Quantum Mechanics: Fall 2018
Midterm Exam: Brief Solutions

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

Some useful facts:

- 1D harmonic oscillator: $\hat{H} = \frac{\hat{p}^2}{2m} + \frac{m\omega^2}{2}\hat{x}^2 = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{m\omega^2}{2}x^2$.
  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 $a > 0$.

- 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 azimuthal angular momentum quantum number; E is the energy eigenvalue.

  - The spherical harmonics are orthonormal, and are eigenfunctions of $\hat{\boldsymbol{L}}^2$ and $\hat{L}_z$.
    $Y_0^0 = \frac{1}{\sqrt{4\pi}}$, $Y_1^0 = \sqrt{\frac{3}{4\pi}}\cos\theta$, $Y_1^{\pm1} = \mp\sqrt{\frac{3}{8\pi}}\sin\theta e^{\pm\mathbb{i}\phi}$, ...

- 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 $(\hat{J}_x \pm \mathbb{i}\hat{J}_y)|j,m\rangle = \sqrt{(j\mp m)(j\pm m+1)}\hbar|j,m\pm1\rangle$.
  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.
    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. (45 points) Consider the 1D harmonic oscillator $\hat{H} = \frac{\hat{p}^2}{2m} + \frac{m\omega^2\hat{x}^2}{2}$.

(a) (5pts) Define observables $\hat{X} = \cos(\theta)\cdot\hat{x} + \sin(\theta)\cdot\frac{\hat{p}}{m\omega}$, $\hat{P} = \cos(\theta)\cdot\hat{p} - \sin(\theta)\cdot m\omega\hat{x}$. Here θ is a real number. *Compute the commutator* $[\hat{X},\hat{P}]$. *Rewrite* $\hat{H}$ *in terms of* $\hat{X}$ *and* $\hat{P}$.

(b) (15pts) Set the initial wavefunction to be $\varphi(x,t=0) = A\cdot\hat{X}\psi_1(x)$. *Solve the normalization constant* A *and the explicit form of this wavefunction. Expand* $\varphi(x,t=0) = \sum_{n=0}^{\infty} c_n\psi_n(x)$, *solve the coefficients* c_n. *Write down the wavefunction* $\varphi(x,t)$ *at time* t. Here ψ_n is the eigenstate of $\hat{H}$ defined on page 1. [Hint: use ladder operators]

(c) (5pts) Measure energy (namely $\hat{H}$) under $\varphi(x,t)$. *What are the possible measurement results and their probabilities?*

(d) (20pts) *Compute the expectation values* $\langle\hat{X}\rangle$, $\langle\hat{P}\rangle$, $\langle\hat{X}^2\rangle$, $\langle\hat{P}^2\rangle$ *in the state* $\varphi(x,t)$. *Check that the uncertainty principle for* $\hat{X},\hat{P}$ *is satisfied, namely* $(\langle\hat{X}^2\rangle - \langle\hat{X}\rangle^2)(\langle\hat{P}^2\rangle - \langle\hat{P}\rangle^2) \geq \frac{1}{4}|\langle[\hat{X},\hat{P}]\rangle|^2$. [Hint: use ladder operators]

Solution: this is essentially the same as Midterm Problem 1 of last year.

(a)

$[\hat{X},\hat{P}] = (\cos\theta)^2[\hat{x},\hat{p}] + (\sin\theta\cdot\cos\theta)\frac{1}{m\omega}[\hat{p},\hat{p}] - (\cos\theta\cdot\sin\theta)m\omega[\hat{x},\hat{x}] - (\sin\theta)^2\frac{1}{m\omega}m\omega[\hat{p},\hat{x}]$

$[\hat{X},\hat{P}] = \mathrm{i}\hbar$

Invert these relations, $\hat{x} = \hat{X}\cos\theta - \frac{1}{m\omega}\hat{P}\sin\theta$, $\hat{p} = \hat{P}\cos\theta + m\omega\hat{X}\sin\theta$.

