PHYS 661 - Quantum Mechanics II

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Homework 6

Problem 1 - 1D δ-potential Revisited

Consider the 3D attractive potential $V(r) = \begin{cases} -V_0, & r < a, \\ 0, & r > a. \end{cases}$

(a) Solve the s-wave ($\ell = 0$) Schrodinger equation exactly and find the scattering phase shift $\delta_0(k)$ as a function of momentum $k = \sqrt{\frac{2m}{\hbar^2}E}$, V_0, and a. (It will be a complicated expression, no need to simplify it.) Find an equation for k such that the phase shift vanishes $\delta_0(k) = 0$ (no need to solve the equation).

(b) Find the equation for bound state energies E in terms of V_0 and a (no need to solve the equation).

(c) Give your best effort to verify Levinson's theorem, that the number of bound states is given by $N_b = \frac{1}{\pi}[\delta(E \to 0) - \delta(E \to \infty)]$.

Solution. (a) For the s-wave ($\ell = 0$) in a spherically symmetric potential, we work with the radial Schrdinger equation

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2 u(R)}{\mathrm{d}r^2} + V(r)u(r) = Eu(r),$$

with the given potential

$$V(r) = \begin{cases} -V_0, & r < a, \\ 0, & r > a. \end{cases}$$

The solution can be split into two regions

- For $r > a$, the radial wave function has the general form
$$u(r) = \frac{\sin(kr + \delta_0)}{\sqrt{kr}}.$$
- For $r < a$, we seek a solution satisfying the boundary conditions. The phase shift $\delta_0(k)$ is determined by the matching condition at $r = a$, which gives
$$\tan(\delta_0) = \frac{k\cot(ka) - \frac{mV_0}{\hbar^2}}{\frac{mV_0}{\hbar^2}ka\cot(ka) - k}.$$

An equation for zero phase shift ($\delta_0 = 0$) is

$$\cot(ka) = \frac{mV_0}{\hbar^2 k}.$$

(b) For bound states, we seek solutions with $E < 0$. The condition for bound states is determined by

$$\tan(k'a) = -\frac{\hbar^2 mk'}{mV_0}, \quad \text{where } k' = \sqrt{-\frac{2mE}{\hbar^2}}.$$

Rearranging, the bound state energy condition becomes

$$\cot(k'a) = -\frac{mV_0}{\hbar^2 k'}.$$

(c) Levinson's theorem states that the number of bound states N_b is related to the phase shift at zero and infinite energy by

$$N_b = \frac{1}{\pi}\left[\delta(E \to 0) - \delta(E \to \infty)\right].$$

From our previous calculations

- At $E \to 0$, $\delta_0 \approx \frac{mV_0 a}{\hbar^2}$.
- At $E \to \infty$, $\delta_0 \to \frac{\pi}{2}$.

Thus, $N_b = \frac{1}{\pi}[\frac{mV_0 a}{\hbar^2} - \frac{\pi}{2}]$. The number of bound states depends on the potential strength V_0, range a, and reduced mass m.

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Problem 2 - Three Angular Momenta
Consider three angular momentum operators $\mathbf{S}, \mathbf{L}, \mathbf{I}$ in the $S = 1$, $L = 2$, $I = \frac{1}{2}$, representations, respectively. Consider also the operator $Q = a\mathbf{S} \cdot \mathbf{L} + b(\mathbf{S} + \mathbf{L}) \cdot \mathbf{I}$ where a, b are scalars.

(a) What is the dimension of the matrix Q? Show that the terms proportional to a, b in Q commute with each other.

(b) Write Q in a block-diagonal form, in terms of a maximum set of commuting observables.

Solution. First, let's calculate the matrix dimension

- $\mathbf{S}$: $S = 1$ representation $\to$ dimension $2S + 1 = 3$.
- $\mathbf{L}$: $L = 2$ representation $\to$ dimension $2L + 1 = 5$.
- $\mathbf{I}$: $I = \frac{1}{2}$ representation $\to$ dimension $2I + 1 = 2$.

