Quantum Mechanics: Fall 2023
Midterm Exam: Brief Solutions

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

Some useful facts: You can use them directly.

- Heisenberg equations of motion: $\frac{\mathrm{d}}{\mathrm{d}t}\langle\hat{O}\rangle = \langle\frac{\partial\hat{O}}{\partial t}\rangle + \frac{\mathrm{i}}{\hbar}\langle[\hat{H},\hat{O}]\rangle$.
- 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, $[\hat{x},\hat{p}] = \mathrm{i}\hbar$, and in position representation $\hat{p} = -\mathrm{i}\hbar\frac{\partial}{\partial x}$. Define $\hat{a}_{\mp} = \sqrt{\frac{m\omega}{2\hbar}}(\hat{x} \pm \mathrm{i}\frac{1}{m\omega}\hat{p}) = \sqrt{\frac{m\omega}{2\hbar}}(x \pm \frac{\hbar}{m\omega}\frac{\partial}{\partial x})$. Then $[\hat{a}_-,\hat{a}_+] = 1$ and $\hat{H} = \hbar\omega\,(\hat{a}_+\hat{a}_- + \frac{1}{2})$. It has a unique ground state $|\psi_0\rangle$ with $\hat{a}_-|\psi_0\rangle = 0$, and excited states $|\psi_n\rangle \equiv \frac{1}{\sqrt{n!}}(\hat{a}_+)^n|\psi_0\rangle$ with energy $E_n = (n+\frac{1}{2})\hbar\omega$. The ground state wavefunction is $\psi_0(x) = (\frac{m\omega}{\pi\hbar})^{1/4}\exp(-\frac{m\omega}{2\hbar}x^2)$.
- $\int_{-\infty}^{+\infty} e^{-x^2/a}\mathrm{d}x = \sqrt{\pi a}$, 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 $-\mathrm{i}\hbar\frac{\partial}{\partial\boldsymbol{r}}$, 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 $\hat{L}_z$. $Y_0^0 = \frac{1}{\sqrt{4\pi}}$, $Y_1^0 = \sqrt{\frac{3}{4\pi}}\cos\theta$, $Y_1^{\pm1} = \mp\sqrt{\frac{3}{8\pi}}\sin\theta e^{\pm\mathrm{i}\phi}$, ...
- Generic angular momentum: $[\hat{J}_x,\hat{J}_y] = \mathrm{i}\hbar\hat{J}_z$, $[\hat{J}_y,\hat{J}_z] = \mathrm{i}\hbar\hat{J}_x$, $[\hat{J}_z,\hat{J}_x] = \mathrm{i}\hbar\hat{J}_y$.
  For eigenstate $|j,m\rangle$ of $\hat{\boldsymbol{J}}^2$ and $\hat{J}_z$, $\hat{\boldsymbol{J}}^2|j,m\rangle = j(j+1)\hbar^2|j,m\rangle$, $\hat{J}_z|j,m\rangle = m\hbar|j,m\rangle$, and $(\hat{J}_x \pm \mathrm{i}\hat{J}_y)|j,m\rangle = \hbar\sqrt{(j\mp m)(j\pm m+1)}|j,m\pm1\rangle$.
  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, $\sigma_x = \begin{pmatrix}0&1\\1&0\end{pmatrix}$, $\sigma_y = \begin{pmatrix}0&-\mathrm{i}\\\mathrm{i}&0\end{pmatrix}$, $\sigma_z = \begin{pmatrix}1&0\\0&-1\end{pmatrix}$. $\sigma_a\sigma_b = \delta_{ab}\mathbb{1}_{2\times2} + \mathrm{i}\sum_c\epsilon_{abc}\sigma_c$.
    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. (35 points) Consider a 1D harmonic oscillator $\hat{H} = \frac{\hat{p}^2}{2m} + \frac{m\omega^2\hat{x}^2}{2}$. (see page 1)

(a) (5pts) The initial wavefunction is $\varphi(x, t=0) = A \cdot (x + \sqrt{\frac{\hbar}{m\omega}})^2 \cdot \exp(-\frac{m\omega}{2\hbar}x^2)$. *Solve A so that $\varphi(x, t=0)$ is normalized.*

(b) (5pts) Measure energy(namely $\hat{H}$) under $\varphi(x, t = 0)$. *What are the possible measurement results, and their corresponding probabilities?*

(c) (5pts) Evolve the state according to the Schrödinger equation by the Hamiltonian $\hat{H}$. *Solve the wavefunction $\varphi(x, t)$ at time t.*

(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 relation for $\hat{x}, \hat{p}$ is satisfied.*

Solution

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

$\varphi(x, t=0) = A \cdot \frac{\hbar}{2m\omega}(\hat{a}_+ + \hat{a}_- + \sqrt{2})^2 (\frac{\pi\hbar}{m\omega})^{1/4}\psi_0$