$\hat{H} = \frac{1}{2m}\hat{P}^2 + \frac{m\omega^2}{2}\hat{X}^2$

(b)

$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}(\hat{a}_- + \hat{a}_+)$, $\hat{p} = -\mathrm{i}\sqrt{\frac{\hbar m\omega}{2}}(\hat{a}_- - \hat{a}_+)$. Then

$\hat{X} = \sqrt{\frac{\hbar}{2m\omega}}(e^{-\mathrm{i}\theta}\hat{a}_- + e^{\mathrm{i}\theta}\hat{a}_+)$, $\hat{P} = -\mathrm{i}\sqrt{\frac{\hbar m\omega}{2}}(e^{-\mathrm{i}\theta}\hat{a}_- - e^{\mathrm{i}\theta}\hat{a}_+)$

$\psi_1(x) = \hat{a}_+\psi_0(x) = (\frac{m\omega}{\hbar\pi})^{1/4}\frac{\sqrt{2}x}{\sqrt{\hbar/m\omega}}\exp(-\frac{x^2}{2\hbar/m\omega})$

$\psi_2(x) = \frac{1}{\sqrt{2!}}(\hat{a}_+)^2\psi_0(x) = \frac{1}{\sqrt{2}}\hat{a}_+\psi_1(x) = (\frac{m\omega}{\hbar\pi})^{1/4}\frac{1}{\sqrt{2}}(\frac{2x^2}{\hbar/m\omega} - 1)\exp(-\frac{x^2}{2\hbar/m\omega})$

$\psi(x,t=0) = A\cdot\sqrt{\frac{\hbar}{2m\omega}}(e^{-\mathrm{i}\theta}\hat{a}_- + e^{\mathrm{i}\theta}\hat{a}_+)\cdot\hat{a}_+\psi_0 = A\sqrt{\frac{\hbar}{2m\omega}}\cdot(e^{-\mathrm{i}\theta}\psi_0 + e^{\mathrm{i}\theta}\sqrt{2}\psi_2)$

Here we have used $\hat{a}_-\hat{a}_+\psi_0 = (1+\hat{a}_+\hat{a}_-)\psi_0 = \psi_0$.

Then $|A|^2\frac{\hbar}{2m\omega}\cdot(1+2) = 1$, we can choose $A = \sqrt{\frac{2m\omega}{3\hbar}}$.

$\psi(x,t=0) = \sqrt{\frac{1}{3}}(\frac{m\omega}{\hbar\pi})^{1/4}(e^{\mathrm{i}\theta}\frac{2x^2}{h/m\omega} + (e^{-\mathrm{i}\theta} - e^{\mathrm{i}\theta}))\exp(-\frac{x^2}{2\hbar/m\omega})$.

$c_0 = \sqrt{\frac{1}{3}}e^{-\mathrm{i}\theta}$, $c_2 = \sqrt{\frac{2}{3}}e^{\mathrm{i}\theta}$, other $c_n = 0$.

$\psi(x,t) = \sum_n c_n e^{-\mathrm{i}E_n t/\hbar}\psi_n(x) = \sqrt{\frac{1}{3}}e^{-\mathrm{i}\theta}e^{-\mathrm{i}\omega t/2}\psi_0(x) + \sqrt{\frac{2}{3}}e^{-\mathrm{i}\theta}e^{-\mathrm{i}\cdot 5\omega t/2}\psi_2(x)$

$= \sqrt{\frac{1}{3}}(\frac{m\omega}{\hbar\pi})^{1/4}(e^{\mathrm{i}\theta}e^{-\mathrm{i}\cdot 5\omega t/2}\frac{2x^2}{h/m\omega} + (e^{-\mathrm{i}\theta}e^{-\mathrm{i}\omega t/2} - e^{\mathrm{i}\theta}e^{-\mathrm{i}\cdot 5\omega t/2}))\exp(-\frac{x^2}{2\hbar/m\omega})$

(c)

$E_0 = \frac{\hbar\omega}{2}$ with probability $|c_0|^2 = \frac{1}{3}$;

$E_2 = \frac{5\hbar\omega}{2}$ with probability $|c_2|^2 = \frac{2}{3}$.

(d)

$\langle\hat{X}\rangle = 0$, $\langle\hat{P}\rangle = 0$.

This can be seen from the fact that $\psi(x,t)$ is an even function of x and $\hat{X}$ and $\hat{P}$ are odd, or that $\hat{X}\psi(x,t)$ and $\hat{P}\psi(x,t)$ will contain only ψ_1 and ψ_3 eigenbasis states.

