Física Quântica I / Mecânica Quântica (2021/22)

Folha de Problemas 9 (Potenciais constantes por partes em 1D)

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— Soluções —

Nota: No final deste conjunto de problemas são listados alguns integrais úteis.

Problema 1 | Poço de potencial infinito I

Uma partícula de massa m é confinada pelo potencial unidimensional seguinte:

$$V(x) = \begin{cases} +\infty, & x < 0 \\ 0, & 0 < x < a \\ +\infty, & x > a \end{cases}, \qquad (a > 0).$$

1. Determine as funções de onda normalizadas $\varphi_n(x)$ que representam os estados estacionários da partícula neste potencial.

2. Represente esquematicamente o gráfico das funções $\varphi_1(x)$ e $\varphi_2(x)$ que correspondem aos dois estados de menor energia. Se existirem, identifique os zeros destas funções.

3. Supondo que o estado da partícula é descrito pela função de onda

$$\psi(x) = \frac{1}{\sqrt{a}} \begin{cases} 1, & 0 < x < a \\ 0, & \text{restantes } x \end{cases},$$

quais são os resultados possíveis numa medição da energia, e quais são as respetivas probabilidades?

4. Qual é a probabilidade de uma medição de energia resultar num valor inferior a $\frac{10\pi^2\hbar^2}{ma^2}$?

Solution

Important note: This potential is zero in the region $0 \leq x \leq a$. This is different from the one discussed in the lectures, which is zero in the region $-a/2 \leq x \leq a/2$. This difference will reflect in the form of the eigenfunctions computed below, which are also different from the ones obtained in the lecture notes. This illustrates why in this type of problem it's very important to, before doing anything else, first draw a sketch of the potential.

1. The normalized wavefunctions are

$$\varphi_n(x) = \begin{cases} \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right), & 0 < x < a \\ 0, & \text{otherwise} \end{cases}$$

where $n = 1, 2, 3, \ldots$ The energies corresponding to each of these states are

$$E_n = \frac{\hbar^2\pi^2 n^2}{2ma^2}.$$

2. Each wavefunction $\varphi_n(x)$ has $n-1$ nodes (zeros), located at the positions

$$x_0 = \frac{a}{n\pi},\, 2\frac{a}{n\pi},\, 3\frac{a}{n\pi}, \ldots, (n-1)\frac{a}{n\pi}.$$

3. The possible outcomes are one of the eigenvalues of the Hamiltonian, which are

$$E_n = \frac{\hbar^2\pi^2 n^2}{2ma^2}, \qquad (n = 1, 2, \ldots)\,.$$

The probability of measuring each specific energy eigenvalue is given, according to the probability postulate (and taking into account that the energy eigenstates of a 1D potential are all non-degenerate), by $p_n = |\langle\varphi_n|\psi\rangle|^2$. The inner product is

$$\begin{aligned}
\langle\varphi_n|\psi\rangle &= \int_{-\infty}^{+\infty} \varphi_n(x)^* \psi(x)\, dx \\
&= \int_0^a \left[\sqrt{\frac{2}{a}} \sin\frac{n\pi x}{a}\right] \left[\frac{1}{\sqrt{a}}\right] dx = \sqrt{\frac{2}{a^2}} \int_0^a \sin\frac{n\pi x}{a}\, dx \\
&= \sqrt{2}\left(\frac{1-\cos n\pi}{n\pi}\right) = \sqrt{2}\left[\frac{1-(-1)^n}{n\pi}\right].
\end{aligned}$$

Therefore, the probabilities are

$$p_n = |\langle\varphi_n|\psi\rangle|^2 = \begin{cases} 0, & n \text{ even} \\ \dfrac{8}{\pi^2 n^2}, & n \text{ odd} \end{cases}$$

[the fact that p_n is zero for n even in the state ψ should be clear by comparing the symmetry of the eigenfunctions $\varphi_n(x)$ relative to the symmetry of $\psi(x)$].

The final answer is therefore that we can only find the energies

$$E_n = \frac{\hbar^2\pi^2 n^2}{2ma^2} \qquad \text{with } n \text{ odd, and probability} \qquad p_n = \frac{8}{\pi^2 n^2}.$$

4. First we look for the state with highest energy, but yet smaller than the given value:

$$\frac{\hbar^2\pi^2 n^2}{2ma^2} < \frac{10\pi^2\hbar^2}{ma^2} \quad \Leftrightarrow \quad n^2 < 20 \quad \Leftrightarrow \quad n \le 4,$$

because n is an integer. Therefore the levels $n = 1, 2, 3, 4$ have energy smaller than the requested value. The probability of obtaining an energy smaller than that is then

$$\sum_{n=1}^{4} p_n = p_1 + p_3 = \frac{8}{\pi^2}\left(1 + \frac{1}{9}\right) = \frac{80}{9\pi^2} \simeq 0.9.$$

Problema 2 | Poço de potencial infinito II

Considere uma partícula confinada pelo potencial infinito seguinte:

$$V(x) = \begin{cases} 0, & |x| \le \frac{a}{2} \\ +\infty & |x| > \frac{a}{2} \end{cases}.$$

Se designarmos por $|\varphi_n\rangle$ o estado estacionário (autoestado do Hamiltoniano) associado à energia E_n, sabemos através dos resultados discutidos nas aulas que

$$E_n = \frac{\hbar^2\pi^2 n^2}{2ma^2} \qquad \text{e} \qquad \varphi_n(x) = \langle x|\varphi_n\rangle = \begin{cases} \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right), & n \text{ par} \\ \sqrt{\frac{2}{a}}\cos\left(\frac{n\pi x}{a}\right), & n \text{ ímpar} \end{cases}.$$

1. Para cada estado estacionário, calcule $\langle\hat{X}\rangle_n$, $\langle\hat{X}^2\rangle_n$, $\langle\hat{P}\rangle_n$, $\langle\hat{P}^2\rangle_n$, onde esta notação significa $\langle\hat{A}\rangle_n \equiv \langle\varphi_n|\hat{A}|\varphi_n\rangle$. *Nota: utilize a simetria sempre que possível e recorra ao Apêndice para os integrais que precisará de calcular.*

2. Calcule o produto das incertezas $\delta X\delta P$ para cada estado estacionário φ_n.

3. Suponha que a partícula é preparada em $t = 0$ no estado

$$|\psi\rangle = \frac{1}{\sqrt{2}}|\varphi_1\rangle + \frac{1}{\sqrt{2}}|\varphi_2\rangle.$$

   Com este estado de partida:

   a) Calcule a função de onda e a distribuição de probabilidade no instante t.

   b) Calcule $\langle\hat{X}\rangle_\psi$ em função do tempo e mostre que varia periodicamente entre $\pm\frac{16a}{9\pi^2}$.

   c) Era de esperar que $\langle\hat{X}\rangle_\psi$ variasse no tempo? Explique.

