University of Hyderabad
School of Physics

M.Sc.-I/IMSc.-III   Quantum Mechanics   **June 27, 2018**

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Solutions to Test-I Problems

§1 Question [1]

Question Show that spin one matrices are given by [8]

$$S_x = \frac{\hbar}{\sqrt{2}}\begin{pmatrix}0 & 1 & 0\\ 1 & 0 & 1\\ 0 & 1 & 0\end{pmatrix}; \quad S_y = \frac{\hbar}{\sqrt{2}}\begin{pmatrix}0 & -i & 0\\ i & 0 & -i\\ 0 & i & 0\end{pmatrix}; \quad S_z = \hbar\begin{pmatrix}1 & 0 & 0\\ 0 & 0 & 0\\ 0 & 0 & -1\end{pmatrix}.$$

Solution The matrix S_z is diagonal because the eigenvectors of S_z are taken as basis. The entries for the S_z matrix are $\hbar, 0, -\hbar$, because spin is 1. Hence

$$S_z = \hbar\begin{pmatrix}1 & 0 & 0\\ 0 & 0 & 0\\ 0 & 0 & -1\end{pmatrix} \tag{1}$$

For S_x, S_y we begin with the identity

$$S_+|m\rangle = \sqrt{s(s+1) - m(m+1)}\hbar|m+1\rangle. \tag{2}$$

and compute action of S_+ on kets $|1\rangle, |0\rangle, |-1\rangle$. Using the above identity we would get

$$S_+|1\rangle = 0, \quad S_+|0\rangle = \sqrt{2}\hbar|1\rangle, S_+|-1\rangle = \sqrt{2}\hbar|0\rangle. \tag{3}$$

Taking scalar product of the above vectors, consecutively, with $|1\rangle, |0\rangle, |-1\rangle$ and using orthonormal property of vectors $|m\rangle$ we get

$$\langle 1|S_+|1\rangle = 0 \qquad \langle 1|S_+|0\rangle = \sqrt{2}\hbar \quad \langle 1|S_+|-1\rangle = 0 \tag{4}$$

$$\langle 0|S_+|1\rangle = 0 \qquad \langle 0|S_+|0\rangle = 0 \quad \langle 0|S_+|-1\rangle = \sqrt{2}\hbar \tag{5}$$

$$\langle -1|S_+|1\rangle = 0 \qquad \langle -1|S_+|0\rangle = \sqrt{2}\hbar \quad \langle -1|S_+|-1\rangle = 0 \tag{6}$$

(7)

Therefore the matrix for S_+ is given by

$$S_+ = \hbar\begin{pmatrix}0 & \sqrt{2} & 0\\ 0 & 0 & \sqrt{2}\\ 0 & 0 & 0\end{pmatrix} \tag{8}$$

Taking adjoint of S_+ we get

$$S_- = \hbar \begin{pmatrix} 0 & 0 & 0 \\ \sqrt{2} & 0 & 0 \\ 0 & \sqrt{2} & 0 \end{pmatrix} \tag{9}$$

Hence using $S_x = \frac{1}{2}(S_+ + S_-), S_y = \frac{1}{2i}(S_+ - iS_-)$, we get the matrices for S_x, S_y

$$S_x = \frac{\hbar}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}; \qquad S_y = \frac{\hbar}{\sqrt{2}} \begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}.$$

§2 Question [2]

Question

For particle in a potential well with a rigid wall (see Fig. 1) [8]

$$V(x) = \begin{cases} \infty, & \text{for } x < 0 \\ 0, & \text{for } 0 \leq x \leq L \\ V_0, & \text{for } x > L, \end{cases} \qquad (10)$$

solve the Schrodinger equation for energy range $0 < E < V_0$ and show that that the bound state energies are given by

$$k \cot kL = -\alpha$$

where

$$k = \sqrt{\frac{2mE}{\hbar^2}}, \qquad \alpha = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}.$$

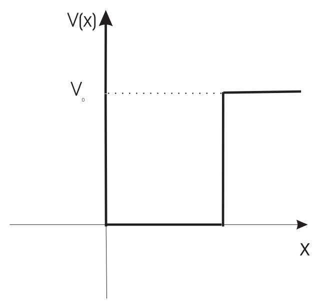

Fig. **1**

Solution in different regions

Region I $(x < 0)$**:** the potential is infinite.Therefore the solution must vanish:

$$u_{\text{I}}(x) = 0 \qquad \text{for } x < 0.$$

Region II $(0 < x < L)$**:** The Schrodinger equation can be cast as

$$-\frac{\hbar^2}{2m}\frac{d^2u}{dx^2} + k^2u = 0.$$

and the solution is given by

$$u_{\text{II}}(x) = A \sin kx + B \cos kx, 0 < x < L.$$

Region III $(0 < x < L)$**:** The Schrodinger equation can be written as

$$-\frac{\hbar^2}{2m}\frac{d^2u}{dx^2} - \alpha^2u = 0.$$

and most general solution has the form

$$u_{\text{III}}(x) = Ce^{-\alpha x} + De^{\alpha x}. \qquad (11)$$

Boundary conditions

- The potential has infinite jump discontinuity at $x = 0$. Therefore the solution $u_{\rm II}(x)$ must vanish at$x = 0$. Hence $B = 0$ and