The total matrix dimension is then $3 \times 5 \times 2 = 30$.
To show the terms commute, we'll examine $\mathbf{S} \cdot \mathbf{L}$ and $(\mathbf{S} + \mathbf{L}) \cdot \mathbf{I}$. We have

$$[\mathbf{S} \cdot \mathbf{L}, (\mathbf{S} + \mathbf{L}) \cdot \mathbf{I}] = 0$$

by the commutation relations of angular momentum operators given by

$$\begin{aligned} [\mathbf{S} \cdot \mathbf{L}, \mathbf{S}_i] = [\mathbf{S} \cdot \mathbf{L}, \mathbf{L}_i] = 0, \\ [\mathbf{S} \cdot \mathbf{L}, \mathbf{I}_i] = 0. \end{aligned}$$

The maximum set of commuting observables includes the total angular momentum squared $\mathbf{J}^2$, the z component of total angular momentum $\mathbf{J}_z$, $\mathbf{I}^2$, and $\mathbf{I}_z$. The total angular momentum is $\mathbf{J} = \mathbf{S} + \mathbf{L}$.
The block-diagonal form will be

$$Q = \bigoplus_{J, M_J, I, M_I} a(\mathbf{S} \cdot \mathbf{L})_{J, M_J} + b(\mathbf{S} + \mathbf{L})_z \cdot \mathbf{I}_z$$

Each block corresponds to a specific set of quantum numbers

$$\begin{aligned} J &= |L - S|, |L - S| + 1, \ldots, L + S \\ M_J &= -J, -J + 1, \ldots, J \\ I &= \frac{1}{2} \\ M_I &= \pm\frac{1}{2} \end{aligned}$$

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Problem 3 - Some Properties of Rotation Generators

(a) Let L_x, L_y, and L_z denote the components of the angular momentum operator. Show that if and operator O satisfies $[O, L_x] = [O, L_y] = 0$, then $[O, L_z] = 0$.

(b) Let $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ denote the Pauli matrices, I the 2×2 identity matrix, and $\mathbf{a}, \mathbf{b} \in \mathbb{R}^3$. Show that

$$(\mathbf{a} \cdot \boldsymbol{\sigma})(\mathbf{b} \cdot \boldsymbol{\sigma}) = \mathbf{a} \cdot \mathbf{b}\mathbb{I} + \mathrm{i}(\mathbf{a} \times \mathbf{b}) \cdot \boldsymbol{\sigma}.$$

(c) We know that any complex 2×2 matrix M_2 can be written in terms of $I, \sigma_x, \sigma_y, \sigma_z$ as a linear combination $M_2 = a_0\mathbb{I} + \mathbf{a} \cdot \boldsymbol{\sigma}$. Show that any complex 3×3 matrix M_3 can be written in terms of I_3, S_x, S_y, S_z where I_3 denotes the 3×3 identity matrix and S_x, S_y, S_z the spin-1 matrices, but that in this case M_3 will not be a linear function of S_x, S_y, S_z. (Hint: Investigate the anticommutators $\{S_i, S_j\}$.) The spin 1 matrices are [in units $\hbar = 1$]

$$S_x = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \quad S_y = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}, \quad S_z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}.$$

Solution. (a) Let's prove that if $[O, L_x] = [O, L_y] = 0$, then $[O, L_z] = 0$.

Recall the angular momentum commutation relations:

$$\begin{aligned} [L_x, L_y] &= \mathrm{i}L_z, \\ [L_y, L_z] &= \mathrm{i}L_x, \\ [L_z, L_x] &= \mathrm{i}L_y. \end{aligned}$$

Assume $[O, L_x] = [O, L_y] = 0$. Consider the commutator $[O, L_z]$. We'll prove this is zero by contradiction.

Expand the commutator using the given conditions and the commutation relations

$$\begin{aligned} [O, L_z] &= [O, L_x L_x^{-1} L_z L_x L_x^{-1}] \\ &= [O, L_x] L_x^{-1} L_z L_x L_x^{-1} + L_x [O, L_x^{-1}] L_z L_x L_x^{-1} + L_x L_x^{-1} [O, L_z] L_x L_x^{-1} \\ &= 0 \cdot L_z + L_x \cdot 0 \cdot L_x L_x^{-1} + L_x L_x^{-1} \cdot 0 \cdot L_x L_x^{-1} \\ &= 0 \end{aligned}$$

Therefore, $[O, L_z] = 0$.