Solution

1. Starting with the position, by symmetry we expect $\langle\hat{X}\rangle$ to be zero. Let's verify that explicitly:

$$\langle\hat{X}\rangle = \int_{-a/2}^{a/2} x\,|\varphi_n(x)|^2\,dx = 0$$

   because $|\varphi_n(x)|^2$ is an even function of x for both n even and n odd. The next expectation value is

$$\langle\hat{X}^2\rangle = \int_{-a/2}^{a/2} x^2\,|\varphi_n(x)|^2\,dx = \frac{2}{a}\begin{cases} \int_{-a/2}^{a/2} x^2\sin^2\left(\frac{n\pi x}{a}\right)dx, & n \text{ even} \\ \int_{-a/2}^{a/2} x^2\cos^2\left(\frac{n\pi x}{a}\right)dx, & n \text{ odd} \end{cases}$$

   Using one of the results from the appendix this becomes

$$\langle\hat{X}^2\rangle = \frac{1}{12}a^2\left(1 - \frac{6}{n^2\pi^2}\right).$$

   The expectation value of the momentum should be zero because the states are described by real eigenfunctions (we saw that in "Folha de Problemas 7"). To see it explicitly here:

$$\begin{aligned} \langle\hat{P}\rangle &= -i\hbar\int_{-a/2}^{+a/2}\varphi_n(x)\varphi_n'(x)dx \\ \text{(for even and odd)} \qquad &= \pm\frac{2i\hbar}{a}\left(\frac{n\pi}{a}\right)\int_{-a/2}^{+a/2}\sin\left(\frac{n\pi x}{a}\right)\cos\left(\frac{n\pi x}{a}\right)dx \\ &= 0 \end{aligned}$$

because the integrand is an odd function.

The last expectation value is

$$\langle \hat{P}^2 \rangle = -\hbar^2 \int_{-a/2}^{+a/2} \varphi_n(x)\varphi_n''(x)dx.$$

But, since for both even and odd n we have

$$\varphi_n''(x) = -\left(\frac{n\pi}{a}\right)^2 \varphi_n(x),$$

the result is simply

$$\langle \hat{P}^2 \rangle = \left(\frac{n\hbar\pi}{a}\right)^2 \int_{-a/2}^{+a/2} [\varphi_n(x)]^2 \, dx = \left(\frac{n\hbar\pi}{a}\right)^2,$$

where we used the fact that the $\varphi_n(x)$ given in the problem are normalized.

2. From the results obtained above

$$\delta X = \sqrt{\langle \hat{X}^2 \rangle - \langle \hat{X} \rangle} = a\sqrt{\frac{1}{12} - \frac{1}{2n^2\pi^2}}, \qquad \text{and} \qquad \delta P = \frac{|n|\,\hbar\pi}{a},$$

and hence

$$\delta X \delta P = \hbar\sqrt{\frac{\pi^2 n^2}{12} - \frac{1}{2}}.$$

Note that the product of these uncertainties increases with n. Its smallest value is

$$\delta X \delta P\bigg|_{\text{min}} = \hbar\sqrt{\frac{\pi^2}{12} - \frac{1}{2}},$$

which is $\geq \hbar/2$, as should always be the case according to Heisenberg's uncertainty relation between the position and momentum observables.

3. The wavefunction that describes the initial state is

$$|\psi(0)\rangle = \frac{1}{\sqrt{2}}|\varphi_1\rangle + \frac{1}{\sqrt{2}}|\varphi_2\rangle \qquad \longrightarrow \qquad \psi(x,0) = \frac{1}{\sqrt{2}}\varphi_1(x) + \frac{1}{\sqrt{2}}\varphi_2(x).$$

a) Recall that the time dependence of the state vector is given by

$$|\psi(t)\rangle = \sum_n \langle \varphi_n|\psi(0)\rangle \, e^{-iE_n t/\hbar} \, |\varphi_n\rangle.$$

Since the initial state $|\psi(0)\rangle$ is already given as a linear combination of energy eigenstates, the time evolved state is simply

$$|\psi(t)\rangle = \frac{e^{-iE_1 t/\hbar}}{\sqrt{2}}|\varphi_1\rangle + \frac{e^{-iE_2 t/\hbar}}{\sqrt{2}}|\varphi_2\rangle.$$

Projecting onto the position basis, we get the corresponding wavefunction:

$$\psi(x,t) = \frac{e^{-iE_1 t/\hbar}}{\sqrt{2}}\varphi_1(x) + \frac{e^{-iE_2 t/\hbar}}{\sqrt{2}}\varphi_2(x), \qquad \text{with} \qquad E_n = \frac{\hbar^2\pi^2 n^2}{2ma^2}.$$

The probability density is

$$\begin{aligned} |\psi(x,t)|^2 &= \frac{1}{2}\left|\varphi_1(x) + e^{-i(E_2-E_1)t/\hbar}\varphi_2(x)\right|^2 \\ &= \frac{1}{2}\,|\varphi_1(x)|^2 + \frac{1}{2}\,|\varphi_2(x)|^2 + \varphi_1(x)\varphi_2(x)\cos\left[\frac{(E_2-E_1)\,t}{\hbar}\right]. \end{aligned}$$

b) The expectation value of the position is given by

$$\langle \hat{X} \rangle = \int_{-a/2}^{+a/2} |\psi(x,t)|^2 \, x \, dx = \cos\left[\frac{(E_2 - E_1)\, t}{\hbar}\right] \int_{-a/2}^{+a/2} \varphi_1(x)\varphi_2(x) x \, dx,$$

where we used the above-derived result

$$\langle \varphi_n | \hat{X} | \varphi_n \rangle = 0$$

to simplify the integrals involving $|\varphi_1(x)|$ and $|\varphi_2(x)|$. The integral that remains is calculated using one of the results listed in the appendix:

$$\int_{-a/2}^{+a/2} \varphi_1(x)\varphi_2(x) x \, dx = \frac{2}{a} \int_{-a/2}^{+a/2} x \cos\left(\frac{\pi x}{a}\right) \sin\left(\frac{2\pi x}{a}\right) dx = \frac{16a}{9\pi^2}.$$

Therefore, the average position is

$$\langle \hat{X} \rangle = \frac{16a}{9\pi^2} \cos\left[\frac{(E_2 - E_1)\, t}{\hbar}\right],$$

which oscillates at a frequency

$$\omega_{21} \equiv \frac{E_2 - E_1}{\hbar} = \frac{3\hbar\pi^2}{2ma^2},$$

between the extremal values $\pm 16a/(9\pi^2)$.

c) The expectation value of an observable in a generic states is constant in time if either (i) the expectation is taken with respect to a stationary state, or (ii) the operator commutes with the Hamiltonian. Condition (i) is not verified because the initial state $\psi(0)$ is not a stationary state (note that a linear combination of stationary states is *not* a stationary state). Condition (ii) is also not satisfied because the Hamiltonian of the particle includes the kinetic energy part $\hat{\mathrm{P}}^2/(2m)$, which does not commute with $\hat{\mathrm{X}}$. Therefore, we necessarily could anticipate that $\langle \hat{X} \rangle$ would vary with time.

