Quantum Mechanics: Fall 2022
Final Exam: Brief Solutions

Possibly useful facts:

- 1D harmonic oscillator: $\hat{H} = \frac{\hat{p}_x^2}{2m} + \frac{m\omega^2}{2}\hat{x}^2 = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{m\omega^2}{2}x^2$.
  $[\hat{x}, \hat{p}_x] = \mathbb{i}\hbar$, and in position representation $\hat{p}_x = -\mathbb{i}\hbar\frac{\partial}{\partial x}$. Define $\hat{a}_\mp = \sqrt{\frac{m\omega}{2\hbar}}(\hat{x} \pm \mathbb{i}\frac{1}{m\omega}\hat{p}_x) = \sqrt{\frac{m\omega}{2\hbar}}(x \pm \frac{\hbar}{m\omega}\frac{\partial}{\partial x})$. 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: $[\hat{J}_x, \hat{J}_y] = \mathbb{i}\hbar\hat{J}_z$, $[\hat{J}_y, \hat{J}_z] = \mathbb{i}\hbar\hat{J}_x$, $[\hat{J}_z, \hat{J}_x] = \mathbb{i}\hbar\hat{J}_y$.
  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 $(\hat{J}_x \pm \mathbb{i}\hat{J}_y)|j,m\rangle = \sqrt{(j\mp m)(j\pm m+1)}\hbar|j,m\pm 1\rangle$.
  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.
    $\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, $\sigma_y = \begin{pmatrix} 0 & -\mathbb{i} \\ \mathbb{i} & 0 \end{pmatrix}$, $\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$.

- (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 $\hat{H}|\psi_n\rangle = E_n|\psi_n\rangle$, E_n is close to $E_n^{(0)}$, then $(E_n - E_n^{(0)})$ is an eigenvalue of "secular equation" matrix, $\langle\psi_{n\beta}^{(0)}|\hat{H}^{(1)}|\psi_{n\alpha}^{(0)}\rangle + \sum_{m, m\neq n}\frac{1}{E_n^{(0)} - E_m^{(0)}}\langle\psi_{n\beta}^{(0)}|\hat{H}^{(1)}|\psi_m^{(0)}\rangle\langle\psi_m^{(0)}|\hat{H}^{(1)}|\psi_{n\alpha}^{(0)}\rangle$ 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.

- Dyson series: Solution to $\frac{\partial}{\partial t}c_n(t) = \sum_m V_{n,m}(t)c_m(t)$ is formally,
  $$c_n(t) = c_n(t=0) + \sum_m \int_0^t V_{n,m}(t')\mathrm{d}t' \cdot c_m(t=0)$$
  $$+ \sum_m \sum_{m'} \int_0^t V_{n,m}(t')\left[\int_0^{t'} V_{m,m'}(t'')\mathrm{d}t''\right]\mathrm{d}t' \cdot c_{m'}(t=0) + \ldots$$

Problem 1. (35 points) Consider a two-dimensional harmonic oscillator, $\hat{H}_0 = (\frac{1}{2m}\hat{p}_x^2 + \frac{m\omega^2}{2}x^2) + (\frac{1}{2m}\hat{p}_y^2 + \frac{m\omega^2}{2}y^2)$. Here $\hat{p}_x = -\mathbb{i}\hbar\partial_x$, $\hat{p}_y = -\mathbb{i}\hbar\partial_y$.

(a) (5pts) *Write down the explicit form of ground state and first excited states wavefunctions.* [Hint: it would be convenient to define ladder operators for the x- and y- parts of $\hat{H}_0$, but the final answer should be explicit functions of x, y].

(b) (10pts) Add a time-independent perturbation $\hat{H}_1 = Vx^2y^2$, where V is a "small" real parameter. *Compute the ground state energy of $\hat{H}_0 + \hat{H}_1$ up to second order of V.*

(c) (5pts) *Compute the correction by $\hat{H}_1$ to the original first excited state energies in (a) to first order of V.*

(d) (5pts*) *Compute the correction to the original first excited states energies to second order of V.* [Hint: degenerate perturbation theory can be avoided]

(e) (10pts) Use the variational method to estimate the ground state energy of $\hat{H} = \hat{H}_0 + \hat{H}_1$. Consider a "variational Hamiltonian" $\hat{H}_\Omega = \frac{1}{2m}\hat{p}_x^2 + \frac{m\Omega^2}{2}x^2 + \frac{1}{2m}\hat{p}_y^2 + \frac{m\Omega^2}{2}y^2$, with "variational parameter" Ω, its normalized ground state is $\psi_{0,\Omega}(x,y)$, *Compute the energy expectation value $E(\Omega) = \langle\psi_{0,\Omega}|(\hat{H}_0 + \hat{H}_1)|\psi_{0,\Omega}\rangle$, then minimize $E(\Omega)$ with respect to Ω to find the best "variational energy".* [Note: this variational ground state energy may not match the result of (b).]

Solution:

(a) Define $\hat{a}_{x,\pm} = \sqrt{\frac{m\omega}{2\hbar}}(\hat{x} \mp \frac{\mathbb{i}}{m\omega}\hat{p}_x)$, $\hat{a}_{y,\pm} = \sqrt{\frac{m\omega}{2\hbar}}(\hat{y} \mp \frac{\mathbb{i}}{m\omega}\hat{p}_y)$, then $[\hat{a}_{i,-}, \hat{a}_{j,+}] = \delta_{i,j}$, $[\hat{a}_{i,-}, \hat{a}_{j,-}] = 0$,

$\hat{H}_0 = \hbar\omega(\hat{a}_{x,+}\hat{a}_{x,-} + \hat{a}_{y,+}\hat{a}_{y,-} + 1)$ is the sum of two independent 1D harmonic oscillators.

