psi^{(0)}_1(x_1)\psi^{(0)}_2(x_2) + \psi^{(0)}_2(x_1)\psi^{(0)}_1(x_2)]$

$= -\frac{1}{\sqrt{2}L}[\cos(\frac{\pi x_1}{2L})\sin(\frac{\pi x_2}{L}) + \sin(\frac{\pi x_1}{L})\cos(\frac{\pi x_2}{2L})] = -\frac{\sqrt{2}}{L}\cos(\frac{\pi x_1}{2L})\cos(\frac{\pi x_2}{2L})[\sin(\frac{\pi x_1}{2L}) + \sin(\frac{\pi x_2}{2L})]$.

$E^{(0)}_{2,2} = E^{(0)}_2 + E^{(0)}_2 = \frac{\hbar^2\pi^2}{8mL^2} \cdot 8$,

$\psi^{(B,0)}_{2,2}(x_1, x_2) = \psi^{(0)}_2(x_1)\psi^{(0)}_2(x_2) = \frac{1}{L}\sin(\frac{\pi x_1}{L})\sin(\frac{\pi x_2}{L})$.

(b)

$E^{(0)}_{1,2} = E^{(0)}_1 + E^{(0)}_2 = \frac{\hbar^2\pi^2}{8mL^2} \cdot 5,$

$\psi^{(F,0)}_{1,2}(x_1, x_2) = \frac{1}{\sqrt{2}}[\psi^{(0)}_1(x_1)\psi^{(0)}_2(x_2) - \psi^{(0)}_2(x_1)\psi^{(0)}_1(x_2)]$

$= -\frac{1}{\sqrt{2}L}[\cos(\frac{\pi x_1}{2L})\sin(\frac{\pi x_2}{L}) - \sin(\frac{\pi x_1}{L})\cos(\frac{\pi x_2}{2L})] = \frac{\sqrt{2}}{L}\cos(\frac{\pi x_1}{2L})\cos(\frac{\pi x_2}{2L})[\sin(\frac{\pi x_1}{2L}) - \sin(\frac{\pi x_2}{2L})].$

$E^{(0)}_{1,3} = E^{(0)}_1 + E^{(0)}_3 = \frac{\hbar^2\pi^2}{8mL^2} \cdot 10,$

$\psi^{(F,0)}_{1,3}(x_1, x_2) = \frac{1}{\sqrt{2}}[\psi^{(0)}_1(x_1)\psi^{(0)}_3(x_2) - \psi^{(0)}_3(x_1)\psi^{(0)}_1(x_2)]$

$= -\frac{1}{\sqrt{2}L}[\cos(\frac{\pi x_1}{2L})\cos(\frac{3\pi x_2}{2L}) - \cos(\frac{3\pi x_1}{2L})\cos(\frac{\pi x_2}{2L})].$

$E^{(0)}_{2,3} = E^{(0)}_2 + E^{(0)}_3 = \frac{\hbar^2\pi^2}{8mL^2} \cdot 13,$

$\psi^{(F,0)}_{2,3}(x_1, x_2) = \frac{1}{\sqrt{2}}[\psi^{(0)}_2(x_1)\psi^{(0)}_3(x_2) - \psi^{(0)}_3(x_1)\psi^{(0)}_2(x_2)]$

$= \frac{1}{\sqrt{2}L}[\sin(\frac{\pi x_1}{L})\cos(\frac{3\pi x_2}{2L}) - \cos(\frac{3\pi x_1}{2L})\sin(\frac{\pi x_2}{L})].$

(c) We just need to compute $\int_{-L}^{0} \mathrm{d}x_1 \int_{-L}^{0} \mathrm{d}x_2\, |\psi(x_1, x_2)|^2$.

For $\psi^{(B,0)}_{1,1}(x_1, x_2)$, the probability is $\big[\int_{-L}^{0} \mathrm{d}x\, |\psi^{(0)}_1(x)|^2\big]^2 = (\frac{1}{2})^2 = \frac{1}{4}$.

