Quantum Mechanics: Fall 2022
Midterm Exam: Brief Solutions

NOTE: Problems start on page 2. Bold symbols are 3-component vectors.

Some useful facts: You can use them directly.

- 1D harmonic oscillator: $\hat{H} = \frac{\hat{p}^2}{2m} + \frac{m\omega^2}{2}\hat{x}^2 = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{m\omega^2}{2}x^2$.
  Here $\hat{x}$ is position operator, $\hat{p}$ is momentum operator, $[\hat{x}, \hat{p}] = \mathbb{i}\hbar$, 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 $\psi_0(x) = (\frac{m\omega}{\pi\hbar})^{1/4}\exp(-\frac{m\omega}{2\hbar}x^2)$.

- $\int_{-\infty}^{+\infty} e^{-x^2/a}\mathrm{d}x = \sqrt{\pi a}$, for $a > 0$. Applying $\frac{\partial}{\partial a}$ can produce $\int_{-\infty}^{+\infty} x^{2n}e^{-x^2/a}\mathrm{d}x$.

- Central potential problem: $\hat{H} = \frac{1}{2m}\hat{\boldsymbol{p}}^2 + V(r)$.
  Here $\hat{\boldsymbol{p}}$ is the 3D momentum $-\mathbb{i}\hbar\frac{\partial}{\partial \boldsymbol{r}}$, and $r = |\boldsymbol{r}|$ is the radius. Under polar coordinates (r, θ, ϕ), the eigenfunctions are generally $\psi_{E,\ell,m} = \frac{u(r)}{r}\cdot Y_\ell^m(\theta, \phi)$, where $Y_\ell^m(\theta, \phi)$ is the spherical harmonics, and $u(r)$ satisfies $-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2u}{\mathrm{d}r^2} + \left[V(r) + \frac{\hbar^2}{2m}\frac{\ell(\ell+1)}{r^2}\right]\cdot u = E\cdot u$. Here $\ell = 0, 1, \ldots$ is the angular momentum quantum number; $m = -\ell, -\ell+1, \ldots, \ell$ is the "magnetic quantum number"; E is the energy eigenvalue.

  - The spherical harmonics are orthonormal, and are eigenfunctions of $\hat{\boldsymbol{L}}^2$ and $\hat{L}_z$. $Y_0^0 = \frac{1}{\sqrt{4\pi}}$, $Y_1^0 = \sqrt{\frac{3}{4\pi}}\cos\theta$, $Y_1^{\pm 1} = \mp\sqrt{\frac{3}{8\pi}}\sin\theta e^{\pm\mathbb{i}\phi}$, $\ldots$.

- 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 $(\hat{J}_x \pm \mathbb{i}\hat{J}_y)|j, m\rangle = \hbar\sqrt{(j \mp m)(j \pm m + 1)}|j, m \pm 1\rangle$.
  Here $2j$ is non-negative integer, $m = -j, -j+1, \ldots, j$.

  - Orbital angular momentum: $\hat{\boldsymbol{L}} \equiv \hat{\boldsymbol{r}} \times \hat{\boldsymbol{p}}$.
  - Spin-1/2: basis states $|\uparrow\rangle$ and $|\downarrow\rangle$. Under this basis, $\hat{S}_a = \frac{\hbar}{2}\sigma_a$, where $\sigma_{x,y,z}$ are Pauli matrices, $\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, $\sigma_y = \begin{pmatrix} 0 & -\mathbb{i} \\ \mathbb{i} & 0 \end{pmatrix}$, $\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$. $\sigma_a\sigma_b = \delta_{ab}\mathbb{1}_{2\times 2} + \mathbb{i}\sum_c \epsilon_{abc}\sigma_c$.
    Generic wavefunction under this basis is $\begin{pmatrix} \psi_\uparrow \\ \psi_\downarrow \end{pmatrix}$, which means $\psi_\uparrow|\uparrow\rangle + \psi_\downarrow|\downarrow\rangle$.

Problem 1. (20 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 $-\frac{L}{2} \le x \le \frac{L}{2}$ with periodic boundary condition for the wavefunction, $\psi(-\frac{L}{2}) = \psi(\frac{L}{2})$, and normalization condition $\int_{x=-\frac{L}{2}}^{\frac{L}{2}} |\psi(x)|^2 \, \mathrm{d}x = 1$.

(a) (5pts) For free particle (no potential energy) with this periodic boundary condition, *write down all the energy eigenvalues and normalized eigenstate wavefunctions.*

(b) (5pts) Include a δ-potential, $-\alpha\,\delta(x)$, where α is a positive parameter. *Draw the qualitative pictures of the ground state, 1st excited, and 2nd excited state wavefunctions.* [NOTE: discussion about 1D bound state properties in lectures may not apply here.]

(c) (10pts) *Derive the equations satisfied by the energy eigenvalues of the ground state and 1st excited states in (b), respectively.*

Solution:

(a) This is basically homework Problem 2.46.

$\psi_n(x) = \frac{1}{\sqrt{L}} e^{\mathrm{i}2\pi n x/L}$, $E_n = \frac{\hbar^2}{2m}(\frac{2\pi n}{L})^2$, n is an integer.

Except $n = 0$ case, all E_n energy level is 2-fold degenerate.

(b)(c)

The boundary condition at $x = 0$ is,

$\psi(-0) = \psi(+0),\ -\frac{\hbar^2}{2m}\frac{\mathrm{d}}{\mathrm{d}x}\psi\Big|_{x=-0}^{+0} - \alpha\psi(0) = 0.$

The "boundary condition" at $x = \pm L/2$ is (there is no real boundary here, eigenstates should be smooth here)

$\psi(-L/2) = \psi(L/2),\ \frac{\mathrm{d}}{\mathrm{d}x}\psi\big|_{x=-L/2} = \frac{\mathrm{d}}{\mathrm{d}x}\psi\big|_{x=L/2}.$

NOTE:

as in Problem 2.46, the argument of non-degenerate eigenstates does not apply;

but the argument about inversion symmetry still applies, eigenstates can be chosen as either even or odd functions;

For odd eigenfunctions, $\psi(0) = 0$, the δ-potential has no effect on the energy eigenvalue etc., and there are no odd bound states, these odd eigenstates are $\psi_{n,\text{odd}} = \sqrt{\frac{2}{L}}\sin(2\pi n x/L)$, with $E_{n,\text{odd}} = E_n$ and $n = 1, 2, \ldots$.