$\hat{X}^2 = \frac{\hbar}{2m\omega}(e^{-\mathrm{i}\theta}\hat{a}_- + e^{\mathrm{i}\theta}\hat{a}_+)^2 = \frac{\hbar}{2m\omega}(e^{-2\mathrm{i}\theta}\hat{a}_-^2 + e^{2\mathrm{i}\theta}\hat{a}_+^2 + 2\hat{a}_+\hat{a}_- + 1)$,

$\hat{P}^2 = -\frac{\hbar m\omega}{2}(e^{-\mathrm{i}\theta}\hat{a}_- - e^{\mathrm{i}\theta}\hat{a}_+)^2 = \frac{\hbar m\omega}{2}(-e^{-2\mathrm{i}\theta}\hat{a}_-^2 - e^{2\mathrm{i}\theta}\hat{a}_+^2 + 2\hat{a}_+\hat{a}_- + 1)$. Then,

$\langle\hat{X}^2\rangle = \frac{\hbar}{2m\omega}\cdot\Big($

$+e^{-2\mathrm{i}\theta}(\sqrt{\frac{1}{3}}e^{-\mathrm{i}\theta}e^{-\mathrm{i}\omega t/2})^*\sqrt{2}(\sqrt{\frac{2}{3}}e^{\mathrm{i}\theta}e^{-\mathrm{i}5\omega t/2})$ $+e^{2\mathrm{i}\theta}(\sqrt{\frac{2}{3}}e^{\mathrm{i}\theta}e^{-\mathrm{i}5\omega t/2})^*\sqrt{2}(\sqrt{\frac{1}{3}}e^{-\mathrm{i}\theta}e^{-\mathrm{i}\omega t/2})$

$+(\sqrt{\frac{1}{3}}e^{-\mathrm{i}\theta}e^{-\mathrm{i}\omega t/2})^*\cdot 1\cdot(\sqrt{\frac{1}{3}}e^{-\mathrm{i}\theta}e^{-\mathrm{i}\omega t/2}) + (\sqrt{\frac{2}{3}}e^{\mathrm{i}\theta}e^{-\mathrm{i}5\omega t/2})^*\cdot 5\cdot(\sqrt{\frac{2}{3}}e^{\mathrm{i}\theta}e^{-\mathrm{i}5\omega t/2})\ \Big)$

$= \frac{\hbar}{2m\omega}\cdot(\frac{11}{3} + \frac{4}{3}\cos(2\omega t))$

$\langle\hat{P}^2\rangle = \frac{\hbar m\omega}{2}\cdot\Big($

$-e^{-2\mathrm{i}\theta}(\sqrt{\frac{1}{3}}e^{-\mathrm{i}\theta}e^{-\mathrm{i}\omega t/2})^*\sqrt{2}(\sqrt{\frac{2}{3}}e^{\mathrm{i}\theta}e^{-\mathrm{i}5\omega t/2})$ $-e^{2\mathrm{i}\theta}(\sqrt{\frac{2}{3}}e^{\mathrm{i}\theta}e^{-\mathrm{i}5\omega t/2})^*\sqrt{2}(\sqrt{\frac{1}{3}}e^{-\mathrm{i}\theta}e^{-\mathrm{i}\omega t/2})$

$+(\sqrt{\frac{1}{3}}e^{-\mathrm{i}\theta}e^{-\mathrm{i}\omega t/2})^*\cdot 1\cdot(\sqrt{\frac{1}{3}}e^{-\mathrm{i}\theta}e^{-\mathrm{i}\omega t/2}) + (\sqrt{\frac{2}{3}}e^{\mathrm{i}\theta}e^{-\mathrm{i}5\omega t/2})^*\cdot 5\cdot(\sqrt{\frac{2}{3}}e^{\mathrm{i}\theta}e^{-\mathrm{i}5\omega t/2})\ \Big)$

$= \frac{\hbar m\omega}{2}\cdot(\frac{11}{3} - \frac{4}{3}\cos(2\omega t))$

Here we have used $\hat{a}_+\hat{a}_-\psi_0 = 0$, $\hat{a}_+\hat{a}_-\psi_2 = 2\psi_2$ (check $\hat{H}$ eigenvalues), $\hat{a}_+^2\psi_0 = \sqrt{2}\psi_2$ (by definition), and $\hat{a}_-^2\psi_2 = \frac{1}{\sqrt{2}}\hat{a}_-^2\hat{a}_+^2\psi_0 = \frac{1}{\sqrt{2}}\hat{a}_-\cdot([\hat{a}_-,\hat{a}_+]\hat{a}_+ + \hat{a}_+[\hat{a}_-,\hat{a}_+] + \hat{a}_+^2\hat{a}_-)\psi_0$ $= \frac{1}{\sqrt{2}}\cdot 2\hat{a}_-\hat{a}_+\psi_0 = \frac{1}{\sqrt{2}}\cdot 2(\hat{a}_+\hat{a}_- + 1)\psi_0 = \sqrt{2}\psi_0$.