$= A \cdot \frac{\hbar}{2m\omega}(\frac{\pi\hbar}{m\omega})^{1/4}(\hat{a}_+ + \hat{a}_- + \sqrt{2})(\psi_1 + 0 + \sqrt{2}\psi_0)$

$= A \cdot \frac{\hbar}{2m\omega}(\frac{\pi\hbar}{m\omega})^{1/4}(\sqrt{2}\psi_2 + \sqrt{2}\psi_1 + \psi_0 + \sqrt{2}\psi_1 + 2\psi_0)$

$= A \cdot \frac{\hbar}{2m\omega}(\frac{\pi\hbar}{m\omega})^{1/4}(\sqrt{2}\psi_2 + 2\sqrt{2}\psi_1 + 3\psi_0)$.

Therefore $|A|^2 \cdot (\frac{\hbar}{2m\omega})^2 (\frac{\pi\hbar}{m\omega})^{1/2} \cdot [(\sqrt{2}^2 + (2\sqrt{2})^2 + 3^2] = 1$,

$|A| = (\frac{m\omega}{\pi\hbar})^{1/4} \cdot \frac{2m\omega}{\hbar} \cdot \frac{1}{\sqrt{19}}$.

Without loss of generality, assume A is real positive hereafter.

(b) by the "measurement postulate", measurement results are

$E_0 = \frac{1}{2}\hbar\omega$, with probability $\frac{9}{19}$;

$E_1 = \frac{3}{2}\hbar\omega$, with probability $\frac{8}{19}$;

$E_2 = \frac{5}{2}\hbar\omega$, with probability $\frac{2}{19}$.

(c) $\varphi(x, t) = A \cdot \frac{\hbar}{2m\omega}(\frac{\pi\hbar}{m\omega})^{1/4}(\sqrt{2}e^{-\mathrm{i}(5/2)\omega t}\psi_2 + 2\sqrt{2}e^{-\mathrm{i}(3/2)\omega t}\psi_1 + 3e^{-\mathrm{i}(1/2)\omega t}\psi_0)$

$= \frac{1}{\sqrt{19}}e^{-\mathrm{i}(1/2)\omega t}(\sqrt{2}e^{-2\mathrm{i}\omega t}\psi_2 + 2\sqrt{2}e^{-\mathrm{i}\omega t}\psi_1 + 3\psi_0)$

(d) use $\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}(\hat{a}_+ + \hat{a}_-)$, and $\hat{p} = \mathbb{i}\sqrt{\frac{\hbar m\omega}{2}}(\hat{a}_- - \hat{a}_+)$,

$\hat{x}\varphi(x,t) = \sqrt{\frac{\hbar}{2m\omega}}\frac{1}{\sqrt{19}}e^{-\mathbb{i}(1/2)\omega t}[(\sqrt{6}e^{-2\mathbb{i}\omega t}\psi_3 + 4e^{-\mathbb{i}\omega t}\psi_2 + 3\psi_1) + (2e^{-2\mathbb{i}\omega t}\psi_1 + 2\sqrt{2}e^{-\mathbb{i}\omega t}\psi_0)]$

$= \sqrt{\frac{\hbar}{2m\omega}}\frac{1}{\sqrt{19}}e^{-\mathbb{i}(1/2)\omega t}[\sqrt{6}e^{-2\mathbb{i}\omega t}\psi_3 + 4e^{-\mathbb{i}\omega t}\psi_2 + (3 + 2e^{-2\mathbb{i}\omega t})\psi_1 + 2\sqrt{2}e^{-\mathbb{i}\omega t}\psi_0)]$

similarly, $\hat{p}\varphi(x,t) = \mathbb{i}\sqrt{\frac{\hbar m\omega}{2}}e^{-\mathbb{i}(1/2)\omega t}[\sqrt{6}e^{-2\mathbb{i}\omega t}\psi_3 + 4e^{-\mathbb{i}\omega t}\psi_2 + (3 - 2e^{-2\mathbb{i}\omega t})\psi_1 - 2\sqrt{2}e^{-\mathbb{i}\omega t}\psi_0)]$

Finally,

$\langle\hat{x}\rangle = \langle\varphi(x,t)|\hat{x}\varphi(x,t)\rangle$

$= \sqrt{\frac{\hbar}{2m\omega}} \cdot \frac{1}{19}[\sqrt{2}e^{2\mathbb{i}\omega t} \cdot 4e^{-\mathbb{i}\omega t} + 2\sqrt{2}e^{\mathbb{i}\omega t} \cdot (3 + 2e^{-2\mathbb{i}\omega t}) + 3 \cdot 2\sqrt{2}e^{-\mathbb{i}\omega t}] =$