For even eigenfunctions, we must have $\frac{\mathrm{d}}{\mathrm{d}x}\psi\big|_{x=-L/2} = \frac{\mathrm{d}}{\mathrm{d}x}\psi\big|_{x=L/2} = 0$.

For even "bound states" with $E = -\frac{\hbar^2\kappa^2}{2m} < 0$, we must have $\psi(x) = A\cdot\cosh[\kappa\cdot(|x|-L/2)]$, the boundary condition at $x = 0$ produces

$$\frac{\hbar^2}{m}\kappa\sinh(\kappa L/2) - \alpha\cosh(\kappa L/2) = 0$$

therefore $\kappa\tanh(\kappa L/2) = \frac{m\alpha}{\hbar^2}$, where $\kappa = \sqrt{-2mE}/\hbar$. The left-hand-side of this equation is a monotonic function of κ, so there is only one "bound state" (the ground state).

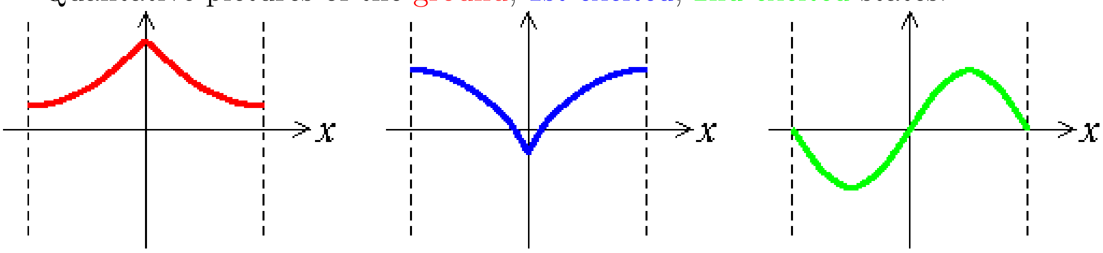
For even eigenstates with $E = \frac{\hbar^2 k^2}{2m} > 0$, we must have $\psi(x) = A\cdot\cos[k\cdot(|x| - L/2)]$, the boundary condition at $x = 0$ produces

$$\frac{\hbar^2}{m}k\sin(kL/2) - \alpha\cos(kL/2) = 0$$

therefore $k\tan(kL/2) = \frac{m\alpha}{\hbar^2}$, where $k = \sqrt{2mE}/\hbar$. There are infinite many solutions to k, the smallest one satisfies $0 < k < \frac{\pi}{L}$, and is the 1st excited state.

The 2nd excited state is the odd solution with $n = 1$, $\psi_{1,\text{odd}} = \sqrt{\frac{2}{L}}\sin(2\pi x/L)$, with wavevector $k = \frac{2\pi}{L}$.

Qualitative pictures of the ground, 1st excited, 2nd excited states:



Problem 2. (20 points) Hydrogen atom has $\hat{H} = \frac{\hat{\mathbf{p}}^2}{2m} - \frac{\hbar^2}{ma}\cdot\frac{1}{r}$, where $a = \frac{4\pi\epsilon_0}{e^2}\cdot\frac{\hbar^2}{m}$ is the Bohr radius. Its energy eigenvalues are $E_n = -\frac{\hbar^2}{2ma^2}\cdot\frac{1}{n^2}$, with eigenstate wavefunction $\psi_{n\ell m}(r,\theta,\phi) = R_{n\ell}(r)Y_\ell^m(\theta,\phi)$. Some special cases of the radial wavefunctions are,
$R_{10}(r) = 2a^{-3/2}e^{-r/a}$, $R_{20}(r) = \frac{1}{\sqrt{2}}a^{-3/2}(1-\frac{r}{2a})e^{-r/2a}$, $R_{21}(r) = \frac{1}{2\sqrt{6}}a^{-3/2}(\frac{r}{a})e^{-r/2a}$.

(a) (10pts) *Compute the expectation value of kinetic energy* $\frac{\hat{\mathbf{p}}^2}{2m}$ *under the state* ψ_{210}.

(b) (10pts) Consider the subspace of 1st excited states, spanned by four basis states $\Psi_1 \equiv \psi_{200}$, $\Psi_2 \equiv \psi_{211}$, $\Psi_3 \equiv \psi_{210}$, $\Psi_4 \equiv \psi_{21,-1}$. *Compute all the matrix elements* $\langle\Psi_i|\hat{z}|\Psi_j\rangle$ *for the z-component of position operator* $\hat{z}$. [Hint: symmetry consideration can dramatically simplify this problem.]

Solution:

(a) $\frac{\hat{\boldsymbol{p}}^2}{2m} = \hat{H} + \frac{\hbar^2}{ma}\cdot\frac{1}{r}$, then

$\langle\psi_{210}|\frac{\hat{\boldsymbol{p}}^2}{2m}|\psi_{210}\rangle = E_2 + \langle\psi_{210}|\frac{\hbar^2}{ma}\cdot\frac{1}{r}|\psi_{210}\rangle = -\frac{\hbar^2}{2ma^2}\cdot\frac{1}{4} + \frac{\hbar^2}{ma}\int_0^\infty \frac{1}{r}\cdot[R_{21}(r)]^2\, r^2\mathrm{d}r$

$= -\frac{\hbar^2}{2ma^2}\cdot\frac{1}{4} + \frac{\hbar^2}{ma}\cdot\frac{1}{24}a^{-3}\int_0^\infty \frac{r}{a^2}e^{-r/a}\, r^2\mathrm{d}r$

$= \frac{\hbar^2}{8ma^2} = -E_2$

NOTE: the fact that $\langle\psi_{210}|\frac{\hat{\boldsymbol{p}}^2}{2m}|\psi_{210}\rangle = -E_2$ can be derived from "virial theorem".