Finally, $(\langle\hat{X}^2\rangle - \langle\hat{X}\rangle^2)(\langle\hat{P}^2\rangle - \langle\hat{P}\rangle^2) = \frac{\hbar^2}{4}[(\frac{11}{3})^2 - (\frac{4}{3})^2\cos^2(2\omega t)] \geq \frac{\hbar^2}{4}[(\frac{11}{3})^2 - (\frac{4}{3})^2]$ $> \frac{1}{4}|\langle[\hat{X},\hat{P}]\rangle|^2 = \frac{\hbar^2}{4}$.

Note: these results can in principle be obtained by directly computing integrals (omitted).

Problem 2. (15 points) Consider the 1D infinite square potential well with a repulsive δ-function potential in the center, $\hat{H} = \frac{\hat{p}^2}{2m} + \alpha \cdot \delta(x) + V(x)$, with $V(x) = \begin{cases} +\infty, & |x| > L; \\ 0, & |x| < L. \end{cases}$ Here α, L are positive constants.

(a) (10pts) *Draw qualitatively the wavefunctions for the ground state, first excited state, and second excited state. What can you say about the properties of these wavefunctions?*

(b) (5pts) *Derive the equations for energy eigenvalues.* Note: you will not be able to solve all the eigenvalues.

Solution

(a)

qualitative features:

eigenstate wavefunctions vanish for $|x| \geq L$ (1pt),

ground state is an even function without node in $|x| < L$ (2pts),

1st excited state is an odd function with only one node in $|x| < L$ (2pts),

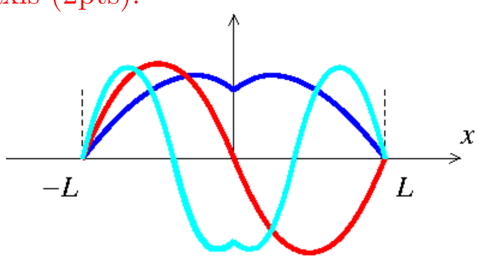
2nd excited state is an even function with two nodes in $|x| < L$ (2pts),

1st excited state is smooth in $|x| < L$, same as the case without δ-function potential (1pt),

ground state and 2nd excited state wavefunctions are continuous in $|x| < L$, but has discontinuous derivative at $x = 0$, a "cusp" pointing toward x-axis (2pts).

Schematic picture of the wavefunctions in $|x| < L$,

for ground state, 1st excited state, 2nd excited state,



(b)

Label the states by $n = 0, 1, \ldots$ in ascending order of energy. Then $E_n = \frac{\hbar^2}{2m} k_n^2$, where k_n is the wavevector in $V(x) = 0$ regions.

For odd n, the n-th excited states are the same as those without the δ-function potential,

$$\psi_n(x) = \begin{cases} 0, & |x| > L; \\ \frac{1}{\sqrt{L}} \cdot \sin(\frac{(n+1)\pi}{2L}(L+x)), & -L < x < L. \end{cases}, \text{ with } k_n = \frac{(n+1)\pi}{2L},\ E_n = \frac{\hbar}{2m}(\frac{(n+1)\pi}{2L})^2.$$

For even n, the eigenstate functions are $\psi_n(x) = \begin{cases} 0, & |x| > L; \\ A_n \cdot \sin(k_n \cdot (L+x)), & -L < x < 0; \\ A_n \cdot \sin(k_n \cdot (L-x)), & 0 < x < L. \end{cases}$

The boundary condition at $x = 0$ produces $-\frac{\hbar^2}{2m}\partial_x \psi_n|_{x=-0}^{+0} + \alpha\psi_n(0) = 0$, or $\frac{\hbar^2}{m}k_n \cdot \cos(k_n L) + \alpha \sin(k_n L) = 0$, or $-\frac{\hbar^2}{mL\alpha} = \frac{\tan(k_n L)}{k_n L}$. The solution to these k_n for even n will be between $\frac{(n+1)\pi}{2L}$ and $\frac{(n+2)\pi}{2L}$, larger than the case without δ-function potential.

