Physics 741 – Graduate Quantum Mechanics 1

Solution Set M

1. **[20] A particle of mass *m* and energy *E* in two dimensions is incident on a plane step function given by**

$$V\left(Q_x,Q_y\right)=\begin{cases}0 & \text{if } Q_x<0,\\ V_0 & \text{if } Q_x>0.\end{cases}$$

The incoming wave has wave function $\psi_{\text{in}}\left(x,y\right)=e^{i\left(k_x x+k_y y\right)}$ **for** $x<0$**.**

(a) [7] Write the Hamiltonian. Determine the energy *E* for the incident wave. Convince yourself that the Hamiltonian has a translation symmetry, and therefore that the transmitted and reflected wave will share something in common with the incident wave (they are all eigenstates of what operator?).

The Hamiltonian, of course, is just

$$H=\frac{p_x^2+p_y^2}{2m}+V\left(x,y\right)=-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)+V\left(x,y\right)$$

The incident wave will therefore have an energy

$$E\psi=H\psi=-\frac{\hbar^2}{2m}\left(\left(ik_x\right)^2+\left(ik_y\right)^2\right)\psi+V\left(x,y\right)\psi=\frac{\hbar^2\left(k_x^2+k_y^2\right)}{2m}\psi\ ,$$

so that $E=\hbar^2\left(k_x^2+k_y^2\right)\big/2m$.

The potential depends on *x*, but is independent of *y*. Therefore, they are eigenstates of the translation operator in the *y*-direction, $T\left(a\hat{y}\right)$, for any *a*. Since this is a continuous symmetry, we can consider small translations, and we define the momentum operator in the *y*-direction P_y in the usual way, and our state must be an eigenstate of this operator as well. Our wave must therefore take the form

$$\psi\left(x,y\right)=e^{ik_y y}X\left(x\right).$$

It remains only to find the function $X(x)$.

(b) [7] Write the general form of the reflected and transmitted wave. Use Schrödinger's equation to solve for the values of the unknown parts of the momentum for each of these waves (assume $k_x^2\hbar^2/2m > V_0$).

If we plug our general solution into Schrödinger's equation, we have

$$Ee^{ik_y y}X(x) = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)\left(e^{ik_y y}X(x)\right)+V(x,y)e^{ik_y y}X(x),$$

$$\frac{\hbar^2\left(k_x^2+k_y^2\right)}{2m}e^{ik_y y}X(x) = \left(\frac{\hbar^2 k_y^2}{2m}-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\right)e^{ik_y y}X(x)+V(x,y)e^{ik_y y}X(x).$$

The exponentials cancel everywhere, and some factors can be cancelled. Solving for the second derivative term, we find

$$\frac{\partial^2 X(x)}{\partial x^2} = \left[\frac{2mV(x,y)}{\hbar^2}-k_x^2\right]X(x).$$

This equation is easy to solve. For *x*<0, the potential is zero, and we are solving $X'' = -k^2 X$ and the solutions are proportional to $e^{\pm ik_x x}$. For $x > 0$, we can define $k_x'^2 = k_x^2 - 2mV_0/\hbar^2$, and we are solving $X'' = -k'^2 X$ and the solutions are proportional to $e^{\pm ik_x' x}$.

The incident wave is $X_I = e^{+ik_x x}$. The wave going the other way in this region must be the reflected wave, $X_R \propto e^{-ik_x x}$. In the other region, the wave proportional to $e^{+ik_x' x}$ is a wave traveling to the right, so we have $X_T \propto e^{+ik_x' x}$. The wave proportional to $e^{-ik_x' x}$ would represent a wave moving to the left from infinity on the right, so this doesn't represent anything in this problem. Reinstating the *y*-dependence, and throwing in some constants of proportionality, our waves are

$$\psi_I = e^{+ik_x x+ik_y y}\ , \qquad \psi_R = Ae^{-ik_x x+ik_y y}\ , \qquad \psi_T = Be^{ik_x' x+ik_y y}$$

(c) [8] Assume the wave function and its derivative are continuous across the boundary *x* = 0. Find the amplitudes for the transmitted and reflected waves, and find the probability *R* of the wave being reflected.

The wave in the region $x < 0$ is given by $\psi_I + \psi_R$, and on the right, by ψ_T. Matching these wave functions and their derivatives in the *x*-direction at the boundary, we have

$$e^{ik_y y} + Ae^{ik_y y} = Be^{ik_y y} \qquad \text{and} \qquad k_x e^{ik_y y} - Ak_x e^{ik_y y} = Bk_x' e^{ik_y y}$$

When we cancel the common phase on both sides of each of these equations, the first equation becomes 1 + *A* = *B*, and substituting this into the second yields

$$k_x - Ak_x = (1+A)k_x'.$$

Rearranging this a bit, we have

$$k_x - k_x' = \left(k_x + k_x'\right) A, \quad A = \frac{k_x - k_x'}{k_x + k_x'} \quad \text{and} \quad B = 1 + A = \frac{2k_x}{k_x + k_x'}$$

The reflected wave function is $\psi_R = Ae^{-ik_x x + ik_y y}$, and this has a probability density of $\left|\psi_R\right|^2 = \left|A\right|^2$, as opposed to the incident wave, which has $\left|\psi_I\right|^2 = 1$, so the probability of reflection is

$$R = A^2 = \left(\frac{k_x - k_x'}{k_x + k_x'}\right)^2 = \left(\frac{k_x - \sqrt{k_x^2 - 2mV_0/\hbar^2}}{k_x + \sqrt{k_x^2 - 2mV_0/\hbar^2}}\right)^2 .$$

2. [15] A particle in three dimensions has Hamiltonian

$$H = \frac{1}{2M}\left(P_x^2 + P_y^2 + P_z^2\right) + \tfrac{1}{4}A\left(Q_x^2 + Q_y^2\right)^2$$

(a) [6] Show that this Hamiltonian has *two* continuous symmetries, and that they commute. Call the corresponding eigenvalues *m* and *k*. Are there any restrictions on *k* and *m*?