(b) Note that $[\hat{z}, \hat{L}_z] = 0$, therefore $\hat{z}$ does not change $\hat{L}_z$ eigenvalue, then $\langle\psi_{n\ell m}|\hat{z}|\psi_{n'\ell'm'}\rangle$ will vanish if $m \neq m'$ [can also be seen from the fact that $\psi^*_{n\ell m} z \psi_{n'\ell'm'} = e^{\mathrm{i}(m'-m)\phi}\cdot f(r,\theta)$]. By this "selection rule", most of the matrix elements $\langle\Psi_i|\hat{z}|\Psi_j\rangle$ are vanishing except for $(i,j) = (1,1)$ or $(1,3)$ or $(2,2)$ or $(3,1)$ or $(3,3)$ or $(4,4)$.

Note that for $\langle\Psi_i|\hat{z}|\Psi_i\rangle = \int |\Psi_i(\boldsymbol{r})|^2 z\, \mathrm{d}^3\boldsymbol{r}$, the integrand is an odd function under $\boldsymbol{r} \to -\boldsymbol{r}$, therefore all diagonal matrix elements $\langle\Psi_i|\hat{z}|\Psi_i\rangle = 0$.

So we only need to evaluate $\langle\Psi_3|\hat{z}|\Psi_1\rangle^* = \langle\Psi_1|\hat{z}|\Psi_3\rangle$

$= \int_0^\infty [R_{20}(r)]^*\cdot r\cdot R_{21}(r)\cdot r^2\mathrm{d}r \times \int_0^\pi \sin\theta\mathrm{d}\theta \int_0^{2\pi}\mathrm{d}\phi\, [(\sqrt{\tfrac{1}{4\pi}})^*\cdot\cos\theta\cdot\sqrt{\tfrac{3}{4\pi}}\cos\theta]$

$= \frac{1}{4\sqrt{3}}\int_0^\infty r\cdot\frac{r}{a}\cdot(1-\frac{r}{2a})a^{-3}e^{-r/a}\, r^2\mathrm{d}r \times \frac{1}{\sqrt{3}} = -3a$

Problem 3. (30 points) Consider three spin-1/2 with spin angular momentum operators $\hat{\boldsymbol{S}}_i$, $i = 1,2,3$ respectively. The entire Hilbert space is the tensor product of the three spin-1/2 Hilbert spaces, with tensor product basis $|S_{1z}\rangle|S_{2z}\rangle|S_{3z}\rangle$. For notation simplicity, label these basis as $|\uparrow\uparrow\uparrow\rangle$, $|\uparrow\uparrow\downarrow\rangle$, $\dots$, $|\downarrow\downarrow\downarrow\rangle$. The spin-1/2 operators extended to the entire Hilbert space are, $\hat{\boldsymbol{S}}_1 = \frac{\hbar}{2}\boldsymbol{\sigma}\otimes\mathbb{1}\otimes\mathbb{1}$, $\hat{\boldsymbol{S}}_2 = \mathbb{1}\otimes\frac{\hbar}{2}\boldsymbol{\sigma}\otimes\mathbb{1}$, $\hat{\boldsymbol{S}}_3 = \mathbb{1}\otimes\mathbb{1}\otimes\frac{\hbar}{2}\boldsymbol{\sigma}$. Here $\mathbb{1}$ are 2×2 identity matrix (identity operator in one spin-1/2 Hilbert space). Define $\hat{\boldsymbol{S}}_{1+2} = \hat{\boldsymbol{S}}_1 + \hat{\boldsymbol{S}}_2$, and $\hat{\boldsymbol{S}}_{1+2+3} = \hat{\boldsymbol{S}}_1 + \hat{\boldsymbol{S}}_2 + \hat{\boldsymbol{S}}_3$.

(a) (10pts) As a standard "addition of angular momentum" problem, *Write down all* *possible combinations of* $\hat{\boldsymbol{S}}^2_{1+2}$ *and* $\hat{S}_{1+2,z}$ *eigenvalues, and their simultaneous eigenstates* $|S_{1+2}, S_{1+2,z}\rangle$ *in terms of the above tensor product basis.*

(b) (10pts) *Show that* $\hat{\boldsymbol{S}}^2_{1+2+3}$ *and* $\hat{S}_{1+2+3,z}$ *and* $\hat{\boldsymbol{S}}^2_{1+2}$ *mutually commute.*

(c) (10pts*) *Solve all possible combinations of the eigenvalues of the three observables in (b), and their simultaneous eigenstates* $|S_{1+2+3}, S_{1+2+3,z}, S_{1+2}\rangle$ *in terms of the tensor product basis.* [Hint: $\hat{\boldsymbol{S}}_{1+2+3} = \hat{\boldsymbol{S}}_{1+2} + \hat{\boldsymbol{S}}_3$ as an addition of angular momentum problem]

Solution:

(a) If we consider only spin 1 and spin 2, this is the standard addition of two spin-1/2 (textbook Example 4.5), and they can form spin triplet($S_{1+2} = 1$) or singlet($S_{1+2} = 0$) states, the simultaneous eigenstates of $\hat{\boldsymbol{S}}^2_{1+2}$ and $\hat{S}_{1+2,z}$ in the two spin-1/2 space are
$|S_{1+2} = 1, S_{1+2,z} = 1\rangle = |\uparrow\uparrow\rangle$,
$|S_{1+2} = 1, S_{1+2,z} = 0\rangle = \frac{1}{2}(|\downarrow\uparrow\rangle + |\uparrow\downarrow\rangle)$,
$|S_{1+2} = 1, S_{1+2,z} = -1\rangle = |\downarrow\downarrow\rangle$,
$|S_{1+2} = 0, S_{1+2,z} = 0\rangle = \frac{1}{2}(|\downarrow\uparrow\rangle - |\uparrow\downarrow\rangle)$.