Problema 3 | Poço de potencial infinito III

Considere uma partícula confinada no seguinte poço de potencial infinito:

$$V(x) = \begin{cases} 0, & 0 < x < a \\ +\infty, & x > a \ \lor \ x < 0 \end{cases}, \qquad (a > 0),$$

e sejam $|\varphi_n\rangle$ os autoestados de energia E_n. Num determinado instante, a função de onda é

$$\psi(x) = \begin{cases} \mathcal{N}\, x\,(a - x)\,, & 0 < x < a \\ 0, & x > a \ \lor \ x < a \end{cases},$$

onde $\mathcal{N}$ é uma constante de normalização.

1. Se a energia for medida neste instante, qual é a probabilidade (p_n) de obtermos cada uma das energias, E_n, dos estados estacionários neste potencial? Calcule o valor numérico de p_n para os 5 estados de menor energia.

2. Esquematize graficamente a função $\psi(x)$ e a função que representa o estado fundamental, $\varphi_1(x)$. Comparando estas duas funções, consegue justificar o tipo de variação de p_n com n obtida na questão anterior?

3. Mostre que, no estado $\psi(x)$, o valor esperado da energia da partícula é

$$\langle \hat{H} \rangle_\psi = \frac{5\hbar^2}{ma^2}.$$

Consegue explicar porque este resultado é próximo da energia do estado fundamental, E_1, tendo em conta o que concluiu nas questões precedentes?

4. Como bónus, este problema permite-nos demonstrar facilmente que

$$\sum_{s=1}^{\infty} \frac{1}{(2s-1)^4} = \frac{\pi^4}{96} \qquad \text{e} \qquad \sum_{s=1}^{\infty} \frac{1}{(2s-1)^6} = \frac{\pi^6}{960}.$$

Demonstre estas duas identidades usando o resultado obtido acima para p_n e recordando que

$$\langle \hat{H} \rangle = \sum_{n=1}^{\infty} p_n E_n \qquad \text{e} \qquad \sum_{n=1}^{\infty} p_n = 1.$$

Solution

Since the questions in this problem require us to know the energy eigenstates, we first determine them. Their wavefunctions will clearly be non-zero only in the region $0 < x < a$, where the general solution for the Schrodinger equation is

$$\varphi(x) = Ae^{ikx} + Be^{-ikx}, \qquad k = \sqrt{\frac{2mE}{\hbar^2}}.$$

Imposing the continuity of $\varphi(x)$ at $x = 0$ and $x = a$ we obtain the two equations

$$A + B = 0 \qquad \text{and} \qquad Ae^{ika} + Be^{-ika} = 0.$$

Combining them we get

$$A \sin(ka) = 0.$$

The solution is either $k = n\pi/a$ and $A \neq 0$, or $A = 0$ and $k \neq 0$. The last one leads to $\varphi(x) = 0$ everywhere, which is the trivial solution we're not interested in. Hence, we are left with the solutions

$$\varphi_n(x) = A \sin(k_n a), \qquad k_n = \frac{n\pi}{a}, \qquad n = 1, 2, \ldots$$

Finally we normalize them obtaining

$$\int_0^a |\varphi_n(x)|^2 = 1 \quad \longrightarrow \quad \varphi_n(x) = \sqrt{\frac{2}{a}} \sin(k_n a), \qquad k_n = \frac{n\pi}{a}, \qquad n = 1, 2, \ldots$$

for $0 \leq x \leq a$, and $\varphi_n(x) = 0$ elsewhere. The respective energy eigenvalues are

$$E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{\hbar^2 \pi^2 n^2}{2ma^2} \qquad n = 1, 2, \ldots$$

1. The probability of obtaining the energy E_n is given, as usual, by

$$p_n = |\langle\varphi_n|\psi\rangle|^2 \,,$$

when the state $|\psi\rangle$ is normalized. So first we determine the proper normalization constant for the given state ψ:

$$\frac{1}{\mathcal{N}^2} = \int_0^a x^2 (a-x)^2 \, dx = \int_0^a \left(a^2x^2 - 2ax^3 + x^4\right) \, dx = a^5 \left(\frac{1}{3} - \frac{1}{2} + \frac{1}{5}\right) = \frac{a^5}{30}.$$

So,

$$\mathcal{N} = \sqrt{\frac{30}{a^5}}.$$

Next we need to calculate the projection of the particle's state on the n-th eigenstate:

$$\langle\varphi_n|\psi\rangle = \int_{-\infty}^{+\infty} dx\, \varphi_n^*(x)\psi(x) = \sqrt{\frac{2\mathcal{N}^2}{a}} \int_0^a x\,(a-x) \sin\left(k_n x\right) \, dx.$$

Using the primitives given in the Appendix, we have

$$\int_0^a x \sin\left(k_n x\right) \, dx = \frac{1}{k_n^2} \Big[\sin k_n x - k_n x \, \cos k_n x\Big|_0^a = -\left(-1\right)^n \frac{a}{k_n},$$

and

$$\begin{aligned}\int_0^a x^2 \sin\left(k_n x\right) \, dx &= \frac{1}{k_n^3} \Big[2k_n x \, \sin(k_n x) + \left(2 - k_n^2 x^2\right) \cos(k_n x)\Big|_0^a \\ &= \frac{1}{k_n^3} \Big[\left(-1\right)^n \left(2 - k_n^2 a^2\right) - 2\Big].\end{aligned}$$

Putting everything together, we arrive at

$$\langle\varphi_n|\psi\rangle = \frac{2}{k_n^3} \sqrt{\frac{2\mathcal{N}^2}{a}} \Big[1 - \left(-1\right)^n\Big],$$

which means that the probabilities are

$$p_n = \begin{cases} \frac{960}{n^6\pi^6}, & n \text{ odd} \\ 0 & n \text{ even} \end{cases}$$

The numerical values for the 5 lowest energy eigenstates are

$$p_1 \simeq 0.9986, \qquad p_2 = 0, \qquad p_3 \simeq 0.0014, \qquad p_4 = 0, \qquad p_5 \simeq 6 \times 10^{-5}.$$

2. The normalized wavefunction and ground state are

$$\psi(x) = \sqrt{\frac{30}{a^5}} x\,(a-x) \,, \qquad \varphi_1(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right) ,$$

in the well region and zero outside. The function $\psi(x)$ is an inverted parabola intersecting the x axis at $x = 0$ and $x = a$, and with maximum value

$$\psi\left(\tfrac{a}{2}\right) = \frac{1}{\sqrt{a}} \sqrt{\frac{30}{16}} \simeq 1.37 \times \frac{1}{\sqrt{a}}$$

When we draw the function $\varphi_1(x)$ we can see that it has a shape that closely follows that of $\psi(x)$, including the maximum value

$$\varphi_1(\tfrac{a}{2}) = \sqrt{\frac{2}{a}} \simeq 1.41 \times \frac{1}{\sqrt{a}}, \qquad \text{which is close to} \quad \psi\left(\tfrac{a}{2}\right) = 1.37 \times \frac{1}{\sqrt{a}}.$$

The two normalized functions $\psi(x)$ and $\varphi_n(x)$ therefore approximately overlap with each other in the entire space, which means that the value of

$$\langle \varphi_1 | \psi \rangle = \int_{-\infty}^{+\infty} dx\, \varphi_0^*(x)\psi(x)$$

is very nearly 1. Consequently, the probability of finding the particle in the ground state is also nearly 1. This, of course, implies that the probability associated with the other eigenstates is very small.