The ground state of $\hat{H}_0$ satisfies $\hat{a}_{x,-}\psi_0(x,y) = \hat{a}_{y,-}\psi_0(x,y) = 0$, and is $\psi_0(x,y) = \psi_0(x)\cdot\psi_0(y) = (\frac{m\omega}{\pi\hbar})^{1/2}e^{-\frac{m\omega}{2\hbar}(x^2+y^2)}$, with $E_{0,0} = E_0 + E_0 = \hbar\omega$. [see Page 1 for 1D harmonic oscillator eigenvalues/states E_n, $\psi_n(x)$]

the first excited states of $\hat{H}_0$ are

$\psi_{1,0}(x,y) = \psi_1(x)\cdot\psi_0(y) = \hat{a}_{x,+}\psi_0(x)\cdot\psi_0(y) = (\frac{m\omega}{\pi\hbar})^{1/2}\sqrt{\frac{2m\omega}{\hbar}}x \cdot e^{-\frac{m\omega}{2\hbar}(x^2+y^2)}$, and

$\psi_{0,1}(x,y) = \psi_0(x)\cdot\psi_1(y) = \psi_0(x)\cdot\hat{a}_{y,+}\psi_0(y) = (\frac{m\omega}{\pi\hbar})^{1/2}\sqrt{\frac{2m\omega}{\hbar}}y\cdot e^{-\frac{m\omega}{2\hbar}(x^2+y^2)}$, with
$E_{1,0} = E_{0,1} = E_0 + E_1 = 2\hbar\omega$.

Generically the eigenstates of $\hat{H}_0$ are
$\psi_{n_x,n_y}(x,y) = \psi_{n_x}(x)\cdot\psi_{n_y}(y) = \frac{1}{\sqrt{n_x!n_y!}}(\hat{a}_{x,+})^{n_x}(\hat{a}_{y,+})^{n_y}\psi_{0,0}(x,y)$, with
$E_{n_x,n_y} = E_{n_x} + E_{n_y} = \hbar\omega(n_x+n_y+1)$, where $n_x, n_y = 0, 1, \ldots$.

(b)
$\hat{x}^2 = \sqrt{\frac{\hbar}{2m\omega}}(\hat{a}_{x,-}+\hat{a}_{x,+})^2 = \frac{\hbar}{2m\omega}(2\hat{a}_{x,+}\hat{a}_{x,-}+1+\hat{a}_{x,+}^2+\hat{a}_{x,-}^2)$,
similarly, $\hat{y}^2 == \frac{\hbar}{2m\omega}(2\hat{a}_{y,+}\hat{a}_{y,-}+1+\hat{a}_{y,+}^2+\hat{a}_{y,-}^2)$,
Then $\hat{H}_1 = V\cdot(\frac{\hbar}{2m\omega})^2\cdot(2\hat{a}_{x,+}\hat{a}_{x,-}+1+\hat{a}_{x,+}^2+\hat{a}_{x,-}^2)(2\hat{a}_{y,+}\hat{a}_{y,-}+1+\hat{a}_{y,+}^2+\hat{a}_{y,-}^2)$
$\hat{H}_1|\psi_{0,0}\rangle = V\cdot(\frac{\hbar}{2m\omega})^2\left[|\psi_{0,0}\rangle+\sqrt{2}|\psi_{2,0}\rangle+\sqrt{2}|\psi_{0,2}\rangle+2|\psi_{2,2}\rangle\right]$

The first order correction to ground state energy is
$E_{0,0}^{(1)} = \langle\psi_{0,0}(x,y)|\hat{H}_1|\psi_{0,0}(x,y)\rangle = V\cdot(\frac{\hbar}{2m\omega})^2$

The second order correction is $\sum_{m,m\neq(0,0)}\frac{|\langle\psi_m|\hat{H}_1|\psi_{(0,0)}\rangle|^2}{E_{0,0}-E_m}$, m can be $(2,0)$, $(0,2)$, and $(2,2)$, note that $E_{2,0} = E_{0,2} = 3\hbar\omega$, and $E_{2,2} = 5\hbar\omega$, the second order correction to ground state energy is
$E_{0,0}^{(2)} = \frac{|V\cdot(\frac{\hbar}{2m\omega})^2\cdot\sqrt{2}|^2}{\hbar\omega-3\hbar\omega} + \frac{|V\cdot(\frac{\hbar}{2m\omega})^2\cdot\sqrt{2}|^2}{\hbar\omega-3\hbar\omega} + \frac{|V\cdot(\frac{\hbar}{2m\omega})^2\cdot 2|^2}{\hbar\omega-5\hbar\omega} = -\frac{3V^2\hbar^3}{16m^4\omega^5}$

(c) The first order secular equation is actually diagonal,
$\langle\psi_{1,0}|\hat{H}_1|\psi_{1,0}\rangle = \langle\psi_{1,0}|V\cdot(\frac{\hbar}{2m\omega})^2(2\hat{a}_{x,+}\hat{a}_{x,-}+1)(2\hat{a}_{y,+}\hat{a}_{y,-}+1)|\psi_{1,0}\rangle = V\cdot(\frac{\hbar}{2m\omega})^2\cdot 3$
similarly, $\langle\psi_{0,1}|\hat{H}_1|\psi_{0,1}\rangle = V\cdot(\frac{\hbar}{2m\omega})^2\cdot 3$,
and the off-diagonal term $\langle\psi_{1,0}|\hat{H}_1|\psi_{0,1}\rangle = 0$, this can be seen from the fact that $\psi_{1,0}$, $\hat{H}_1$, $\psi_{0,1}$ are odd, even, even functions of x respectively.