Including spin 3, the eigenstates of $\hat{\boldsymbol{S}}^2_{1+2}$ and $\hat{S}_{1+2,z}$ just become 2-fold degenerate $|S_{1+2}, S_{1+2,z}\rangle|S_{3z}\rangle$, where $S_{3z} =\uparrow, \downarrow$.

The results are summarized in the following table,

S_{1+2}	$S_{1+2,z}$	$\hat{\boldsymbol{S}}^2_{1+2}$ eigenvalue	$\hat{S}_{1+2,z}$ eigenvalue	states
1	1	$2\hbar^2$	$\hbar$	$\|\uparrow\uparrow\uparrow\rangle$ $\|\uparrow\uparrow\downarrow\rangle$
1	0	$2\hbar^2$	0	$\frac{1}{\sqrt{2}}(\|\downarrow\uparrow\uparrow\rangle + \|\uparrow\downarrow\uparrow\rangle)$ $\frac{1}{\sqrt{2}}(\|\downarrow\uparrow\downarrow\rangle + \|\uparrow\downarrow\downarrow\rangle)$
1	-1	$2\hbar^2$	$-\hbar$	$\|\uparrow\uparrow\uparrow\rangle$ $\|\uparrow\uparrow\downarrow\rangle$
0	0	0	0	$\frac{1}{\sqrt{2}}(\|\downarrow\uparrow\uparrow\rangle - \|\uparrow\downarrow\uparrow\rangle)$ $\frac{1}{\sqrt{2}}(\|\downarrow\uparrow\downarrow\rangle - \|\uparrow\downarrow\downarrow\rangle)$

(b) use
$[\hat{S}_{1+2+3,a}, \hat{S}_{1+2,b}] = \sum_c \mathrm{i}\hbar\epsilon_{abc}\hat{S}_{1+2,c}$,

$[\hat{S}_{1+2+3,a}, \hat{S}_{1+2+3,b}] = \sum_c \mathbb{i}\hbar\epsilon_{abc}\hat{S}_{1+2+3,c}$,
and $[\hat{A}\hat{B}, \hat{C}] = \hat{A}[\hat{B}, \hat{C}] + [\hat{A}, \hat{C}]\hat{B}$.

we have
$[\hat{S}_{1+2+3,a}, \hat{\boldsymbol{S}}^2_{1+2}] = \sum_b [\hat{S}_{1+2+3,a}, \hat{S}^2_{1+2,b}]$
$= \sum_{b,c}(\mathbb{i}\hbar\epsilon_{abc}\hat{S}_{1+2,c}\hat{S}_{1+2,b} + \mathbb{i}\hbar\epsilon_{abc}\hat{S}_{1+2,b}\hat{S}_{1+2,c}) = \sum_{b,c}(\mathbb{i}\hbar\epsilon_{abc}\hat{S}_{1+2,c}\hat{S}_{1+2,b} + \mathbb{i}\hbar\epsilon_{acb}\hat{S}_{1+2,c}\hat{S}_{1+2,b})$
$= \sum_{b,c}(\mathbb{i}\hbar\hat{S}_{1+2,c}\hat{S}_{1+2,b}(\epsilon_{abc} + \epsilon_{acb}) = 0$.

in particular $[\hat{S}_{1+2+3,z}, \hat{\boldsymbol{S}}^2_{1+2}] = 0$,

similarly we have $[\hat{S}_{1+2+3,z}, \hat{\boldsymbol{S}}^2_{1+2+3}] = 0$,

finally $[\hat{\boldsymbol{S}}^2_{1+2+3}, \hat{\boldsymbol{S}}^2_{1+2}] = \sum_a [\hat{S}^2_{1+2+3,a}, \hat{\boldsymbol{S}}^2_{1+2}] = 0$.

(c) In the subspace spanned by $|S_{1+2} = 0, S_{1+2,z} = 0\rangle|S_{3z}\rangle$, this is the "addition of two spins of $S_{1+2} = 0$ and $S_3 = \frac{1}{2}$", so the total spin quantum number must be $S_{1+2+3} = \frac{1}{2}$, and obviously,
$|S_{1+2+3} = \frac{1}{2}, S_{1+2+3,z} = +\frac{1}{2}, S_{1+2} = 0\rangle = |S_{1+2} = 0, S_{1+2,z} = 0\rangle|S_{3z} =\uparrow\rangle$,
$|S_{1+2+3} = \frac{1}{2}, S_{1+2+3,z} = -\frac{1}{2}, S_{1+2} = 0\rangle = |S_{1+2} = 0, S_{1+2,z} = 0\rangle|S_{3z} =\downarrow\rangle$,

In the subspace spanned by $|S_{1+2} = 1, S_{1+2,z}\rangle|S_{3z}\rangle$, this is the "addition of two spins of $S_{1+2} = 1$ and $S_3 = \frac{1}{2}$", the total spin quantum number can be $S_{1+2+3} = \frac{1}{2}$ or $\frac{3}{2}$, the relevant C.-G. coefficients have been used in homework Problem 4.40,

The $S_{1+2+3} = \frac{3}{2}$ states are (up to overall phase factor),

$|S_{1+2+3} = \frac{3}{2}, S_{1+2+3,z} = +\frac{3}{2}, S_{1+2} = 1\rangle = |S_{1+2} = 1, S_{1+2,z} = 1\rangle|S_{3z} =\uparrow\rangle$,

$|S_{1+2+3} = \frac{3}{2}, S_{1+2+3,z} = +\frac{1}{2}, S_{1+2} = 1\rangle$
$= \frac{1}{\sqrt{3}}(\sqrt{2}|S_{1+2} = 1, S_{1+2,z} = 0\rangle|S_{3z} =\uparrow\rangle + |S_{1+2} = 1, S_{1+2,z} = 1\rangle|S_{3z} =\downarrow\rangle)$,

$|S_{1+2+3} = \frac{3}{2}, S_{1+2+3,z} = -\frac{1}{2}, S_{1+2} = 1\rangle$
$= \frac{1}{\sqrt{3}}(\sqrt{2}|S_{1+2} = 1, S_{1+2,z} = 0\rangle|S_{3z} =\downarrow\rangle + |S_{1+2} = 1, S_{1+2,z} = -1\rangle|S_{3z} =\uparrow\rangle)$,

