Problem Set 8 Solutions

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March 27, 2025

Question 1(a): Ground State and First Excited State of the 3D Isotropic Harmonic Oscillator

Hamiltonian and Separation of Variables

The Hamiltonian for the 3D isotropic harmonic oscillator is:

$$\hat{H} = \frac{\hat{p}_x^2 + \hat{p}_y^2 + \hat{p}_z^2}{2m} + \frac{1}{2}m\omega^2(x^2 + y^2 + z^2). \tag{1}$$

Because it *separates* into a sum of three identical 1D harmonic oscillators, the wavefunction can be written as a product:

$$\Psi_{n_x,n_y,n_z}(x,y,z) = \psi_{n_x}(x)\,\psi_{n_y}(y)\,\psi_{n_z}(z), \tag{2}$$

where each $\psi_n(x)$ is the standard 1D harmonic oscillator solution.

1D Review

1D ground state:

$$\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \exp\left[-\tfrac{m\omega}{2\hbar}\,x^2\right]. \tag{3}$$

1D first excited state:

$$\psi_1(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \sqrt{2}\,\alpha\,x\,\exp\left[-\tfrac{m\omega}{2\hbar}\,x^2\right] \quad \text{where} \quad \alpha = \left(\frac{m\omega}{\hbar}\right)^{1/2}. \tag{4}$$

Ground State in 3D

For $n_x = n_y = n_z = 0$, the 3D ground state is:

$$\Psi_{0,0,0}(x,y,z) = \psi_0(x)\,\psi_0(y)\,\psi_0(z) = \left(\frac{m\omega}{\pi\hbar}\right)^{3/4} \exp\left[-\frac{m\omega}{2\hbar}(x^2+y^2+z^2)\right]. \tag{5}$$

First Excited States in 3D

The energy in 3D is $\hbar\omega\,(n_x+n_y+n_z+\frac{3}{2})$. The first excited level occurs when $n_x+n_y+n_z=1$. That yields three possible combinations:

$$\begin{aligned}(n_x,n_y,n_z)&=(1,0,0),\\(n_x,n_y,n_z)&=(0,1,0),\\(n_x,n_y,n_z)&=(0,0,1).\end{aligned}$$

Thus we have three degenerate first-excited states:

$$\begin{aligned}\Psi_{1,0,0}(x,y,z)&=\psi_1(x)\,\psi_0(y)\,\psi_0(z),\\\Psi_{0,1,0}(x,y,z)&=\psi_0(x)\,\psi_1(y)\,\psi_0(z),\\\Psi_{0,0,1}(x,y,z)&=\psi_0(x)\,\psi_0(y)\,\psi_1(z),\end{aligned}$$

all with energy $E=\frac{5}{2}\hbar\omega$.

Final Results

- **Ground State:**

$$\Psi_{0,0,0}(x,y,z)=\left(\frac{m\omega}{\pi\hbar}\right)^{3/4}\exp\Big[-\frac{m\omega}{2\hbar}(x^2+y^2+z^2)\Big]. \tag{6}$$

- **First-Excited States (3-fold degenerate):**

$$\begin{aligned}\Psi_{1,0,0}(x,y,z)&=\psi_1(x)\,\psi_0(y)\,\psi_0(z),\\\Psi_{0,1,0}(x,y,z)&=\psi_0(x)\,\psi_1(y)\,\psi_0(z),\\\Psi_{0,0,1}(x,y,z)&=\psi_0(x)\,\psi_0(y)\,\psi_1(z),\end{aligned}$$

- **Energy at first-excited level:** $E=\frac{5}{2}\hbar\omega$.

Question 1(b): Energy and Degeneracy of the 3D Isotropic Harmonic Oscillator

Energy of the n-th Excited State

For a 1D harmonic oscillator, the energy levels are

$$E_n^{(1\mathrm{D})}=\hbar\omega\Big(n+\tfrac{1}{2}\Big),\quad n=0,1,2,\ldots \tag{7}$$

In 3D, we have three independent 1D oscillators, so the total energy is

$$E_{n_x,n_y,n_z} = \hbar\omega\Big(n_x + n_y + n_z + \tfrac{3}{2}\Big). \tag{8}$$

Defining $n = n_x + n_y + n_z$, the n-th excited level has energy

$$\boxed{E_n = \hbar\omega\big(n + \tfrac{3}{2}\big).} \tag{9}$$

Degeneracy of the n-th Excited State

The states with $n_x + n_y + n_z = n$ share the same energy E_n. The number of nonnegative integer solutions to $n_x + n_y + n_z = n$ is

$$\binom{n+3-1}{3-1} = \binom{n+2}{2} = \frac{(n+1)(n+2)}{2}. \tag{10}$$

Hence, the degeneracy is

$$\boxed{g_n = \frac{(n+1)(n+2)}{2}.} \tag{11}$$

Construction Using Raising Operators

Let $a_i, a_i^\dagger$ be the annihilation and creation operators for each Cartesian direction $i = 1, 2, 3$. The 3D ground state $|\psi_0\rangle$ satisfies

$$a_i\,|\psi_0\rangle = 0, \quad i = 1, 2, 3. \tag{12}$$

Then any excited state with quantum numbers (n_x, n_y, n_z) can be built by applying the appropriate creation operators:

$$|n_x, n_y, n_z\rangle \;\propto\; (a_1^\dagger)^{n_x}\,(a_2^\dagger)^{n_y}\,(a_3^\dagger)^{n_z}\;|\psi_0\rangle\,. \tag{13}$$

