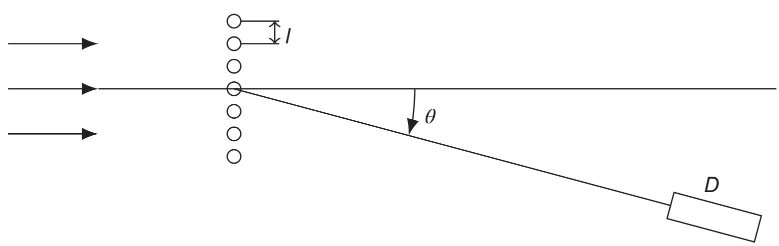
1

Solutions to the Exercises of Chapter I (Complement K_I). Waves and Particles. Introduction to the Fundamental Ideas of Quantum Mechanics

1.1 Interference and Diffraction with a Beam of Neutrons

Statement

A beam of neutrons of mass M_n ($M_n \simeq 1.67 \times 10^{-27}$ kg), of constant velocity and energy E, is incident on a linear chain of atomic nuclei, arranged in a regular fashion as shown in the figure (these nuclei could be, for example, those of a long linear molecule). We call l the distance between two consecutive nuclei, and d, their size ($d \ll l$). A neutron detector D is placed far away, in a direction which makes an angle of θ with the direction of the incident neutrons.



a. Describe qualitatively the phenomena observed at D when the energy E of the incident neutrons is varied.

b. The counting rate, as a function of E, presents a resonance about $E = E_1$. Knowing that there are no other resonances for $E < E_1$, show that one can determine l. Calculate l for $\theta = 30°$ and $E_1 = 1.3 \times 10^{-20}$ joule.

c. At about what value of E must we begin to take the finite size of the nuclei into account?

Comments

In this exercise, we will exploit wave–particle duality and liken this experiment to one very similar in which light passes through a grating.

Light is naturally described in terms of (electromagnetic) waves, but wave–particle duality allows us to also describe it as a beam of photons. Let us therefore imagine

Solution Manual to Accompany Volume I of Quantum Mechanics by Cohen-Tannoudji, Diu and Laloë, First Edition. Guillaume Merle, Oliver J. Harper and Philippe Ribière.

a beam of light (of wavelength λ) arriving on a grating comprised of wires of width d and spacing l and picture the diffracted light or the probability of arrival of the photons on a screen placed at infinity.

Each wire creates a diffraction pattern, the characteristic angle governing the size of each diffraction spot is $\theta_{\text{diffraction}} \simeq \dfrac{\lambda}{d}$.

The various waves that are diffracted by the wires are coherent with each other and can hence interfere. The characteristic angle for interferences is around $\theta_{\text{interferences}} \simeq \dfrac{\lambda}{l}$.

Since $l > d$, the diffraction pattern is larger than the interference pattern. Interferences, therefore, appear as a modulation of the light intensity within each diffraction spot.

In this experiment, the beam is made up of neutrons that we assume to be independent of each other. We must therefore reason by analogy with the beam of light. Here, the grating is substituted by a linear chain of atomic nuclei.

Wave–particle duality is a difficult reality to comprehend. The notion of wave packets, limited in space (the coherence length in wave optics, *i.e.* for photons) and time, helps us to visualize this process: the wave packet associated with each particle (here neutrons) can diffract and interfere, by passing through several slits at once.

Solution

A beam of neutrons of mass M_n ($M_n \simeq 1.67 \times 10^{-27}$ kg), of constant velocity and energy E, is incident on a linear chain of atomic nuclei, arranged in a regular fashion as shown in the figure (these nuclei could be, for example, those of a long linear molecule). We call l the distance between two consecutive nuclei, and d, their size ($d \ll l$). A neutron detector D is placed far away, in a direction which makes an angle of θ with the direction of the incident neutrons.

a. Describe qualitatively the phenomena observed at D when the energy E of the incident neutrons is varied.

   We assume the neutrons are free neutrons. Each neutron exhibits wave-like behavior. In a similar way to what is well known in wave optics, the neutrons are diffracted by the nuclei as photons are diffracted by a grating. The corresponding wavelength of a neutron can be calculated using:

$$E = \frac{p^2}{2M_n} = \frac{(\hbar k)^2}{2M_n} = \frac{(2\pi\hbar)^2}{2M_n\lambda^2} \Leftrightarrow \lambda = \frac{2\pi\hbar}{\sqrt{2M_nE}}$$

   Assuming that the detector is placed at infinity, the angle between two consecutive interference fringes is $\theta_{\text{interferences}} \simeq \dfrac{\lambda}{l}$ and the characteristic diffraction angle due to a single slit is $\theta_{\text{diffraction}} \simeq \dfrac{\lambda}{d}$. Increasing the energy E, therefore, leads to a decrease in wavelength λ and the interference fringes move closer together as for the diffraction pattern of light. Conversely, decreasing E increases the wavelength λ and the interference fringes move further apart. By varying E, the scale of interference and diffraction changes but not the overall aspect. Their relative position is still the same.

b. The counting rate, as a function of E, presents a resonance about $E = E_1$. Knowing that there are no other resonances for $E < E_1$, show that one can determine l. Calculate l for $\theta = 30°$ and $E_1 = 1.3 \times 10^{-20}$ joule.