$= \sqrt{\frac{\hbar}{2m\omega}} \cdot \frac{1}{19} \cdot 20\sqrt{2}\cos(\omega t)$,

$\langle\hat{p}\rangle = \langle\varphi(x,t)|\hat{p}\varphi(x,t)\rangle$

$= \mathbb{i}\sqrt{\frac{\hbar m\omega}{2}} \cdot \frac{1}{19}[\sqrt{2}e^{2\mathbb{i}\omega t} \cdot 4e^{-\mathbb{i}\omega t} + 2\sqrt{2}e^{\mathbb{i}\omega t} \cdot (3 - 2e^{-2\mathbb{i}\omega t}) - 3 \cdot 2\sqrt{2}e^{-\mathbb{i}\omega t}] =$

$= -\sqrt{\frac{\hbar m\omega}{2}} \cdot \frac{1}{19} \cdot 20\sqrt{2}\sin(\omega t)$

$\langle\hat{x}^2\rangle = \langle\hat{x}\varphi(x,t)|\hat{x}\varphi(x,t)\rangle$

$= \frac{\hbar}{2m\omega} \cdot \frac{1}{19}[(\sqrt{6})^2 + 4^2 + |(3 + 2e^{-2\mathbb{i}\omega t})|^2 + (2\sqrt{2})^2]$

$= \frac{\hbar}{2m\omega} \cdot \frac{1}{19} \cdot [43 + 12\cos(2\omega t)]$

$\langle\hat{p}^2\rangle = \langle\hat{p}\varphi(x,t)|\hat{p}\varphi(x,t)\rangle$

$= \frac{\hbar m\omega}{2} \cdot \frac{1}{19}[(\sqrt{6})^2 + 4^2 + |(3 - 2e^{-2\mathbb{i}\omega t})|^2 + (2\sqrt{2})^2]$

$= \frac{\hbar}{2m\omega} \cdot \frac{1}{19} \cdot [43 - 12\cos(2\omega t)]$

Then

$\sigma_{\hat{x}}^2 = \langle\hat{x}^2\rangle - \langle\hat{x}\rangle^2 = \frac{\hbar}{2m\omega} \cdot \frac{19\times[43+12\cos(2\omega t)]-800\cos^2(\omega t)}{361} = \frac{\hbar}{2m\omega} \cdot \frac{417-172\cos(2\omega t)}{361}$,

$\sigma_{\hat{p}}^2 = \langle\hat{p}^2\rangle - \langle\hat{p}\rangle^2 = \frac{\hbar m\omega}{2} \cdot \frac{19\times[43-12\cos(2\omega t)]-800\sin^2(\omega t)}{361} = \frac{\hbar m\omega}{2} \cdot \frac{417+172\cos(2\omega t)}{361}$,

so uncertainty relation $\sigma_{\hat{x}}^2 \cdot \sigma_{\hat{p}}^2 = \frac{\hbar^2}{4} \cdot \frac{417^2-172^2\cos^2(2\omega t)}{361^2} \geq \frac{\hbar^2}{4} \cdot \frac{417^2-172^2}{361^2} = \frac{\hbar^2}{4} \cdot \frac{144305}{130321} > \frac{\hbar^2}{4}$ is still satisfied.

NOTE: $\langle\hat{x}\rangle$ and $\langle\hat{p}\rangle$ can also be solved by Heisenberg equations of motion.

From $\frac{\mathrm{d}}{\mathrm{d}t}\langle\hat{x}\rangle = \frac{1}{m}\langle\hat{p}\rangle$, $\frac{\mathrm{d}}{\mathrm{d}t}\langle\hat{p}\rangle = -m\omega^2\langle\hat{p}\rangle$, we have

$\langle\hat{x}\rangle(t) = \langle\hat{x}\rangle(t=0)\cos(\omega t) + \frac{1}{m\omega}\langle\hat{p}\rangle(t=0)\sin(\omega t)$,

$\langle\hat{p}\rangle(t) = \langle\hat{p}\rangle(t=0)\cos(\omega t) - m\omega\langle\hat{x}\rangle(t=0)\sin(\omega t)$,

Problem 2. (15 points) Consider $\hat{H} = \frac{\hat{p}^2}{2m} + \frac{\hbar^2}{2m} \cdot \beta_1 \cdot [\delta(x-L) + \delta(x+L)] - \frac{\hbar^2}{2m} \cdot \beta_2 \cdot \delta(x)$. Here m, β_1, β_2, L are positive constants, δs are Dirac δ-functions.