$|S_{1+2+3} = \frac{3}{2}, S_{1+2+3,z} = -\frac{3}{2}, S_{1+2} = 1\rangle = |S_{1+2} = 1, S_{1+2,z} = -1\rangle|S_{3z} =\downarrow\rangle$, The $S_{1+2+3} = \frac{1}{2}$ states are (up to overall phase factor),

$$|S_{1+2+3} = \tfrac{1}{2}, S_{1+2+3,z} = +\tfrac{1}{2}, S_{1+2} = 1\rangle$$
$$= \tfrac{1}{\sqrt{3}}(|S_{1+2} = 1, S_{1+2,z} = 0\rangle|S_{3z} =\uparrow\rangle - \sqrt{2}|S_{1+2} = 1, S_{1+2,z} = 1\rangle|S_{3z} =\downarrow\rangle),$$

$$|S_{1+2+3} = \tfrac{1}{2}, S_{1+2+3,z} = -\tfrac{1}{2}, S_{1+2} = 1\rangle$$
$$= \tfrac{1}{\sqrt{3}}(\sqrt{2}|S_{1+2} = 1, S_{1+2,z} = -1\rangle|S_{3z} =\uparrow\rangle - |S_{1+2} = 1, S_{1+2,z} = 0\rangle|S_{3z} =\downarrow\rangle),$$

The results are summarized in the following table,

$\hat{\boldsymbol{S}}^2_{1+2+3}$	$\hat{S}_{1+2+3,z}$	$\hat{\boldsymbol{S}}^2_{1+2}$	state
$\frac{3}{4}\hbar^2$	$+\frac{\hbar}{2}$	0	$\frac{1}{\sqrt{2}}(\lvert\downarrow\uparrow\uparrow\rangle - \lvert\uparrow\downarrow\uparrow\rangle)$
$\frac{3}{4}\hbar^2$	$-\frac{\hbar}{2}$	0	$\frac{1}{\sqrt{2}}(\lvert\downarrow\uparrow\downarrow\rangle - \lvert\uparrow\downarrow\downarrow\rangle)$
$\frac{15}{4}\hbar^2$	$+\frac{3\hbar}{2}$	$2\hbar^2$	$\lvert\uparrow\uparrow\uparrow\rangle$
$\frac{15}{4}\hbar^2$	$+\frac{1\hbar}{2}$	$2\hbar^2$	$\frac{1}{\sqrt{3}}(\lvert\downarrow\uparrow\uparrow\rangle + \lvert\uparrow\downarrow\uparrow\rangle + \lvert\uparrow\uparrow\downarrow\rangle)$
$\frac{15}{4}\hbar^2$	$-\frac{1\hbar}{2}$	$2\hbar^2$	$\frac{1}{\sqrt{3}}(\lvert\downarrow\downarrow\uparrow\rangle + \lvert\downarrow\uparrow\downarrow\rangle + \lvert\uparrow\downarrow\downarrow\rangle)$
$\frac{15}{4}\hbar^2$	$-\frac{3\hbar}{2}$	$2\hbar^2$	$\lvert\downarrow\downarrow\downarrow\rangle$
$\frac{3}{4}\hbar^2$	$+\frac{1\hbar}{2}$	$2\hbar^2$	$\frac{1}{\sqrt{6}}(\lvert\downarrow\uparrow\uparrow\rangle + \lvert\uparrow\downarrow\uparrow\rangle - 2\lvert\uparrow\uparrow\downarrow\rangle)$
$\frac{3}{4}\hbar^2$	$-\frac{1\hbar}{2}$	$2\hbar^2$	$\frac{1}{\sqrt{6}}(2\lvert\downarrow\downarrow\uparrow\rangle - \lvert\uparrow\downarrow\uparrow\rangle - \lvert\uparrow\uparrow\downarrow\rangle)$

Problem 4. (30 points) Consider the 1D harmonic oscillator $\hat{H} = \frac{\hat{p}^2}{2m} + \frac{m\omega^2}{2}\hat{x}^2 = \hbar\omega\left(\hat{a}_+\hat{a}_- + \frac{1}{2}\right)$ (see page 1). Define a new Hamiltonian $\hat{H}' = \hat{H} + \frac{\Delta}{2}\cdot(\hat{a}_+\hat{a}_+ + \hat{a}_-\hat{a}_-)$, where Δ is a small real parameter ($|\Delta| \ll \hbar\omega$).

(a) (5pts) *Write down the ground state energy E_0' and wave function $\psi_0'(x)$ of $\hat{H}'$.* [Hint: rewrite $\hat{H}'$ in terms of $\hat{x}$, $\hat{p}$]

(b) (10pts**) Expand ψ_0' as a linear combination of eigenbasis ψ_n of $\hat{H}$ (see page 1), $|\psi_0'\rangle = \sum_{n=0}^{\infty} c_n|\psi_n\rangle$. *Try to compute all c_n.* [Hint: c_0 can be computed by inner product; try to derive some recursion relation, compute the first few c_n and guess the general expression; or by analogy to coherent state, guess that $|\psi_0'\rangle = c_0\exp(\alpha\hat{a}_+\hat{a}_+)|\psi_0\rangle$ and solve α]

(c) (5pts) Let the initial state be $\psi(x, t = 0) = \psi_0'(x)$. Evolve it by $\hat{H}$ (not $\hat{H}'$), namely $\mathrm{i}\hbar\frac{\partial}{\partial t}\psi(x,t) = \hat{H}\psi(x,t)$. *Measure $\hat{H}$ under the state $\psi(x,t)$, what are the possible* *measurement results and their corresponding probabilities.*

(d) (10pts**) *Evaluate expectation values* $\langle \hat{x} \rangle$, $\langle \hat{p} \rangle$, $\langle \hat{x}^2 \rangle$, $\langle \hat{p}^2 \rangle$, *under the state* $\psi(x,t)$ *defined in (c). Show that the uncertainty relation* $\sigma_{\hat{x}}^2 \cdot \sigma_{\hat{p}}^2 \geq \frac{\hbar^2}{4}$ *is still satisfied.*

Solution:

(a) $\hat{H}' = (\frac{1}{2m} - \frac{\Delta}{2m\hbar\omega})\hat{p}^2 + (\frac{m\omega^2}{2} + \frac{m\omega\Delta}{2\hbar})\hat{x}^2$ is still a harmonic oscillator,

$\hat{H}' = \frac{\hat{p}^2}{2m'} + \frac{m'\omega'^2}{2}\hat{x}^2$, with $m' = \frac{m}{1-\Delta/\hbar\omega}$, $\omega' = \omega\sqrt{1-(\frac{\Delta}{\hbar\omega})^2}$.