Problem 3. (40 points) Consider a 3D harmonic oscillator $\hat{H} = \frac{1}{2m}\hat{\boldsymbol{p}}^2 + \frac{m\omega^2}{2}\hat{\boldsymbol{r}}^2$. Here m, ω are positive constants. It can be views as three copies of independent 1D harmonic oscillators, $\hat{H} = (\frac{\hat{p}_x^2}{2m} + \frac{m\omega^2\hat{x}^2}{2}) + (\frac{\hat{p}_y^2}{2m} + \frac{m\omega^2\hat{y}^2}{2}) + (\frac{\hat{p}_z^2}{2m} + \frac{m\omega^2\hat{z}^2}{2})$. Define ladder operators, $\hat{a}_{i,\pm} = \sqrt{\frac{m\omega}{2\hbar}}(\hat{r}_i \mp \mathbb{i}\frac{\hat{p}_i}{m\omega})$, for $i = x, y, z$ respectively. Then $[\hat{a}_{i,-}, \hat{a}_{j,+}] = \delta_{i,j}$. $\hat{H}$ has a unique normalized ground state $\varphi_0(\boldsymbol{r})$, satisfying $\hat{a}_{i,-}\varphi_0 = 0$. The first excited states are 3-fold degenerate, their orthonormal wavefunctions are $\varphi_{1,x} = \hat{a}_{x,+}\varphi_0$, $\varphi_{1,y} = \hat{a}_{y,+}\varphi_0$, $\varphi_{1,z} = \hat{a}_{z,+}\varphi_0$.

(a) (5pts) *Write down the wavefunctions of φ_0, $\varphi_{1,x}$, $\varphi_{1,y}$, $\varphi_{1,z}$ in terms of Cartesian coordinates x, y, z.*

(b) (15pts) *Evaluate the matrix elements of the orbital angular momentum operators $\hat{L}_x$, $\hat{L}_y$, $\hat{L}_z$ between the three states $\varphi_{1,x}$, $\varphi_{1,y}$, $\varphi_{1,z}$, namely $(L_k)_{ij} \equiv \langle\varphi_{1,i}|\hat{L}_k|\varphi_{1,j}\rangle$ for $i, j, k = x, y, z$. Check that the three 3×3 matrices L_k satisfy the commutation relation between angular momentum operators.* [Hint: act the operators on the states and represent the results as linear combinations, computation may be simplified by cyclic permutations of x, y, z]

(c) (5pts) $\hat{H}$, $\hat{\boldsymbol{L}}^2$, $\hat{L}_z$ mutually commute. *Find normalized linear combinations of φ_0, $\varphi_{1,x}$, $\varphi_{1,y}$, $\varphi_{1,z}$, so that they are simultaneous eigenstates of $\hat{H}$, $\hat{\boldsymbol{L}}^2$ and $\hat{L}_z$. Write down the corresponding eigenvalues.* [Hint: rewrite the states in terms of spherical harmonics]

(d) (5pts) Consider a spin-$\frac{1}{2}$ particle with spinor wavefunction $\psi(\boldsymbol{r}) \equiv \begin{pmatrix} \psi_\uparrow(\boldsymbol{r}) \\ \psi_\downarrow(\boldsymbol{r}) \end{pmatrix}$ (see page 1). Suppose $\psi_\uparrow$ and $\psi_\downarrow$ are linear combinations of φ_0, $\varphi_{1,x}$, $\varphi_{1,y}$, $\varphi_{1,z}$. Define the total angular momentum $\hat{\boldsymbol{J}} = \hat{\boldsymbol{L}} + \hat{\boldsymbol{S}}$. Then $\hat{\boldsymbol{J}}^2$ and $\hat{\boldsymbol{L}}^2$ and $\hat{J}_z$ mutually commute, and can have simultaneous eigenstate $\psi_{j,\ell,m}$ with eigenvalues $j(j+1)\hbar^2$ and $\ell(\ell+1)\hbar^2$ and $m\hbar$, respectively. *What are the possible total angular momentum quantum number j?*

(e) (10pts) *For the lowest possible j in (d), write down all the normalized spinor wavefunction $\psi_{j,\ell,m}$, in terms of φ_0, $\varphi_{1,x}$, $\varphi_{1,y}$, $\varphi_{1,z}$.*

Solution

(a)

Use separation of variable in the Cartesian coordinates, and previous result for $\psi_1 = \hat{a}_+\psi_0$,

$\varphi_0 = \psi_0(x)\psi_0(y)\psi_0(z) = (\frac{m\omega}{\hbar\pi})^{3/4}\exp(-\frac{x^2+y^2+z^2}{2\hbar/m\omega})$,