It is no surprise then that the probability p_n decays very abruptly with n (it decays as $\propto n^{-6}$), reflecting the fact that the initial wavefunction is almost coinciding with the lowest eigenstate, and that its overlap with higher eigenstates will be very small due to the oscillating nature of their wavefunctions.

In addition, it should be clear why $p_n = 0$ for even n, since the corresponding eigenfunctions $\varphi_n(x)$ for those cases are anti-symmetric with respect to the center, whereas $\psi(x)$ is symmetric.

3. The expectation value of the energy can be calculated from the expectation of the square of the momentum:

$$\begin{aligned}\langle \hat{H} \rangle = \frac{\langle \hat{P}^2 \rangle}{2m} &= \frac{-\hbar^2}{2m} \int_{-\infty}^{+\infty} \psi^*(x)\, \frac{d^2\psi(x)}{dx^2}\, dx = \frac{\hbar^2 \mathcal{N}^2}{m} \int_0^{+a} x\,(a-x)\, dx \\ &= \frac{\hbar^2 \mathcal{N}^2}{m} \left[\frac{a^3}{2} - \frac{a^3}{3} \right] = \frac{5\hbar^2}{ma^2}.\end{aligned}$$

As always, since we have calculated the probabilities p_n in an earlier question, we could have also obtained this expectation value from

$$\langle \hat{H} \rangle = \sum_{n=1}^{\infty} p_n E_n.$$

Now, note that

$$E_n p_n = \frac{\hbar^2 \pi^2 n^2}{2ma^2} \times \frac{960}{n^6 \pi^6} = \frac{480\hbar^2}{2\pi^4 ma^2} \times \frac{1}{n^4}, \qquad (n \text{ odd}),$$

which decays rapidly with n. Hence, in this particular problem, keeping only the largest term in the sum above will be a good approximation:

$$p_1 E_1 = \frac{480\hbar^2}{2\pi^4 ma^2} = 0.986 \left(\frac{5\hbar^2}{ma^2} \right) \simeq \langle \hat{H} \rangle.$$

Again, this is no surprise because, as discussed above, the wavefunction $\psi(x)$ almost completely overlaps with that of the ground state.

4. To prove the first result, we notice that, if the expectation value $\langle \hat{H} \rangle$ is expressed directly in terms of the probabilities, we have

$$\langle E \rangle = \sum_{n=1}^{\infty} p_n E_n.$$

Since $p_n = 0$ for n even, we need only to sum over the odd integers n. For that, we write $n = 2s-1$ and note that for $s = 1, 2, 3, \dots$ we get all the odd integers n. Therefore we can write the above as

$$\langle E \rangle = \sum_{n=1}^{\infty} p_n E_n = \frac{960\hbar^2\pi^2}{2m\pi^6 a^2} \sum_{s=1}^{\infty} \frac{1}{(2s-1)^4}.$$

Combining this with the result of the previous question, we can conclude that

$$\frac{960\hbar^2\pi^2}{2m\pi^6 a^2} \sum_{s=1}^{\infty} \frac{1}{(2s-1)^4} = \frac{5\hbar^2}{ma^2} \qquad \Leftrightarrow \qquad \sum_{s=1}^{\infty} \frac{1}{(2s-1)^4} = \frac{\pi^4}{96} \qquad \boxdot$$

To obtain the second result we use the normalization condition on the probabilities:

$$\sum_{n=1}^{\infty} p_n = 1.$$

Replacing here the p_n obtained earlier and performing the same substitution $n = 2s-1$, this equation becomes

$$1 = \frac{960}{\pi^6} \sum_{s=1}^{\infty} \frac{1}{(2s-1)^6} \qquad \Leftrightarrow \qquad \sum_{s=1}^{\infty} \frac{1}{(2s-1)^6} = \frac{\pi^6}{960} \qquad \boxdot$$

Comment: Notice that the eigenfunctions obtained above for this infinite well are

$$\varphi_n(x) = \sqrt{\frac{2}{a}} \sin(k_n a),$$

irrespective of whether n is even or odd. If this appears to you to be different from what we derived in the lectures for the eigenfunctions of the infinite potential well, notice that the potential well is defined here from $0 < x < a$, whereas in the lectures we defined the potential in the interval $-a/2 < x < a/2$. Consequently the wavefunctions have to be different, but you can check that the ones here are just a simple translation of the ones in the lecture notes. Of course the energies are the same, irrespective of where the centre of the potential is.

Problema 4 | Periodicidade do movimento num poço de potencial infinito

Considere uma partícula confinada num poço de potencial infinito de largura L, e uma qualquer função de onda $\psi(x)$ que especifica o estado da partícula no instante $t = 0$.

1. Escreva a expressão geral que descreve a evolução temporal da função de onda, $\psi(x,t)$, em termos dos estados estacionários deste problema.

2. Mostre que essa função de onda é periódica no tempo; isto é,

$$\psi(x,t+T)=\psi(x,t), \qquad \text{onde} \qquad T=\frac{4mL^2}{\pi\hbar}.$$

3. Note que este período se pode escrever como $T=2\pi/\omega_1$, onde $\omega_1\equiv E_1/\hbar$ é a frequência mais pequena deste sistema. Explique qualitativamente porque é esta frequência em particular que determina o período do movimento.