The path difference between two consecutive "slits" is $\delta = l \sin\theta$, and a resonance will occur for $\delta = n\lambda$ with $n \in \mathbb{Z}$. Hence:

$$l \sin\theta = n\lambda = n\frac{2\pi\hbar}{\sqrt{2M_n E_1}} \Leftrightarrow n = l\sin\theta\frac{\sqrt{2M_n E_1}}{2\pi\hbar}$$

according to the results from question a. As there is no other resonance for $E < E_1$, the first resonance occurs for $E = E_1$ and so n is minimal and equals 1. We deduce:

$$l\sin\theta = \frac{2\pi\hbar}{\sqrt{2M_n E_1}} \Leftrightarrow l = \frac{2\pi\hbar}{\sqrt{2M_n E_1}\sin\theta} \simeq 2\,\text{Å}$$

c. At about what value of E must we begin to take the finite size of the nuclei into account?

The finite size of the nuclei must be taken into account once $\lambda \sim l$, which corresponds to energies such that:

$$E = \frac{(2\pi\hbar)^2}{2M_n\lambda^2} \sim \frac{(2\pi\hbar)^2}{2M_n l^2} = \frac{E_1}{4}$$

since

$$E_1 = \frac{(2\pi\hbar)^2}{2M_n l^2 \sin^2\theta} \sim \frac{4(2\pi\hbar)^2}{2M_n l^2}$$

1.2 Bound State of a Particle in a "Delta Function Potential"

Statement

Consider a particle whose Hamiltonian H [operator defined by formula (D-10) of Chapter I] is:

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} - \alpha\delta(x)$$

where α is a positive constant whose dimensions are to be found.

a. Integrate the eigenvalue equation of H between $-\varepsilon$ and $+\varepsilon$. Letting ε approach 0, show that the derivative of the eigenfunction $\varphi(x)$ presents a discontinuity at $x = 0$ and determine it in terms of α, m, and $\varphi(0)$.

b. Assume that the energy E of the particle is negative (bound state). $\varphi(x)$ can then be written:

$$x < 0 \quad \varphi(x) = A_1 e^{\rho x} + A_1' e^{-\rho x}$$

$$x > 0 \quad \varphi(x) = A_2 e^{\rho x} + A_2' e^{-\rho x}$$

Express the constant ρ in terms of E and m. Using the results of the preceding question, calculate the matrix M defined by:

$$\begin{pmatrix} A_2 \\ A_2' \end{pmatrix} = M \begin{pmatrix} A_1 \\ A_1' \end{pmatrix}$$

Then, using the condition that $\varphi(x)$ must be square-integrable, find the possible values of the energy. Calculate the corresponding normalized wave functions.

c. Plot these wave functions on a graph. Give an order of magnitude for their width Δx.

d. What is the probability $\overline{\mathrm{d}\mathscr{P}}(p)$ that a measurement of the momentum of the particle in one of the normalized stationary states calculated above will give a result included between p and $p + \mathrm{d}p$? For what value of p is this probability maximum? In what domain, of dimension Δp, does it take on non-negligible values? Give an order of magnitude for the product $\Delta x \cdot \Delta p$.

Comments

This exercise deals with a "limited" potential: an infinitely deep well, but infinitely narrow, a Dirac well. (Beware: the Dirac function is not dimensionless, hence the dimensional analysis question in the preamble.)

Before starting to solve this exercise, it is important to enquire what the application of classical mechanics to this situation would yield. Since the particle energy is negative, classical mechanics dictates that the particle stay trapped in the Dirac potential well, so is localized at $x = 0$ in a bound state.

Let us now adopt a quantum approach. This Hamiltonian yields very interesting results and interpretations using straightforward calculations in terms of very few different spatial zones, meaning that there are fewer A_i constants to determine.

However, the interface conditions (or continuity conditions) either side of the well are not known *a priori*. They must therefore be established by starting with a known and finite situation (question a).

The rest of the exercise is based on the usual approach and constitutes a superb exercise for implementing fundamental notions of quantum mechanics and additionally offers an interpretation of analytical results.

Solution

Consider a particle whose Hamiltonian H [operator defined by formula (D-10) of Chapter I] is:

$$H = -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} - \alpha\delta(x)$$

where α is a positive constant whose dimensions are to be found.

The Hamiltonian H is the total energy operator (since $H\varphi(x) = E\varphi(x)$) whose dimensions are thus an energy. In addition, we know that $\int_{-\infty}^{+\infty} \delta(x)\mathrm{d}x = 1$, and $\delta(x)$ has dimensions of inverse length. The α constant, therefore, has dimensions of an energy multiplied by length and corresponds to the area under the curve of the delta function.

a. Integrate the eigenvalue equation of H between $-\varepsilon$ and $+\varepsilon$. Letting ε approach 0, show that the derivative of the eigenfunction $\varphi(x)$ presents a discontinuity at $x = 0$ and determine it in terms of α, m, and $\varphi(0)$.