Therefore

$E_0' = \frac{1}{2}\hbar\omega' = \frac{1}{2}\hbar\omega\sqrt{1-(\frac{\Delta}{\hbar\omega})^2}$,

$\psi_0'(x) = (\frac{m'\omega'}{\pi\hbar})^{1/4} e^{-\frac{m'\omega'}{2\hbar}x^2} = (\frac{1+\Delta/\hbar\omega}{1-\Delta/\hbar\omega})^{1/8}(\frac{m\omega}{\pi\hbar})^{1/4}\exp(-\sqrt{\frac{1+\Delta/\hbar\omega}{1-\Delta/\hbar\omega}}\frac{m\omega}{2\hbar}x^2)$

(b) $c_n \equiv \langle \psi_n | \psi_0' \rangle$.

Note $\psi_n(x)$ is an odd function for odd n, while $\psi_0'(x)$ is even, then $c_n = 0$ for odd n.

So $\psi_0' = \sum_{k=0}^{\infty} c_{2k}|\psi_{2k}\rangle$.

$c_0 \equiv \langle \psi_0 | \psi_0' \rangle = \int (\frac{m'\omega'}{\pi\hbar})^{1/4} e^{-\frac{m'\omega'}{2\hbar}x^2} \cdot (\frac{m\omega}{\pi\hbar})^{1/4} e^{-\frac{m\omega}{2\hbar}x^2}\,\mathrm{d}x$

$= [\frac{4m'\omega' m\omega}{(m'\omega'+m\omega)^2}]^{1/4} = (\frac{4\sqrt{1-(\Delta/\hbar\omega)^2}}{(\sqrt{1-\Delta/\hbar\omega}+\sqrt{1+\Delta/\hbar\omega})^2})^{1/4}$

$= [1-(\frac{\sqrt{1+\Delta/\hbar\omega}-\sqrt{1-\Delta/\hbar\omega}}{\sqrt{1-\Delta/\hbar\omega}+\sqrt{1+\Delta/\hbar\omega}})^2]^{1/4} = [1-(\frac{\Delta/\hbar\omega}{1+\sqrt{1-(\Delta/\hbar\omega)^2}})^2]^{1/4}$

Method #1:

Consider $\hat{H}'|\psi_0'\rangle = E_0'|\psi_0'\rangle$, namely

$\sum_{k=0}^{\infty}\left[\hbar\omega(2k+\frac{1}{2})c_{2k}|\psi_{2k}\rangle + \frac{\Delta}{2}c_{2k}\sqrt{(2k+2)(2k+1)}|\psi_{2k+2}\rangle + \frac{\Delta}{2}c_{2k}\sqrt{(2k)(2k-1)}|\psi_{2k-2}\rangle\right.$

$= E_0'\sum_{k=0}^{\infty} c_{2k}|\psi_{2k}\rangle$.

Therefore,

$$\hbar\omega(2k+\frac{1}{2})c_{2k} + \frac{\Delta}{2}c_{2k-2}\sqrt{(2k)(2k-1)} + \frac{\Delta}{2}c_{2k+2}\sqrt{(2k+2)(2k+1)} = E_0' c_{2k} \qquad (*)$$

$c_2 = -\frac{1}{\Delta/\sqrt{2}} \cdot c_0 \cdot (\frac{1}{2}\hbar\omega - \frac{1}{2}\hbar\omega') = -c_0 \cdot \frac{1}{\sqrt{2}} \cdot \frac{\Delta}{\hbar\omega+\hbar\omega'}$ (use $\omega^2 - \omega'^2 = \Delta^2/\hbar^2$)

$c_4 = \frac{1}{\sqrt{3}\Delta} \cdot [c_2 \cdot (\frac{1}{2}\hbar\omega' - \frac{5}{2}\hbar\omega) - \frac{\Delta}{2} \cdot \sqrt{2}c_0] = \frac{1}{\sqrt{3}\Delta} \cdot c_0 \cdot \frac{\Delta}{\sqrt{2}} \cdot \frac{\frac{3}{2}\hbar\omega - \frac{3}{2}\hbar\omega'}{\hbar\omega+\hbar\omega'} = c_0 \cdot \frac{\sqrt{3}}{\sqrt{8}} \cdot \frac{\Delta^2}{(\hbar\omega+\hbar\omega')^2}$

By mathematical induction, one can show that $c_{2k} = c_0 \cdot (-1)^k\sqrt{\frac{(2k-1)!!}{(2k)!!}} \cdot (\frac{\Delta}{\hbar\omega+\hbar\omega'})^k$.