Solution

1. We can recall the general solution for the time-evolved state vector expanded in terms of the energy eigenstates $|\varphi_n\rangle$:

$$|\psi(0)\rangle=\sum_n c_n|\varphi_n\rangle \qquad \longrightarrow \qquad |\psi(t)\rangle=\sum_n c_n e^{-iE_nt/\hbar}|\varphi_n\rangle.$$

Therefore, projecting this into the position basis we get the time evolved wavefunction in terms of the energy eigenfunctions:

$$\psi(x,t)\equiv\langle x|\psi(x,t)\rangle=\sum_n c_n e^{-iE_nt/\hbar}\langle x|\varphi_n\rangle=\sum_n c_n e^{-iE_nt/\hbar}\varphi_n(x).$$

2. To see whether the time evolution of the particle within this potential well is periodic we seek a possible solution for $\psi(x,t+T)=\psi(x,t)$. For example, considering the basis-independent expansion of the state

$$|\psi(t)\rangle=\sum_n c_n e^{-iE_nt/\hbar}|\varphi_n\rangle,$$

this periodicity condition amounts to the following

$$|\psi(t+T)\rangle-|\psi(t)\rangle=0 \qquad \Leftrightarrow \qquad \sum_n c_n\left(e^{-iE_nT/\hbar}-1\right)|\varphi_n\rangle=0.$$

Now, since in the infinite potential well all states are bound states (and, in addition, non-degenerate), the set of all the eigenstates $\{|\varphi_1\rangle,|\varphi_2\rangle,\dots\}$ constitutes a complete and orthonormal basis for the Hilbert space of the particle. In particular they are all linearly independent of each other, which means that the above condition is only satisfied if *all* the coefficients

$$c_n\left(e^{-iE_nT/\hbar}-1\right)=0 \qquad \text{for all } n.$$

Moreover, since we want to show this for a general state, we should not assume anything regarding c_n, and hence the condition becomes

$$e^{-iE_nT/\hbar}=1 \qquad \text{for all } n.$$

When can we satisfy this for all n? For that to happen we must have

$$\frac{E_nT}{\hbar}=2\pi\times\text{integer}$$

for all n. Recall that the energies for the infinite potential well are

$$E_n = \frac{\hbar^2 \pi^2 n^2}{2mL^2}.$$

and so

$$\frac{E_n T}{\hbar} = 2\pi n^2 \left(\frac{\hbar \pi T}{4mL^2}\right).$$

Clearly, if $T = 4mL^2/\pi\hbar$, the condition is satisfied for all n, because n^2 is an integer.

3. The period $T = 2\pi/\omega_1$ is easy to understand if one looks at the general expression for the time-evolved state

$$|\psi(t)\rangle = \sum_n c_n e^{-iE_n t/\hbar} |\varphi_n\rangle$$

This expression says that the time-evolved state consists of a linear combination of stationary states, where the coefficient of each is a periodic function of time: $\exp(-iE_n t/\hbar)$. For each level n the corresponding frequency is $\omega_n = \frac{E_n}{\hbar}$, and obviously the period associated with each of these coefficients is

$$T_n = \frac{2\pi}{\omega_n} = \frac{4mL^2}{\hbar \pi n^2}.$$

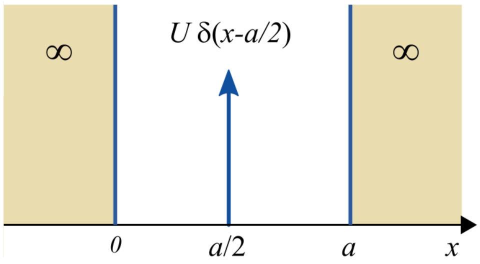
We then have a sum of many periodic functions, each with its own period T_n. But you can see that

$$T_1 = 4T_2 = 9T_3 = 16T_4 = \cdots = n^2 T_n = \ldots$$

which means that all periods are integer fractions of the fundamental one, T_1 (or, equivalently, that the frequencies ω_n will be integer harmonics of the smallest one, ω_1). Consequently, the overall period of the wavefunction will have to be the largest of these. Hence, the wavefunction will be periodic with period T_1.

Problema 5 | Poço de potencial infinito com delta repulsivo

Um poço de potencial infinito confina uma partícula à região do espaço $0 \leq x \leq a$. A partícula está ainda sob influência de uma barreira de potencial repulsiva com a forma $V(x) = U\,\delta(x - a/2)$ localizada no centro dessa região, sendo $U > 0$. O potencial total sentido pela partícula é, então, o seguinte:



$$V(x) = \begin{cases} +\infty, & x < 0 \vee x > a, \\ U\,\delta\left(x - \frac{a}{2}\right), & 0 \leq x \leq a. \end{cases}$$

1. Mostre que a solução geral da eq. de Schrödinger independente do tempo tem a forma

$$\psi(x) = \begin{cases} A\sin(kx), & 0 \le x < \frac{a}{2}, \\ B\sin\bigl[k(x-a)\bigr], & \frac{a}{2} < x \le a, \end{cases} \qquad (A, B \text{ constantes}).$$

2. Indique as condições fronteira para $\psi(x)$ e $\psi'(x)$ em $x = \frac{a}{2}$. *(Recorde que a presença da função delta de Dirac impõe uma condição fronteira diferente da usual neste ponto.)*

3. Obtenha a equação transcendente cuja solução determina as energias dos estados estacionários desta partícula em função dos parâmetros U e a.

4. Se remover a função delta de Dirac (isto é, tomando $U \to 0$), o que acontece à energia da partícula no estado fundamental: aumenta ou diminui? Justifique qualitativamente esse resultado.

Solution

Before starting, we note that this potential has 4 different regions which need to be considered separately:

$$\text{region I}: \ x < 0, \quad \text{region II}: \ 0 \le x \le \frac{a}{2}, \quad \text{region III}: \ \frac{a}{2} < x < a, \quad \text{region IV}: \ x > a.$$

We should also note that **the presence of a Dirac-delta potential creates a special situation**, because the potential is strictly infinite at $x = a/2$, but this region where $V(x) = +\infty$ has zero width (the potential is $+\infty$ at precisely, and only, $x = a/2$). In this case the wavefunction can remain finite (as opposed to being forced to zero), but its derivative is discontinuous (because the potential has an infinite discontinuity at $x = a/2$).

To understand what happens to the derivative of the wavefunction at this point, let us begin with the time-independent Schrödinger equation that we need to solve,

$$-\frac{\hbar^2}{2m}\psi''(x) + V(x)\,\psi(x) = E\,\psi(x). \tag{5.1}$$

We now choose some arbitrary point $x = x_0$ and integrate this equation in an infinitesimal vicinity of the point x_0:

$$-\frac{\hbar^2}{2m}\int_{x_0-\varepsilon}^{x_0+\varepsilon} \psi''(x)\,dx + \int_{x_0-\varepsilon}^{x_0+\varepsilon} V(x)\,\psi(x)\,dx = E\int_{x_0-\varepsilon}^{x_0+\varepsilon} \psi(x)\,dx, \tag{5.2}$$

where $\varepsilon \approx 0$ is an infinitesimal constant that we shall take to zero in the end. Recalling basic calculus,

$$\int_{x_0-\varepsilon}^{x_0+\varepsilon} \psi''(x)\,dx = \psi'(x_0+\varepsilon) - \psi'(x_0-\varepsilon).$$