(a) (5pts) *Draw qualitatively the picture of bound states (if they exist).*

(b) (5pts*) *Derive the equation for bound states energy E.* [Hint: use symmetry]

(c) (5pts**) From the result of (b), *determine the conditions on β_1, β_2, L so that bound states exist.* [Hint: consider the extreme case with $E \sim -0$]

Solution

for eigenstates, the boundary condition at $x = \pm L$ is $\psi(\pm L - 0) = \psi(\pm L + 0)$, $-\partial_x \psi|_{x=\pm L-0}^{\pm L+0} + \beta_1 \psi(\pm L) = 0$, so there should be a "cusp" pointing toward x-axis at $x = \pm L$;

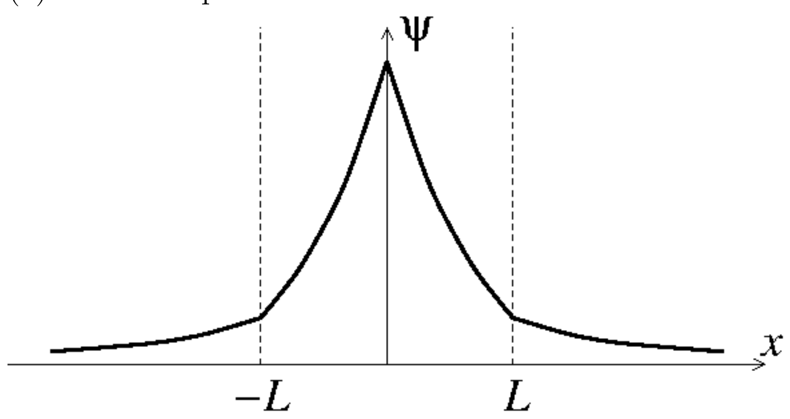
the boundary conditions at $x = 0$ is $\psi(-0) = \psi(+0)$, $-\partial_x \psi|_{x=-0}^{+0} - \beta_2 \psi(0) = 0$, so there should be a "cusp" pointing away from x-axis at $x = 0$.

the potential has inversion symmetry, $V(-x) = V(x)$, therefore eigenstates can be chosen as either even or odd function,

there will NOT be odd bound states, because for odd $\psi_{\text{odd}}(x)$, $\langle \psi_{\text{odd}} | V(x) | \psi_{\text{odd}} \rangle = \frac{\hbar^2}{2m} \cdot \beta_1 (|\psi_{\text{odd}}(-L)|^2 + |\psi_{\text{odd}}(L)|^2) \geq 0$, therefore the energy for odd states are positive, and cannot be bound state.

consider $E = -\frac{\hbar^2 \kappa^2}{2m} < 0$ with $\kappa = \frac{\sqrt{-2mE}}{\hbar} > 0$, the bound state wavefunctions must be $\propto e^{-\kappa x}$ for $x > L$ region, and $\propto e^{\kappa x}$ for $x < -L$ region

(a) schematic picture



(b) consider the following even wavefunction, $\psi(x) = \begin{cases} Ae^{\kappa|x|} + Be^{-\kappa|x|}, & |x| < L; \\ Ce^{-\kappa(|x|-L)}, & |x| > L. \end{cases}$,

the boundary condition at $x = L$ produces

$Ae^{\kappa L} + Be^{-\kappa L} = C,$

$\kappa C + (\kappa Ae^{\kappa L} - \kappa Be^{-\kappa L}) + \beta_1 C = 0,$

the boundary condition at $x = 0$ produces (continuity of ψ is already satisfied)

$-2(\kappa A - \kappa B) - \beta_2(A + B) = 0$

these can be rearranged into $\begin{pmatrix} e^{\kappa L} & e^{-\kappa L} & -1 \\ \kappa e^{\kappa L} & -\kappa e^{-\kappa L} & (\kappa + \beta_1) \\ -(2\kappa + \beta_2) & (2\kappa - \beta_2) & 0 \end{pmatrix} \begin{pmatrix} A \\ B \\ C \end{pmatrix} = 0$

To have nonzero solutions to A, B, C, the 3×3 coefficient matrix must be singular, namely its determinant must vanish, the determinant is (Laplace expansion by the last row)

$-(2\kappa + \beta_2) \cdot e^{-\kappa L}[(\kappa + \beta_1) - \kappa] - (2\kappa - \beta_2) \cdot e^{\kappa L}[(\kappa + \beta_1) - (-\kappa)]]$

$= e^{\kappa L}(\beta_2 - 2\kappa)(\beta_1 + 2\kappa) - e^{-\kappa L}(\beta_2 + 2\kappa)\beta_1$

So the equation for $\kappa = \sqrt{-2mE}/\hbar$ is

$e^{2\kappa L} = \frac{(\beta_2+2\kappa)\beta_1}{(\beta_2-2\kappa)(\beta_1+2\kappa)}$

A positive solution of κ to this equation corresponds to a bound state.

