Quantum Mechanics: Fall 2018
Final Exam: Brief Solutions

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

Possibly useful facts:

- 1D harmonic oscillator: $\hat{H} = \frac{\hat{p}^2}{2m} + \frac{m\omega^2}{2}\hat{x}^2 = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{m\omega^2}{2}x^2$.
  $[\hat{x}, \hat{p}] = \mathbb{i}\hbar$, and in position representation $\hat{p} = -\mathbb{i}\hbar\frac{\partial}{\partial x}$. Define $\hat{a}_\mp = \sqrt{\frac{m\omega}{2\hbar}}(\hat{x} \pm \mathbb{i}\frac{1}{m\omega}\hat{p}) = \sqrt{\frac{m\omega}{2\hbar}}(x \pm \frac{\hbar}{m\omega}\frac{\partial}{\partial x})$. 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.

- (Degenerate) Time-independent perturbation theory: $\hat{H} = \hat{H}^{(0)} + \hat{H}^{(1)}$. Denote the (degenerate) orthonormal eigenstates of $\hat{H}^{(0)}$ by $|\psi^{(0)}_{n\alpha}\rangle$, $\hat{H}^{(0)}|\psi^{(0)}_{n\alpha}\rangle = E^{(0)}_n|\psi_{n\alpha}\rangle$.
  Suppose $\hat{H}|\psi_n\rangle = E_n|\psi_n\rangle$, with E_n close to $E^{(0)}_n$, then $(E_n - E^{(0)}_n)$ is the eigenvalue of "secular equation", $\langle\psi^{(0)}_{n\beta}|\hat{H}^{(1)}|\psi^{(0)}_{n\alpha}\rangle + \sum_{m, m\neq n}\frac{1}{E^{(0)}_n - E^{(0)}_m}\langle\psi^{(0)}_{n\beta}|\hat{H}^{(1)}|\psi^{(0)}_m\rangle\langle\psi^{(0)}_m|\hat{H}^{(1)}|\psi^{(0)}_{n\alpha}\rangle$ 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 $E^{(0)}_n$. 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 $z = x + (-a_1)x^2 + (2a_1^2 - a_2)x^3 + (-5a_1^3 + 5a_1 a_2 - a_3)x^4 + O(x^5)$.

- Change of variables: if $x'_i = \sum_j A_{ij}x_j$, where A is a non-singular constant matrix. Then $\frac{\partial}{\partial x'_i} = \sum_j (A^{-1})_{ji}\frac{\partial}{\partial x_j}$, where A^{-1} is the inverse matrix of A.

Problem 1. (20 points) Consider a non-relativistic particle moving on a ring of radius R. Label the points on the ring by polar angle θ, the wavefunction as a function of θ must be periodic, $\psi(\theta+2\pi)=\psi(\theta)$, with normalizaiton $\int_{-\pi}^{\pi}|\psi(\theta)|^2 d\theta = 1$. The free particle Hamiltonian is $\hat{H}^{(0)} = \frac{\hat{p}^2}{2m} = -\frac{\hbar^2}{2mR^2}(\frac{\partial}{\partial\theta})^2$. Add a δ-function perturbation $\hat{H}^{(1)} = \alpha\cdot\delta(\theta)$, where α is a "small" parameter, $\alpha > 0$. The full Hamiltonian is $\hat{H} = \hat{H}^{(0)} + \hat{H}^{(1)}$.

(a) (5pts) *Write down the eigenvalues $E_n^{(0)}$ and normalized eigenstates $\psi_n^{(0)}(\theta)$ 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 $\hat{H}$ for $-2\pi \le \theta \le 2\pi$, and describe its properties.* [Hint: be careful about the "boundary conditions"]

(d) (5pts*) Denote the exact ground state energy of $\hat{H}$ by $\frac{\hbar^2k^2}{2mR^2}$. *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]

Solution

The perturbation should be understood as periodic "comb function", $\sum_{n\in\mathbb{Z}}\alpha\cdot\delta(\theta-2\pi n)$. if we do not restrict ourselves in $-\pi\le\theta\le\pi$.

(a) $\hat{H}^{(0)} = \frac{\hat{p}^2}{2m}$ commutes with $\hat{p} = -\mathbb{i}\frac{\hbar}{R}\partial_\theta$. Eigenstates of $\hat{p}$ are eigenstates of $\hat{H}^{(0)}$.

Periodic eigenfunctions of $-\mathbb{i}\partial_\theta$ are $e^{\mathbb{i}n\theta}$ with integer n.

So the eigenstates and eigenvalues of $\hat{H}^{(0)}$ can be chosen as

$\psi_n^{(0)}(\theta) = \frac{1}{\sqrt{2\pi}}e^{\mathbb{i}n\theta}$, with $E_n^{(0)} = \frac{\hbar^2n^2}{2mR^2}$, for integer n.

Note: n and $-n$ complex basis states are degenerate (for $n\ne 0$).

We can also choose real basis,

$\psi_0^{(0)} = \frac{1}{\sqrt{2\pi}}$ with $E_0^{(0)} = 0$, and

$\psi_{nc}^{(0)}(\theta) = \frac{1}{\sqrt{\pi}}\cos(n\theta)$, and $\psi_{ns}^{(0)}(\theta) = \frac{1}{\sqrt{\pi}}\sin(n\theta)$, with $E_n^{(0)} = \frac{\hbar^2n^2}{2mR^2}$, for $n = 1, 2, \ldots$.

(b) The original ground state has $n=0$, unperturbed ground state energy is $E_0^{(0)}=0$.

First order correction to ground state energy is
$E_0^{(1)}=\langle\psi_0^{(0)}|\hat{H}^{(1)}|\psi_0^{(0)}\rangle=\int_{-\pi}^{\pi}(\frac{1}{\sqrt{2\pi}})^*\cdot\alpha\cdot\delta(\theta)\cdot\frac{1}{\sqrt{2\pi}}\,\mathrm{d}\theta=\frac{\alpha}{2\pi}$.

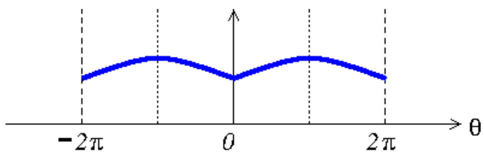
Second order correction to ground state energy is $E_0^{(2)}=\sum_{n,n\neq 0}\frac{|\langle\psi_0^{(0)}|\hat{H}^{(1)}|\psi_n^{(0)}\rangle|^2}{E_0^{(0)}-E_n^{(0)}}$, the matrix element is $\langle\psi_0^{(0)}|\hat{H}^{(1)}|\psi_n^{(0)}\rangle=\int_{-\pi}^{\pi}(\frac{1}{\sqrt{2\pi}})^*\cdot\alpha\cdot\delta(\theta)\cdot\frac{e^{in\theta}}{\sqrt{2\pi}}\,\mathrm{d}\theta=\frac{\alpha}{2\pi}$, so
$E_0^{(2)}=-2|\frac{\alpha}{2\pi}|^2\frac{2mR^2}{\hbar^2}\sum_{n=1}^{\infty}\frac{1}{n^2}=-\frac{\alpha^2 mR^2}{\pi^2\hbar^2}\sum_{n=1}^{\infty}\frac{1}{n^2}=-\frac{\alpha^2 mR^2}{6\hbar^2}$.