The first order secular equation (under $|\psi_{1,0}\rangle$, $\psi_{0,1}\rangle$ basis) is $3V\cdot(\frac{\hbar}{2m\omega})^2\cdot\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}$,
so it does not lift the degeneracy, and produce first order energy shift $3V\cdot(\frac{\hbar}{2m\omega})^2$ for both first excited states.

(d) naively we need to compute the 2nd order secular equation $[i,j = (1,0),(0,1)]$,

$\sum_m \frac{\langle\psi_i|\hat{H}_1|\psi_m\rangle\langle\psi_m|\hat{H}_1|\psi_j\rangle}{E_{1,0}^{(0)}-E_m^{(0)}}$,

however it is easy to see that this matrix is diagonal and proportional to identity matrix,

note that $\psi_{1,0}$ is odd function of x, $\psi_{0,1}$ is even function of x, $\hat{H}_1$ is even function of x, therefore the above term is nonzero only if ψ_i, ψ_m, ψ_j have the same parity under $x \to -x$, then we need $i = j = (1,0)$ or $(0,1)$,

and by the $x \leftrightarrow y$ symmetry, the $i = j = (1,0)$ and $i = j = (0,1)$ terms should equal,

alternatively, we can work within the subspaces of even(odd) functions of x (because $\hat{H}_0 + \hat{H}_1$ is even function of x), within each of these subspaces, there is no degeneracy for the $E = 2\hbar\omega$ level.

similar to the 2nd order perturbation term for ground state, compute first

$\hat{H}_1|\psi_{1,0}\rangle = V \cdot (\frac{\hbar}{2m\omega})^2 \left[3|\psi_{1,0}\rangle + \sqrt{6}|\psi_{3,0}\rangle + 3\sqrt{2}|\psi_{1,2}\rangle + 2\sqrt{3}|\psi_{3,2}\rangle\right]$,

the 2nd order correction to 1st excited state energy is

$E_{(1,0)}^{(2)} = E_{(0,1)}^{(2)} = |V \cdot (\frac{\hbar}{2m\omega})^2|^2 \cdot [\frac{|\sqrt{6}|^2}{-2\hbar\omega} + \frac{|3\sqrt{2}|^2}{-2\hbar\omega} + \frac{|2\sqrt{3}|^2}{-4\hbar\omega}] = -\frac{15V^2\hbar^3}{16m^4\omega^5}$

(e)

$\hat{H}_0 + \hat{H}_1 = \hat{H}_\Omega + \frac{m(\omega^2-\Omega^2)}{2}(x^2+y^2) + Vx^2y^2$.

Note that $\langle\psi_{0,\Omega}|x^2|\psi_{0,\Omega}\rangle = \langle\psi_{0,\Omega}|y^2|\psi_{0,\Omega}\rangle = \frac{\hbar}{2m\Omega}$,

$E(\Omega) = \hbar\Omega + \frac{m(\omega^2-\Omega^2)}{2}(\frac{\hbar}{2m\Omega} \times 2) + V(\frac{\hbar}{2m\Omega})^2 = \frac{1}{2}(\hbar\Omega + \hbar\frac{\omega^2}{\Omega}) + V(\frac{\hbar}{2m\Omega})^2$

let $\frac{\mathrm{d}E}{\mathrm{d}\Omega} = \frac{\hbar}{2}(1 - \frac{\omega^2}{\Omega^2}) - \frac{V\hbar^2}{2m^2\Omega^3} = 0$

assume $\frac{\omega}{\Omega} = 1 + a_1V + a_2V^2 + O(V^3)$, the above equation becomes

$\frac{\hbar}{2}[-2a_1V - (2a_2 + a_1^2)V^2 + O(V^3)] - \frac{\hbar^2}{2m^2\omega^3}V[1 + 3a_1V + (3a_1^2 + 3a_2)V^2 + O(V^3)] = 0$, then

$a_1 = -\frac{\hbar}{2m^2\omega^3}$, $a_2 = -\frac{a_1^2}{2} - 3\frac{\hbar^2}{2m^2\omega^3}a_1 = \frac{5}{8}(\frac{\hbar}{m^2\omega^3})^2$

So best variational parameter is

$\Omega \approx \omega \cdot [1 - a_1V + (a_1^2 - a_2)V^2 + O(V^3)] = \omega \cdot [1 + \frac{\hbar}{2m^2\omega^3}V - \frac{3}{8}(\frac{\hbar}{m^2\omega^3})^2V^2 + O(V^3)]$

Best variational energy is

$E(\Omega) \approx \frac{\hbar\omega}{2}[2 + a_1^2V^2 + O(V^3)] + V\frac{\hbar^2}{4m^2\omega^2}[1 + 2a_1V + (a_1^2 + 2a_2)V^2 + O(V^3)]$

$\approx \hbar\omega + V\frac{\hbar^2}{4m^2\omega^2} - V^2\frac{\hbar^4}{8m^4\omega^5} + O(V^3)$

The first order variational energy is consistent with perturbation theory, but second order term is higher than perturbation theory result.

Problem 2. (25 points) Consider a non-relativistic particle of mass m moving on a ring of circumference L. This can be viewed as a 1D problem defined on x-axis with periodic boundary condition for the wavefunction, $\psi(x+L)=\psi(x)$, and normalization condition $\int_{x=-\frac{L}{2}}^{\frac{L}{2}} |\psi(x)|^2\,\mathrm{d}x = 1$.

