Quantum Mechanics III — Epiphany Term 2009

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Homework 2 – due 26 February 2009

1. A particle of mass m in one dimenion is subject to the potential

$$V(x) = \begin{cases} V_1 & (x < 0) \\ 0 & (0 < x < L) \\ V_2 & (x > L) \end{cases}$$

where $V_2 > V_1 > 0$.

(a) In each of the following regions of energy E, determine if there may be states (i.e. eigenstates of the Hamiltonian), and if so, if they are confined states or scattering states: $E < 0$, $0 < E < V_1$, $V_1 < E < V_2$, $E > V_2$.

(b) In each of the regions where there may be states: if they are scattering states, determine the reflection and transmission coefficients for particles incoming from the left (from $x = -\infty$), and if they are confined states, derive the algebraic equation (involving the variable E and the parameters V_1, V_2, L, m) that fixes the energy levels.

Answer

(a) $E < 0$: no states, because E is smaller than the minimum of the potential. $0 < E < V_1$: bound states, because E is between the minimum of the potential and the minimum of the asymptotic values of the potential. $V_1 < E < V_2$: scattering states, because E is larger than the minimum of the asymptotic values of the potential (which is V_1 here). $E > V_2$: scattering states, same reason.

(b) For $V_1 < E < V_2$: we have scattering states without any transmission, since in the region $x > L$, the wave function is exponentially decreasing. Hence $T = 0$, and a calculation would give a reflection coefficient $R = 1$, since the formula $R + T = 1$ is always valid. No need to calculate it explicitly!

Consider $E > V_2$. We write the wave function for $x < 0$ as ψ_1, that of $0 < x < L$ as ψ_0, and that of $x > L$ as ψ_2. Then, we immediately have, since the potential is flat in the three regions,

$$\begin{aligned} \psi_1(x) &= Ae^{ip_1x/\hbar} + Be^{-ip_1x/\hbar}, \quad p_1 = \sqrt{2m(E - V_1)} > 0 \\ \psi_0(x) &= C\sin(p_0x/\hbar) + D\cos(p_0x/\hbar), \quad p_0 = \sqrt{2mE} > 0 \\ \psi_2(x) &= Ee^{ip_2x/\hbar}, \quad p_2 = \sqrt{2m(E - V_2)} > 0 \end{aligned}$$

In the first region, we put both the incident and the reflected waves. In the second region, we also have both right-moving and left-moving waves, but we wrote them in terms of sine and cosine functions instead for convenience. In the third region, we only have transmitted waves.

The continuity equations at $x = 0$ give

$$\begin{array}{rcl} \psi_1(0) = \psi_0(0) & \Rightarrow & A + B = D \\ \psi_1'(0) = \psi_0'(0) & \Rightarrow & ip_1(A - B) = p_0 C \end{array} \tag{1}$$

and those at $x = L$ give

$$\begin{array}{rcl} \psi_0(0) = \psi_2(0) & \Rightarrow & Cs + Dc = Ee \\ \psi_0'(0) = \psi_2'(0) & \Rightarrow & p_0(Cc - Ds) = ip_2 Ee \end{array} \tag{2}$$

where we define for convenience

$$s \equiv \sin(p_0 L/\hbar), \quad c \equiv \cos(p_0 L/\hbar), \quad e \equiv e^{ip_2 L/\hbar} \tag{3}$$

Putting the continuity equations together by eliminating the intermediate constants C and D (which only have to do with the waves in the region $0 < x < L$, hence are not directly involved in the calculation of R and T), we get

$$\begin{array}{rcl} \frac{ip_1}{p_0}(A - B)s + (A + B)c & = & Ee \\ ip_1(A - B)c + p_0(A + B)s & = & ip_2 Ee \end{array}$$

We write that as a matrix equation for the vector $\begin{pmatrix} A \\ B \end{pmatrix}$:

$$\begin{pmatrix} \frac{ip_1}{p_0}s + c & -\frac{ip_1}{p_0}s + c \\ ip_1 c - p_0 s & -ip_1 c - p_0 s \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix} = Ee \begin{pmatrix} 1 \\ ip_2 \end{pmatrix}$$