Here we have used $\sum_{n=1}^{\infty}\frac{1}{n^2}=\frac{\pi^2}{6}$, which can be obtained by taking $x\to 0$ limit in the given formula $\sum_{n=1}^{\infty}\frac{1}{x^2-n^2}=\frac{\pi x\cos(\pi x)-\sin(\pi x)}{2x^2\sin(\pi x)}$.

Finally, $E_0\approx 0+\frac{\alpha}{2\pi}-\frac{\alpha^2 mR^2}{6\hbar^2}$.

(c) The exact ground state wavefunction can be chosen real, and

- has no nodes (2pts);
- is continuous, but has discontinuous derivative (a "cusp" toward θ-axis) at $\theta=0 \mod 2\pi$ (2pts);
- symmetric under inversion around $\theta=n\pi$ (1pts).



(d) As suggested by the picture in (c), $\psi_0(\theta)=\begin{cases}A\cdot\cos[k(\theta+\pi)], & -\pi\leq\theta<0;\\ A\cdot\cos[k(\theta-\pi)], & 0<\theta\leq\pi.\end{cases}$ where A is the normalization constant. The energy is $\frac{\hbar^2k^2}{2mR^2}$, of the same form as free particle.

The boundary condition at the δ-function is $-\frac{\hbar^2}{2mR^2}\partial_\theta\psi\Big|_{\theta=0-0}^{\theta=0+0}+\alpha\psi(0)=0$, this leads to $\frac{\hbar^2}{mR^2}k\sin(k\pi)=\alpha\cos(k\pi)$, or, $(k\pi)\cdot\tan(k\pi)=\frac{\alpha\pi mR^2}{\hbar^2}$.

Expand the left-hand-side of this equation into power series of $k\pi$, use $\frac{1}{\cos(x)}\approx 1+\frac{x^2}{2}+O(x^4)$ from page 1, we have $(k\pi)^2+\frac{(k\pi)^4}{3}+O((k\pi)^6)=\frac{\alpha\pi mR^2}{\hbar^2}$, use the "series inversion" formula on page 1, $(k\pi)^2\approx(\frac{\alpha\pi mR^2}{\hbar^2})-\frac{1}{3}(\frac{\alpha\pi mR^2}{\hbar^2})^2+O(\alpha^3)$.

Finally the approximate ground state energy is $\frac{\hbar^2k^2}{2mR^2}=\frac{\hbar^2}{2mR^2\pi^2}(k\pi)^2$
$\approx\frac{\hbar^2}{2mR^2\pi^2}\cdot[(\frac{\alpha\pi mR^2}{\hbar^2})-\frac{1}{3}(\frac{\alpha\pi mR^2}{\hbar^2})^2+O(\alpha^3)]=\frac{\alpha}{2\pi}-\frac{\alpha^2 mR^2}{6\hbar^2}+O(\alpha^3)$.

This matches the perturbation theory result in (b).

Problem 2. (30 points) Consider two identical particles in the ring defined in Problem 1. The free particle Hamiltonian is $\hat{H}^{(0)}=\frac{\hat{p}_1^2}{2m}+\frac{\hat{p}_2^2}{2m}=-\frac{\hbar^2}{2mR^2}[(\frac{\partial}{\partial\theta_1})^2+(\frac{\partial}{\partial\theta_2})^2]$. Subscripts $_1$ and $_2$ label the two particles. If they are distinguishable, the orthonormal eigenstates of $\hat{H}_0$ can be chosen as $\psi_{n_1,n_2}^{(0)}(\theta_1;\theta_2)=\psi_{n_1}^{(0)}(\theta_1)\cdot\psi_{n_2}^{(0)}(\theta_2)$, with energy eigenvalue $E_{n_1,n_2}^{(0)}=E_{n_1}^{(0)}+E_{n_2}^{(0)}$. Here $E_n^{(0)}$ and $\psi_n^{(0)}(\theta)$ are defined in Problem 1(a). For identical particles, $\psi(\theta_1;\theta_2)$ must satisfy certain permutation symmetry. The normalization is $\int_{-\pi}^{\pi}\int_{-\pi}^{\pi}|\psi(\theta_1;\theta_2)|^2\,\mathrm{d}\theta_1\mathrm{d}\theta_2 = 1$.

(a) (10pts) *Write down the energies and ORTHONORMAL eigenstate wavefunctions for two BOSONS for the lowest THREE energy levels of* $\hat{H}^{(0)}$. [Note: may have degeneracy]

(b) (10pts) *Write down the energies and ORTHONORMAL eigenstate wavefunctions for two FERMIONS for the lowest THREE energy levels of* $\hat{H}^{(0)}$. [Note: may have degeneracy]

(c) (5pts) *In the ground state(s) of two FERMIONS in (b), compute the probability that the two particles are in the same quadrant, namely the probability of* $\cos(\theta_1-\theta_2) > 0$.

(d) (5pts) Add perturbation $\hat{H}^{(1)} = \alpha\cdot[\delta(\theta_1)+\delta(\theta_2)]$, where α is a "small" real parameter. *Compute the ground state(s) energy of* $\hat{H} = \hat{H}^{(0)} + \hat{H}^{(1)}$ *for two FERMIONS under 1st order perturbation.* [Hint: you might need degenerate perturbation theory]

Solution

(a) For two bosons, wavefunctions $\psi^{(\mathrm{B})}(\theta_1;\theta_2)$ are symmetric, $\psi^{(\mathrm{B})}(\theta_1;\theta_2) = \psi^{(\mathrm{B})}(\theta_2;\theta_1)$.

The orthonormal basis can be chosen as

$\psi^{(\mathrm{B},0)}_{i,i}(\theta_1;\theta_2) = \psi^{(0)}_i(\theta_1)\psi^{(0)}_i(\theta_2)$ with $E^{(0)}_{i,i} = E^{(0)}_i + E^{(0)}_i$; and

$\psi^{(\mathrm{B},0)}_{i,j}(\theta_1;\theta_2) = \frac{1}{\sqrt{2}}[\psi^{(0)}_i(\theta_1)\psi^{(0)}_j(\theta_2) + \psi^{(0)}_i(\theta_1)\psi^{(0)}_j(\theta_2)]$ with $E^{(0)}_{i,j} = E^{(0)}_i + E^{(0)}_j$, for $i \neq j$.