(a) (5pts) For free particle, $\hat{H}_0 = \frac{\hat{p}^2}{2m}$, with this periodic boundary condition, *write down all the energy eigenvalues $E_n^{(0)}$ and normalized eigenstate wavefunctions $\psi_n^{(0)}(x)$.*

(b) (5pts) Consider a δ-potential whose position moves with constant speed v, on x-axis this can be represented by a moving "comb" function, it is a time-dependent perturbation, $V(x,t) = \alpha\sum_{j=-\infty}^{\infty}\delta(x-vt-jL)$, here $\alpha>0$. Assume the solution to $\mathbb{i}\hbar\frac{\partial}{\partial t}|\psi\rangle = [\hat{H}_0+V(x,t)]|\psi\rangle$ is $|\psi\rangle = \sum_n c_n(t)e^{-\mathbb{i}E_n^{(0)}t/\hbar}|\psi_n^{(0)}\rangle$, *Derive the differential equations satisfied by $c_n(t)$.* [Note: the result should not contain unknown variables(matrix elements).]

(c) (10pts) *Compute the transition probability from ground state of $\hat{H}_0$ to first excited state(s) of $\hat{H}_0$ over time t, under the perturbation in (b), to lowest non-trivial order of α.*

(d) (5pts*) Convert the problem $\mathbb{i}\hbar\frac{\partial}{\partial t}\psi(x,t) = [-\frac{\hbar^2}{2m}\partial_x^2 + V(x,t)]\psi(x,t)$ to a problem with time-independent Hamiltonian by "Galilean boost". Change variable x to $\tilde{x} = x - vt$, define $\tilde{\psi}(\tilde{x},t) = \psi(x,t)$. *Derive the Schrödinger equation satisfied by $\tilde{\psi}$. Derive the algebraic equation satisfied by the ground state energy $\tilde{E}_0$* [Note: the equation for $\tilde{E}_0$ cannot be explicitly solved.]

Solution

(a)

this is the same as a midterm problem,

$E_n^{(0)} = \frac{\hbar^2}{2m}(\frac{2\pi n}{L})^2$, $\psi_n^{(0)}(x) = \frac{1}{\sqrt{L}}e^{\mathbb{i}\frac{2\pi n}{L}x}$

n is an integer.

(b)

$\mathbb{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}c_n(t) = \sum_m e^{\mathbb{i}\omega_{nm}t}\langle\psi_n^{(0)}|V(x,t)|\psi_m^{(0)}\rangle\cdot c_m(t)$

Here $\omega_{nm} = \frac{E_n^{(0)} - E_m^{(0)}}{\hbar} = \frac{2\pi^2\hbar}{mL^2}(n^2 - m^2)$,

$\langle \psi_n^{(0)} | V(x,t) | \psi_m^{(0)} \rangle = \int_{x=-L/2}^{L/2} \alpha \sum_{j=-\infty}^{\infty} \delta(x - vt - jL) \cdot \frac{1}{L} e^{\mathbb{i}\frac{2\pi(m-n)x}{L}} \, \mathrm{d}x$

$= \alpha \cdot \frac{1}{L} \exp(\mathbb{i}\frac{2\pi}{L}(m-n)vt)$, [generically there is one and only one j such that $-L/2 \le x - vt - jL < L/2$]

(c) To first order, transition probability is

$$P_{m\to n}(t) = \left| \int_0^t \frac{1}{\mathbb{i}\hbar} e^{\mathbb{i}\omega_{nm}t} \langle \psi_n^{(0)} | V(x,t) | \psi_m^{(0)} \rangle \, \mathrm{d}t \right|^2 = \frac{\alpha^2}{\hbar^2 L^2} \frac{4\sin(\frac{\omega_{nm} + \frac{2\pi}{L}(m-n)v}{2}t)}{[\omega_{nm} + \frac{2\pi}{L}(m-n)v]^2}$$

Let $m = 0$, $n = \pm 1$, the transition probability from ground to first excited states are

$P_{0\to 1}(t) = \frac{\alpha^2}{\hbar^2 L^2} \frac{4\sin((\frac{\pi^2\hbar}{mL^2} - \frac{\pi}{L}v)t)}{(\frac{2\pi^2\hbar}{mL^2} - \frac{2\pi}{L}v)^2}$, $P_{0\to -1}(t) = \frac{\alpha^2}{\hbar^2 L^2} \frac{4\sin((\frac{\pi^2\hbar}{mL^2} + \frac{\pi}{L}v)t)}{(\frac{2\pi^2\hbar}{mL^2} + \frac{2\pi}{L}v)^2}$

(d)

$(\frac{\partial\tilde\psi}{\partial t})_{\tilde x} = (\frac{\partial\psi}{\partial t})_x + (\frac{\partial\psi}{\partial x})_t (\frac{\partial x}{\partial t})_{\tilde x} = (\frac{\partial\psi}{\partial t})_x + (\frac{\partial\psi}{\partial x})_t \cdot v$,

$(\frac{\partial\tilde\psi}{\partial\tilde x})_t = (\frac{\partial\psi}{\partial x})_t$

$\mathbb{i}\hbar\frac{\partial}{\partial t}\tilde\psi(\tilde x, t) + v \cdot \mathbb{i}\hbar\frac{\partial}{\partial\tilde x}\tilde\psi(\tilde x, t) = [-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial\tilde x^2} + \tilde V(\tilde x)]\tilde\psi(\tilde x, t)$,

here $\tilde V(\tilde x) = V(x,t) = \alpha \sum_j \delta(\tilde x - jL)$,

then $\tilde H = \frac{\hat{\tilde p}^2}{2m} + v \cdot \hat{\tilde p} + \tilde V(\tilde x)$