For $\psi^{(F,0)}_{1,2}(x_1, x_2)$, the probability is

$\big[\int_{-L}^{0} \mathrm{d}x\, |\psi^{(0)}_1(x)|^2\big]\big[\int_{-L}^{0} \mathrm{d}x\, |\psi^{(0)}_2(x)|^2\big] - \big|\int_{-L}^{0} \mathrm{d}x\, (\psi^{(0)}_1(x))^*\psi^{(0)}_2(x)\big|^2 = \frac{1}{2}\cdot\frac{1}{2} - |\frac{4}{3\pi}|^2 = \frac{1}{4} - \frac{16}{9\pi^2}.$

(d) The energy of $\hat{H}^{(0)}$ does not depend on spin, and will be the same as those in (a). The wavefunctions can be chosen as products of orbital wavefunction $\psi(x_1, x_2)$ and spin wavefunction $\chi(s_1, s_2)$. Denote $\chi(s_1, s_2)$ by 4-component vector, $\begin{pmatrix} \chi(\uparrow;\uparrow) \\ \chi(\uparrow;\downarrow) \\ \chi(\downarrow;\uparrow) \\ \chi(\downarrow;\downarrow) \end{pmatrix}$. Define

$$\chi_{S=1,S_z=1} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix};\ \chi_{S=1,S_z=0} = \begin{pmatrix} 0 \\ \sqrt{1/2} \\ \sqrt{1/2} \\ 0 \end{pmatrix};\ \chi_{S=1,S_z=-1} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix};\ \chi_{S=0,S_z=0} = \begin{pmatrix} 0 \\ \sqrt{1/2} \\ -\sqrt{1/2} \\ 0 \end{pmatrix}.$$

The $S = 1$ spin wavefunctions are symmetric with respect to exchange of s_1, s_2, then the corresponding orbital wavefunctions should be symmetric with respect to exchange of x_1, x_2; the $S = 0$ spin wavefunction is anti-symmetric, then the corresponding orbital wavefunctions should also be anti-symmetric with respect to exchange of x_1, x_2.

$E^{(0)}_{1,1} = E^{(0)}_1 + E^{(0)}_1 = \frac{\hbar^2\pi^2}{8mL^2}\cdot 2$ (3-fold degenerate),
$\psi^{(B,0)}_{1,1,S_z}(x_1,s_1,x_2,s_2) = \psi^{(B,0)}_{1,1}(x_1,x_2)\chi_{S=1,S_z}(s_1,s_2)$, for $S_z = -1, 0, +1$.

$E^{(0)}_{1,2} = E^{(0)}_1 + E^{(0)}_2 = \frac{\hbar^2\pi^2}{8mL^2}\cdot 5$ (4-fold degenerate),
$\psi^{(B,0)}_{1,2,S=0}(x_1,s_1,x_2,s_2) = \psi^{(F,0)}_{1,2}(x_1,x_2)\chi_{S=0,S_z=0}(s_1,s_2)$, and
$\psi^{(B,0)}_{1,2,S=1,S_z}(x_1,s_1,x_2,s_2) = \psi^{(B,0)}_{1,2}(x_1,x_2)\chi_{S=1,S_z}(s_1,s_2)$, for $S_z = -1, 0, +1$.

$E^{(0)}_{2,2} = E^{(0)}_2 + E^{(0)}_2 = \frac{\hbar^2\pi^2}{8mL^2}\cdot 8$ (3-fold degenerate),
$\psi^{(B,0)}_{2,2,S_z}(x_1,s_1,x_2,s_2) = \psi^{(B,0)}_{2,2}(x_1,x_2)\chi_{S=1,S_z}(s_1,s_2)$, for $S_z = -1, 0, +1$.

(e) Method #1: use degenerate perturbation theory for 2-particle states,
$\hat{H}^{(1)} = \frac{\lambda}{2}[e^{-ikx_1}\hat{S}_{1+} + e^{ikx_1}\hat{S}_{1-} + e^{-ikx_2}\hat{S}_{2+} + e^{ikx_2}\hat{S}_{2-}]$, under the 4-component spinor wavefunction basis, $\hat{H}^{(1)}$ is a 4×4 matrix function, $H^{(1)} = \frac{\lambda\hbar}{2}\begin{pmatrix} 0 & e^{-ikx_2} & e^{-ikx_1} & 0 \\ e^{ikx_2} & 0 & 0 & e^{-ikx_1} \\ e^{ikx_1} & 0 & 0 & e^{-ikx_2} \\ 0 & e^{ikx_1} & e^{ikx_2} & 0 \end{pmatrix}$

The 3×3 matrix for the first order secular equation is, $\langle\psi^{(B,0)}_{1,1,S_z}|\hat{H}^{(1)}|\psi^{(B,0)}_{1,1,S'_z}\rangle \equiv \int dx_1 \int dx_2\, [\psi^{(B)}_{1,1}(x_1,x_2)]^* \cdot [\chi^\dagger_{S=1,S_z}\cdot H^{(1)}\cdot\chi_{S=1,S'_z}]\cdot\psi^{(B)}_{1,1}(x_1,x_2)$,
here $S_z, S'_z = +1, 0, -1$ are row and column indices respectively.