On the other hand, since $\psi(x)$ must be continuous everywhere, in the limit $\varepsilon \to 0$, we have

$$\int_{x_0-\varepsilon}^{x_0+\varepsilon} V(x)\,\psi(x)\,dx \simeq \psi(x_0)\int_{x_0-\varepsilon}^{x_0+\varepsilon} V(x)\,dx,$$

and

$$\int_{x_0-\varepsilon}^{x_0+\varepsilon} \psi(x)\,dx \simeq \psi(x_0)\int_{x_0-\varepsilon}^{x_0+\varepsilon} dx = 2\varepsilon\,\psi(x_0).$$

Substituting all this in eq. (5.2) above, we get

$$-\frac{\hbar^2}{2m}\Big[\psi'(x_0+\varepsilon)-\psi'(x_0-\varepsilon)\Big]+\psi(x_0)\int_{x_0-\varepsilon}^{x_0+\varepsilon}V(x)\,dx=\xcancel{2\varepsilon\,E\,\psi(x_0)}^{\,0},$$

where the last term goes to 0 in the limit $\varepsilon \to 0$. Rearranging what remains, we have

$$\psi'(x_0+\varepsilon)-\psi'(x_0-\varepsilon)=\frac{2m\psi(x_0)}{\hbar^2}\int_{x_0-\varepsilon}^{x_0+\varepsilon}V(x)\,dx. \tag{5.3}$$

Here's what this result means:

- The left-hand side contains the discontinuity in the derivative of the wavefunction at the point x_0. This is because, in the limit $\varepsilon \to 0$, $\psi'(x_0+\varepsilon)$ becomes the value of the derivative as we approach the point x_0 from the right, and $\psi'(x_0-\varepsilon)$ is the derivative as we approach x_0 from the left.

- Suppose the potential is discontinuous at the point x_0, but this discontinuity is finite; in other words, suppose

  $$V(x_0+\varepsilon)=V_+, \qquad V(x_0-\varepsilon)=V_-, \qquad \text{with } V_+-V_- \text{ finite.}$$

  In this case, the integral in eq. (5.3) evaluates to

  $$\int_{x_0-\varepsilon}^{x_0+\varepsilon}V(x)\,dx=\int_{x_0}^{x_0+\varepsilon}V(x)\,dx+\int_{x_0-\varepsilon}^{x_0}V(x)\,dx\simeq\varepsilon\,(V_+-V_-)\quad\xrightarrow[\varepsilon\to0]{}\quad 0.$$

  This, of course implies that eq. (5.3) reduces to

  $$\psi'(x_0+\varepsilon)-\psi'(x_0-\varepsilon)=0\qquad\xrightarrow[\varepsilon\to0]{}\qquad\psi'(x_0^+)=\psi'(x_0^-).$$

  This means that $\psi'(x)$ is continuous at $x = x_0$. In other words, we have derived that:

  $\psi'(x)$ is continuous at any finite discontinuity of the potential.

- The situation where $V(x)$ is continuous at x_0 is just a particular case of the above, with $V_+ = V_-$. The wavefunction is continuous as well.

- Suppose, instead, that there is **a Dirac-delta term** in the potential at $x = x_0$; for example, suppose that $V(x) = U\,\delta(x-x_0)$ near x_0. In this case, the integral in eq. (5.3) becomes

  $$\int_{x_0-\varepsilon}^{x_0+\varepsilon}V(x)\,dx=U\int_{x_0-\varepsilon}^{x_0+\varepsilon}\delta(x-x_0)\,dx=U.$$

  The boundary condition on the derivative then becomes

  $$\psi'(x_0+\varepsilon)-\psi'(x_0-\varepsilon)=\frac{2mU\psi(x_0)}{\hbar^2}. \tag{5.4}$$

  This expression tells us that the amount of discontinuity in $\psi'(x)$ depends on both U and $\psi(x_0)$. It also tells us that

  every time we encounter a Dirac-delta potential at some point x_0, we must use the relation (5.4) to set the correct boundary conditions on the derivative of the wavefunction at x_0.

We now move on to the responses to the questions in this problem.

1. In the regions where the potential is infinite ($x < 0$ or $x > a$), we must have $\psi(x) = 0$, for exactly the same reasons we discussed in the case of the infinite potential well (see lecture notes). The presence of the Dirac-delta potential at $x = a/2$ defines two regions that must be treated separately: the region $0 \le x \le a/2$ and the region $a/2 \le x \le a$. In each of these there will be physical solutions to the time-independent Schrödinger equation with $E > 0$. (There are no solutions with $E < 0$ because the absolute minimum of the potential is $V_{\text{min}} = 0$; physical solutions never exist with energy below the absolute minimum of any potential.) In these regions, the general solution will therefore take the form

$$\psi(x) = \begin{cases} Fe^{ikx} + Ge^{-ikx}, & 0 \le x \le \frac{a}{2} \\ Ce^{ikx} + De^{-ikx}, & \frac{a}{2} \le x \le a \end{cases}, \qquad k \equiv \sqrt{\frac{2mE}{\hbar^2}}.$$

   Since $\psi(x)$ must be continuous everywhere, we must have $\psi(0) = \psi(a) = 0$. In the left region this implies

$$\psi(0) = 0: \qquad F + G = 0 \qquad \Rightarrow \quad \psi(x) = F\left(e^{ikx} - e^{-ikx}\right) = A\,\sin(kx).$$

   (In the last step we simply re-wrote the overall factor $2iF$ as a normalization constant A.) In the right region,

$$\psi(a) = 0: \qquad Ce^{ika} + De^{-ika} = 0 \qquad \Rightarrow \quad \psi(x) = -De^{ikx-2ika} + De^{-ikx} = B\,\sin[k(x-a)].$$

   (The constants A and B simply substitute the initially introduced F, G, C, D).

2. The wavefunction itself should be continuous everywhere. In the vicinity of $x = a/2$ the potential is

$$V(x) = U\delta(x - \tfrac{a}{2}),$$

   which means that we should use the relation (5.4) discussed above to obtain the correct boundary condition for the derivative at this point. In this particular problem, the derivative must be discontinuous at $x = a/2$ by the amount

$$\psi'(\tfrac{a}{2}^{+}) - \psi'(\tfrac{a}{2}^{-}) = \frac{2mU}{\hbar^2}\,\psi(\tfrac{a}{2}).$$

3. From question 1, we know that the solution in the two regions has the form

$$\psi(x) = \begin{cases} A\sin(kx), & 0 \le x < \frac{a}{2} \\ B\sin\big[k(x-a)\big], & \frac{a}{2} < x \le a \end{cases}, \qquad (A, B \text{ constants}).$$