In order to invert the matrix, we need its determinant, which is very simple:

$$\begin{array}{rcl} \det & = & \left(\frac{ip_1}{p_0}s + c\right)(-ip_1 c - p_0 s) - \left(-\frac{ip_1}{p_0}s + c\right)(ip_1 c - p_0 s) \\ & = & 2i\mathrm{Im}\left[\left(\frac{ip_1}{p_0}s + c\right)(-ip_1 c - p_0 s)\right] \\ & = & -2ip_1 \end{array} \tag{4}$$

using $s^2 + c^2 = 1$. Then,

$$\begin{pmatrix} A \\ B \end{pmatrix} = -\frac{1}{2ip_1} \begin{pmatrix} -ip_1 c - p_0 s & \frac{ip_1}{p_0}s - c \\ -ip_1 c + p_0 s & \frac{ip_1}{p_0}s + c \end{pmatrix} Ee \begin{pmatrix} 1 \\ ip_2 \end{pmatrix}$$

In particular, we find

$$A = -\frac{Ee}{2ip_1}\left(-i(p_1+p_2)c - \frac{p_0^2+p_1p_2}{p_0}s\right)$$

so that

$$\begin{aligned}|A|^2 &= \frac{|E|^2}{4p_1^2}\left((p_1+p_2)^2c^2 + \left(\frac{p_0^2+p_1p_2}{p_0}\right)^2 s^2\right) \\ &= \frac{|E|^2}{4p_1^2}\left(4p_1p_2 + (p_1-p_2)^2c^2 + \left(\frac{p_0^2-p_1p_2}{p_0}\right)^2 s^2\right)\end{aligned}$$

where we used $|e| = 1$. Hence, the transmission coefficient is

$$T = \frac{|E|^2 p_2}{|A|^2 p_1} = \frac{4p_1p_2}{4p_1p_2 + U}$$

where

$$U = (p_1-p_2)^2c^2 + \left(\frac{p_0^2-p_1p_2}{p_0}\right)^2 s^2.$$

The reflection coefficient is simply

$$R = 1 - T = \frac{U}{4p_1p_2+U}$$

Note that the only cases where there can be pure transmission (where $U = 0$) are when both of the following equations are satisfied:

$$p_1 = p_2, \quad \sin(p_0L/\hbar) = 0$$

Finally, consider the case $0 < E < V_1$ (the bound states). The starting point is the following form of the wave function in the various regions, satisfying the condition of a vanishing wave function at $\pm\infty$:

$$\begin{aligned}\psi_1(x) &= Ae^{q_1x/\hbar}, \quad q_1 = \sqrt{2m(V_1-E)} > 0 \\ \psi_0(x) &= B\sin(p_0x/\hbar) + C\cos(p_0x/\hbar), \quad p_0 = \sqrt{2mE} > 0 \\ \psi_2(x) &= De^{-q_2x/\hbar}, \quad q_2 = \sqrt{2m(V_2-E)} > 0\end{aligned}$$

The continuity equations give

$$\begin{aligned}A &= C \\ q_1A &= p_0B\end{aligned}$$

and

$$\begin{aligned}Bs + Cc &= Df \\ p_0(Bc - Cs) &= -q_2Df \end{aligned} \tag{5}$$

where s and c are as before, and where $f = e^{-q_2 L/\hbar}$. Putting these equations together, we find

$$\begin{aligned} \frac{q_1}{p_0}s + c &= \frac{Df}{A} \\ q_1 c - p_0 s &= -q_2 \frac{Df}{A} \end{aligned} \tag{6}$$

so that, eliminating D in order to obtain an equation that does not involve any coefficients (just the energy variable remains)

$$p_0(q_1 + q_2)c + (q_1 q_2 - p_0^2)s = 0$$

which gives

$$\tan(p_0 L/\hbar) = \frac{p_0(q_1 + q_2)}{p_0^2 - q_1 q_2}$$

This is the algebraic equation that determines the possible values of energy, recalling that

$$p_0 = \sqrt{2mE}, \quad q_1 = \sqrt{2m(V_1 - E)}, \quad q_2 = \sqrt{2m(V_2 - E)}$$