For given $\tilde E > -\frac{mv^2}{2}$, define $\tilde p_\pm = -mv \pm \sqrt{2m\tilde E + m^2v^2}$,

assume $\tilde\psi = Ae^{\mathbb{i}\tilde p_+ x/\hbar} + Be^{\mathbb{i}\tilde p_- x/\hbar}$, for $0 < x < L$,

the boundary condition at $x = 0$ is

$\tilde\psi(+0) = \tilde\psi(L-0)$,

$-\frac{\hbar^2}{2m}[\frac{\partial\tilde\psi}{\partial\tilde x}|_{x=+0} - \frac{\partial\tilde\psi}{\partial\tilde x}|_{x=L-0}] + \alpha\tilde\psi(0) = 0$,

namely, $A \cdot (1 - e^{\mathbb{i}\tilde p_+ L/\hbar}) + B \cdot (1 - e^{\mathbb{i}\tilde p_- L/\hbar}) = 0$,

$-\frac{\hbar}{2m}[\mathbb{i}\tilde p_+ A \cdot (1 - e^{\mathbb{i}\tilde p_+ L/\hbar}) + \mathbb{i}\tilde p_- B \cdot (1 - e^{\mathbb{i}\tilde p_- L/\hbar})] = -\alpha(A + B)$

solve B in terms of A from first equation, plug into second equation,

$\frac{\hbar}{2m}\mathbb{i}(\tilde p_+ - \tilde p_-)(1 - e^{\mathbb{i}\tilde p_+ L/\hbar})A = \alpha\frac{e^{\mathbb{i}\tilde p_+ L/\hbar} - e^{\mathbb{i}\tilde p_- L/\hbar}}{(1 - e^{\mathbb{i}\tilde p_- L/\hbar})} \cdot A$

Finally, $\frac{\hbar}{m}\sqrt{2m\tilde E + m^2v^2} = -\alpha \cdot \frac{\sin(\sqrt{2m\tilde E + m^2v^2} \cdot L/\hbar)}{2\sin(\tilde p_+ L/2\hbar)\sin(\tilde p_- L/2\hbar)}$

Note: when $v = 0$, this problem basically reduces to midterm Problem 1(c).

Problem 3. (25 points) Consider two identical particles in 1D harmonic potential, with Hamiltonian $\hat{H}_0 = \frac{1}{2m}(\hat{p}_1^2 + \hat{p}_2^2) + \frac{m\omega^2}{2}(x_1^2 + x_2^2)$. Subscripts $_1$ and $_2$ label the two particles. $\hat{p}_1 = -\mathbb{i}\hbar\frac{\partial}{\partial x_1}$, $\hat{p}_2 = -\mathbb{i}\hbar\frac{\partial}{\partial x_2}$.

(a) (5pts) For two identical spinless BOSONS under $\hat{H}_0$, *write down the normalized ground state(s) and first excited state(s), and second excited state(s) wavefunctions, and corresponding energies.*

(b) (5pts) For two identical spinless FERMIONS under $\hat{H}_0$, *write down the normalized ground state(s) and first excited state(s), and second excited state(s) wavefunctions, and corresponding energies.*

(c) (10pts) For spin-1/2 BOSONS and FERMIONS under $\hat{H}_0$, *write down the normalized ground state(s) and first excited state(s), and corresponding energies, for the boson/fermion cases respectively.*

(d) (5pts*) Add a perturbation $\hat{H}_1 = \lambda \cdot (\hat{p}_1 + \hat{p}_2) \cdot (\hat{S}_{1x} + \hat{S}_{2x})$, here λ is a "small" real parameter. *Compute the corrections to all the FERMION case energies in (c) to lowest nontrivial order of* λ

Solution

(a)

Ground state

$\psi_{0,0}^{(B,spinless)}(x_1, x_2) = \psi_0(x_1)\psi_0(x_2) = (\frac{m\omega}{\pi\hbar})^{1/2}\exp(-\frac{m\omega}{2\hbar}(x_1^2 + x_2^2))$,

$E_{0,0} = E_0 + E_0 = \hbar\omega$,

First excited state

$\psi_{0,1}^{(B,spinless)}(x_1, x_2) = \sqrt{\frac{1}{2}}[\psi_0(x_1)\psi_1(x_2) + \psi_1(x_1)\psi_0(x_2)]$

$= \sqrt{\frac{m\omega}{\hbar}}(x_1 + x_2) \cdot (\frac{m\omega}{\pi\hbar})^{1/2}\exp(-\frac{m\omega}{2\hbar}(x_1^2 + x_2^2))$,

$E_{0,1} = E_0 + E_1 = 2\hbar\omega$,

Second excited states

$\psi_{0,2}^{(B,spinless)}(x_1, x_2) = \sqrt{\frac{1}{2}}[\psi_0(x_1)\psi_2(x_2) + \psi_2(x_1)\psi_0(x_2)]$

$= [\frac{m\omega}{\hbar}(x_1^2 + x_2^2) - 1] \cdot (\frac{m\omega}{\pi\hbar})^{1/2} \exp(-\frac{m\omega}{2\hbar}(x_1^2 + x_2^2)),$

and $\psi_{1,1}^{(B,spinless)}(x_1, x_2) = \psi_1(x_1)\psi_1(x_2) = 2(\frac{m\omega}{\hbar})x_1 x_2 \cdot (\frac{m\omega}{\pi\hbar})^{1/2} \exp(-\frac{m\omega}{2\hbar}(x_1^2 + x_2^2)),$