From the $(*)$ equation,

$$c_{2k+2} = \frac{2}{\sqrt{(2k+2)(2k+1)\Delta}} \cdot [c_{2k} \cdot (\tfrac{1}{2}\hbar\omega' - (2k+\tfrac{1}{2})\hbar\omega) - \tfrac{\Delta}{2} \cdot \sqrt{(2k)(2k-1)}c_{2k-2}]$$
$$= -\frac{2}{\sqrt{(2k+2)(2k+1)\Delta}} \cdot c_{2k} \cdot [((2k+\tfrac{1}{2})\hbar\omega - \tfrac{1}{2}\hbar\omega') - \tfrac{\Delta}{2} \cdot \tfrac{\hbar\omega+\hbar\omega'}{\Delta} \cdot (2k)]$$
$$= -\frac{2}{\sqrt{(2k+2)(2k+1)\Delta}} \cdot c_{2k} \cdot \tfrac{2k+1}{2} \cdot (\hbar\omega - \hbar\omega') = -\sqrt{\tfrac{2k+1}{2k+2}(\tfrac{\Delta}{\hbar\omega+\hbar\omega'})} \cdot c_{2k}$$
$$= c_0 \cdot (-1)^{k+1}\sqrt{\tfrac{(2k+1)!!}{(2k+2)!!}} \cdot (\tfrac{\Delta}{\hbar\omega'+\hbar\omega})^{k+1}$$

(not required) As a consistency check,
$\sum_k |c_{2k}|^2 = |c_0|^2 \sum_k \frac{(2k+1)!!}{(2k+2)!!}(\frac{\Delta}{\hbar\omega'+\hbar\omega})^{2k} = |c_0|^2 \cdot [1-(\frac{\Delta}{\hbar\omega'+\hbar\omega})^2]^{-1/2} = 1$

Method #2:

use the guessed form $|\psi_0'\rangle = c_0 \exp(\alpha\hat{a}_+\hat{a}_+)|\psi_0\rangle$
$= c_0 \sum_{k=0}^{\infty} \frac{\alpha^k}{k!}(\hat{a}_+)^{2k}|\psi_0\rangle = c_0 \sum_{k=0}^{\infty} \frac{\alpha^k}{k!}\sqrt{(2k)!}|\psi_{2k}\rangle = c_0 \sum_{k=0}^{\infty}(\frac{\alpha}{2})^k \sqrt{\frac{(2k-1)!!}{(2k)!!}}|\psi_{2k}\rangle$

define ladder operators for $\hat{H}'$, $\hat{a}'_\pm = \sqrt{\frac{m'\omega'}{2\hbar}}(\hat{x} \mp \frac{\mathrm{i}}{m'\omega'}\hat{p})$, then $\hat{a}'_-|\psi_0'\rangle = 0$.

$\hat{a}'_-$ is a linear combination of $\hat{a}_\pm$,

$\hat{a}'_- = \frac{1}{2}(\sqrt{\frac{m'\omega'}{m\omega}} + \sqrt{\frac{m\omega}{m'\omega'}})\hat{a}'_- + \frac{1}{2}(\sqrt{\frac{m'\omega'}{m\omega}} - \sqrt{\frac{m\omega}{m'\omega'}})\hat{a}'_+$

define
$u = \frac{1}{2}(\sqrt{\frac{m'\omega'}{m\omega}} + \sqrt{\frac{m\omega}{m'\omega'}}) = \frac{m'\omega'+m\omega}{2\sqrt{m'\omega' m\omega}}$,
$v = \frac{1}{2}(\sqrt{\frac{m'\omega'}{m\omega}} - \sqrt{\frac{m\omega}{m'\omega'}}) = \frac{m'\omega'-m\omega}{2\sqrt{m'\omega' m\omega}}$,

Then $\hat{a}'_-|\psi_0'\rangle = (u\hat{a}_- + v\hat{a}_+)c_0 \sum_{k=0}^{\infty}(\frac{\alpha}{2})^k \sqrt{\frac{(2k-1)!!}{(2k)!!}}|\psi_{2k}\rangle$
$= c_0 \sum_{k=0}^{\infty}(\frac{\alpha}{2})^k \sqrt{\frac{(2k-1)!!}{(2k)!!}}(u\sqrt{2k}|\psi_{2k-1}\rangle + v\sqrt{2k+1}|\psi_{2k+1}\rangle)$
$= c_0 \sum_{k=0}^{\infty}(\frac{\alpha}{2})^k \sqrt{\frac{(2k+1)!!}{(2k)!!}}(\frac{\alpha}{2} \cdot u + v)|\psi_{2k+1}\rangle$

Therefore $\alpha = -2 \cdot \frac{v}{u} = -2 \cdot \frac{m'\omega'-m\omega}{m'\omega'+m\omega} = -2 \cdot \frac{\sqrt{1+\Delta/\hbar\omega}-\sqrt{1-\Delta/\hbar\omega}}{\sqrt{1+\Delta/\hbar\omega}+\sqrt{1-\Delta/\hbar\omega}}$
$= -2 \cdot \frac{2\Delta/\hbar\omega}{2+2\sqrt{1-(\Delta/\hbar\omega)^2}} = -2 \cdot \frac{\Delta}{\hbar\omega+\hbar\omega'}$

$c_n = c_0(\frac{\alpha}{2})^k \sqrt{\frac{(2k-1)!!}{(2k)!!}} = c_0(-1)^k \sqrt{\frac{(2k-1)!!}{(2k)!!}}(\frac{\Delta}{\hbar\omega+\hbar\omega'})^k$.

From $1 = \sum_k |c_{2k}|^2 = |c_0|^2 \sum_{k=0}^{\infty} \frac{(2k-1)!!}{(2k)!!}(\frac{\Delta}{\hbar\omega+\hbar\omega'})^{2k} = |c_0|^2[1-(\frac{\Delta}{\hbar\omega+\hbar\omega'})^2]^{-1/2}$, we get
$c_0 = [1-(\frac{\Delta}{\hbar\omega+\hbar\omega'})^2]^{1/4}$.

(c) $|\psi(x,t)\rangle = \sum_{k=0}^{\infty} c_{2k}e^{-\mathrm{i}E_{2k}t/\hbar}|\psi_{2k}\rangle = \sum_{k=0}^{\infty} c_{2k}e^{-\mathrm{i}(2k+\frac{1}{2})\omega t}|\psi_{2k}\rangle$,

therefore possible $\hat{H}$ measurement results are $(2k+\frac{1}{2})\hbar\omega$,
with probability $|c_{2k}|^2 = [1-(\frac{\Delta}{\hbar\omega'+\hbar\omega})^2]^{1/2}\frac{(2k+1)!!}{(2k+2)!!}(\frac{\Delta}{\hbar\omega'+\hbar\omega})^{2k}$.