   The boundary conditions for $\psi(x)$ and $\psi'(x)$ at $x = a/2$ lead to

$$\psi(\tfrac{a}{2}^{+}) = \psi(\tfrac{a}{2}^{-}): \qquad B = -A$$

$$\psi'(\tfrac{a}{2}^{+}) - \psi'(\tfrac{a}{2}^{-}) = \frac{2mU}{\hbar^2}\psi(\tfrac{a}{2}): \qquad -kA\cos(\tfrac{ka}{2}) - kA\cos(\tfrac{ka}{2}) = \frac{2mU}{\hbar^2}A\sin(\tfrac{ka}{2}),$$

   or, rearranging, the last expression,

$$k\,\cot\left(\tfrac{ka}{2}\right) = -\frac{mU}{\hbar^2}. \tag{5.5}$$

The roots, k_n, of this equation determine the bound-state energies, which correspond to the values

$$E_n = \frac{\hbar^2 k_n^2}{2m}.$$

4. If $U = 0$, we have a simple infinite potential well, for which the ground state energy is

$$E_{\text{gs}}^{(0)} = \frac{\hbar^2 \pi^2}{2ma^2}.$$

At finite U, the ground state energy corresponds to the solution of the above equation (5.5) with the lowest k. Note that, on the one hand, the right-hand side of (5.5) is independent of k; on the other hand, since k and U are positive, the equation

$$k\,\cot(\tfrac{ka}{2}) = -\frac{mU}{\hbar^2}$$

can only be satisfied when $\cot(\frac{ka}{2}) < 0$. The lowest interval of k where that happens is

$$\cot(\tfrac{ka}{2}) < 0 \qquad \Rightarrow \qquad \frac{\pi}{2} < \frac{ka}{2} < \pi \qquad \Leftrightarrow \qquad \frac{\pi}{a} < k < \frac{2\pi}{a}.$$

(as usual, making a graphical sketch of the two sides of the transcendental equation will help visualize this more easily). Consequently, the first solution of (5.5) will occur for a certain $k = k_{\text{gs}}$ in this range, and the corresponding energy then satisfies

$$E_{\text{gs}} = \frac{\hbar^2 k_{\text{gs}}^2}{2m} > \frac{\hbar^2 \pi^2}{2ma^2} = E_{\text{gs}}^{(0)} \qquad (\text{because } k_{\text{gs}} > \frac{\pi}{a}).$$

Since $E_{\text{gs}} > E_{\text{gs}}^{(0)}$, the ground state energy decreases when $U \to 0$. In fact, for any finite U, E_{gs} will decrease whenever U decreases, which can be easily seen by graphically representing the transcendental equation (5.5).

Problema 6 | Energias dos estados ligados num poço de potencial finito

Considere o potencial seguinte em uma dimensão

$$V(x) = \begin{cases} 0, & |x| < a, \\ V_0, & |x| > a, \end{cases} \qquad (V_0 > 0).$$

1. Obtenha a equação transcendente cuja solução determina as energias dos estados ligados desta partícula em função de V_0 e a.

2. Mostre que, no limite $V_0 \to +\infty$, essa equação é facilmente solúvel analiticamente, e que obtém as energias dos estados estacionários num poço de potencial infinito.

Solution

1. From the shape of the potential well, we can conclude that bound solutions can only exist in the range $0 < E < V_0$. In addition, the potential is symmetric with respect to the origin. Since the bound state energies in 1D are always non-degenerate, we can consider separately the solutions that yield even and odd wavefunctions, and, in addition, we need only to consider what happens in one half of the x axis.

   Even solutions — The possible physical solutions of the Schrodinger equation that are even with respect to the origin have the general form

   $$\psi(x) = \begin{cases} A\cos kx, & 0 < x < a \\ Be^{-\lambda x} & x > a \end{cases}$$

   where

   $$k = \sqrt{2mE}/\hbar, \qquad \lambda = \sqrt{2m\,(V_0 - E)}/\hbar,$$

   and their derivative is

   $$\psi'(x) = \begin{cases} -Ak\sin kx, & 0 < x < a \\ -\lambda Be^{-\lambda x} & x > a \end{cases}$$

   The matching condition at $x = a$ requires

   $$\frac{\psi'(a^+)}{\psi(a^+)} = \frac{\psi'(a^-)}{\psi(a^-)} \qquad \Leftrightarrow \qquad \lambda = k\,\tan(ka).$$

   Odd solutions — The possible physical solutions of the Schrodinger equation that are odd with respect to the origin have the general form

   $$\psi(x) = \begin{cases} C\,\sin kx, & 0 < x < a \\ D\,e^{-\lambda x} & x > a \end{cases}$$

   where

   $$k = \sqrt{2mE}/\hbar, \qquad \lambda = \sqrt{2m\,(V_0 - E)}/\hbar,$$

   and their derivative is

   $$\psi'(x) = \begin{cases} Ck\cos kx, & 0 < x < a \\ -\lambda De^{-\lambda x} & x > a \end{cases}$$

   The matching condition at $x = a$ requires, again, that

   $$\frac{\psi'(a^+)}{\psi(a^+)} = \frac{\psi'(a^-)}{\psi(a^-)} \qquad \Leftrightarrow \qquad \lambda = -k\,\cot(ka).$$

   Therefore, the equations that determine the bound state energies are

   $$\lambda = k\,\tan(ka) \qquad \text{and} \qquad \lambda = -k\,\cot(ka).$$

   If we replace λ and k by their definitions, these equations read

   $$\sqrt{\frac{V_0 - E}{E}} = \tan\left(\frac{\sqrt{2mE}a}{\hbar}\right) \qquad \text{and} \qquad \sqrt{\frac{V_0 - E}{E}} = -\cot\left(\frac{\sqrt{2mE}a}{\hbar}\right).$$

2. For finite V_0 the equations cannot be solved analytically. In the limit $V_0 \to +\infty$ the equations become

$$\tan\frac{\sqrt{2mE}a}{\hbar} = +\infty \qquad \text{and} \qquad \cot\frac{\sqrt{2mE}a}{\hbar} = -\infty$$

which have the following respective solutions

$$\frac{\sqrt{2mE}a}{\hbar} = \frac{p\pi}{2} \quad (p \text{ odd}) \qquad \text{and} \qquad \frac{\sqrt{2mE}a}{\hbar} = s\pi \quad (s = 1, 2, 3, \dots)\,.$$

If we multiply both sides by 2, this reads

$$\frac{2a\sqrt{2mE}}{\hbar} = n\pi \quad (n \text{ odd}) \qquad \text{and} \qquad \frac{2a\sqrt{2mE}}{\hbar} = n\pi \quad (n \text{ even})\,.$$

These two equations mean that we will have a solution whenever

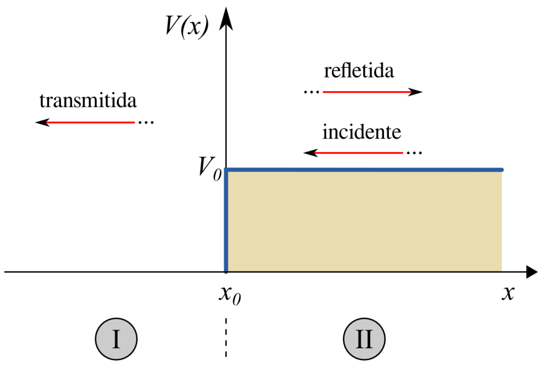
$$\frac{2a\sqrt{2mE}}{\hbar} = n\pi \qquad \text{or} \qquad E_n = \frac{\hbar^2 n^2 \pi^2}{2m(2a)^2}, \qquad n = 1, 2, 3, \dots$$

These are precisely the energy levels of an infinite potential well of width $2a$. This is what we could expect because, in the limit $V_0 \to +\infty$, the potential becomes an infinite well of width $2a$.