Consistency check: when $L \to +\infty$, this should reduce to a single attractive δ-potential, $-\frac{\hbar^2}{2m} \cdot \beta_2\delta(x)$, and the solution is $\kappa = \beta_2/2$.

(c) Take logarithm of the result equation of (b),

$2\kappa L = \log \frac{(1+2\kappa/\beta_2)}{(1-2\kappa/\beta_2)(1+2\kappa/\beta_1)}$,

there is a trivial (unphysical) solution $2\kappa = 0$,

consider the threshold case when a $E \approx -0$ bound state just appears (by *e.g.* increasing β_2 from 0), then κ is infinitesimally small, expand the above equation in terms of (2κ),

$L \cdot (2\kappa) = \frac{2}{\beta_2} \cdot (2\kappa) - \frac{1}{\beta_1} \cdot (2\kappa) + \frac{1}{2\beta_1^2} \cdot (2\kappa)^2 + O((2\kappa)^3),$

for (2κ) to have positive solution, we need $L - \frac{2}{\beta_2} + \frac{1}{\beta_1} > 0$, or

$\beta_2 > \frac{2\beta_1}{L\beta_1+1}$

Consistency check: when $L \to 0$, this reduces to a single δ-potential, $\frac{\hbar^2}{2m} \cdot (2\beta_1 - \beta_2)\delta(x)$, then we need $\beta_2 > 2\beta_1$ to have bound state.

NOTE(not required): to be rigorous, we should prove that there is at most one nontrivial solution of κ, this can be seen from the fact that $\log \frac{(1+2\kappa/\beta_2)}{(1-2\kappa/\beta_2)(1+2\kappa/\beta_1)}$ is a convex function

with respect to 2κ, then a straight line $L \cdot (2\kappa)$ can have at most two intersection points with $\log \frac{(1+2\kappa/\beta_2)}{(1-2\kappa/\beta_2)(1+2\kappa/\beta_1)}$, this convexity can be seen from
$\frac{\mathrm{d}^2}{\mathrm{d}t^2}[\log \frac{(1+t/\beta_2)}{(1-t/\beta_2)(1+t/\beta_1)}] = \frac{1}{\beta_2^2}[\frac{1}{(1-t/\beta_2)^2} - \frac{1}{(1+t/\beta_2)^2}] + \frac{1}{\beta_1^2} \cdot \frac{1}{(1+t/\beta_1)^2} > 0$ for $t > 0$.

Problem 3. (35 points) Electron in hydrogen atom has $\hat{H} = \frac{\hat{\boldsymbol{p}}^2}{2m} - \frac{\hbar^2}{ma} \cdot \frac{1}{r}$, 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) (5pts) Consider the orbital wave function $\psi(\boldsymbol{r}) = A \cdot (x+y+z) \cdot e^{-r/2a}$. *Solve A so that ψ is normalized.*

(b) (15pts) Under the state $\psi(\boldsymbol{r})$ in (a), *compute expectations of orbital angular momentum operators $\langle \hat{L}_x \rangle$, $\langle \hat{L}_y \rangle$, $\langle \hat{L}_z \rangle$.*

(c) (15pts*) Electron has $S = \frac{1}{2}$ spin angular momentum. Define its total angular momentum operator $\hat{\boldsymbol{J}} \equiv \hat{\boldsymbol{L}} + \hat{\boldsymbol{S}}$. Suppose the combined orbital and spin state is $|\psi(\boldsymbol{r})\rangle |\downarrow\rangle$, measure $\hat{\boldsymbol{J}}^2$ and $\hat{J}_z$ under this state. *What are the possible measurement results, namely combinations (α, β) of eigenvalues α for $\hat{\boldsymbol{J}}^2$ and β for $\hat{J}_z$, and corresponding probability $P_{\alpha,\beta}$, and the collapsed state $|\hat{\boldsymbol{J}}^2 = \alpha, \hat{J}_z = \beta\rangle$ in terms of orbital wavefunctions and spin-1/2 $|\uparrow\rangle, |\downarrow\rangle$ basis?*

Solution

(a) Method #1: represent $\psi(\boldsymbol{r})$ by spherical harmonics (thus by $\psi_{n\ell m}$ eigenbasis),

$\psi(\boldsymbol{r}) = A \cdot re^{-r/2a}(\sin\theta\cos\phi + \sin\theta\sin\phi + \cos\theta)$

$= A \cdot [\sqrt{\frac{8\pi}{3}} \cdot \frac{1}{2}(-Y_1^1 + Y_1^{-1}) + \sqrt{\frac{8\pi}{3}} \cdot \frac{\mathrm{i}}{2}(Y_1^1 + Y_1^{-1}) + \sqrt{\frac{4\pi}{3}} \cdot Y_1^0]$