$\varphi_{1,x} = \psi_1(x)\psi_0(y)\psi_0(z) = (\frac{m\omega}{\hbar\pi})^{3/4}\frac{\sqrt{2}x}{\sqrt{\hbar/m\omega}}\exp(-\frac{x^2+y^2+z^2}{2\hbar/m\omega})$,

$\varphi_{1,y} = \psi_0(x)\psi_1(y)\psi_0(z) = (\frac{m\omega}{\hbar\pi})^{3/4}\frac{\sqrt{2}y}{\sqrt{\hbar/m\omega}}\exp(-\frac{x^2+y^2+z^2}{2\hbar/m\omega})$,

$\varphi_{1,z} = \psi_0(x)\psi_0(y)\psi_1(z) = (\frac{m\omega}{\hbar\pi})^{3/4}\frac{\sqrt{2}z}{\sqrt{\hbar/m\omega}}\exp(-\frac{x^2+y^2+z^2}{2\hbar/m\omega})$,

(b)

You can directly apply $\hat{L}_x = -\mathbb{i}\hbar(y\partial_z - z\partial_y)$, $\hat{L}_y = -\mathbb{i}\hbar(z\partial_x - x\partial_z)$, $\hat{L}_z = -\mathbb{i}\hbar(x\partial_y - y\partial_x)$, on the results of (a), note that the orbital angular momentum operator is independent of radius $r = \sqrt{x^2+y^2+z^2}$, so you can just apply these operators on the prefactors in front of $\exp(-\frac{r^2}{2\hbar/m\omega})$.

Or you can rewrite $\hat{L}_{x,y,z}$ into ladder operators, $\hat{L}_x = \hbar(-\mathbb{i}\hat{a}_{y,+}\hat{a}_{z,-} + \mathbb{i}\hat{a}_{z,+}\hat{a}_{y,-})$, $\hat{L}_y = \hbar(-\mathbb{i}\hat{a}_{z,+}\hat{a}_{x,-} + \mathbb{i}\hat{a}_{x,+}\hat{a}_{z,-})$, $\hat{L}_z = \hbar(-\mathbb{i}\hat{a}_{x,+}\hat{a}_{y,-} + \mathbb{i}\hat{a}_{y,+}\hat{a}_{x,-})$, and use $\hat{a}_{i,-}\psi_n(r_i) = \sqrt{n}\psi_{n-1}(r_i)$, and $\hat{a}_{i,+}\psi_n(r_i) = \sqrt{n+1}\psi_{n+1}(r_i)$, for $i = x, y, z$.

Under the basis of $\varphi_{1,x}$, $\varphi_{1,y}$, $\varphi_{1,z}$,

$$L_x = \hbar\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -\mathbb{i} \\ 0 & \mathbb{i} & 0 \end{pmatrix}, L_y = \hbar\begin{pmatrix} 0 & 0 & \mathbb{i} \\ 0 & 0 & 0 \\ -\mathbb{i} & 0 & 0 \end{pmatrix}, L_z = \hbar\begin{pmatrix} 0 & -\mathbb{i} & 0 \\ \mathbb{i} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

It is straightforward to check that they satisfy the commutation relations between angular momentum operators (steps omitted).

(c)

	$\hat{H}$	$\hat{\boldsymbol{L}}^2$	$\hat{L}_z$
$\varphi_{\ell=0,\ell_z=0} = \varphi_0 = \sqrt{4\pi}(\frac{m\omega}{\hbar\pi})^{3/4} \cdot Y_0^0(\theta,\phi) \cdot e^{-\frac{r^2}{2\hbar/m\omega}}$	$\hbar\omega \cdot \frac{3}{2}$	0	0
$\varphi_{\ell=1,\ell_z=0} = \varphi_{1,z} = \sqrt{\frac{4\pi}{3}}(\frac{m\omega}{\hbar\pi})^{3/4} \cdot Y_1^0(\theta,\phi) \cdot \frac{\sqrt{2}r}{\sqrt{h/m\omega}} e^{-\frac{r^2}{2\hbar/m\omega}}$	$\hbar\omega \cdot \frac{5}{2}$	$2\hbar^2$	0
$\varphi_{\ell=1,\ell_z=+1} = \frac{1}{\sqrt{2}}(-\varphi_{1,x} - \mathbb{i}\varphi_{1,y}) = \sqrt{\frac{4\pi}{3}}(\frac{m\omega}{\hbar\pi})^{3/4} \cdot Y_1^1(\theta,\phi) \cdot \frac{\sqrt{2}r}{\sqrt{h/m\omega}} e^{-\frac{r^2}{2\hbar/m\omega}}$	$\hbar\omega \cdot \frac{5}{2}$	$2\hbar^2$	$\hbar$
$\varphi_{\ell=1,\ell_z=-1} = \frac{1}{\sqrt{2}}(\varphi_{1,x} - \mathbb{i}\varphi_{1,y}) = \sqrt{\frac{4\pi}{3}}(\frac{m\omega}{\hbar\pi})^{3/4} \cdot Y_1^{-1}(\theta,\phi) \cdot \frac{\sqrt{2}r}{\sqrt{h/m\omega}} e^{-\frac{r^2}{2\hbar/m\omega}}$	$\hbar\omega \cdot \frac{5}{2}$	$2\hbar^2$	$-\hbar$