We can use either the complex basis or the real basis for single particle states. The results are summarized in the following table.

energy	complex basis	real basis
0	$\psi^{(\mathrm{B},0)}_{0,0} = \frac{1}{2\pi}$	$\psi^{(\mathrm{B},0)}_{0,0} = \frac{1}{2\pi}$
$\frac{\hbar^2}{2mR^2}$	$\psi^{(\mathrm{B},0)}_{0,1} = \frac{1}{2\pi}\frac{1}{\sqrt{2}}(e^{\mathrm{i}\theta_1}+e^{\mathrm{i}\theta_2})$, $\psi^{(\mathrm{B},0)}_{0,-1} = \frac{1}{2\pi}\frac{1}{\sqrt{2}}(e^{-\mathrm{i}\theta_1}+e^{-\mathrm{i}\theta_2})$.	$\psi^{(\mathrm{B},0)}_{0,1c} = \frac{1}{\sqrt{2\pi}}\frac{1}{\sqrt{2}}(\cos\theta_1+\cos\theta_2)$, $\psi^{(\mathrm{B},0)}_{0,1s} = \frac{1}{\sqrt{2\pi}}\frac{1}{\sqrt{2}}(\sin\theta_1+\sin\theta_2)$.
$\frac{\hbar^2}{2mR^2}\cdot 2$	$\psi^{(\mathrm{B},0)}_{1,1} = \frac{1}{2\pi}e^{\mathrm{i}(\theta_1+\theta_2)}$, $\psi^{(\mathrm{B},0)}_{1,-1} = \frac{1}{2\pi}\frac{1}{\sqrt{2}}(e^{\mathrm{i}(\theta_1-\theta_2)}+e^{\mathrm{i}(\theta_2-\theta_1)})$, $\psi^{(\mathrm{B},0)}_{-1,-1} = \frac{1}{2\pi}e^{-\mathrm{i}(\theta_1+\theta_2)}$.	$\psi^{(\mathrm{B},0)}_{1c,1c} = \frac{1}{\pi}\cos\theta_1\cos\theta_2$, $\psi^{(\mathrm{B},0)}_{1c,1s} = \frac{1}{\pi}\frac{1}{\sqrt{2}}(\cos\theta_1\sin\theta_2+\sin\theta_1\cos\theta_2)$, $\psi^{(\mathrm{B},0)}_{1s,1s} = \frac{1}{\pi}\sin\theta_1\sin\theta_2$,

(b) For two fermions, wavefunctions $\psi^{(\mathrm{F})}(\theta_1;\theta_2) = \psi^{(\mathrm{F})}(\theta_2;\theta_1)$ are anti-symmetric.

The orthonormal basis can be chosen as

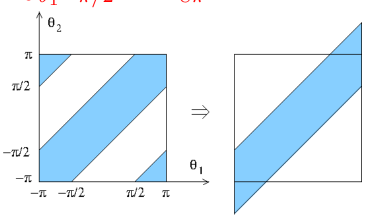
$\psi_{i,j}^{(\mathrm{F},0)}(\theta_1;\theta_2) = \frac{1}{\sqrt{2}}[\psi_i^{(0)}(\theta_1)\psi_j^{(0)}(\theta_2) - \psi_i^{(0)}(\theta_1)\psi_j^{(0)}(\theta_2)]$ with $E_{i,j}^{(0)} = E_i^{(0)} + E_j^{(0)}$, for $i \neq j$.

The results are summarized in the following table.

energy	complex basis	real basis
$\frac{\hbar^2}{2mR^2}$	$\psi_{0,1}^{(\mathrm{F},0)} = \frac{1}{2\pi}\frac{1}{\sqrt{2}}(e^{\mathrm{i}\theta_1} - e^{\mathrm{i}\theta_2})$, $\psi_{0,-1}^{(\mathrm{F},0)} = \frac{1}{2\pi}\frac{1}{\sqrt{2}}(e^{-\mathrm{i}\theta_1} - e^{-\mathrm{i}\theta_2})$.	$\psi_{0,1c}^{(\mathrm{F},0)} = \frac{1}{\sqrt{2}\pi}\frac{1}{\sqrt{2}}(\cos\theta_1 - \cos\theta_2)$, $\psi_{0,1s}^{(\mathrm{F},0)} = \frac{1}{\sqrt{2}\pi}\frac{1}{\sqrt{2}}(\sin\theta_1 - \sin\theta_2)$.
$\frac{\hbar^2}{2mR^2}\cdot 2$	$\psi_{1,-1}^{(\mathrm{F},0)} = \frac{1}{2\pi}\frac{1}{\sqrt{2}}(e^{\mathrm{i}(\theta_1-\theta_2)} - e^{\mathrm{i}(\theta_2-\theta_1)})$	$\psi_{1c,1s}^{(\mathrm{F},0)} = \frac{1}{\pi}\frac{1}{\sqrt{2}}(\cos\theta_1\sin\theta_2 - \sin\theta_1\cos\theta_2)$
$\frac{\hbar^2}{2mR^2}\cdot 4$	$\psi_{0,2}^{(\mathrm{F},0)} = \frac{1}{2\pi}\frac{1}{\sqrt{2}}(e^{2\mathrm{i}\theta_1} - e^{2\mathrm{i}\theta_2})$, $\psi_{0,-2}^{(\mathrm{F},0)} = \frac{1}{2\pi}\frac{1}{\sqrt{2}}(e^{-2\mathrm{i}\theta_1} - e^{-2\mathrm{i}\theta_2})$.	$\psi_{0,2c}^{(\mathrm{F},0)} = \frac{1}{\sqrt{2}\pi}\frac{1}{\sqrt{2}}(\cos(2\theta_1) - \cos(2\theta_2))$, $\psi_{0,2s}^{(\mathrm{F},0)} = \frac{1}{\sqrt{2}\pi}\frac{1}{\sqrt{2}}(\sin(2\theta_1) - \sin(2\theta_2))$.

(c) The probability is $\int_{-\pi}^{\pi}\mathrm{d}\theta_1\int_{\theta_1-\pi/2}^{\theta_1+\pi/2}\mathrm{d}\theta_2\,|\psi^{(\mathrm{F})}(\theta_1;\theta_2)|^2$.

For two fermions, the two ground state wavefunctions $\psi_{0,1}^{(\mathrm{F},0)}$ and $\psi_{0,-1}^{(\mathrm{F},0)}$ are complex conjugate to each other, so produce the same result, $\int_{-\pi}^{\pi}\mathrm{d}\theta_1\int_{\theta_1-\pi/2}^{\theta_1+\pi/2}\mathrm{d}\theta_2\,\frac{1}{8\pi^2}[2-2\cos(\theta_2-\theta_1)]$ $= 2\pi\cdot\frac{1}{8\pi^2}(2\pi-4) = \frac{1}{2}-\frac{1}{\pi}$.



Note that the wavefunction is periodic with respect to both θ_1 and θ_2, so we can use the integration region $\theta_1 - \frac{\pi}{2} < \theta_2 < \theta_1 + \frac{\pi}{2}$ (blue region in the figure).

The real basis $\psi_{0,1c}^{(\mathrm{F},0)}$ and $\psi_{0,1s}^{(\mathrm{F},0)}$ also produce the same result. In fact any linear combinations between them will produce the same result, because the two-fermion ground state wavefunction is always of the form, $\sin(\frac{\theta_1-\theta_2}{2})\cdot\psi(\frac{\theta_1+\theta_2}{2})$.

This probability is much smaller than distinguishable (un-entangled) particle case, with wavefunction $\psi_{n_1}(\theta_1)\psi_{n_2}(\theta_2)$, which will trivially give probability $\frac{1}{2}$ for $\theta_1 - \frac{\pi}{2} < \theta_2 < \theta_1 + \frac{\pi}{2}$.

(d) Use the $\psi_{0,1}^{(\mathrm{F},0)}$ and $\psi_{0,-1}^{(\mathrm{F},0)}$ ground state basis in (b), denote them by $|\phi_{0;1}^{(\mathrm{F},0)}\rangle$ and $|\phi_{0;2}^{(\mathrm{F},0)}\rangle$, the 1st order secular equation matrix is $(i,j=1,2)$, $\langle\phi_{0;j}^{(\mathrm{F},0)}|\hat{H}^{(1)}|\phi_{0;i}^{(\mathrm{F},0)}\rangle = \begin{pmatrix}\frac{\alpha}{\pi} & \frac{\alpha}{2\pi}\\ \frac{\alpha}{2\pi} & \frac{\alpha}{\pi}\end{pmatrix}$.