The eigenvalue equation of H is:

$$H\varphi(x) = E\varphi(x) \Leftrightarrow -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\varphi(x)}{\mathrm{d}x^2} - \alpha\delta(x)\varphi(x) = E\varphi(x)$$

Integrating this equation between $-\varepsilon$ et $+\varepsilon$ yields:

$$-\frac{\hbar^2}{2m}\int_{-\varepsilon}^{+\varepsilon}\frac{\mathrm{d}^2\varphi(x)}{\mathrm{d}x^2}\mathrm{d}x - \alpha\int_{-\varepsilon}^{+\varepsilon}\delta(x)\varphi(x)\mathrm{d}x = E\int_{-\varepsilon}^{+\varepsilon}\varphi(x)\mathrm{d}x$$

$$\Leftrightarrow -\frac{\hbar^2}{2m}\left[\frac{\mathrm{d}\varphi(+\varepsilon)}{\mathrm{d}x} - \frac{\mathrm{d}\varphi(-\varepsilon)}{\mathrm{d}x}\right] - \alpha\varphi(0) = E\int_{-\varepsilon}^{+\varepsilon}\varphi(x)\mathrm{d}x$$

$$\Leftrightarrow \frac{\mathrm{d}\varphi(+\varepsilon)}{\mathrm{d}x} - \frac{\mathrm{d}\varphi(-\varepsilon)}{\mathrm{d}x} = -\frac{2m\alpha}{\hbar^2}\varphi(0) - \frac{2mE}{\hbar^2}\int_{-\varepsilon}^{+\varepsilon}\varphi(x)\mathrm{d}x$$

Letting ε approach 0, we find:

$$\lim_{\varepsilon\to 0}\left[\frac{\mathrm{d}\varphi(+\varepsilon)}{\mathrm{d}x} - \frac{\mathrm{d}\varphi(-\varepsilon)}{\mathrm{d}x}\right] = -\frac{2m\alpha}{\hbar^2}\varphi(0)$$

and the derivative of the eigenfunction $\varphi(x)$ presents a discontinuity at $x = 0$ equal to $-\frac{2m\alpha}{\hbar^2}\varphi(0)$.

b. Assume that the energy E of the particle is negative (bound state). $\varphi(x)$ can then be written:

$$x < 0 \quad \varphi(x) = A_1 e^{\rho x} + A_1' e^{-\rho x}$$
$$x > 0 \quad \varphi(x) = A_2 e^{\rho x} + A_2' e^{-\rho x}$$

Express the constant ρ in terms of E and m. Using the results of the preceding question, calculate the matrix M defined by:

$$\begin{pmatrix} A_2 \\ A_2' \end{pmatrix} = M \begin{pmatrix} A_1 \\ A_1' \end{pmatrix}$$

Then, using the condition that $\varphi(x)$ must be square-integrable, find the possible values of the energy. Calculate the corresponding normalized wave functions.

Thanks to the relation established in the preceding question, the wave functions either side of the Dirac well can be calculated, without the knowledge of an expression for the function in the well. This way, we avoid introducing two additional constants that are necessary in a well of finite depth and width. Let us set:

$$x < 0 \quad \varphi_{\mathrm{I}}(x) = A_1 e^{\rho x} + A_1' e^{-\rho x}$$
$$x > 0 \quad \varphi_{\mathrm{II}}(x) = A_2 e^{\rho x} + A_2' e^{-\rho x}$$

with $\rho = \sqrt{\frac{-2mE}{\hbar^2}}$ since the eigenvalue equation of H, for $x < 0$ and $x > 0$, is:

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\varphi(x)}{\mathrm{d}x^2} - E\varphi(x) = 0 \Leftrightarrow \frac{\mathrm{d}^2\varphi(x)}{\mathrm{d}x^2} - \frac{-2mE}{\hbar^2}\varphi(x) = 0$$
$$\Leftrightarrow \frac{\mathrm{d}^2\varphi(x)}{\mathrm{d}x^2} - \rho^2\varphi(x) = 0$$

as we assume $E < 0$. Firstly, the function $\varphi(x)$ is continuous at $x = 0$, so:

$$\varphi_{\mathrm{I}}(0) = \varphi_{\mathrm{II}}(0) \Leftrightarrow A_1 + A_1' = A_2 + A_2'$$

Secondly, according to the results of the previous question, $\frac{\mathrm{d}\varphi(x)}{\mathrm{d}x}$ presents a discontinuity at $x = 0$ equal to $-\frac{2m\alpha}{\hbar^2}\varphi(0)$, so:

$$\frac{\mathrm{d}\varphi_{\mathrm{II}}(0)}{\mathrm{d}x} - \frac{\mathrm{d}\varphi_{\mathrm{I}}(0)}{\mathrm{d}x} = -\frac{2m\alpha}{\hbar^2}\varphi(0) \Leftrightarrow \rho(A_2 - A_2' - A_1 + A_1') = -\frac{2m\alpha}{\hbar^2}(A_1 + A_1')$$

Hence

$$\begin{cases} A_2 + A_2' = A_1 + A_1' \\ A_2 - A_2' = \left(1 - \frac{2m\alpha}{\rho\hbar^2}\right)A_1 - \left(1 + \frac{2m\alpha}{\rho\hbar^2}\right)A_1' \end{cases}$$

$$\Leftrightarrow \begin{cases} A_2 = \left(1 - \frac{m\alpha}{\rho\hbar^2}\right)A_1 - \frac{m\alpha}{\rho\hbar^2}A_1' \\ A_2' = \frac{m\alpha}{\rho\hbar^2}A_1 + \left(1 + \frac{m\alpha}{\rho\hbar^2}\right)A_1' \end{cases}$$