$E_{0,2} = E_{1,1} = 3\hbar\omega,$

(b)

Ground state

$\psi_{0,1}^{(F,spinless)}(x_1, x_2) = \sqrt{\frac{1}{2}}[\psi_0(x_1)\psi_1(x_2) - \psi_1(x_1)\psi_0(x_2)]$

$= \sqrt{\frac{m\omega}{\hbar}}(x_2 - x_1) \cdot (\frac{m\omega}{\pi\hbar})^{1/2} \exp(-\frac{m\omega}{2\hbar}(x_1^2 + x_2^2)),$

$E_{0,1} = E_0 + E_1 = 2\hbar\omega,$

First excited state

$\psi_{0,2}^{(F,spinless)}(x_1, x_2) = \sqrt{\frac{1}{2}}[\psi_0(x_1)\psi_2(x_2) - \psi_2(x_1)\psi_0(x_2)]$

$= \frac{m\omega}{\hbar}(x_2^2 - x_1^2) \cdot (\frac{m\omega}{\pi\hbar})^{1/2} \exp(-\frac{m\omega}{2\hbar}(x_1^2 + x_2^2)),$

$E_{0,2} = E_0 + E_2 = 3\hbar\omega,$

Second excited states

$\psi_{0,3}^{(F,spinless)}(x_1, x_2) = \sqrt{\frac{1}{2}}[\psi_0(x_1)\psi_3(x_2) - \psi_3(x_1)\psi_0(x_2)],$

and $\psi_{1,2}^{(F,spinless)}(x_1, x_2) = \sqrt{\frac{1}{2}}[\psi_1(x_1)\psi_2(x_2) - \psi_2(x_1)\psi_1(x_2)],$

$E_{0,3} = E_{1,2} = 4\hbar\omega,$

(c)

Represent the bases as (spinless particle bases)*(spin singlet/triplets).

The involved spin wavefunctions are

$|S = 0, S_z = 0\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle|\downarrow\rangle - |\downarrow\rangle|\uparrow\rangle),$

$|S = 1, S_z = 1\rangle = |\uparrow\rangle|\uparrow\rangle,$

$|S = 1, S_z = 0\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle|\downarrow\rangle + |\downarrow\rangle|\uparrow\rangle),$

$|S = 0, S_z = -1\rangle = |\downarrow\rangle|\downarrow\rangle,$

For spin-1/2 bosons,

ground state is $\psi_{0,0}^{B,spinless}(x_1, x_2) \otimes |S = 1, S_z\rangle$, for $S_z = -1, 0, +1$, with $E_{0,0} = \hbar\omega$,

first excited states are $\psi_{1,0}^{B,spinless}(x_1, x_2) \otimes |S = 1, S_z\rangle$, for $S_z = -1, 0, +1$, or $\psi_{1,0}^{F,spinless}(x_1, x_2) \otimes |S = 0, S_z = 0\rangle$, with $E_{1,0} = 2\hbar\omega$

For spin-1/2 fermions,

ground state is $\psi_{0,0}^{B,spinless}(x_1, x_2) \otimes |S = 0, S_z = 0\rangle$, with $E_{0,0} = \hbar\omega$, first excited states are $\psi_{1,0}^{F,spinless}(x_1, x_2) \otimes |S = 1, S_z\rangle$, for $S_z = -1, 0, +1$, or $\psi_{1,0}^{B,spinless}(x_1, x_2) \otimes |S = 0, S_z = 0\rangle$, with $E_{1,0} = 2\hbar\omega$

(d)

The entire Hamiltonian $\hat{H}_0 + \hat{H}_1$ commutes with $(\hat{\boldsymbol{S}}_1 + \hat{\boldsymbol{S}}_2)^2$ and $(\hat{S}_{1x} + \hat{S}_{2x})$,

it would be convenient to change the spin wavefunction basis in (c) to $|S = 0, S_x = 0\rangle$, and $|S = 1, S_x = -1, 0, 1\rangle$.

We don't need the explicit form of these spin wavefunctions.

By considering the subspaces with fixed S and S_x quantum numbers, we can avoid degenerate perturbation theory. In this subspace, $\hat{H}_1 = \lambda \cdot (\hat{p}_1 + \hat{p}_2) \cdot \hbar S_x$.

For two spin-1/2 fermion ground state, $\psi_{0,0}^{B,spinless}(x_1, x_2) \otimes |S = 0, S_x = 0\rangle$, in the $S = 0$ and $S_x = 0$ subspace, $\hat{H}_1$ completely vanishes, perturbation to all order vanishes, energy correction is 0.

Similarly, For first excited state $\psi_{0,1}^{B,spinless}(x_1, x_2) \otimes |S = 0, S_x = 0\rangle$, perturbation to all order vanishes, energy correction is 0.

For first excited state $\psi_{0,1}^{F,spinless}(x_1, x_2) \otimes |S = 1, S_x = 0\rangle$, perturbation to all order vanishes, energy correction is 0.

For first excited state $\psi_{0,1}^{F,spinless}(x_1, x_2) \otimes |S = 1, S_x = 1\rangle$, $\hat{H}_1 = \lambda \cdot (\hat{p}_1 + \hat{p}_2) \cdot \hbar$, we can use 2nd order perturbation theory to compute the energy correction, or consider $\hat{H}_0 + \hat{H}_1 = \frac{1}{2m}(\hat{p}_1 + \lambda\hbar m)^2 + \frac{m\omega^2}{2}x_1^2 + \frac{1}{2m}(\hat{p}_2 + \lambda\hbar m)^2 + \frac{m\omega^2}{2}x_2^2 - m\lambda^2\hbar^2$, it's easy to see all energy levels in this $S_x = 1$ subspace are shifted by $-m\lambda^2\hbar^2$, so this state's energy correction is $-m\lambda^2\hbar^2$.