Here $\langle\psi_{0,1}^{(\mathrm{F},0)}|\hat{H}^{(1)}|\psi_{0,1}^{(\mathrm{F},0)}\rangle = \langle\psi_{0,-1}^{(\mathrm{F},0)}|\hat{H}^{(1)}|\psi_{0,-1}^{(\mathrm{F},0)}\rangle$
$= \int_{-\pi}^{\pi}\mathrm{d}\theta_1\int_{-\pi}^{\pi}\mathrm{d}\theta_2\,\frac{1}{8\pi^2}[2-2\cos(\theta_2-\theta_1)]\cdot\alpha\cdot[\delta(\theta_1)+\delta(\theta_2)]$
$= 2\cdot\int_{-\pi}^{\pi}\mathrm{d}\theta\,\frac{1}{8\pi^2}(2-2\cos\theta)\cdot\alpha = \frac{\alpha}{\pi}$.

And $\langle\psi_{0,1}^{(\mathrm{F},0)}|\hat{H}^{(1)}|\psi_{0,-1}^{(\mathrm{F},0)}\rangle^* = \langle\psi_{0,-1}^{(\mathrm{F},0)}|\hat{H}^{(1)}|\psi_{0,1}^{(\mathrm{F},0)}\rangle = \int_{-\pi}^{\pi}\mathrm{d}\theta_1\int_{-\pi}^{\pi}\mathrm{d}\theta_2\,\frac{1}{8\pi^2}(e^{\mathrm{i}\theta_1}-e^{\mathrm{i}\theta_2})^2\cdot\alpha\cdot[\delta(\theta_1)+\delta(\theta_2)] = 2\cdot\int_{-\pi}^{\pi}\mathrm{d}\theta\,\frac{1}{8\pi^2}(e^{\mathrm{i}\theta}-1)^2\cdot\alpha = \frac{\alpha}{2\pi}$.

So the 1st order correction to ground state energy is $\frac{\alpha}{\pi}\pm\frac{\alpha}{2\pi} = \frac{\alpha}{2\pi}$ and $\frac{3\alpha}{2\pi}$.

In fact the $\psi_{0,1s}^{(\mathrm{F},0)}$ and $\psi_{0,1c}^{(\mathrm{F},0)}$ states are just the eigenstates of this 1st order secular equation.

Problem 3. (15 points) Consider a 1D harmonic oscillator $\hat{H}_0 = \frac{\hat{p}^2}{2m} + \frac{m\omega^2}{2}\hat{x}^2$, with a time-dependent perturbation, $\hat{V}(t) = -f \cdot [\cos(\Omega t)\cdot \hat{x} - \sin(\Omega t)\cdot \frac{\hat{p}}{m\omega}]$. Here m, ω, f, Ω are positive constants, f is a "small" parameter. The full Hamiltonian is $\hat{H} = \hat{H}_0 + \hat{V}(t)$.

(a) (5pts) Suppose $\psi(x,t) = \sum_n c_n(t)\cdot e^{-\mathbb{i}E_n t/\hbar}\cdot \psi_n(x)$ satisfy the Schrödinger equation $\mathbb{i}\hbar\frac{\partial}{\partial t}\psi = \hat{H}\psi$. Here $E_n = \hbar\omega(n+\frac{1}{2})$ and $\psi_n(x)$ are eigenvalues and normalized eigenfunctions of $\hat{H}_0$ (see page 1). *Derive the differential equations for the coefficients $c_n(t)$ in terms of given quantities.* [Hint: use the ladder operators to compute the matrix elements.]

(b) (5pts) Suppose the initial state is $\psi(x, t=0) = \psi_0(x)$. *Compute the transition probability $P_{0\to 1}(t) \equiv |c_1(t)|^2$ for the lowest non-trivial order of f.*

(c) (5pts) With the same initial conditions of (b), *compute $P_{0\to 0}(t) \equiv |c_0(t)|^2$ to second order of f.* [Hint: result of (b) will be useful, keep terms up to appropriate order in $c_0(t)$]

Solution

This is similar to Problem 2 of Final Exam of 2017. Use $\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}(\hat{a}_- + \hat{a}_+)$, $\hat{p} = -\mathbb{i}m\omega\sqrt{\frac{\hbar}{2m\omega}}(\hat{a}_- - \hat{a}_+)$, then $\hat{V}(t) = -f\sqrt{\frac{\hbar}{2m\omega}}(e^{\mathbb{i}\Omega t}\hat{a}_- + e^{-\mathbb{i}\Omega t}\hat{a}_+)$.

(a) This equation has been given in the Summary.

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

For the perturbation considered here, the matrix element is

$\langle\psi_n|\hat{V}(t)|\psi_m\rangle = -f\sqrt{\frac{\hbar}{2m\omega}}(e^{\mathbb{i}\Omega t}\delta_{n+1,m}\sqrt{m} + e^{-\mathbb{i}\Omega t}\delta_{n,m+1}\sqrt{n})$.

$\frac{\mathrm{d}}{\mathrm{d}t}c_n(t) = \frac{\mathbb{i}f}{\sqrt{2m\omega\hbar}}[e^{-\mathbb{i}(\omega-\Omega)t}\sqrt{n+1}c_{n+1}(t) + e^{\mathbb{i}(\omega-\Omega)t}\sqrt{n}c_{n-1}(t)]$.

For $n=0$ the right-hand-side has only one term, $\frac{\mathrm{d}}{\mathrm{d}t}c_n(t) = \frac{\mathbb{i}f}{\sqrt{2m\omega\hbar}}e^{-\mathbb{i}(\omega-\Omega)t}c_1(t)$.

(b) The initial condition is $c_0(t=0) = 1$ and $c_{n>0}(t=0) = 0$.

Use $\frac{\mathrm{d}}{\mathrm{d}t}c_1(t) = \frac{\mathbb{i}f}{\sqrt{2m\omega\hbar}}\cdot(e^{-\mathbb{i}(\omega-\Omega)t}\sqrt{2}c_2(t) + e^{\mathbb{i}(\omega-\Omega)t}c_0(t))$,

approximate $c_2(t) \sim 0$ and $c_0(t) \sim 1$ on the right-hand-side.

$c_1(t) \approx \int_0^t \mathrm{d}t\, \frac{\mathbb{i}f}{\sqrt{2m\omega\hbar}}e^{\mathbb{i}(\omega-\Omega)t} = \frac{f}{(\omega-\Omega)\sqrt{2m\omega\hbar}}(e^{\mathbb{i}(\omega-\Omega)t} - 1)$,

$P_{0\to 1}(t) = |c_1(t)|^2 \approx \frac{f^2}{2m\omega\hbar}\frac{4\sin^2(\frac{(\omega-\Omega)t}{2})}{(\omega-\Omega)^2}$.

(c) Method #1: $c_0(t)$ contains $O(1)$ term, so we need to keep up to $O(f^2)$ term in $c_0(t)$, in order to get accurate $O(f^2)$ terms in $|c_0(t)|^2$.