Finally,

$$\begin{pmatrix} A_2 \\ A_2' \end{pmatrix} = \begin{pmatrix} 1 - \frac{m\alpha}{\rho\hbar^2} & -\frac{m\alpha}{\rho\hbar^2} \\ \frac{m\alpha}{\rho\hbar^2} & 1 + \frac{m\alpha}{\rho\hbar^2} \end{pmatrix} \begin{pmatrix} A_1 \\ A_1' \end{pmatrix}$$

and the expression of matrix M such that

$$\begin{pmatrix} A_2 \\ A_2' \end{pmatrix} = M \begin{pmatrix} A_1 \\ A_1' \end{pmatrix}$$

is

$$M = \begin{pmatrix} 1 - \frac{m\alpha}{\rho\hbar^2} & -\frac{m\alpha}{\rho\hbar^2} \\ \frac{m\alpha}{\rho\hbar^2} & 1 + \frac{m\alpha}{\rho\hbar^2} \end{pmatrix}$$

In order to be square-integrable, $\varphi(x)$ must be bounded when $x \to \pm\infty$, which implies $A_1' = A_2 = 0$ so

$$\begin{pmatrix} 0 \\ A_2' \end{pmatrix} = \begin{pmatrix} 1 - \dfrac{m\alpha}{\rho\hbar^2} & -\dfrac{m\alpha}{\rho\hbar^2} \\ \dfrac{m\alpha}{\rho\hbar^2} & 1 + \dfrac{m\alpha}{\rho\hbar^2} \end{pmatrix} \begin{pmatrix} A_1 \\ 0 \end{pmatrix}$$

which implies the two conditions:

$$\frac{m\alpha}{\rho\hbar^2} = 1 \text{ and } A_2' = A_1 = A$$

The possible energy values are given by:

$$\rho = \frac{m\alpha}{\hbar^2} = \sqrt{\frac{-2mE}{\hbar^2}} \Rightarrow \frac{-2mE}{\hbar^2} = \frac{m^2\alpha^2}{\hbar^4} \Leftrightarrow E = -\frac{m\alpha^2}{2\hbar^2}$$

and there is a unique bound state whose energy is $E = -\dfrac{m\alpha^2}{2\hbar^2}$. The value of A can be calculated using the normalization condition of the eigenfunction $\varphi(x)$:

$$\int_{-\infty}^{0} |\varphi_{\mathrm{I}}(x)|^2 \mathrm{d}x + \int_{0}^{+\infty} |\varphi_{\mathrm{II}}(x)|^2 \mathrm{d}x = 1$$

$$\Leftrightarrow |A|^2 \int_{-\infty}^{0} e^{2\rho x} \mathrm{d}x + |A|^2 \int_{0}^{+\infty} e^{-2\rho x} \mathrm{d}x = 1$$

$$\Leftrightarrow |A|^2 \left[\frac{1}{2\rho} + \frac{1}{2\rho}\right] = 1 \Leftrightarrow A = \sqrt{\rho} e^{i\varphi} = \sqrt{\frac{m\alpha}{\hbar^2}} e^{i\varphi}$$

Setting $\varphi = 0$ so that A is real and positive, there is only one normalized wave function such that:

$$x < 0 \quad \varphi_{\mathrm{I}}(x) = \sqrt{\frac{m\alpha}{\hbar^2}} e^{\frac{m\alpha}{\hbar^2} x}$$

$$x > 0 \quad \varphi_{\mathrm{II}}(x) = \sqrt{\frac{m\alpha}{\hbar^2}} e^{-\frac{m\alpha}{\hbar^2} x}$$

which can be written in a simplified form:

$$\varphi(x) = \sqrt{\frac{m\alpha}{\hbar^2}} e^{-\frac{m\alpha}{\hbar^2} |x|}$$

The functions $\varphi_{\mathrm{I}}(x)$ and $\varphi_{\mathrm{II}}(x)$ are both decreasing exponential functions since $E < 0$. It is indeed a bound state, the probability for the particle to be found at infinity is vanishing, and it stays in the vicinity of the Dirac well and nominally explores the zone that is “forbidden” by classical mechanics.

c. Plot these wave functions on a graph. Give an order of magnitude for their width Δx.

The wave function determined in question b is represented in Figure 1.1.

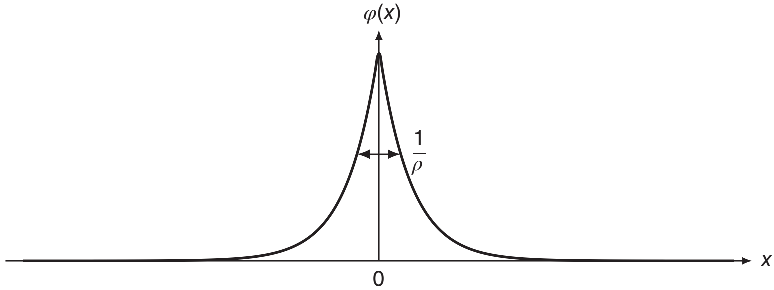


Figure 1.1 Graphic representation of the wave function determined in question b.