The 3×3 matrix $[\chi^\dagger_{S=1,S_z}\cdot H^{(1)}\cdot\chi_{S=1,S'_z}]$ is, $\frac{\lambda\hbar}{2\sqrt{2}}\begin{pmatrix} 0 & e^{-ikx_1}+e^{-ikx_2} & 0 \\ e^{ikx_1}+e^{ikx_2} & 0 & e^{-ikx_1}+e^{-ikx_2} \\ 0 & e^{ikx_1}+e^{ikx_2} & 0 \end{pmatrix}$

Finally, $\langle\psi^{(B,0)}_{1,1,S_z}|\hat{H}^{(1)}|\psi^{(B,0)}_{1,1,S'_z}\rangle = I_1\cdot\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$, where
$I_1 = \frac{\lambda\hbar}{2}\int_{-L}^{L} dx_1 \int_{-L}^{L} dx_2\, \frac{1}{L^2}\cos^2(\frac{\pi x_1}{2L})\cos^2(\frac{\pi x_2}{2L})\frac{1}{\sqrt{2}}[\cos(kx_1)+\cos(kx_2)] = \frac{\sqrt{2}\lambda\hbar}{2}\frac{\pi^2}{\pi^2-k^2L^2}\frac{\sin(kL)}{kL}$.

The first order secular equation has eigenvalues $+\sqrt{2}I_1, 0, -\sqrt{2}I_1$.

Finally the first order ground state energies are
$E_{1,1,(1)} \approx E^{(0)}_{1,1} + \sqrt{2}I_1 = \frac{\hbar^2\pi^2}{8mL^2}\cdot 2 + \lambda\hbar\frac{\pi^2}{\pi^2-k^2L^2}\frac{\sin(kL)}{kL}$;
$E_{1,1,(2)} \approx E^{(0)}_{1,1} = \frac{\hbar^2\pi^2}{8mL^2}\cdot 2$;
$E_{1,1,(3)} \approx E^{(0)}_{1,1} - \sqrt{2}I_1 = \frac{\hbar^2\pi^2}{8mL^2}\cdot 2 - \lambda\hbar\frac{\pi^2}{\pi^2-k^2L^2}\frac{\sin(kL)}{kL}$.

Method #2: solve approximate single particle ground state energies first,

The single particle Hamiltonian for one spin-1/2 boson is,
$\hat{H}_{\text{1-particle}} = \hat{H}^{(0)}_{\text{1-particle}} + \hat{H}^{(1)}_{\text{1-particle}} = [-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V_0(x)] + \frac{\lambda}{2}\cdot[e^{-\mathbb{i}kx}\hat{S}_+ + e^{\mathbb{i}kx}\hat{S}_-]$.

The unperturbed single particle eigenstates are 2-fold degenerate, $|\psi^{(0)}_n, \uparrow\rangle$ and $|\psi^{(0)}_n, \downarrow\rangle$, for energy $E^{(0)}_n$.

The perturbation $\hat{H}^{(1)}_{\text{1-particle}} = \frac{\lambda}{2}\cdot[e^{-\mathbb{i}kx}\hat{S}_+ + e^{\mathbb{i}kx}\hat{S}_-]$ can be viewed as a 2×2 matrix, $\frac{\lambda\hbar}{2}\begin{pmatrix} 0 & e^{-\mathbb{i}kx} \\ e^{\mathbb{i}kx} & 0 \end{pmatrix}$ for 2-component spin-1/2 spinor wavefunctions $[|\uparrow\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, |\downarrow\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}]$.

The first order secular equation 2×2 matrix is $\langle \psi^{(0)}_1, S_z|\hat{H}^{(1)}_{\text{1-particle}}|\psi^{(0)}_1, S'_z\rangle$
$= \int \mathrm{d}x \left(|\psi^{(0)}_1(x)|^2 \cdot \frac{\lambda\hbar}{2}\begin{pmatrix} 0 & e^{-\mathbb{i}kx} \\ e^{\mathbb{i}kx} & 0 \end{pmatrix}\right) = \int_{-L}^{L} \mathrm{d}x \left(\frac{1}{L}\cos^2(\frac{\pi x}{2L})\cdot\frac{\lambda\hbar}{2}\begin{pmatrix} 0 & e^{-\mathbb{i}kx} \\ e^{\mathbb{i}kx} & 0 \end{pmatrix}\right)$
$= \frac{\lambda\hbar}{2}\frac{\pi^2}{\pi^2-k^2L^2}\frac{\sin(kL)}{kL}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, here $S_z, S'_z = \uparrow, \downarrow$ are row and column indices respectively. It has eigenvalues $\pm\frac{\lambda\hbar}{2}\frac{\pi^2}{\pi^2-k^2L^2}\frac{\sin(kL)}{kL}$ for eigenvectors $\chi_{(1)}(s) = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}$, and $\chi_{(2)}(s) = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}$, respectively.