Use $\frac{\mathrm{d}}{\mathrm{d}t}c_n(t) = \frac{\mathrm{i}f}{\sqrt{2m\omega\hbar}}e^{-\mathrm{i}(\omega-\Omega)t}c_1(t)$. Plug in the solution of $c_1(t)$ from (b).

$c_0(t) - c_0(0) \approx \int_0^t \mathrm{d}t\, \frac{\mathrm{i}f}{\sqrt{2m\omega\hbar}}e^{-\mathrm{i}(\omega-\Omega)t} \cdot \frac{f}{(\omega-\Omega)\sqrt{2m\omega\hbar}}(e^{\mathrm{i}(\omega-\Omega)t} - 1) = \frac{f^2}{2m\omega\hbar}(\frac{\mathrm{i}t}{\omega-\Omega} - \frac{e^{-\mathrm{i}(\omega-\Omega)t}-1}{(\omega-\Omega)^2})$.

Then $c_0(t) \approx 1 + \frac{f^2}{2m\omega\hbar}(\frac{\mathrm{i}t}{\omega-\Omega} - \frac{e^{-\mathrm{i}(\omega-\Omega)t}-1}{(\omega-\Omega)^2})$.

Note that the imaginary part of $c_0(t)$ has terms of $O(f^2)$ or higher, so to get $|c_0(t)|^2$ accurate to $O(f^2)$, we only need to compute the square of real part of $c_0(t)$ above.

$P_{0\to 0}(t) = |c_0(t)|^2 \approx (1 + \frac{f^2}{2m\omega\hbar}\frac{\cos((\omega-\Omega)t)-1}{(\omega-\Omega)^2})^2 \approx 1 + 2\cdot\frac{f^2}{2m\omega\hbar}\frac{\cos((\omega-\Omega)t)-1}{(\omega-\Omega)^2}$
$= 1 - \frac{f^2}{2m\omega\hbar}\frac{4\sin^2(\frac{(\omega-\Omega)t}{2})}{(\omega-\Omega)^2}$.

Method #2: use $\sum_{n=0}^{\infty} P_{0\to n}(t) = 1$, then $P_{0\to 0}(t) = 1 - P_{0\to 1}(t) - P_{0\to 2}(t) - \ldots$.

By mathematical induction, it is easy to see that under the initial condition in (b), $c_n(t)$ is of $O(f^n)$ or higher order, therefore $P_{0\to n}(t)$ is of $O(f^{2n})$ order.

So up to $O(f^2)$ order, $P_{0\to 0}(t) \approx 1 - P_{0\to 1}(t) = 1 - \frac{f^2}{2m\omega\hbar}\frac{4\sin^2(\frac{(\omega-\Omega)t}{2})}{(\omega-\Omega)^2}$.

Problem 4 (15 points) Consider a 1D anharmonic oscillator $\hat{H} = \frac{\hat{p}^2}{2m} + \frac{m\omega^2}{2}\hat{x}^2 + \frac{U}{4}\hat{x}^4$, here m, ω, U are positive constants. U is a "small" parameter.

(a) (5pts) Consider $\hat{H}_\Omega^{(0)} = \frac{\hat{p}^2}{2m} + \frac{m\Omega^2}{2}\hat{x}^2$, with normalized ground state $\psi_{0,\Omega}(x)$, parametrized by a positive "variational" parameter Ω. *Compute* $E(\Omega) \equiv \langle\psi_{0,\Omega}|\hat{H}|\psi_{0,\Omega}\rangle$. [Hint: $\hat{H} = \hat{H}_\Omega^{(0)} + \frac{m(\omega^2-\Omega^2)}{2}\hat{x}^2 + \frac{U}{4}\hat{x}^4$, use Gaussian integrals or ladder operators.]

(b) (5pts*) You may not be able to solve $\frac{\partial}{\partial\Omega}E(\Omega) = 0$ exactly. *Solve* Ω *approximately up to 2nd order of* U*, and therefore obtain the minimal* $E(\Omega)$ *to 2nd order of* U. [Hint: assume $\Omega = \omega\cdot(1+z)$ with small z, some facts on page 1 will be useful]

(c) (5pts*) Treat the $\frac{U}{4}\hat{x}^4$ term by perturbation theory. *Compute the ground state energy of* $\hat{H}$ *to 2nd order of* U. [Hint: use ladder operators, this may not match the result in (b)]

Solution

(a) Use $\hat{H} = \hat{H}_\Omega^{(0)} + \frac{m(\omega^2-\Omega^2)}{2}\hat{x}^2 + \frac{U}{4}\hat{x}^4$, and $\hat{H}_\Omega^{(0)}|\psi_{0,\Omega}\rangle = \frac{\hbar\Omega}{2}|\psi_{0,\Omega}\rangle$.

$E(\Omega) = \langle\psi_{0,\Omega}|\hat{H}|\psi_{0,\Omega}\rangle = \frac{1}{2}\hbar\Omega + \frac{m(\omega^2-\Omega^2)}{2}\cdot\langle\psi_{0,\Omega}|\hat{x}^2|\psi_{0,\Omega}\rangle + \frac{U}{4}\cdot\langle\psi_{0,\Omega}|\hat{x}^4|\psi_{0,\Omega}\rangle$
$= \frac{1}{2}\hbar\Omega + \frac{m(\omega^2-\Omega^2)}{2}\cdot\frac{\hbar}{2m\Omega} + \frac{U}{4}\cdot 3(\frac{\hbar}{2m\Omega})^2 = \frac{1}{4}\hbar\Omega + \frac{1}{4}\hbar\frac{\omega^2}{\Omega} + \frac{U}{4}\cdot 3(\frac{\hbar}{2m\Omega})^2$.

Here $\langle\psi_{0,\Omega}|\hat{x}^{2n}|\psi_{0,\Omega}\rangle = \int_{-\infty}^{\infty} x^{2n}(\frac{m\omega}{\hbar\pi})^{-1/2}\exp[-x^2/(2\cdot\frac{\hbar}{2m\omega})]\,\mathrm{d}x$
$= (\frac{m\omega}{\hbar\pi})^{-1/2}\cdot(2n)!!\cdot(\frac{\hbar}{2m\omega})^n\cdot\sqrt{2\pi\cdot\frac{\hbar}{2m\omega}} = (2n)!!\cdot(\frac{\hbar}{2m\omega})^n$.

(b) $\frac{\partial}{\partial\Omega}E(\Omega) = 0$ is, $\frac{\hbar}{4} - \frac{\hbar\omega^2}{4\Omega^2} - \frac{3U}{8}\frac{\hbar^2}{m^2\Omega^3} = 0$.

Define $\Omega = \omega\cdot(1+z)$, multiply both sides of this equation by $\frac{2}{\hbar}(\Omega/\omega)^3$, we have,
$\frac{1}{2}[(1+z)^3-(1+z)] = \frac{3U}{4}\frac{\hbar}{m^2\omega^3}$, or, $z + \frac{3}{2}z^2 + \frac{1}{2}z^3 = (\frac{3U}{4}\frac{\hbar}{m^2\omega^3})$.

The right-hand-side is a dimensionless small number. Use "series inversion" on page 1,
$z \approx (\frac{3U}{4}\frac{\hbar}{m^2\omega^3}) - \frac{3}{2}(\frac{3U}{4}\frac{\hbar}{m^2\omega^3})^2 + O(U^3)$.