Defining Δx as the full width at half maximum, we find:

$$\varphi(x) = \frac{1}{2}\sqrt{\frac{m\alpha}{\hbar^2}} \Leftrightarrow \sqrt{\frac{m\alpha}{\hbar^2}}e^{-\rho|x|} = \frac{1}{2}\sqrt{\frac{m\alpha}{\hbar^2}} \Leftrightarrow -\rho|x| = -\ln 2 \Leftrightarrow |x| = \frac{\ln 2}{\rho}$$

and therefore

$$\Delta x = \frac{2\ln 2}{\rho} \simeq \frac{1.39}{\rho} \sim \frac{1}{\rho}$$

This result is consistent with the idea that the particle only explores the "forbidden" zone over a distance of the order of $\frac{1}{\rho} = \frac{\hbar^2}{m\alpha}$ (the dimensional analysis of ρ shows it to be an inverse length).

d. What is the probability $\overline{\mathrm{d}\mathscr{P}}(p)$ that a measurement of the momentum of the particle in one of the normalized stationary states calculated above will give a result included between p and $p + \mathrm{d}p$? For what value of p is this probability maximum? In what domain, of dimension Δp, does it take on non-negligible values? Give an order of magnitude for the product $\Delta x \cdot \Delta p$.

The eigenfunction in momentum space is the Fourier transform of the eigenfunction in position space, *i.e.*

$$\begin{aligned}
\overline{\varphi}(p) &= \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{+\infty}\varphi(x)e^{-ipx/\hbar}\mathrm{d}x \\
&= \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{0}\varphi_{\mathrm{I}}(x)e^{-ipx/\hbar}\mathrm{d}x + \frac{1}{\sqrt{2\pi\hbar}}\int_{0}^{+\infty}\varphi_{\mathrm{II}}(x)e^{-ipx/\hbar}\mathrm{d}x \\
&= \frac{A}{\sqrt{2\pi\hbar}}\int_{-\infty}^{0}e^{\rho x}e^{-ipx/\hbar}\mathrm{d}x + \frac{A}{\sqrt{2\pi\hbar}}\int_{0}^{+\infty}e^{-\rho x}e^{-ipx/\hbar}\mathrm{d}x \\
&= \frac{A}{\sqrt{2\pi\hbar}}\int_{-\infty}^{0}e^{(\rho-ip/\hbar)x}\mathrm{d}x + \frac{A}{\sqrt{2\pi\hbar}}\int_{0}^{+\infty}e^{-(\rho+ip/\hbar)x}\mathrm{d}x \\
&= \frac{A}{\sqrt{2\pi\hbar}}\left[\frac{e^{(\rho-ip/\hbar)x}}{\rho-\frac{ip}{\hbar}}\right]_{-\infty}^{0} + \frac{A}{\sqrt{2\pi\hbar}}\left[-\frac{e^{-(\rho+ip/\hbar)x}}{\rho+\frac{ip}{\hbar}}\right]_{0}^{+\infty}
\end{aligned}$$

$$\overline{\varphi}(p) = \frac{A}{\sqrt{2\pi\hbar}}\left(\frac{\hbar}{\rho\hbar - ip} + \frac{\hbar}{\rho\hbar + ip}\right) = \frac{1}{\sqrt{2\pi\hbar}}\frac{2\rho A\hbar^2}{p^2 + \rho^2\hbar^2}$$

The probability $\overline{\mathrm{d}\mathscr{P}}(p)$ that a measurement of the momentum of the particle in the unique normalized stationary state calculated in question b yields a result included between p and $p + \mathrm{d}p$ is

$$\overline{\mathrm{d}\mathscr{P}}(p) = |\overline{\varphi}(p)|^2\mathrm{d}p = \left(\frac{1}{\sqrt{2\pi\hbar}}\frac{2\rho A\hbar^2}{p^2 + \rho^2\hbar^2}\right)^2\mathrm{d}p$$

This probability is maximal for $p = 0$ for which

$$\overline{\mathrm{d}\mathscr{P}}(0) = \frac{2A^2}{\pi\hbar\rho^2}\mathrm{d}p$$

Defining Δp as the full width at half maximum of $\overline{\mathrm{d}\mathscr{P}}(p)$, we find

$$\begin{aligned}\overline{\mathrm{d}\mathscr{P}}(p) = \frac{A^2}{\pi\hbar\rho^2}\mathrm{d}p \Leftrightarrow \left(\frac{1}{\sqrt{2\pi\hbar}}\frac{2\rho A\hbar^2}{p^2 + \rho^2\hbar^2}\right)^2 &= \frac{A^2}{\pi\hbar\rho^2}\\ \Leftrightarrow \frac{2\rho^2A^2\hbar^4}{\pi\hbar\left(p^2 + \rho^2\hbar^2\right)^2} &= \frac{A^2}{\pi\hbar\rho^2}\\ \Leftrightarrow (p^2 + \rho^2\hbar^2)^2 &= 2\rho^4\hbar^4\\ \Leftrightarrow p^2 = (\sqrt{2} - 1)\rho^2\hbar^2 &\Leftrightarrow p = \pm\sqrt{\sqrt{2} - 1}\rho\hbar\end{aligned}$$

hence

$$\Delta p = 2\sqrt{\sqrt{2} - 1}\rho\hbar \simeq 0.644\rho\hbar \sim \rho\hbar$$

We finally find:

$$\Delta x \cdot \Delta p \sim \hbar$$

which is of the order of magnitude of the Heisenberg limit. The fact that $\Delta x \cdot \Delta p \sim \hbar$ shows that this problem is only solvable quantum mechanically, since the particle explores an area in space, outside the Dirac well, which is "forbidden" by classical mechanics. Trying to localize the particle within the Dirac peak, *i.e.* the "authorized zone" according to classical mechanics, is not compatible with Heisenberg's principle, which is at the heart of quantum mechanics.