Therefore the first order single particle ground state energies are
$E_{1,(1)} = E^{(0)}_1 + \frac{\lambda\hbar}{2}\frac{\pi^2}{\pi^2-k^2L^2}\frac{\sin(kL)}{kL}$, and $E_{1,(2)} = E^{(0)}_1 - \frac{\lambda\hbar}{2}\frac{\pi^2}{\pi^2-k^2L^2}\frac{\sin(kL)}{kL}$,
with corresponding approximate eigenstates $\psi_{1,(i)}(x,s) = \psi^{(0)}_1(x)\chi_{(i)}(s)$, $i = 1, 2$.

From the perturbed single particle ground states, we can construct perturbed two boson ground states,
$E_{1,1,(1)} = E_{1,(1)} + E_{1,(1)} = \frac{\hbar^2\pi^2}{8mL^2}\cdot 2 + \lambda\hbar\frac{\pi^2}{\pi^2-k^2L^2}\frac{\sin(kL)}{kL}$, for $\psi_{1,(1)}(x_1,s_1)\psi_{1,(1)}(x_2,s_2)$;
$E_{1,1,(2)} = E_{1,(1)} + E_{1,(2)} = \frac{\hbar^2\pi^2}{8mL^2}\cdot 2$, for $\frac{1}{\sqrt{2}}[\psi_{1,(1)}(x_1,s_1)\psi_{1,(2)}(x_2,s_2) + \psi_{1,(2)}(x_1,s_1)\psi_{1,(1)}(x_2,s_2)]$;
$E_{1,1,(3)} = E_{1,(2)} + E_{1,(2)} = \frac{\hbar^2\pi^2}{8mL^2}\cdot 2 - \lambda\hbar\frac{\pi^2}{\pi^2-k^2L^2}\frac{\sin(kL)}{kL}$, for $\psi_{1,(2)}(x_1,s_1)\psi_{1,(2)}(x_2,s_2)$.

(f) use Method #2 for (e), compute the 2nd order secular equation for single particle, solve the 2nd order perturbed ground state energies for single particle, and then construct the two boson ground states.

the matrix for secular equation up to 2nd order is,
$\langle\psi^{(0)}_1, S_z|\hat{H}^{(1)}_{\text{1-particle}}|\psi^{(0)}_1, S'_z\rangle + \sum_{n>1}\sum_{S''_z}\frac{\langle\psi^{(0)}_1,S_z|\hat{H}^{(1)}_{\text{1-particle}}|\psi^{(0)}_n,S''_z\rangle\langle\psi^{(0)}_n,S''_z|\hat{H}^{(1)}_{\text{1-particle}}|\psi^{(0)}_1,S'_z\rangle}{E^{(0)}_1 - E^{(0)}_n}$,

$$\langle\psi_1^{(0)}, S_z|\hat{H}^{(1)}_{\text{1-particle}}|\psi_n^{(0)}, S_z''\rangle = \int \mathrm{d}x \left([\psi_1^{(0)}(x)]^*\psi_n^{(0)}(x)\cdot\frac{\lambda\hbar}{2}\begin{pmatrix}0 & e^{-\mathbb{i}kx}\\ e^{\mathbb{i}kx} & 0\end{pmatrix}\right).$$

If n is even positive integer,

$$\langle\psi_1^{(0)}, S_z|\hat{H}^{(1)}_{\text{1-particle}}|\psi_n^{(0)}, S_z''\rangle = \int_{-L}^{L}\mathrm{d}x\,\frac{1}{L}\left(\cos(\tfrac{\pi x}{2L})(-1)^{n/2}\sin(\tfrac{n\pi x}{2L})\cdot\frac{\lambda\hbar}{2}\begin{pmatrix}0 & e^{-\mathbb{i}kx}\\ e^{\mathbb{i}kx} & 0\end{pmatrix}\right)$$