Plug this back into the formula of $E(\Omega)$, the minimal variational energy is
$\min[E(\Omega)] = \frac{\hbar\omega}{4}((1+z)+\frac{1}{1+z}) + \frac{3U}{16}\frac{\hbar^2}{m^2\omega^2}\frac{1}{(1+z)^2} \approx \frac{\hbar\omega}{4}(2+z^2) + \frac{3U}{16}\frac{\hbar^2}{m^2\omega^2}(1-2z) + O(U^3)$
$\approx \hbar\omega\cdot[\frac{1}{2} + \frac{1}{4}\cdot(\frac{3U}{4}\frac{\hbar}{m^2\omega^3}) - \frac{1}{4}\cdot(\frac{3U}{4}\frac{\hbar}{m^2\omega^3})^2 + O(U^3)$.

(c) Denote the orthonormal eigenstates of "unperturbed" Hamiltonian $\hat{H}^{(0)} \equiv \frac{\hat{p}^2}{2m} + \frac{m\omega^2}{2}\hat{x}^2$ by $|\psi_n\rangle$, with energy $E_n^{(0)} = \hbar\omega\cdot(n+\frac{1}{2})$ (see page 1).

The original ground state is $|\psi_0\rangle$.

The perturbation is $\hat{H}^{(1)} \equiv \frac{U}{4}\hat{x}^4 = \frac{U}{4}(\frac{\hbar}{2m\omega})^2(\hat{a}_- + \hat{a}_+)^4$.

Then $\hat{H}^{(1)}|\psi_0\rangle = \frac{U}{4}(\frac{\hbar}{2m\omega})^2(\hat{a}_-+\hat{a}_+)^3|\psi_1\rangle = \frac{U}{4}(\frac{\hbar}{2m\omega})^2(\hat{a}_-+\hat{a}_+)^2(|\psi_0\rangle + \sqrt{2}|\psi_2\rangle)$
$= \frac{U}{4}(\frac{\hbar}{2m\omega})^2(\hat{a}_-+\hat{a}_+)(3|\psi_1\rangle + \sqrt{6}|\psi_3\rangle) = \frac{U}{4}(\frac{\hbar}{2m\omega})^2(3|\psi_0\rangle + 6\sqrt{2}|\psi_2\rangle + \sqrt{24}|\psi_4\rangle)$.

Therefore the first order correction is $\langle\psi_0|\hat{H}^{(1)}|\psi_0\rangle = \frac{U}{4}(\frac{\hbar}{2m\omega})^2\cdot 3 = \frac{\hbar\omega}{4}\cdot(\frac{3U}{4}\frac{\hbar}{m^2\omega^3})$.

The second order correction is $\frac{|\langle\psi_2|\hat{H}^{(1)}|\psi_0\rangle|^2}{E_0^{(0)}-E_2^{(0)}} + \frac{|\langle\psi_4|\hat{H}^{(1)}|\psi_0\rangle|^2}{E_0^{(0)}-E_4^{(0)}} = (\frac{U}{4}(\frac{\hbar}{2m\omega})^2)^2\cdot[\frac{(6\sqrt{2})^2}{-2\hbar\omega} + \frac{(\sqrt{24})^2}{-4\hbar\omega}]$
$= -\hbar\omega\cdot\frac{7}{24}\cdot(\frac{3U}{4}\frac{\hbar}{m^2\omega^3})^2$

Finally, the perturbative expansion result for the ground state energy is,
$E_0 \approx \hbar\omega\cdot[\frac{1}{2} + \frac{1}{4}\cdot(\frac{3U}{4}\frac{\hbar}{m^2\omega^3}) - \frac{7}{24}\cdot(\frac{3U}{4}\frac{\hbar}{m^2\omega^3})^2]$.

The first order term matches the variational result. But second order term does not match, and is slightly lower than the variational result as expected.

Problem 5 (10 points) Consider one spin-1/2 moment $\hat{\boldsymbol{S}}$ (see page 1), with the Hamiltonian $\hat{H} = -B\cdot\hat{S}_x$. Here B is a positive constant. Let the initial state be $|\psi(t=0)\rangle = |\uparrow\rangle$. Evolve this state under $\hat{H}$ from $t=0$ to time t.

(a) (5pts) *Solve the state $|\psi(t)\rangle$ in terms of $|\uparrow\rangle, |\downarrow\rangle$. Measure $\hat{S}_z$ under $|\psi(t)\rangle$. What are the possible measurement results λ and their corresponding probabilities P_λ?*

(b) (5pts) (Quantum Zeno effect) During this time t, measure N times the observable $\hat{S}_z$, at time $t_n = \frac{n}{N}t$, for $n = 1, 2, \ldots, N$. After each measurement, we have a probability distribution $P_\lambda(n)$. *Derive a recursion relation between $P_\lambda(n+1)$ and $P_\lambda(n)$, then solve $P_\lambda(N)$ exactly.* [Hint: it may be helpful to write the recursion relation in matrix-vector form. The $N \to +\infty$ limit should produce the quantum Zeno effect.]

Solution

(a) $\hat{H}$ is $-\frac{B\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ under the $|\uparrow\rangle, |\downarrow\rangle$ basis.

It has eigenvalues $E_{1,2} = \mp\frac{B\hbar}{2}$ with eigenstates $|\psi_{1,2}\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle \pm |\downarrow\rangle)$.

$|\psi(t=0)\rangle = |\uparrow\rangle = \frac{1}{\sqrt{2}}|\psi_1\rangle + \frac{1}{\sqrt{2}}|\psi_2\rangle$, then $|\psi(t)\rangle = \frac{1}{\sqrt{2}}e^{-\mathrm{i}E_1t/\hbar}|\psi_1\rangle + \frac{1}{\sqrt{2}}e^{-\mathrm{i}E_2t/\hbar}|\psi_2\rangle$ $= \frac{1}{\sqrt{2}}e^{\mathrm{i}Bt/2}|\psi_1\rangle + \frac{1}{\sqrt{2}}e^{-\mathrm{i}Bt/2}|\psi_2\rangle = \cos(Bt/2)|\uparrow\rangle + \mathrm{i}\sin(Bt/2)|\downarrow\rangle$.

Measurement of $\hat{S}_z$ will produce:

$\lambda = +\frac{\hbar}{2}$, with probability $P_{+\frac{\hbar}{2}} = \cos^2(Bt/2)$, collapsed state $|\uparrow\rangle$; or
$\lambda = -\frac{\hbar}{2}$, with probability $P_{-\frac{\hbar}{2}} = \sin^2(Bt/2)$, collapsed state $|\downarrow\rangle$.