1.3 Transmission of a "Delta Function" Potential Barrier

Statement

Consider a particle placed in the same potential as in the preceding exercise. The particle is now propagating from left to right along the *Ox* axis, with a positive energy *E*.

a. Show that a stationary state of the particle can be written:

$$\begin{cases} \text{if} \quad x < 0 \quad \varphi(x) = e^{ikx} + Ae^{-ikx} \\ \text{if} \quad x > 0 \quad \varphi(x) = Be^{ikx} \end{cases}$$

where k, A, and B are constants which are to be calculated in terms of the energy E, of m, and of α (watch out for the discontinuity in $\frac{d\varphi}{dx}$ at $x = 0$).

b. Set $-E_L = -\frac{m\alpha^2}{2\hbar^2}$ (bound state energy of the particle). Calculate, in terms of the dimensionless parameter $\frac{E}{E_L}$, the reflection coefficient R and the transmission coefficient T of the barrier. Study their variations with respect to E; what happens when $E \to \infty$? How can this be interpreted? Show that, if the expression of T is extended for negative values of E, it diverges when $E \to -E_L$, and discuss this result.

Comments

This exercise follows on from exercise 2 and cannot be undertaken independently.

Unlike the previous exercise, the energy of the particle is positive, which allows the particle to explore all of space. The particle has sufficient energy to freely move in and outside the well.

From a classical point of view, what can be said about a beam of particles encountering a potential well? It is important to take some time to ask the question, to (re)familiarize oneself with the classical result and thus better appreciate the subtlety of the quantum result. If it is difficult to imagine a Dirac well, it is possible to imagine one that is very narrow albeit finite.

Classical particles stemming from $-\infty$ encounter the well and enter it (increasing their kinetic energy in doing so). They have enough energy to exit the well and then continue to propagate toward increasing x, toward $+\infty$ (having lost the excess kinetic energy on leaving the well). To conclude, all classical particles continue on their path, exactly as if the well did not exist. All of them enter and exit the well, and the energies outside the well, before or after, are the same.

The aim of this exercise is to calculate the transmission rate quantum mechanically and to compare it with the classical result: $T_{\text{classical}} = 100\%$.

Solution

Consider a particle placed in the same potential as in the preceding exercise. The particle is now propagating from left to right along the Ox axis, with a positive energy E.

a. Show that a stationary state of the particle can be written:

$$\begin{cases} \text{if} \quad x < 0 \quad \varphi(x) = e^{ikx} + Ae^{-ikx} \\ \text{if} \quad x > 0 \quad \varphi(x) = Be^{ikx} \end{cases}$$

where k, A, and B are constants which are to be calculated in terms of the energy E, of m, and of α (watch out for the discontinuity in $\frac{\mathrm{d}\varphi}{\mathrm{d}x}$ at $x = 0$).

To the left of the potential barrier ($x < 0$), $V(x) = 0$ and the eigenvalue equation of H is

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\varphi(x)}{\mathrm{d}x^2} - E\varphi(x) = 0 \Leftrightarrow \frac{\mathrm{d}^2\varphi(x)}{\mathrm{d}x^2} + \frac{2mE}{\hbar^2}\varphi(x) = 0 \Leftrightarrow \frac{\mathrm{d}^2\varphi(x)}{\mathrm{d}x^2} + k^2\varphi(x) = 0$$

setting $k = \sqrt{\frac{2mE}{\hbar^2}}$ (*i.e.* $E = \frac{p^2}{2m}$ as for a classical particle) since we assume $E > 0$, and the eigenfunction can thus be written $\varphi(x) = A' e^{ikx} + Ae^{-ikx}$.

To the right of the potential barrier ($x > 0$), $V(x) = 0$ still holds so the eigenfunction can also be written $\varphi(x) = Be^{ikx} + B' e^{-ikx}$.

In addition, the particle is propagating from left to right so $B' = 0$ as no reflection is possible beyond $x = 0$. Without any obstacle, the particles continue their path in $x > 0$, with increasing x hence $B \neq 0$, but no wave is reflected in $x > 0$, in the direction of decreasing x. Likewise, we must take $A \neq 0$ to account for any reflection on the barrier, in which case particles propagate in $x < 0$, in the direction of decreasing x and we can choose $A' = 1$ (relating to incident particles in $x < 0$, propagating along increasing x) since having a normalized wave function allows us to already fix one constant to the value of our choice. In summary:

$$\begin{cases} \text{if} \quad x < 0 \quad \varphi_{\mathrm{I}}(x) = e^{ikx} + Ae^{-ikx} \\ \text{if} \quad x > 0 \quad \varphi_{\mathrm{II}}(x) = Be^{ikx} \end{cases}$$

with $k = \sqrt{\frac{2mE}{\hbar^2}}$. Firstly, the eigenfunction $\varphi(x)$ is continuous at $x = 0$, so

$$\varphi_{\mathrm{I}}(0) = \varphi_{\mathrm{II}}(0) \Leftrightarrow 1 + A = B$$

Secondly, the eigenfunction's first derivative is discontinuous at $x = 0$ due to the delta function, and we showed in exercise 2 that this discontinuity equals $-\frac{2m\alpha}{\hbar^2}\varphi(0)$. Therefore:

$$\frac{\mathrm{d}\varphi_{\mathrm{II}}(0)}{\mathrm{d}x} - \frac{\mathrm{d}\varphi_{\mathrm{I}}(0)}{\mathrm{d}x} = -\frac{2m\alpha}{\hbar^2}\varphi(0) \Leftrightarrow ik(B - 1 + A) = -\frac{2m\alpha}{\hbar^2}B$$