Hence, the n-th excited state $(n = n_x + n_y + n_z)$ can be written in the form

$$\boxed{(a_1^\dagger)^{n_1}(a_2^\dagger)^{n_2}(a_3^\dagger)^{n_3}\,|\psi_0\rangle \quad \text{with} \quad n_1 + n_2 + n_3 = n.} \tag{14}$$

Summary for Part (b)

- **Energy:** $E_n = \hbar\omega(n + \frac{3}{2})$.
- **Degeneracy:** $g_n = \frac{(n+1)(n+2)}{2}$.
- **Raising-Operator Representation:** states in the n-th manifold are generated by distributing n creation-operator actions among the three coordinates.

Question 2: Hermiticity Conditions in Spherical Coordinates (Expanded Explanation)

We have the operator

$$\hat{A} = r\frac{\partial^2}{\partial r^2} + a\frac{\partial}{\partial r} + \frac{1}{r}\Big(\frac{\partial^2}{\partial \theta^2} + b\,\cot(\theta)\,\frac{\partial}{\partial \theta}\Big), \tag{15}$$

where $a, b \in \mathbb{C}$. We want to find for which values of a, b this operator is Hermitian in $L^2(\mathbb{R}^3)$ with the measure $r^2 \sin\theta\, dr\, d\theta\, d\phi$. The assumption is that wavefunctions vanish sufficiently fast as $r \to 0, r \to \infty$, and that everything is well-behaved at $\theta = 0, \theta = \pi$.

Why Hermiticity Requires Integration by Parts

To say $\hat{A}$ is Hermitian, we require

$$\int (\phi^* \hat{A}\,\psi)\,d^3x = \int ((\hat{A}\,\phi)^*\,\psi)\,d^3x \quad \text{for all } \phi, \psi \in L^2(\mathbb{R}^3), \tag{16}$$

where $d^3x = r^2 \sin\theta\, dr\, d\theta\, d\phi$. If boundary terms from integration by parts fail to vanish or if the form of $\hat{A}$ does not match its adjoint, Hermiticity fails.

Step 1: Radial Part in Detail

Consider the radial piece:

$$\hat{A}_r = r\,\frac{\partial^2}{\partial r^2} \;+\; a\,\frac{\partial}{\partial r}. \tag{17}$$

Integration Setup: We look at the radial integral (suppressing angular variables for the moment):

$$\int_0^\infty dr\, r^2\, \phi^*(r)\,\Big(r\,\psi''(r) + a\,\psi'(r)\Big),$$

where $\psi'(r) = \frac{d\psi}{dr}$. We assume boundary conditions such that $\phi, \psi \to 0$ as $r \to 0$ or ∞, so that boundary terms vanish.

Integration by Parts: 1. First, note that $r\,\psi''(r)$ can produce terms of the form $\frac{d}{dr}\big(r\,\psi'(r)\big)$ etc. Doing a full integration by parts carefully indicates that the operator becomes self-adjoint only if the coefficient in front of $\frac{\partial}{\partial r}$ is real. 2. Similarly, the usual radial part of the Laplacian in spherical coordinates is known to be self-adjoint if it looks like $\frac{1}{r^2}\frac{d}{dr}\big(r^2\frac{d}{dr}\big)$. Written out, that equates to certain terms that match $\hat{A}_r$ only if a is real.

Conclusion from radial part: $a \in \mathbb{R}$.

Step 2: Angular Part in Detail

Now consider the angular part:

$$\frac{1}{r}\Big(\frac{\partial^2}{\partial\theta^2} + b\,\cot(\theta)\,\frac{\partial}{\partial\theta}\Big). \tag{18}$$

Focusing on integration over $\theta \in [0, \pi]$ with measure $\sin\theta\, d\theta$ (and also integrating over ϕ, but that part is trivial if $\hat{A}$ does not depend on ϕ):

$$\int_0^\pi d\theta\, \sin\theta\, \phi^*(\theta)\Big(\psi_\theta''(\theta) + b\,\cot(\theta)\,\psi_\theta'(\theta)\Big),$$

where $\psi_\theta'(\theta) = \frac{\partial\psi}{\partial\theta}$. The standard angular part of the Laplacian is

$$\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\Big(\sin\theta\,\frac{\partial}{\partial\theta}\Big) = \frac{\partial^2}{\partial\theta^2} + \cot(\theta)\,\frac{\partial}{\partial\theta}. \tag{19}$$

Clearly, that forces the coefficient of $\cot(\theta)\,\frac{\partial}{\partial\theta}$ to be exactly 1. If $b \neq 1$, we get a mismatch that leads to leftover factors or boundary terms, breaking Hermiticity. Also, for it to be truly self-adjoint, we want b real as well.

Conclusion from angular part: $b = 1$ (and real).

Final Conclusion

Thus, the operator $\hat{A}$ will be Hermitian exactly if

$$\boxed{a \in \mathbb{R}, \quad b = 1.} \tag{20}$$

That mirrors the known structure of the radial and angular parts of the Laplacian in spherical coordinates and ensures no boundary terms survive under integration by parts.