(b)

The evolution from probability distribution of n-th measurement to that of $(n+1)$-th measurement is described by the following table.

n-th measurement	$\lambda = +\frac{\hbar}{2}$		$\lambda = -\frac{\hbar}{2}$	
probabilities	$P_{+\frac{\hbar}{2}}(n)$		$P_{-\frac{\hbar}{2}}(n)$	
state at $t_n + 0$	collapsed to $\vert\uparrow\rangle$		collapsed to $\vert\downarrow\rangle$	
state at $t_{n+1} - 0$	$\cos(\frac{Bt}{2N})\vert\uparrow\rangle + \mathrm{i}\sin(\frac{Bt}{2N})\vert\downarrow\rangle$		$\mathrm{i}\sin(\frac{Bt}{2N})\vert\uparrow\rangle + \cos(\frac{Bt}{2N})\vert\downarrow\rangle$	
$(n+1)$-th measurement	$\lambda = +\frac{\hbar}{2}$,	$\lambda = -\frac{\hbar}{2}$	$\lambda = +\frac{\hbar}{2}$	$\lambda = -\frac{\hbar}{2}$
probabilities	$P_{+\frac{\hbar}{2}}(n)\cos^2(\frac{Bt}{2N})$	$P_{+\frac{\hbar}{2}}(n)\sin^2(\frac{Bt}{2N})$	$P_{-\frac{\hbar}{2}}(n)\sin^2(\frac{Bt}{2N})$	$P_{-\frac{\hbar}{2}}(n)\cos^2(\frac{Bt}{2N})$

To get the time evolution result from $|\uparrow\rangle$ at $t_n + 0$ to $t_{n+1} - 0$, over time duration $\frac{t}{N}$, we can use the $|\psi(t)\rangle$ in (a) with t replaced by $\frac{t}{N}$.

The time evolution of $|\downarrow\rangle$ over time duration $\frac{t}{N}$ can be solved in similar way.

This produce the recursion relation

$$\begin{pmatrix} P_{+\frac{\hbar}{2}}(n+1) \\ P_{-\frac{\hbar}{2}}(n+1) \end{pmatrix} = \begin{pmatrix} \cos^2(\frac{Bt}{2N}), & \sin^2(\frac{Bt}{2N}) \\ \sin^2(\frac{Bt}{2N}), & \cos^2(\frac{Bt}{2N}) \end{pmatrix} \begin{pmatrix} P_{+\frac{\hbar}{2}}(n) \\ P_{-\frac{\hbar}{2}}(n) \end{pmatrix}$$

Therefore $\begin{pmatrix} P_{+\frac{\hbar}{2}}(N) \\ P_{-\frac{\hbar}{2}}(N) \end{pmatrix} = W^N \cdot \begin{pmatrix} 1 \\ 0 \end{pmatrix}$, where $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$ is $\begin{pmatrix} P_{+\frac{\hbar}{2}}(0) \\ P_{-\frac{\hbar}{2}}(0) \end{pmatrix}$, and $W = \begin{pmatrix} \cos^2(\frac{Bt}{2N}), & \sin^2(\frac{Bt}{2N}) \\ \sin^2(\frac{Bt}{2N}), & \cos^2(\frac{Bt}{2N}) \end{pmatrix}$.
[Side remark: this is similar to a "Markov chain"]

Change to basis that diagonalize this 2×2 matrix, we have
$P_{+\frac{\hbar}{2}}(n+1) + P_{-\frac{\hbar}{2}}(n+1) = [\cos^2(\frac{Bt}{2N}) + \sin^2(\frac{Bt}{2N})] \cdot [P_{+\frac{\hbar}{2}}(n) + P_{-\frac{\hbar}{2}}(n)]$,
therefore $P_{+\frac{\hbar}{2}}(N) + P_{-\frac{\hbar}{2}}(N) = 1^N \cdot [P_{+\frac{\hbar}{2}}(0) + P_{-\frac{\hbar}{2}}(0)] = 1$ (should be expected); and
$P_{+\frac{\hbar}{2}}(n+1) - P_{-\frac{\hbar}{2}}(n+1) = [\cos^2(\frac{Bt}{2N}) - \sin^2(\frac{Bt}{2N})] \cdot [P_{+\frac{\hbar}{2}}(n) - P_{-\frac{\hbar}{2}}(n)]$,
therefore $P_{+\frac{\hbar}{2}}(N) - P_{-\frac{\hbar}{2}}(N) = [1 - 2\sin^2(\frac{Bt}{2N})]^N \cdot [P_{+\frac{\hbar}{2}}(0) - P_{-\frac{\hbar}{2}}(0)] = [1 - 2\sin^2(\frac{Bt}{2N})]^N$.

Finally, $P_{+\frac{\hbar}{2}}(N) = \frac{1}{2} + \frac{1}{2}[1 - 2\sin^2(\frac{Bt}{2N})]^N$, $P_{-\frac{\hbar}{2}}(N) = \frac{1}{2} - \frac{1}{2}[1 - 2\sin^2(\frac{Bt}{2N})]^N$.

In the limit $N \to \infty$, $[1 - 2\sin^2(\frac{Bt}{2N})]^N \to [1 - \frac{B^2t^2}{2N^2}]^N \to e^{-\frac{B^2t^2}{2N}} \to 1$, then $P_{+\frac{\hbar}{2}}(N) \to 1$.

Problem 6 (10 points) Consider $2n$ spin-1/2 moments $\hat{\boldsymbol{S}}_i$, labeled by $i = 1, 2, \ldots, 2n$. Here n is a positive integer.

(a) (5pts) *What are the possible total spin angular momentum quantum number S, namely possible eigenvalues of $(\sum_i \hat{\boldsymbol{S}})^2 = \hbar^2 S(S+1)$?*

(b) (5pts**) *How many linearly independent spin singlet (total-spin-0) states can these $2n$ spin-1/2 make? (for generic n)* [Examples:
$n = 1$, then $\mathbf{\frac{1}{2}} \otimes \mathbf{\frac{1}{2}} = \mathbf{0} \oplus \mathbf{1}$, the only singlet state is $\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$;
$n = 2$, then $\mathbf{\frac{1}{2}} \otimes \mathbf{\frac{1}{2}} \otimes \mathbf{\frac{1}{2}} \otimes \mathbf{\frac{1}{2}} = (\mathbf{0} \oplus \mathbf{1}) \otimes (\mathbf{0} \oplus \mathbf{1}) = (\mathbf{0} \otimes \mathbf{0}) \oplus (\mathbf{0} \otimes \mathbf{1}) \oplus (\mathbf{1} \otimes \mathbf{0}) \oplus (\mathbf{1} \otimes \mathbf{1})$
$= \mathbf{0} \oplus \mathbf{1} \oplus \mathbf{1} \oplus (\mathbf{0} \oplus \mathbf{1} \oplus \mathbf{2})$, there are two linearly independent spin singlet states,
$\frac{1}{2}(|\uparrow\downarrow\uparrow\downarrow\rangle - |\uparrow\downarrow\downarrow\uparrow\rangle - |\downarrow\uparrow\uparrow\downarrow\rangle + |\downarrow\uparrow\downarrow\uparrow\rangle)$, and
$\frac{1}{2\sqrt{3}}(2|\uparrow\uparrow\downarrow\downarrow\rangle - |\uparrow\downarrow\uparrow\downarrow\rangle - |\uparrow\downarrow\downarrow\uparrow\rangle - |\downarrow\uparrow\uparrow\downarrow\rangle - |\downarrow\uparrow\downarrow\uparrow\rangle + 2|\downarrow\downarrow\uparrow\uparrow\rangle)$.]

[Hint: consider the dimensions of Hilbert spaces of fixed total $S_z = \sum_i \hat{S}_{i,z}$, total-spin-0 states $|\psi\rangle$ should satisfy $(\sum_i \hat{S}_{i,+})|\psi\rangle = 0$]

Solution

(a) By the Clebsch-Gordon theorem about "addition of angular momentum", from the examples in (b), use mathematical induction, we have: for $2n$ spin-1/2, the total spin angular momentum quantum number S can be any integer between (including) 0 and n, $S = 0$ or 1 or $\ldots$ or n.