NOTE: be careful that $Y_1^1(\theta,\phi) = -\sqrt{\frac{3}{8\pi}}\sin\theta \cdot e^{\mathbb{i}\phi}$ (see page 1), in order to conform with the Condon-Shortley convention. This is important later in (e).

You can also diagonalize the L_z matrix in (b) to get the last two states. Note that there $L_x^2 + L_y^2 + L_z^2 = 2\hbar^2 \mathbb{1}_{3\times 3}$, which means $\varphi_{1,i}$ are eigenstates of $\hat{\boldsymbol{L}}^2$ with eigenvalue $2\hbar^2$. The phases of these states can be fixed by the Condon-Shortley convention, and the fact that $L_+ = L_x + \mathbb{i}L_y = \begin{pmatrix} 0 & 0 & -1 \\ 0 & 0 & -\mathbb{i} \\ 1 & \mathbb{i} & 0 \end{pmatrix}$ under the $\varphi_{1,i}$ basis.

(d) ℓ quantum number is 0 for φ_0 state, the j quantum number can be $\frac{1}{2}$;
ℓ quantum number is 1 for $\varphi_{1,i}$ states, the j quantum number can be $\frac{1}{2}$ and $\frac{3}{2}$.

(e) for $\ell = 0$ and $j = \frac{1}{2}$ case,

$$\psi_{j=\frac{1}{2},\ell=0,m=+\frac{1}{2}} = \varphi_{\ell=0,\ell_z=0}|\uparrow\rangle = \begin{pmatrix} \varphi_0 \\ 0 \end{pmatrix}, \ \psi_{j=\frac{1}{2},\ell=0,m=-\frac{1}{2}} = \varphi_{\ell=0,\ell_z=0}|\downarrow\rangle = \begin{pmatrix} 0 \\ \varphi_0 \end{pmatrix},$$

for $\ell = 1$ and $j = \frac{1}{2}$ case,
let $\psi_{j=\frac{1}{2},\ell=1,m=+\frac{1}{2}} = c_1\varphi_{\ell=1,\ell_z=0}|\uparrow\rangle + c_2\varphi_{\ell=1,\ell_z=1}|\downarrow\rangle$, apply $\hat{J}_+ = \hat{L}_+ + \hat{S}_+$ on it, the result should vanish, then we have $c_1 \cdot (\sqrt{2}\varphi_{\ell=1,\ell_z=1}|\uparrow\rangle + 0) + c_2 \cdot (0 + \varphi_{\ell=1,\ell_z=1}|\uparrow\rangle) = 0$, or $\sqrt{2}c_1 + c_2 = 0$. Note that here we have used the Condon-Shortley convention for the ladder operators, so we must get the relative phases between $\varphi_{\ell=1,\ell_z}$ correctly in (c).

We can choose $c_1 = \sqrt{\frac{1}{3}}$ and $c_2 = -\sqrt{\frac{2}{3}}$,

$$\psi_{j=\frac{1}{2},\ell=1,m=+\frac{1}{2}} = \sqrt{\frac{1}{3}}\varphi_{\ell=1,\ell_z=0}|\uparrow\rangle - \sqrt{\frac{2}{3}}\varphi_{\ell=1,\ell_z=1}|\downarrow\rangle = \frac{1}{\sqrt{3}}\begin{pmatrix} \varphi_{1,z} \\ \varphi_{1,x} + \mathbb{i}\varphi_{1,y} \end{pmatrix}.$$

apply $\hat{J}_- = \hat{L}_- + \hat{S}_-$ on $\psi_{j=\frac{1}{2},\ell=1,m=+\frac{1}{2}}$, we get

$$\psi_{j=\frac{1}{2},\ell=1,m=-\frac{1}{2}} = \sqrt{\frac{2}{3}}\varphi_{\ell=1,\ell_z=-1}|\uparrow\rangle - \sqrt{\frac{1}{3}}\varphi_{\ell=1,\ell_z=0}|\downarrow\rangle = \frac{1}{\sqrt{3}}\begin{pmatrix} \varphi_{1,x} - \mathbb{i}\varphi_{1,y} \\ -\varphi_{1,z} \end{pmatrix}.$$