(d) Obviously that $\psi(x,t)$ is an even function of x, therefore
$\langle\hat{x}\rangle = 0$ and $\langle\hat{p}\rangle = 0$ under $\psi(x,t)$.

$\hat{x}^2 = \frac{\hbar}{2m\omega}(2\hat{a}_+\hat{a}_- + 1 + \hat{a}_+\hat{a}_+ + \hat{a}_-\hat{a}_-)$,

$\hat{p}^2 = \frac{\hbar m\omega}{2}(2\hat{a}_+\hat{a}_- + 1 - \hat{a}_+\hat{a}_+ - \hat{a}_-\hat{a}_-)$,

so we just need to evaluate $\langle\psi(x,t)|2\hat{a}_+\hat{a}_- + 1|\psi(x,t)\rangle$, and $\langle\psi(x,t)|\hat{a}_+\hat{a}_+ + \hat{a}_-\hat{a}_-|\psi(x,t)\rangle$,

$\langle\psi(x,t)|2\hat{a}_+\hat{a}_- + 1|\psi(x,t)\rangle = \sum_{k=0}^{\infty}|c_{2k}|^2\cdot(2\cdot 2k+1)$

$= \langle\psi(x,t=0)|2\hat{a}_+\hat{a}_- + 1|\psi(x,t=0)\rangle = \langle\psi_0'|2\hat{a}_+\hat{a}_- + 1|\psi_-'\rangle$

from $2\hat{a}_+\hat{a}_- + 1 = \frac{2}{\hbar\omega}(\frac{\hat{p}^2}{2m} + \frac{m\omega^2}{2}\hat{x}^2)$,

and $\langle\psi_0'|\hat{x}^2|\psi_-'\rangle = \frac{\hbar}{2m'\omega'}$, $\langle\psi_0'|\hat{p}^2|\psi_-'\rangle = \frac{\hbar m'\omega'}{2}$,

we have $\langle\psi(x,t)|2\hat{a}_+\hat{a}_- + 1|\psi(x,t)\rangle = \frac{m'\omega'}{2m\omega} + \frac{m\omega}{2m'\omega'} = \frac{1}{2}(\sqrt{\frac{1+\Delta/\hbar\omega}{1-\Delta/\hbar\omega}} + \sqrt{\frac{1-\Delta/\hbar\omega}{1+\Delta/\hbar\omega}}])$

$= \frac{1}{\sqrt{1-(\Delta/\hbar\omega)^2}}$

Note that all c_{2k} are real numbers, $\langle\psi(x,t)|\hat{a}_+\hat{a}_+ + \hat{a}_-\hat{a}_-|\psi(x,t)\rangle$

$= \sum_{k=0}^{\infty}[c_{2k+2}^*\sqrt{(2k+2)(2k+1)}c_{2k}e^{2\mathrm{i}\omega t} + c_{2k}^*\sqrt{(2k+1)(2k+2)}c_{2k+2}e^{-2\mathrm{i}\omega t}]$

$= \sum_{k=0}^{\infty}2\sqrt{(2k+2)(2k+1)}c_{2k}c_{2k+2}\cos(2\omega t)$

$= \langle\psi(x,t=0)|\hat{a}_+\hat{a}_+ + \hat{a}_-\hat{a}_-|\psi(x,t=0)\rangle\cdot\cos(2\omega t) = \langle\psi_0'|\hat{a}_+\hat{a}_+ + \hat{a}_-\hat{a}_-|\psi_0'\rangle\cdot\cos(2\omega t)$

$\hat{a}_+\hat{a}_+ + \hat{a}_-\hat{a}_- = \frac{2}{\Delta}[\hat{H}' - \hbar\omega(\hat{a}_+\hat{a}_- + \frac{1}{2})]$

therefore $\langle\psi_0'|\hat{a}_+\hat{a}_+ + \hat{a}_-\hat{a}_-|\psi_0'\rangle = \frac{2}{\Delta}[\frac{\hbar\omega'}{2} - \hbar\omega(\frac{m'\omega'}{4m\omega} + \frac{m\omega}{4m'\omega'})]$

$= \frac{\hbar\omega}{\Delta}(\sqrt{1-(\Delta/\hbar\omega)^2} - \frac{1}{2}[\sqrt{\frac{1+\Delta/\hbar\omega}{1-\Delta/\hbar\omega}} + \sqrt{\frac{1-\Delta/\hbar\omega}{1+\Delta/\hbar\omega}}])$

$= \frac{\hbar\omega}{\Delta}[\sqrt{1-(\Delta/\hbar\omega)^2} - \frac{1}{\sqrt{1-(\Delta/\hbar\omega)^2}}] = -\frac{\Delta}{\hbar\omega}\cdot\frac{1}{\sqrt{1-(\Delta/\hbar\omega)^2}}$

Finally,

$\langle\psi(x,t)|\hat{x}^2|\psi(x,t)\rangle = \frac{\hbar}{2m\omega}\frac{1}{\sqrt{1-(\Delta/\hbar\omega)^2}}[1 - \frac{\Delta}{\hbar\omega}\cos(2\omega t)]$,

$\langle\psi(x,t)|\hat{p}^2|\psi(x,t)\rangle = \frac{\hbar m\omega}{2}\frac{1}{\sqrt{1-(\Delta/\hbar\omega)^2}}[1 + \frac{\Delta}{\hbar\omega}\cos(2\omega t)]$,

The uncertainty relation is still satisfied,

$\sigma_x^2\cdot\sigma_p^2 = \langle\hat{x}^2\rangle\cdot\langle\hat{p}^2\rangle = \frac{\hbar^2}{4}\frac{1}{1-(\Delta/\hbar\omega)^2}[1 - (\frac{\Delta}{\hbar\omega})^2\cos^2(2\omega t)]$

$\geq \frac{\hbar^2}{4}\frac{1}{1-(\Delta/\hbar\omega)^2}[1 - (\frac{\Delta}{\hbar\omega})^2] = \frac{\hbar^2}{4}$