(b) Method #1: count the dimensions of subspaces of certain total S_z.

Suppose the Hilbert space of $2n$ spin-1/2 is divided into m_0 sets of total-spin-0 states(singlets) plus m_1 sets of total-spin-1 states(triplets) (each set of spin triplet contains $3 = 2 \cdot 1 + 1$ states) plus $\ldots$ plus m_n sets of total-spin-n states (each set of total-spin-n states contains $2n+1$ states),

$$\underbrace{\tfrac{\mathbf{1}}{\mathbf{2}} \otimes \cdots \otimes \tfrac{\mathbf{1}}{\mathbf{2}}}_{2n} = \underbrace{\mathbf{0} \oplus \cdots \oplus \mathbf{0}}_{m_0} \oplus \underbrace{\mathbf{1} \oplus \cdots \oplus \mathbf{1}}_{m_1} \oplus \cdots \oplus \underbrace{\boldsymbol{n} \oplus \cdots \oplus \boldsymbol{n}}_{m_n} \qquad (*)$$

Compute the dimensions of subspaces with certain $S_z = \sum_{i=1}^{2n} S_{i,z}$ in two different ways.

- Consider the right-hand-side of the above $(*)$ expression.

  Each of the subspaces on the right-hand-side (spanned by states with certain total spin quantum number S and total $S_z = -S, \ldots, S$) will contribute a linearly independent total $S_z = 0$ state $|S, S_z = 0\rangle$, so the dimension of total $S_z = 0$ Hilbert space is $\dim[\mathcal{H}_{S_z=0}] = m_0 + m_1 + \cdots + m_n$.

  But only the subspaces with total spin quantum number $S \geq 1$ will contribute a linearly independent $|S, S_z = \hbar\rangle$ state, so the dimension of total $S_z = \hbar$ subspace is $\dim[\mathcal{H}_{S_z=\hbar}] = m_1 + \cdots + m_n$.

- Consider the left-hand-side of the above $(*)$ expression.

  The 2^{2n} basis of the entire Hilbert space can be chosen as the S_z tensor product basis $|S_{1,z}, S_{2,z}, \ldots, S_{2n,z}\rangle$.

  For total $S_z = 0$, there must be n up-spin($S_{i,z} = +\frac{\hbar}{2}$) and n down-spin($S_{i,z} = -\frac{\hbar}{2}$), so $\dim[\mathcal{H}_{S_z=0}] = \binom{2n}{n} = \frac{(2n)!}{n!n!}$.

  For total $S_z = \hbar$, there must be $(n+1)$ up-spin and $(n-1)$ down-spin, so $\dim[\mathcal{H}_{S_z=\hbar}] = \binom{2n}{n+1} = \frac{(2n)!}{(n+1)!(n-1)!}$.

Finally, the number of total-spin-0 states is

$m_0 = \dim[\mathcal{H}_{S_z=0}] - \dim[\mathcal{H}_{S_z=\hbar}] = \binom{2n}{n} - \binom{2n}{n+1} = \frac{(2n)!}{(n+1)!n!}$.

[Side remark: this is related to the "hook length formula" in representation theory.]

Method #2: try to "solve" $\sum_i \hat{S}_{i,+}|\psi\rangle = 0$.

Define the total ladder operators $\hat{S}_\pm = \sum_{i=1}^{2n} \hat{S}_{i,\pm}$. And $\hat{S}_a = \sum_{i=1}^{2n} \hat{S}_{i,a}$.

Denote the basis $|S_{1,z}, \ldots, S_{2n,z}\rangle$ with $\sum_i S_{i,z} = 0$ by $|\psi_\alpha\rangle$, $\alpha = 1, \ldots, \binom{2n}{n}$.

Denote the basis $|S_{1,z}, \ldots, S_{2n,z}\rangle$ with $\sum_i S_{i,z} = \hbar$ by $|\phi_\beta\rangle$, $\beta = 1, \ldots, \binom{2n}{n+1}$.

A non-vanishing state $|\psi\rangle$ is total-spin-0 if and only if $\hat{S}_+|\psi\rangle = 0$ and $(\sum_i \hat{S}_{i,z})|\psi\rangle = 0$.

Expand $|\psi\rangle$ by S_z-basis. Then $|\psi\rangle = \sum_\alpha c_\alpha |\psi_\alpha\rangle$, contains only those $\sum_i S_{i,z} = 0$ states.

Note that $\hat{S}_+|\psi_\alpha\rangle$ is a linear combination of $|\phi_\beta\rangle$ states, $\hat{S}_+|\psi_\alpha\rangle = \sum_\beta |\phi_\beta\rangle \cdot (S_+)_{\beta,\alpha}$.

Here $(S_+)_{\beta,\alpha} = \langle\phi_\beta|\hat{S}_+|\psi_\alpha\rangle$ is a $\binom{2n}{n+1} \times \binom{2n}{n}$ rectangular matrix. It is actually $\hbar$ times a "(0-1)-matrix", each matrix element can be only 0 or $\hbar$.

For a total-spin-0 state $|\psi\rangle$, we have $\hat{S}_+|\psi\rangle = \sum_\alpha \sum_\beta |\phi_\beta\rangle (S_+)_{\beta,\alpha} c_\alpha = 0$. Therefore $\sum_\alpha (S_+)_{\beta,\alpha} c_\alpha = 0$ for each β. The number of linearly independent solutions to this set of linear equations is [number of variables, $\binom{2n}{n}$]$-$rank(S_+), where rank(S_+) is the "rank" of the rectangular matrix $(S_+)_{\beta,\alpha}$.

We still need to prove that rank(S_+) is the smaller dimension $\binom{2n}{n+1}$, namely there is no non-trivial solution to d_β from the linear equations $\sum_\beta d_\beta (S_+)_{\beta,\alpha} = 0$ for each α. We can prove this by contradiction: if there is a non-trivial solution d_β, then $\sum_\beta (S_-)_{\alpha,\beta} d_\beta^* = 0$ for every α, here $(S_-)_{\alpha,\beta} = \langle\psi_\alpha|\hat{S}_-|\phi_\beta\rangle = [(S_+)_{\beta,\alpha}]^*$, define $|\phi\rangle = \sum_\beta d_\beta^* |\phi_\beta\rangle$, then $\hat{S}_-|\phi\rangle = 0$ and $\hat{S}_z|\phi\rangle = \hbar|\phi\rangle$, therefore $\hat{\boldsymbol{S}}^2|\phi\rangle = [\hat{S}_z(\hat{S}_z - \hbar) + \hat{S}_+\hat{S}_-]|\phi\rangle = 0$, however $\langle\phi|\hat{\boldsymbol{S}}^2|\phi\rangle = \langle\phi|[\hat{S}_z(\hat{S}_z + \hbar) + \hat{S}_-\hat{S}_+]|\phi\rangle \geq \langle\phi|[\hat{S}_z(\hat{S}_z + \hbar)]|\phi\rangle = 2\hbar^2\langle\phi|\phi\rangle > 0$. This contradiction proves that there is no such state $|\phi\rangle$, so the rank of $(S_+)_{\beta,\alpha}$ is indeed $\binom{2n}{n+1}$.