First, it is obvious that the potential is independent of Q_z, and therefore there is a continuous translation symmetry in this direction. Secondly, it is easy to see that rotation about the *z*-axis leaves the Hamiltonian unchanged. Specifically, define a set of rotated operators

$$\begin{aligned} Q_x' &= Q_x \cos\theta - Q_y \sin\theta \\ Q_y' &= Q_y \cos\theta + Q_x \sin\theta \end{aligned}$$

Then if we treat the potential as $V(x, y) = \tfrac{1}{4}A\left(x^2 + y^2\right)^2$, then we have

$$\begin{aligned} V\left(Q_x', Q_y'\right) &= \tfrac{1}{4}A\left[\left(Q_x \cos\theta - Q_y \sin\theta\right)^2 + \left(Q_y \cos\theta + Q_x \sin\theta\right)^2\right]^2 \\ &= \tfrac{1}{4}A\begin{bmatrix} Q_x^2 \cos^2\theta - 2Q_xQ_y \cos\theta\sin\theta + Q_y^2 \sin\theta \\ +Q_y^2 \cos^2\theta + 2Q_xQ_y \cos\theta\sin\theta + Q_x^2 \sin^2\theta \end{bmatrix}^2 \\ &= \tfrac{1}{4}A\left(Q_x^2 + Q_y^2\right)^2 = V\left(Q_x, Q_y\right) \end{aligned}$$

Because we have translation symmetry in the *z*-direction and rotation about the *z*-axis, our Hamiltonian will commute with the generators of these groups, P_z and L_z. Our energy eigenstates can also be chosen to be eigenstates of these operators, and we will have

$$P_z\left|\phi\right\rangle = \hbar k\left|\phi\right\rangle \qquad \text{and} \qquad L_z\left|\phi\right\rangle = \hbar m\left|\phi\right\rangle$$

As argued in class, the eigenvalue *m* is forced to be an integer.

(b) [9] What would be an appropriate set of coordinates for writing the eigenstates of this Hamiltonian? Write the eigenstates as a product of three functions (which I call *Z, R,* and Φ), and give me the explicit form of two of these functions.

Clearly, z is a good coordinate to use, since our eigenstates of the Hamiltonian are eigenstates of P_z. However, since they are also eigenstates of L_z, it seems like a good idea to change coordinates to cylindrical coordinates (ρ,ϕ,z), which are related to Cartesian coordinates by

$$\begin{aligned} x &= \rho\cos\phi \\ y &= \rho\sin\phi \\ z &= z \end{aligned} \qquad \text{or} \qquad \begin{aligned} \rho &= \sqrt{x^2+y^2} \\ \phi &= \tan^{-1}(y/x) \\ z &= z \end{aligned}$$

If we write our wave function in terms of these coordinates, and assume it factors, we have

$$\psi(\rho,\phi,z) = R(\rho)\Phi(\phi)Z(z)$$

If we demand that this be an eigenstate of P_z with eigenvalue $\hbar k$, then we find

$$\hbar k Z(z) = P_z Z(z) = \frac{\hbar}{i}\frac{\partial}{\partial z}Z(z) \qquad \text{so that} \qquad Z(z) = e^{ikz}$$

Similarly, if we demand that $\psi(\rho,\phi,z)$ be an eigenstate of L_z with eigenvalue $\hbar m$, then we find

$$\hbar m\Phi(\phi) = L_z\Phi(\phi) = \frac{\hbar}{i}\frac{\partial}{\partial\phi}\Phi(\phi) \qquad \text{so that} \qquad \Phi(\phi) = e^{im\phi}$$

There is a certain arbitrariness in normalization, and the choices we have made have perhaps not been the best, but up to a constant, we therefore find

$$\psi(\rho,\phi,z) = R(\rho)e^{ikz+im\phi}.$$

If we wished, we could now easily write an explicit equation for the radial function R. Writing the Laplacian that is implicit in the kinetic term in the Hamiltonian in cylindrical coordinates, we find

$$H\psi = -\frac{\hbar^2}{2M}\left(\frac{\partial^2\psi}{\partial\rho^2} + \frac{1}{\rho}\frac{\partial\psi}{\partial\rho} + \frac{1}{\rho^2}\frac{\partial^2\psi}{\partial\phi^2} + \frac{\partial^2\psi}{\partial z^2}\right) + \tfrac{1}{4}A\left(\rho^2\right)^2\psi$$

Plugging in our explicit form for the wave function, and using Schrödinger's equation $H\psi = E\psi$, we have

$$ER = -\frac{\hbar^2}{2M}\left(\frac{d^2R}{d\rho^2} + \frac{1}{\rho}\frac{dR}{d\rho}\right) + \left[\frac{\hbar^2k^2}{2M} + \frac{\hbar^2m^2}{2M\rho^2} + \tfrac{1}{4}A\rho^4\right]R\,.$$