Similarly, for first excited state $\psi_{0,1}^{F,spinless}(x_1, x_2) \otimes |S = 1, S_x = -1\rangle$, $\hat{H}_1 = -\lambda \cdot (\hat{p}_1 + \hat{p}_2) \cdot \hbar$, energy correction is $-m\lambda^2\hbar^2$.

Problem 4. (15 points*) For two spin-1/2 moments under static magnetic field along z-direction, $\hat{H}_0 = -\gamma B_0 \cdot (\hat{S}_{1z} + \hat{S}_{2z})$. Turn on a small rotating transverse field,

$\hat{V}(t) = -\gamma B_1 \cdot [\cos(\omega t)(\hat{S}_{1x} + \hat{S}_{2x}) - \sin(\omega t)(\hat{S}_{1y} + \hat{S}_{2y})]$.

(a) (10pts*) *By time-dependent perturbation theory, compute the transition probability from the ground state of* $\hat{H}_0$ *to the highest energy state of* $\hat{H}_0$*, over time* t*, to lowest nontrivial order of* B_1*.*

(b) (5pts**) Suppose the two spin-1/2 moments have interactions, $\hat{H}_0 = -\gamma B_0 \cdot (\hat{S}_{1z} + \hat{S}_{2z}) + J\hat{\boldsymbol{S}}_1 \cdot \hat{\boldsymbol{S}}_2$. Here $J > 0$. *Redo the calculation in (a).*

Problem

This is similar to a homework problem 11.29.

(a)

Method #1:

Eigenstates and energies of $\hat{H}_0$ are listed below

n	state ψ_n	$\hat{H}_0$ eigenvalue E_n
0	$\lvert\uparrow\rangle\lvert\uparrow\rangle$	$-\gamma B_0 \hbar$
1	$\lvert\downarrow\rangle\lvert\downarrow\rangle$	$\gamma B_0 \hbar$
2	$\lvert\uparrow\rangle\lvert\downarrow\rangle$	0
3	$\lvert\downarrow\rangle\lvert\uparrow\rangle$	0

Assume $\psi(t) = \sum_n c_n(t) e^{-\mathrm{i}E_n t/\hbar}|\psi_n\rangle$, then [similar to Problem 2(b)],

$\mathrm{i}\hbar \frac{\mathrm{d}}{\mathrm{d}t} c_n(t) = \sum_m e^{\mathrm{i}\omega_{nm}t} \langle\psi_n|\hat{V}(t)|\psi_m\rangle \cdot c_m(t)$, where $\omega_{nm} = \frac{E_n - E_m}{\hbar}$,

the formal solution is the Dyson series on page 1.

Note that $\hat{V}(t) = -\gamma B_1 \cdot [\cos(\omega t)(\hat{S}_{1x} + \hat{S}_{2x}) - \sin(\omega t)(\hat{S}_{1y} + \hat{S}_{2y})]$

$= -\frac{1}{2}\gamma B_1 (e^{\mathrm{i}\omega t}\hat{S}_{1+} + e^{-\mathrm{i}\omega t}\hat{S}_{1-} + e^{\mathrm{i}\omega t}\hat{S}_{2+} + e^{-\mathrm{i}\omega t}\hat{S}_{2-})$

Then $\langle\psi_2|\hat{V}(t)|\psi_0\rangle = \langle\psi_3|\hat{V}(t)|\psi_0\rangle = \langle\psi_1|\hat{V}(t)|\psi_2\rangle = \langle\psi_1|\hat{V}(t)|\psi_3\rangle = -\frac{1}{2}\gamma B_1 \hbar e^{-\mathrm{i}\omega t}$,

The lowest nontrivial order term that contribute to transition from state "0" to "1" would be two 2nd order processes, $0 \to 2 \to 1$ and $0 \to 3 \to 1$, note that we need to add the amplitudes of these two processes, then take absolute value square to get probability,

Each of these two processes has amplitude

$(\frac{-\mathrm{i}}{\hbar})^2 \int_0^t \mathrm{d}t_1 \int_0^{t_1} \mathrm{d}t_2 e^{-\mathrm{i}\gamma B_0 t_1}(-\frac{1}{2}\gamma B_1 \hbar e^{-\mathrm{i}\omega t_1}) \cdot e^{-\mathrm{i}\gamma B_0 t_2}(-\frac{1}{2}\gamma B_1 \hbar e^{-\mathrm{i}\omega t_2})$

Use $\int_0^t \mathrm{d}t_1 \int_0^{t_1} \mathrm{d}t_2 f(t_1) f(t_2) = \frac{1}{2}[\int_0^t \mathrm{d}t_1 f(t_1)]^2$,

the total transition amplitude is

$(\frac{-\mathrm{i}}{\hbar})^2[\int_0^t \mathrm{d}t_1 e^{-\mathrm{i}\gamma B_0 t_1}(-\frac{1}{2}\gamma B_1 \hbar e^{-\mathrm{i}\omega t_1})]^2 = (\frac{\gamma B_1}{2})^2(\frac{e^{-\mathrm{i}(\gamma B_0+\omega)t_1}-1}{\gamma B_0+\omega})^2$

The lowest nontrivial order of $P_{0\to 1}(t) = (\gamma B_1)^4 \cdot \frac{\sin^4(\frac{\gamma B_0+\omega}{2}t)}{(\gamma B_0+\omega)^4}$

NOTE: you can also use the basis in (b), which are also eigenbasis for $\hat{H}_0$ here, then there is only one 2nd order process, $|\uparrow\uparrow\rangle \to |\frac{1}{\sqrt{2}}(\uparrow\downarrow + \downarrow\uparrow)\rangle \to |\downarrow\downarrow\rangle$.