Since $B = 1 + A$ according to the continuity condition, the previous equation becomes:

$$2ikA = -\frac{2m\alpha}{\hbar^2}(1 + A) \Leftrightarrow \left(\frac{2m\alpha}{\hbar^2} + 2ik\right)A = -\frac{2m\alpha}{\hbar^2}$$

or in other words

$$A = -\frac{m\alpha}{m\alpha + ik\hbar^2} = -\frac{m\alpha}{m\alpha + i\hbar\sqrt{2mE}}$$

which finally yields

$$B = 1 + A = \frac{i\hbar\sqrt{2mE}}{m\alpha + i\hbar\sqrt{2mE}}$$

b. Set $-E_L = -\frac{m\alpha^2}{2\hbar^2}$ (bound state energy of the particle). Calculate, in terms of the dimensionless parameter $\frac{E}{E_L}$, the reflection coefficient R and the transmission coefficient T of the barrier. Study their variations with respect to E; what happens when $E \to \infty$? How can this be interpreted? Show that, if the expression of T is extended for negative values of E, it diverges when $E \to -E_L$, and discuss this result.

The reflection coefficient of the barrier is

$$R = \left|\frac{A}{1}\right|^2 = |A|^2 = \frac{m^2\alpha^2}{m^2\alpha^2 + 2mE\hbar^2} = \frac{1}{1 + \frac{2E\hbar^2}{m\alpha^2}} = \frac{1}{1 + \frac{E}{E_L}}$$

and the transmission coefficient is

$$T = \left|\frac{B}{1}\right|^2 = |B|^2 = \frac{2mE\hbar^2}{m^2\alpha^2 + 2mE\hbar^2} = \frac{\frac{2E\hbar^2}{m\alpha^2}}{1 + \frac{2E\hbar^2}{m\alpha^2}} = \frac{\frac{E}{E_L}}{1 + \frac{E}{E_L}}$$

It is easy to verify $R + T = 1$ representing the energy conservation either side of the barrier. As the energy E is assumed positive, the forms of R and T as functions of E are represented in Figure 1.2.

When $E \to \infty$, $\frac{E}{E_L} \to \infty$ and therefore $R \to 0$ and $T \to 1$: if the energy is sufficiently great to render the potential barrier negligible, then the particle crosses the barrier as if it did not exist.

If we extend the expression of T to negative values of E, T diverges when $1 + \frac{E}{E_L} \to 0 \Leftrightarrow E \to -E_L$. This divergence indicates the existence of a bound

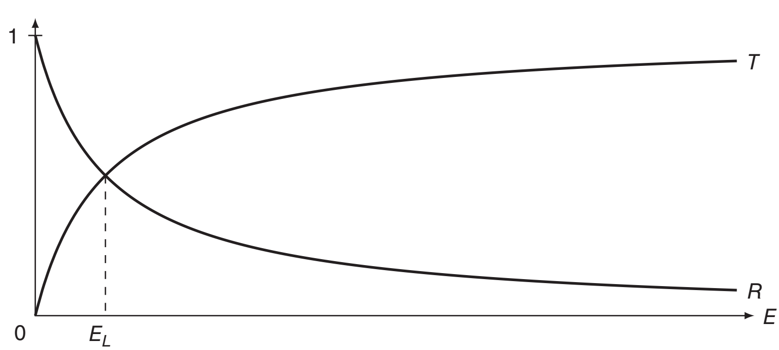


Figure 1.2 Representative curves of R and T as functions of E.

state whose energy equals $-E_L$, as bound states correspond to the poles of the transmission coefficient T.

Let us now compare the quantum and classical results. We can already state that T is not systematically $100\% = T_{\text{classical}}$. This is an important result. Even if particles have enough energy to cross the potential barrier (from a classical point of view), some are reflected back. In quantum mechanics, a given particle of enough energy, therefore, has a probability R to go backward, which is unimaginable in classical mechanics given the shape of the potential. Experimentally, in very similar conditions such as a neutron encountering a nucleus, the predictions of quantum mechanics are verified. Particles do indeed "bounce" in a quantum manner.

If in terms of particles, this experiment seems difficult to conceive, or is at least counter-intuitive, it is not so in terms of "waves". A wave encountering a pane of glass is indeed partly reflected and partly transmitted.

Finally, let us note that when $E \to \infty$, *i.e.* when $E \gg E_l$, then $T \to 1$, which is pertinent. If the barrier is insignificant, undetectable by the highly energetic particle, then particles do not interact with the potential well and continue as before.