$= A \cdot \sqrt{\frac{4\pi}{3}} \cdot (-e^{-\mathrm{i}\pi/4}Y_1^1 + Y_1^0 + e^{\mathrm{i}\pi/4}Y_1^{-1}) \cdot re^{-r/2a}$

$= A \cdot \sqrt{\frac{4\pi}{3}} \cdot 2\sqrt{6}a^{5/2}[-e^{-\mathrm{i}\pi/4}\psi_{2,1,1} + \psi_{2,1,0} + e^{\mathrm{i}\pi/4}\psi_{2,1,-1}]$

therefore $1 = |A|^2 \cdot 4\pi \cdot (2\sqrt{6}a^{5/2})^2 \cdot (|-e^{-\mathrm{i}\pi/4}|^2 + |1|^2 + |e^{\mathrm{i}\pi/4}|^2) = |A|^2 \cdot 96\pi a^5$,

$|A| = \sqrt{\frac{1}{96\pi}}a^{-5/2}$

Method #2: directly compute $\int |\psi(\boldsymbol{r}|^2 \,\mathrm{d}^3\boldsymbol{r} = |A|^2 \int (x+y+z)^2 e^{-r/a} \,\mathrm{d}^3\boldsymbol{r}$,

expand $(x+y+z)^2$, the cross terms do not contribute (*e.g.* $xye^{-r/a}$ is odd under $x \to -x$), so the integral is $\int (x^2+y^2+z^2)e^{-r/a}\,\mathrm{d}^3\boldsymbol{r}$

$= 4\pi \cdot \int_0^\infty r^2 e^{-r/a} \cdot r^2\,\mathrm{d}r = 4\pi \cdot a^5 \cdot \Gamma(5) = 4\pi \cdot a^5 \cdot 24 = 96\pi a^5$

(b) The wavefunction is invariant under cyclic permutation $x \to y \to z \to x$ [a 120° rotation about $(1,1,1)$ direction], therefore the three expectation values $\langle \hat{L}_x\rangle, \langle \hat{L}_y\rangle, \langle \hat{L}_z\rangle$ should equal.

Method #1: direct computation of expectation values using eigenbasis $\psi_{n\ell m}$,

under the $\psi_{2,1,m}$ basis $(m = 1, 0, -1)$,

$\psi(\boldsymbol{r})$ is $\frac{1}{\sqrt{3}}\begin{pmatrix} -e^{-\mathbb{i}\pi/4} \\ 1 \\ e^{\mathbb{i}\pi/4} \end{pmatrix}$

$\hat{L}_z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$,

$\hat{L}_x = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$,

$\hat{L}_y = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & -\mathbb{i} & 0 \\ \mathbb{i} & 0 & -\mathbb{i} \\ 0 & \mathbb{i} & 0 \end{pmatrix}$,

It is then straightforward to compute the expectation values (by vector-matrix-vector product), $\langle\psi|\hat{L}_z|\psi\rangle = \langle\psi|\hat{L}_x|\psi\rangle = \langle\psi|\hat{L}_y|\psi\rangle = 0.$

Method #2: apply $\hat{L}_a$ in Cartesian coordinates,

$\hat{L}_z = -\mathbb{i}\hbar(x\partial_y - y\partial_x)$,

then $\hat{L}_z\psi(\boldsymbol{r}) = -\mathbb{i}\hbar \cdot [(x\partial_y - y\partial_x)(x+y+z)] \cdot e^{-r/2a}$

$= -\mathbb{i}\hbar \cdot (x-y) \cdot e^{-r/2a}$,

Note that here we have used the fact that $\hat{L}_z f(r) = 0$ for any function f depending on radius r only.

then $\langle \hat{L}_z\rangle = -\mathbb{i}\hbar \int (x+y+z)(x-y)e^{-r/a}\,\mathrm{d}^3\boldsymbol{r}$,

by the considerations in (a) Method #2,

$\langle \hat{L}_z\rangle = -\mathbb{i}\hbar \int (x^2-y^2)e^{-r/a}\,\mathrm{d}^3\boldsymbol{r} = 0$ (use cyclic permutation symmetry $x \to y \to z \to x$)

Method #3:

$\hat{L}_{x,y,z}$ are hermitian operators, so their expectation values should be real,

but $\psi(\boldsymbol{r})$ is a real function, so the integrand in $\langle \hat{L}_z \rangle = \int \psi(\boldsymbol{r})^* [(-\mathrm{i}\hbar)(x\partial_y - y\partial_x)\psi(\boldsymbol{r}] \, \mathrm{d}^3\boldsymbol{r}$ is pure imaginary, and the integral should be pure imaginary,

this contraction shows that $\langle \hat{L}_z \rangle$ (and similarly $\langle \hat{L}_{x,y} \rangle$) must vanish under real wave function $\psi(\boldsymbol{r})$.