Method #2: brute-force diagonalization for the $\ell = 1$ case,

under the $\varphi_{1,x}|\uparrow\rangle$, $\varphi_{1,x}|\downarrow\rangle$, $\varphi_{1,y}|\uparrow\rangle$, $\varphi_{1,y}|\downarrow\rangle$, $\varphi_{1,z}|\uparrow\rangle$, $\varphi_{1,z}|\downarrow\rangle$, basis,

$$\hat{\boldsymbol{J}}^2 = \hat{\boldsymbol{L}}^2 \otimes \mathbb{1}_S + \mathbb{1}_L \otimes \hat{\boldsymbol{S}}^2 + 2\sum_{i=x,y,z} \hat{L}_i \otimes \hat{S}_i = \hbar^2 \begin{pmatrix} \frac{11}{4} & 0 & -\mathrm{i} & 0 & 0 & 1 \\ 0 & \frac{11}{4} & 0 & \mathrm{i} & -1 & 0 \\ \mathrm{i} & 0 & \frac{11}{4} & 0 & 0 & -\mathrm{i} \\ 0 & -\mathrm{i} & 0 & \frac{11}{4} & -\mathrm{i} & 0 \\ 0 & -1 & 0 & \mathrm{i} & \frac{11}{4} & 0 \\ 1 & 0 & \mathrm{i} & 0 & 0 & \frac{11}{4} \end{pmatrix}.$$

The matrix elements in cyan, blue, red, are from $\hat{L}_x \otimes \hat{S}_x$, $\hat{L}_y \otimes \hat{S}_y$, $\hat{L}_z \otimes \hat{S}_z$, respectively.

This is actually two decoupled 3×3 matrices, rearrange the basis into $\varphi_{1,x}|\uparrow\rangle$, $\varphi_{1,y}|\uparrow\rangle$, $\varphi_{1,z}|\downarrow\rangle$, $\varphi_{1,x}|\downarrow\rangle$, $\varphi_{1,y}|\downarrow\rangle$, $\varphi_{1,z}|\uparrow\rangle$, this matrix becomes

$$\hbar^2 \begin{pmatrix} \frac{11}{4} & -\mathrm{i} & 1 & 0 & 0 & 0 \\ \mathrm{i} & \frac{11}{4} & -\mathrm{i} & 0 & 0 & 0 \\ 1 & \mathrm{i} & \frac{11}{4} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{11}{4} & \mathrm{i} & -1 \\ 0 & 0 & 0 & -\mathrm{i} & \frac{11}{4} & -\mathrm{i} \\ 0 & 0 & 0 & -1 & \mathrm{i} & \frac{11}{4} \end{pmatrix}.$$

We just need to find out the normalized eigenvectors corresponding to eigenvalue $\frac{3}{4}\hbar^2$. This eigenvector for the top-left 3×3 block is the null vector for $\begin{pmatrix} 2 & -\mathrm{i} & 1 \\ \mathrm{i} & 2 & -\mathrm{i} \\ 1 & \mathrm{i} & 2 \end{pmatrix}$, which is proportional to the minors for the elements of the top row, $\begin{pmatrix} 2\cdot 2 - (-\mathrm{i})\cdot \mathrm{i} \\ -(\mathrm{i}\cdot 2 - (-\mathrm{i})\cdot 1) \\ \mathrm{i}\cdot\mathrm{i} - 2\cdot 1 \end{pmatrix} = \begin{pmatrix} 3 \\ -3\mathrm{i} \\ -3 \end{pmatrix}$. This corresponds to the $\psi_{j=\frac{1}{2},\ell=1,m=-\frac{1}{2}}$ state.

The eigenvector for the bottom-right 3×3 block can be obtained in similar way, which corresponds to the $\psi_{j=\frac{1}{2},\ell=1,m=+\frac{1}{2}}$ state.