Problema 7 | Degrau de potencial

O degrau de potencial é definido como

$$V(x) = \begin{cases} 0, & x < 0, \\ V_0, & x > 0, \end{cases} \qquad (V_0 > 0).$$



Na ilustração acima, $x_0 = 0$.

1. Calcule os coeficientes de transmissão e reflexão para um feixe de partículas com energia $E > V_0$, e incidente da *direita* (veja as setas na figura). Compare estes coeficientes com os que foram derivados nas aulas para partículas incidentes da *esquerda*.

2. Se uma partícula se propagar vinda da esquerda ($x = -\infty$) com $E < V_0$ em direção ao degrau de potencial, haverá uma região $x \gtrsim 0$ na qual a função de onda é finita (penetração da barreira de potencial). Determine a função de onda e a corrente de probabilidade na região $x > 0$. Mostre que, apesar de a função de onda ser finita, a corrente de probabilidade é nula nessa região.

3. Porque é que o resultado anterior implica que a probabilidade de reflexão tem de ser 1 para partículas incidentes da esquerda com $E < V_0$?

Solution

Before starting, let us establish the wavenumbers needed in each region. The Schrödinger equation for this problem is, as usual,

$$\psi''(x) = -\frac{2m(E-V)}{\hbar^2}\psi(x)$$

Since the potential is piecewise constant in regions I and II, we can write the above as

$$\text{Region I}: \qquad \psi''(x) = -k^2\psi(x) \qquad (E>0)$$

$$\begin{aligned}\text{Region II}: \qquad &\psi''(x) = -q^2\psi(x) \qquad (E>V_0)\\ &\psi''(x) = +\lambda^2\psi(x) \qquad (E<V_0)\end{aligned}$$

where the wavenumbers k, q, and λ are defined as

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

1. Since the beam is coming from the far right, the general solution of the above equation for this scattering problem will be

$$\psi(x) = \begin{cases} Ae^{iqx} + Be^{-iqx}, & x>0 \\ Ce^{-ikx}, & x<0 \end{cases}$$

The incoming current is the one associated with the term Be^{-iqx}, since this is the one that represents a wave traveling to the left, and the reflected current is associated with the term Ae^{iqx} in the wavefunction. Therefore, the reflection and transmission coefficients will be

$$R = \frac{j_\mathrm{r}}{j_\mathrm{i}} = \frac{q\,|A|^2}{q\,|B|^2} = \frac{|A|^2}{|B|^2}, \qquad T = \frac{j_\mathrm{t}}{j_\mathrm{i}} = \frac{k\,|C|^2}{q\,|B|^2}.$$

The ratios of A and C to B are obtained from the matching conditions of $\psi(x)$ and $\psi'(x)$ at the potential discontinuity:

$$\begin{aligned}\psi'(0^+) = \psi'(0^-) &\quad\longrightarrow\quad iq(A-B) = -ikC\\ \psi(0^+) = \psi(0^-) &\quad\longrightarrow\quad A+B = C\end{aligned}$$

which leads to

$$\frac{A}{B} = \frac{q-k}{q+k} \quad\Rightarrow\quad R = \left|\frac{q-k}{q+k}\right|^2, \qquad \frac{C}{B} = \frac{2q}{k+q} \quad\Rightarrow\quad T = \frac{4kq}{(k+q)^2}.$$

Substituting the definitions of k and q, these coefficients can be written explicitly in terms of the particles' energy:

$$R = \frac{\left(1-\sqrt{1-\frac{V_0}{E}}\right)^2}{\left(1+\sqrt{1-\frac{V_0}{E}}\right)^2}, \qquad T = \frac{4\sqrt{1-\frac{V_0}{E}}}{\left(1+\sqrt{1-\frac{V_0}{E}}\right)^2}.$$

Comment: If you compare these results with what is obtained when the particles are coming from the left in the regime $E > V_0$, you will see that R and T are the same in both cases.

2. When the particle is coming from the left with $E < V_0$, the wavefunction in the region $x > 0$ will have the form

$$\psi(x) = Ce^{-\lambda x}, \qquad \lambda = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}},$$

where C is a constant that we, for now, do not calculate explicitly. The probability current density is defined as

$$j(x) = \frac{\hbar}{2mi}\left[\psi^*(x)\frac{d\psi(x)}{dx} - \psi(x)\frac{d\psi^*(x)}{dx}\right].$$

In that region, the current density will be

$$j(x) = \frac{\hbar\,|C|^2}{2mi}\left[-\lambda e^{-2\lambda x} + \lambda e^{-2\lambda x}\right] = 0.$$

We could have anticipated this result because the wavefunction is real in this region, which means that the difference of the two terms in the definition of the current vanishes, irrespective of the specific form of the wavefunction.

Therefore, even though there is a finite probability of finding the particle beyond $x = 0$, namely

$$\mathcal{P}(x > 0) = |C|^2 \int_0^\infty e^{-2\lambda x} dx > 0,$$

the probability current density is zero.

3. The reflection and transmission coefficients are defined as the ratios of the reflected and transmitted currents to the incoming current, respectively. Since the current density is conserved everywhere, the fact that $j = 0$ for $x > 0$ necessarily means that all the current remains on the left side of the potential step ($x < 0$). This implies that the magnitude of the incoming and reflected currents must be the same. Therefore the reflection coefficient should be exactly 1.

Apêndice — Integrais potencialmente úteis

Envolvendo funções trigonométricas:

$$\int x \sin x \, dx = \sin x - x \, \cos x,$$

$$\int x^2 \sin x \, dx = 2x \, \sin x + \left(2 - x^2\right) \, \cos x,$$

$$\int_{-a/2}^{+a/2} x^2 \sin^2 \left(\frac{n\pi x}{a}\right) \, dx = \int_{-a/2}^{+a/2} x^2 \cos^2 \left(\frac{n\pi x}{a}\right) \, dx = \frac{1}{24} a^3 \left[1 + \frac{(-1)^n 6}{n^2 \pi^2}\right],$$

$$\int_{-a/2}^{+a/2} x \cos\left(\frac{\pi x}{a}\right) \sin\left(\frac{2\pi x}{a}\right) \, dx = \frac{8a^2}{9\pi^2}.$$