(c) This is similar to Homework Problem 4.40(b),

denote $\psi_{21,m}$ by $|1, m\rangle$ hereafter ($m = 1, 0, -1$),

denote the total angular momentum eigenbasis by $|j, j_z\rangle$ hereafter, here j can be $\frac{1}{2}$ or $\frac{3}{2}$, $j_z = -j, -j+1, \ldots, j$.

the derivation of the following results (C-G coefficients) is omitted here,

$|j = \frac{3}{2}, j_z = -\frac{3}{2}\rangle = |1, -1\rangle|\downarrow\rangle$,

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

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

$|j = \frac{3}{2}, j_z = \frac{3}{2}\rangle = |1, 1\rangle|\uparrow\rangle$,

$|j = \frac{1}{2}, j_z = -\frac{1}{2}\rangle = \frac{1}{\sqrt{3}}(|1, 0\rangle|\downarrow\rangle - \sqrt{2}|1, -1\rangle|\uparrow\rangle)$,

$|j = \frac{1}{2}, j_z = \frac{1}{2}\rangle = \frac{1}{\sqrt{3}}(\sqrt{2}|1, 1\rangle|\downarrow\rangle - |1, 0\rangle|\uparrow\rangle)$,

then $|\psi(\boldsymbol{r})\rangle|\downarrow\rangle = \frac{1}{\sqrt{3}}[-e^{-\mathrm{i}\pi/4}|1, 1\rangle|\downarrow\rangle + |1, 0\rangle|\downarrow\rangle + e^{\mathrm{i}\pi/4}|1, -1\rangle|\downarrow\rangle]$
$= -\frac{e^{-\mathrm{i}\pi/4}}{3}|j = \frac{3}{2}, j_z = \frac{1}{2}\rangle - \frac{\sqrt{2}e^{-\mathrm{i}\pi/4}}{3}|j = \frac{1}{2}, j_z = \frac{1}{2}\rangle + \frac{\sqrt{2}}{3}|j = \frac{3}{2}, j_z = -\frac{1}{2}\rangle$
$+ \frac{1}{3}|j = \frac{1}{2}, j_z = -\frac{1}{2}\rangle + \frac{e^{\mathrm{i}\pi/4}}{\sqrt{3}}|j = \frac{3}{2}, j_z = -\frac{3}{2}\rangle$

The measurement results are summarized in the following table,

(α, β)	$P_{\alpha,\beta}$	$\lvert \hat{\boldsymbol{J}}^2 = \alpha, \hat{J}_z = \beta \rangle$
$(\frac{15}{4}\hbar^2, \frac{1}{2}\hbar)$	$\frac{1}{9}$	$\frac{1}{\sqrt{3}}(\psi_{21,1}\lvert\downarrow\rangle + \sqrt{2}\lvert\psi_{21,0}\lvert\uparrow\rangle)$
$(\frac{3}{4}\hbar^2, \frac{1}{2}\hbar)$	$\frac{2}{9}$	$\frac{1}{\sqrt{3}}(\sqrt{2}\psi_{21,1}\lvert\downarrow\rangle - \lvert\psi_{21,0}\lvert\uparrow\rangle)$
$(\frac{15}{4}\hbar^2, -\frac{1}{2}\hbar)$	$\frac{2}{9}$	$\frac{1}{\sqrt{3}}(\sqrt{2}\psi_{21,0}\lvert\downarrow\rangle + \lvert\psi_{21,-1}\lvert\uparrow\rangle)$
$(\frac{3}{4}\hbar^2, -\frac{1}{2}\hbar)$	$\frac{1}{9}$	$\frac{1}{\sqrt{3}}(\psi_{21,0}\lvert\downarrow\rangle - \sqrt{2}\lvert\psi_{21,-1}\lvert\uparrow\rangle)$
$(\frac{15}{4}\hbar^2, -\frac{3}{2}\hbar)$	$\frac{1}{3}$	$\psi_{21,-1}\lvert\downarrow\rangle$

Here we have used $\alpha = j(j+1)\hbar^2$, $\beta = j_z\hbar$.

Problem 4. (15 points) Consider a particle in combined harmonic potential and finite square well potential, $\hat{H} = \frac{\hat{p}^2}{2m} + V(x)$, $V(x) = \begin{cases} \frac{m\omega^2}{2}x^2, & |x| < a; \\ \frac{m\omega^2}{2}x^2 + V_0, & |x| > a \end{cases}$. Here m, ω, a, V_0 are positive constants.