Method #2:

this is two copies of the same single spin-1/2 problem,

$\hat{H}_{0,\text{single}} = -\gamma B_0 \hat{S}_z$, and

$\hat{V}_{\text{single}}(t) = -\gamma B_1 \cdot [\cos(\omega t)\hat{S}_x - \sin(\omega t)\hat{S}_y] = -\frac{1}{2}\gamma B_1(e^{\mathrm{i}\omega t}\hat{S}_+ + e^{-\mathrm{i}\omega t}\hat{S}_-)$

The transition probability for single spin-1/2 from lowest energy to highest energy state is (keep only the first order term in amplitude),

$P_{\uparrow\to\downarrow}(t) = |\frac{-\mathrm{i}}{\hbar}\int_0^t e^{-\mathrm{i}\gamma B_0 t}(-\frac{1}{2}\gamma B_1 \hbar e^{-\mathrm{i}\omega t})\,\mathrm{d}t|^2 = (\gamma B_1)^2 \cdot \frac{\sin^2(\frac{\gamma B_0+\omega}{2}t)}{(\gamma B_0+\omega)^2}$.

The transition probability for the two spin-1/2 system from lowest energy to highest energy state is

$P_{\uparrow\uparrow\to\downarrow\downarrow}(t) = [P_{\uparrow\to\downarrow}(t)]^2 = (\gamma B_1)^4 \cdot \frac{\sin^4(\frac{\gamma B_0+\omega}{2}t)}{(\gamma B_0+\omega)^4}$,

(b) Eigenstates and energies of $\hat{H}_0$ are listed below

n	state ψ_n	$\hat{H}_0$ eigenvalue E_n
0	$\lvert S=1, S_z=1\rangle = \lvert\uparrow\rangle\lvert\uparrow\rangle$	$-\gamma B_0\hbar + \frac{J\hbar^2}{4}\hbar$
1	$\lvert S=1, S_z=-1\rangle = \lvert\downarrow\rangle\lvert\downarrow\rangle$	$\gamma B_0\hbar + \frac{J\hbar^2}{4}\hbar$
2	$\lvert S=1, S_z=0\rangle = \frac{1}{\sqrt{2}}(\lvert\uparrow\rangle\lvert\downarrow\rangle + \lvert\downarrow\rangle\lvert\uparrow\rangle)$	$0 + \frac{J\hbar^2}{4}$
3	$\lvert S=0, S_z=0\rangle = \frac{1}{\sqrt{2}}(\lvert\uparrow\rangle\lvert\downarrow\rangle - \lvert\downarrow\rangle\lvert\uparrow\rangle)$	$0 - \frac{3J\hbar^2}{4}$

The highest energy state is always state "1"

If $J\hbar^2 > \gamma B_0\hbar$, the ground state is state "3".

If $J\hbar^2 < \gamma B_0\hbar$, the ground state is state "0".

Relevant matrix elements are $\langle\psi_2|\hat{V}(t)|\psi_0\rangle = \langle\psi_1|\hat{V}(t)|\psi_2\rangle = -\frac{1}{\sqrt{2}}\gamma B_1\hbar e^{-\mathrm{i}\omega t}$, and $\langle\psi_3|\hat{V}(t)|\psi_0\rangle = \langle\psi_1|\hat{V}(t)|\psi_3\rangle = \langle\psi_2|\hat{V}(t)|\psi_3\rangle = 0$

the last three vanishing matrix elements can be seen from some "selection rules": $\hat{V}(t)$ commutes with $(\hat{\boldsymbol{S}}_1 + \hat{\boldsymbol{S}}_2)^2$, so $\hat{V}(t)$ cannot change total spin quantum number S; or $\hat{V}(t)$ is symmetric under exchange of spin labels (subscripts $_1$ and $_2$), spin single state $|\psi_3\rangle$ is anti-symmetric, and spin triplet states $|\psi_{0,1,2}\rangle$ are symmetric.

If $J\hbar^2 > \gamma B_0 \hbar$, the ground state is state "3", the transition probability from ground state to highest energy state (in fact, to any other state) is vanishing, because there is no matrix elements connecting state "3" to other states.

If $J\hbar^2 < \gamma B_0 \hbar$, the ground state is state "0", the lowest nontrivial contribution to transition amplitude is a 2nd order process, $0 \to 2 \to 1$, with the same amplitude as that in (a), $(\frac{-\mathbb{i}}{\hbar})^2 \int_0^t \mathrm{d}t_1 \int_0^{t_1} \mathrm{d}t_2 e^{-\mathbb{i}\gamma B_0 t_1}(-\frac{1}{\sqrt{2}}\gamma B_1 \hbar e^{-\mathbb{i}\omega t_1}) \cdot e^{-\mathbb{i}\gamma B_0 t_2}(-\frac{1}{\sqrt{2}}\gamma B_1 \hbar e^{-\mathbb{i}\omega t_2})$. So in this case the lowest nontrivial order of $P_{0\to 1}(t) = (\gamma B_1)^4 \cdot \frac{\sin^4(\frac{\gamma B_0 + \omega}{2} t)}{(\gamma B_0 + \omega)^4}$