(b) For any ordinary vectors $\mathbf{a}$, $\mathbf{b} \in \mathbb{R}^3$, we have

$$\begin{aligned}
(\mathbf{a}\cdot\boldsymbol{\sigma})(\mathbf{b}\cdot\boldsymbol{\sigma}) &= \sum_j \sigma_j a_j \sum_k \sigma_k b_k \\
&= \sum_j \sum_k \sigma_j \sigma_k a_j b_k \\
&= \sum_j \sum_k \left(\delta_{jk} + \mathrm{i}\sum_l \epsilon_{jkl}\sigma_l\right) a_j b_k \\
&= \sum_j \sum_k \delta_{jk} a_j b_k + \mathrm{i}\sum_j \sum_k \sum_l \epsilon_{jkl}\sigma_l a_j b_k \\
&= \sum_j a_j b_j + \mathrm{i}\sum_l \sigma_l \left(\sum_j \sum_k \epsilon_{jkl} a_j b_k\right) \\
&= (\mathbf{a}\cdot\mathbf{b}) + \mathrm{i}\sum_l \sigma_l (\mathbf{a}\times\mathbf{b}) \\
&= (\mathbf{a}\cdot\mathbf{b})\,\mathbb{I} + \mathrm{i}\boldsymbol{\sigma}\cdot(\mathbf{a}\times\mathbf{b}).
\end{aligned}$$

Therefore,

$$(\mathbf{a}\cdot\boldsymbol{\sigma})(\mathbf{b}\cdot\boldsymbol{\sigma}) = (\mathbf{a}\cdot\mathbf{b})\,\mathbb{I} + \mathrm{i}\boldsymbol{\sigma}\cdot(\mathbf{a}\times\mathbf{b}).$$

(c) Calculating the anticommutators of the spin-1 matrices, we have

$$\begin{aligned}
\{S_x, S_y\} &= S_x S_y + S_y S_x = \mathrm{i}S_z, \\
\{S_y, S_z\} &= S_y S_z + S_z S_y = \mathrm{i}S_x, \\
\{S_z, S_x\} &= S_z S_x + S_x S_z = \mathrm{i}S_y.
\end{aligned}$$

Calculating the squares of these matrices, we have

$$S_x^2 = S_y^2 = S_z^2 = 2\mathbb{I}_3 - \frac{1}{3}(S_x^2 + S_y^2 + S_z^2)$$

Consider a general 3×3 complex matrix M_3. We can write it as

$$M_3 = a_0\mathbb{I}_3 + a_x S_x + a_y S_y + a_z S_z + b_x S_x^2 + b_y S_y^2 + b_z S_z^2 + c_{xy}\{S_x, S_y\} + c_{yz}\{S_y, S_z\} + c_{zx}\{S_z, S_x\},$$

where a_0, a_x, a_y, a_z, b_x, b_y, b_z, c_{xy}, c_{yz}, and c_{zx} are complex coefficients.
We can now rewrite the previous as

$$M_3 = a_0\mathbb{I}_3 + a_x S_x + a_y S_y + a_z S_z + (b_x + b_y + b_z)\left(2\mathbb{I}_3 - \frac{1}{3}(S_x^2 + S_y^2 + S_z^2)\right) + \mathrm{i}(c_{xy}S_z + c_{yz}S_x + c_{zx}S_y)$$

This can be further simplified to

$$M_3 = (a_0 + 2(b_x + b_y + b_z))I_3 + (a_x - \mathrm{i}c_{yz})S_x + (a_y - \mathrm{i}c_{zx})S_y + (a_z - \mathrm{i}c_{xy})S_z - \frac{1}{3}(b_x + b_y + b_z)(S_x^2 + S_y^2 + S_z^2)$$

This expression shows that any 3×3 complex matrix can indeed be written in terms of $\mathbb{I}_3$, S_x, S_y, and S_z. However, it's not a linear function of S_x, S_y, and S_z because of the presence of the squared terms S_x^2, S_y^2, and S_z^2.

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