$$= (-1)^{n/2}\cdot\frac{\lambda\hbar}{4}\left(\frac{\sin((k-\frac{(n+1)\pi}{2L})L)}{(k-\frac{(n+1)\pi}{2L})L}+\frac{\sin((k-\frac{(n-1)\pi}{2L})L)}{(k-\frac{(n-1)\pi}{2L})L}-\frac{\sin((k+\frac{(n-1)\pi}{2L})L)}{(k+\frac{(n-1)\pi}{2L})L}-\frac{\sin((k+\frac{(n+1)\pi}{2L})L)}{(k+\frac{(n+1)\pi}{2L})L}\right)\begin{pmatrix}0 & -\mathbb{i}\\ \mathbb{i} & 0\end{pmatrix}$$

$$= \frac{\lambda\hbar}{2}\cdot(kL)\cos(kL)\left(\frac{1}{k^2L^2-(n-1)^2\pi^2/4}-\frac{1}{k^2L^2-(n+1)^2\pi^2/4}\right)\begin{pmatrix}0 & -\mathbb{i}\\ \mathbb{i} & 0\end{pmatrix}$$

If n is odd and $n>1$,

$$\langle\psi_1^{(0)}, S_z|\hat{H}^{(1)}_{\text{1-particle}}|\psi_n^{(0)}, S_z''\rangle = \int_{-L}^{L}\mathrm{d}x\,\frac{1}{L}\left(\cos(\tfrac{\pi x}{2L})(-1)^{(n-1)/2}\cos(\tfrac{n\pi x}{2L})\cdot\frac{\lambda\hbar}{2}\begin{pmatrix}0 & e^{-\mathbb{i}kx}\\ e^{\mathbb{i}kx} & 0\end{pmatrix}\right)$$

$$= (-1)^{(n-1)/2}\cdot\frac{\lambda\hbar}{4}\left(\frac{\sin((k-\frac{(n+1)\pi}{2L})L)}{(k-\frac{(n+1)\pi}{2L})L}+\frac{\sin((k-\frac{(n-1)\pi}{2L})L)}{(k-\frac{(n-1)\pi}{2L})L}+\frac{\sin((k+\frac{(n-1)\pi}{2L})L)}{(k+\frac{(n-1)\pi}{2L})L}+\frac{\sin((k+\frac{(n+1)\pi}{2L})L)}{(k+\frac{(n+1)\pi}{2L})L}\right)\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}$$

$$= \frac{\lambda\hbar}{2}\cdot(kL)\sin(kL)\left(\frac{1}{k^2L^2-(n-1)^2\pi^2/4}-\frac{1}{k^2L^2-(n+1)^2\pi^2/4}\right)\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}$$

The 2nd order secular equation is $I_{1,\text{1-particle}}\cdot\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}+I_{2,\text{1-particle}}\cdot\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}$, where

$I_{1,\text{1-particle}} = \frac{\lambda\hbar}{2}\frac{\pi^2}{\pi^2-k^2L^2}\frac{\sin(kL)}{kL}$ solved in (e),

$I_{2,\text{1-particle}} = [\frac{\lambda\hbar}{2}\cdot(kL)]^2\Big\{\sum_{m=1}^{\infty}\cos^2(kL)\left(\frac{1}{k^2L^2-(2m-1)^2\pi^2/4}-\frac{1}{k^2L^2-(2m+1)^2\pi^2/4}\right)^2$
$+\sum_{m=1}^{\infty}\sin^2(kL)\left(\frac{1}{k^2L^2-(2m)^2\pi^2/4}-\frac{1}{k^2L^2-(2m+2)^2\pi^2/4}\right)^2\Big\}.$

The eigenvalues are $\pm I_1+I_2$, with same eigenvectors $\chi_{(1,2)}$ as those in (e). So the single particle ground state energies up to λ^2 order are $E_{1,(1,2)} = \frac{\hbar^2\pi^2}{8mL^2}\pm I_1+I_2$.

The two boson ground state energies are

$E_{1,1,(1)} = E_{1,(1)}+E_{1,(1)} = \frac{\hbar^2\pi^2}{8mL^2}\cdot 2+2I_{1,\text{1-particle}}+2I_{2,\text{1-particle}}$;
$E_{1,1,(2)} = E_{1,(1)}+E_{1,(2)} = \frac{\hbar^2\pi^2}{8mL^2}\cdot 2+2I_{2,\text{1-particle}}$;
$E_{1,1,(3)} = E_{1,(2)}+E_{1,(2)} = \frac{\hbar^2\pi^2}{8mL^2}\cdot 2-2I_{1,\text{1-particle}}+2I_{2,\text{1-particle}}$.