(a) (9pts) *Draw qualitatively the wave functions for the ground state, 1st excited state, and 2nd excited state. Describe their properties (list as many as you can)*

(b) (4pts) Use subscripts $_{\text{in}}$ and $_{\text{out}}$ to denote variables in $|x| < a$ and $|x| > a$ regions respectively, and $_{\text{in/out}}$ for both cases simultaneously. Consider the stationary Schrödinger equation $\hat{H}\psi = E\psi$, define $\xi = \sqrt{\frac{m\omega}{\hbar}}x$, $K_{\text{in}} = \frac{2E}{\hbar\omega}$, $K_{\text{out}} = \frac{2(E-V_0)}{\hbar\omega}$ then $\frac{\mathrm{d}^2}{\mathrm{d}\xi^2}\psi = [\xi^2 - K_{\text{in/out}}] \cdot \psi$, for $|x| < a$ and $|x| > a$ regions respectively. Assume $\psi(\xi) = h_{\text{in/out}}(\xi) \cdot e^{-\xi^2/2}$, then $[\frac{\mathrm{d}^2}{\mathrm{d}\xi^2} - 2\xi\frac{\mathrm{d}}{\mathrm{d}\xi} + K_{\text{in/out}} - 1] \cdot h_{\text{in/out}} = 0$. Consider the eigenstates in (a), assume $h_{\text{in/out}}(\xi) = \sum_{j=0}^{\infty} c_{\text{in/out},j}\xi^j$ for $\xi \geq 0$. *Derive the recursion relation for $c_{in/out,j}$, write down the boundary condition at $x = a$ in terms of $c_{in/out,j}$ (involving infinite series).*

(c) (2pts**) The recursion relation for $c_{\text{in/out},j}$ in (b) is almost the same as the original harmonic oscillator. But the eigenstate energies are not the original eigenvalues of harmonic oscillator without finite square well potentials, therefore the series for $h_{\text{in/out}}$ will not be truncated to finite order. *How can this reconcile with the requirement that ψ should be normalizable?*

Solution

(a) They look almost the same as original harmonic oscillator eigenstates, with the following properties:

(i) smooth, even at $x = \pm a$;

(ii) ground and 2nd excited states are even, 1st excited state is odd;

(iii) ground state has no node, 1st excited state has a simple node at $x = 0$, 2nd excited state has two nodes;

(iv) (not required) they all behave as $\sim \exp(-\frac{m\omega}{2\hbar}x^2)$ as $x \to \pm\infty$

(b) the recursion relations are exactly the same as those of the original harmonic oscillator,

$c_{\text{in/out},j+2} = c_{\text{in/out},j} \cdot \frac{2j+1-K_{\text{in/out}}}{(j+1)(j+2)}$

the boundary condition should be $\psi|_{x=a-0} = \psi|_{x=a+0}$, and $\frac{\mathrm{d}\psi}{\mathrm{d}x}|_{x=a-0} = \frac{\mathrm{d}\psi}{\mathrm{d}x}|_{x=a+0}$,

this is equivalent to $h_{\text{in}}(\sqrt{\frac{m\omega}{\hbar}}a) = h_{\text{out}}(\sqrt{\frac{m\omega}{\hbar}}a)$, and $\frac{\mathrm{d}h_{\text{in}}}{\mathrm{d}\xi}|_{xi=\sqrt{\frac{m\omega}{\hbar}}a} = \frac{\mathrm{d}h_{\text{out}}}{\mathrm{d}\xi}|_{xi=\sqrt{\frac{m\omega}{\hbar}}a}$,

namely, $\sum_j c_{\text{in},j}(\sqrt{\frac{m\omega}{\hbar}}a)^j = \sum_j c_{\text{out},j}(\sqrt{\frac{m\omega}{\hbar}}a)^j$, and
$\sum_j c_{\text{in},j} \cdot j \cdot (\sqrt{\frac{m\omega}{\hbar}}a)^{j-1} = \sum_j c_{\text{out},j} \cdot j \cdot (\sqrt{\frac{m\omega}{\hbar}}a)^{j-1}$,

(c)

for generic λ, both solutions (even and odd functions) to $[-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \frac{m\omega^2}{2}x^2]f(x) = \lambda \cdot f(x)$, are not normalizable, and behave as $\exp(\frac{m\omega}{2\hbar}x^2)$ as $x \to \pm\infty$,

for the finite region $-a < x < a$, we just use the even or odd solution for $\lambda = E$,

for the region $a < x$, we use a combination of the even and odd solutions for $\lambda = E - V_0$, such that it behaves as $\exp(-\frac{m\omega}{2\hbar}x^2)$ as $x \to +\infty$ (this combination will hehave as $\exp(+\frac{m\omega}{2\hbar}x^2)$ as $x \to -\infty$, but we are not using it there)

for the region $x < -a$, we just use the even or odd image of $a < x$ region

the functions used in each region, if extended to the entire x-axis, will not be normalizable, similar to the bound state for attractive δ-potential