$$u_{\rm II}(x) = A \sin kx, \qquad 0 < x < L.$$

- The wave function should not become infinite as $x \to \infty$. From (11) we get $D = 0$. Therefore

$$u_{\rm III}(x) = Ce^{\alpha x}$$

- The solution and its derivative must be continuous at $x = L$. This gives two conditions

$$u_{\rm II}(x)|_{x=L} = u_{\rm III}(x)|_{x=L} \implies A \sin kL = Ce^{-\alpha L}, \tag{12}$$
$$u'_{\rm II}(x)|_{x=L} = u'_{\rm III}(x)|_{x=L} \implies Ak \cos kL = -C\alpha e^{\alpha L}. \tag{13}$$

It is easily seen that the above conditions imply that nontrivial solution exists if

$$\boxed{k \cot kL = -\alpha}.$$

§3 Question [3]

§3.1 Definitions of Reflection and Transmission

§3.1.1 Potential properties at $\pm\infty$

We shall define reflection and transmission coefficients for a particle incident on a potential which tends to constant values [2]

$$V(x) \to \begin{cases} V_1 & \text{as } x \to -\infty, \\ V_2 & \text{as } x \to +\infty. \end{cases}$$

§3.1.2 Set up solution for $E > V_!, V_2$

Since the potential becomes constant at large distances,the particle travels like free particle with momenta $p_{1,2}^2 = \sqrt{2m(E - V_{1,2})}$. The wave function for large distances is therefore given by

$$\psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx}, & \text{as } x \to -\infty, \\ Ce^{iqx} + De^{-iqx}, & \text{as } x \to \infty. \end{cases} \tag{14}$$

where

$$k = p_1/\hbar = \sqrt{\frac{2m(E - V_1)}{\hbar^2}}, \qquad q = p_2/\hbar = \sqrt{\frac{2m(E - V_2)}{\hbar^2}}. \tag{15}$$

§3.1.3 Assume incident wave comes from $-\infty$

For a beam incident from the left, we can identify the incident, reflected and transmitted waves as follows.

Wave Type	Wave function	Flux
Incident beam	Ae^{ikx}	$\frac{\hbar k}{m}\lvert A^2\rvert$
Reflected beam	Be^{-ikx}	$\frac{\hbar k}{m}\lvert B^2\rvert$
Transmitted beam	Ce^{iqx}	$\frac{\hbar q}{m}\lvert C^2\rvert$

§3.1.4 Apply boundary condition for $x \to \infty$

The last column in the table shows the flux as computed using probability current

$$J = \frac{\hbar}{2im}\left\{\psi^*(x)\frac{d\psi}{dx} - \psi(x)\frac{d\psi^*}{dx}\right\} \tag{16}$$

There should be no wave travelling to the left in the transmission region. This means that $D = 0$.

§3.1.5 Define reflection and transmission coefficients

The reflection and transmission coefficients are computed as ratios of corresponding fluxes with the flux of the incident beam.

$$\text{Transmission coefficient} = \frac{\text{Flux of transmitted wave}}{\text{Flux of incident wave}} = \frac{|B|^2}{|A|^2} \tag{17}$$

$$\text{Reflection coefficient} = \frac{\text{Flux of reflected wave}}{\text{Flux of incident wave}} = \frac{q}{k}\frac{|C|^2}{|A|^2} \tag{18}$$

§3.2 Probability conservation implies $T + R = 1$

The state of system corresponding to wave function $u_E(x)$, solution of time independent Schrodinger equation for energy E, has time dependence given by

$$Hu_E(x) = Eu_E(x) \Longrightarrow \text{ wave function at time } t = \psi(x,t) = u_E(x)e^{-iEt/\hbar}. \tag{19}$$

Hence the probability density, as given by $\rho(x,t) = |\psi(x,t)|^2 = |u_E(x)|^2$, is independent of time. In fact the probability current $j(x,t)$ is also independent of time. Hence the probability conservation equation of continuity (in one dimension) takes the form

$$\frac{\partial \rho}{\partial t} + \frac{\partial j}{\partial x} = 0 \Longrightarrow \frac{\partial j}{\partial x} = 0 \tag{20}$$

Therefore $j(x,t)$ is independent of x also. We therefore compute the flux density at large distances using the wave function at large distance in Eq.(14)

$$j(-\infty) = \frac{\hbar k}{m}(|A|^2 - |B|^2), \tag{21}$$

$$j(+\infty) = \frac{\hbar q}{m}(|C|^2 - |D|^2) = \frac{\hbar q}{m}|C|^2, \qquad \because D = 0 \tag{22}$$

and equate the values at $+\infty$ and $-\infty$:

$$j(-\infty) = j(+\infty) \Longrightarrow \frac{\hbar k}{m}(|A|^2 - |B|^2) = \frac{\hbar q}{m}|C|^2 \tag{23}$$

The last relation can be rearranged to give $T + R = 1$.