1.4 Bound State of a Particle in a "Delta Function Potential", Fourier Analysis

Statement

Return to exercise 2, using this time the Fourier transform.

a. Write the eigenvalue equation of H and the Fourier transform of this equation. Deduce directly from this the expression for $\overline{\varphi}(p)$, the Fourier transform of $\varphi(x)$, in terms of p, E, α, and $\varphi(0)$. Then show that only one value of E, a negative one, is possible. Only the bound state of the particle, and not the ones in which it propagates, is found by this method; why? Then calculate $\varphi(x)$ and show that one can find in this way all the results of exercise 2.

b. The average kinetic energy of the particle can be written (*cf*. Chap. III):

$$E_k = \frac{1}{2m} \int_{-\infty}^{+\infty} p^2 |\overline{\varphi}(p)|^2 \mathrm{d}p$$

Show that, when $\overline{\varphi}(p)$ is a "sufficiently smooth" function, we also have:

$$E_k = -\frac{\hbar^2}{2m} \int_{-\infty}^{+\infty} \varphi^*(x) \frac{\mathrm{d}^2\varphi}{\mathrm{d}x^2} \mathrm{d}x$$

These formulas enable us to obtain, in two different ways, the energy E_k for a particle in the bound state calculated in a. What result is obtained? Note that, in this case, $\varphi(x)$ is not "regular" at $x = 0$, where its derivative is discontinuous. It is then necessary to differentiate $\varphi(x)$ in the sense of distributions, which introduces a contribution of the point $x = 0$ to the sought average value we are looking for. Interpret this contribution physically: consider a square well, centered at $x = 0$, whose width a approaches 0 and whose depth V_0 approaches infinity (so that $aV_0 = \alpha$), and study the behavior of the wave function in this well.

Comments

This exercise follows on from exercise 2 and cannot be undertaken independently. All results and comments from exercise 2 are now assumed to be understood and will not be proven again. The approach here is more technical, but the final interpretation should be compared with that of exercise 2.

At the end of the exercise, a final step of reasoning is proposed in order to better comprehend the results. Once more, the case of a finite well is studied along with its end behavior in terms of a Dirac well by taking the limit. This is an interesting approach albeit not always easy to interpret and rather technical.

Solution

Return to exercise 2, using this time the Fourier transform.

a. Write the eigenvalue equation of H and the Fourier transform of this equation. Deduce directly from this the expression for $\overline{\varphi}(p)$, the Fourier transform of $\varphi(x)$, in terms of p, E, α, and $\varphi(0)$. Then show that only one value of E, a negative one, is possible. Only the bound state of the particle, and not the ones in which it propagates, is found by this method; why? Then calculate $\varphi(x)$ and show that one can find in this way all the results of exercise 2.

The eigenvalue equation of H is

$$H\varphi(x) = E\varphi(x) \Leftrightarrow -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\varphi(x)}{\mathrm{d}x^2} - \alpha\delta(x)\varphi(x) = E\varphi(x)$$

According to equation (38a) of Appendix I, the Fourier transform of this equation is

$$-\frac{\hbar^2}{2m}\left(\frac{ip}{\hbar}\right)^2\overline{\varphi}(p) - \frac{\alpha}{\sqrt{2\pi\hbar}}\int_{-\infty}^{+\infty}\delta(x)\varphi(x)e^{-ipx/\hbar}\mathrm{d}x = E\overline{\varphi}(p)$$

that is

$$\frac{p^2}{2m}\overline{\varphi}(p) - \frac{\alpha\varphi(0)}{\sqrt{2\pi\hbar}} = E\overline{\varphi}(p)$$

from which we can deduce

$$\overline{\varphi}(p) = \frac{1}{\sqrt{2\pi\hbar}}\frac{\alpha\varphi(0)}{\frac{p^2}{2m} - E} = \frac{1}{\sqrt{2\pi\hbar}}\frac{2m\alpha\varphi(0)}{p^2 - 2mE}$$

However, norm conservation is a property of Fourier transforms, so

$$\int_{-\infty}^{+\infty}|\overline{\varphi}(p)|^2\mathrm{d}p = 1 \Leftrightarrow \frac{2m^2\alpha^2\varphi^2(0)}{\pi\hbar}\int_{-\infty}^{+\infty}\frac{\mathrm{d}p}{(p^2 - 2mE)^2} = 1$$

Let us undertake a partial fraction decomposition of $\frac{1}{(p^2 - 2mE)^2}$:

- If $E > 0$, the state is not bound, the particle can explore all of space and the corresponding harmonic wave cannot be normalized.
- If $E < 0$:

$$\begin{aligned}\frac{1}{(p^2-2mE)^2} &= \frac{1}{\left[p^2-(i\sqrt{-2mE})^2\right]^2}\\ &= \frac{1}{(p+i\sqrt{-2mE})^2(p-i\sqrt{-2mE})^2}\\ &= \frac{\alpha}{p+i\sqrt{-2mE}} + \frac{\beta}{(p+i\sqrt{-2mE})^2}\\ &\quad + \frac{\alpha^*}{p-i\sqrt{-2mE}} + \frac{\beta^*}{(p-i\sqrt{-2mE})^2}\end{aligned}$$

We then write:

$$\begin{aligned}\alpha &= \left[\frac{\mathrm{d}}{\mathrm{d}p}\left(\frac{1}{(p-i\sqrt{-2mE})^2}\right)\right]_{p=-i\sqrt{-2mE}}\\ &= \left[-\frac{2}{(p-i\sqrt{-2mE})^3}\right]_{p=-i\sqrt{-2mE}}\\ &= \frac{i}{4(-2mE)^{3/2}}\\ \beta &= \left[\frac{1}{(p-i\sqrt{-2mE})^2}\right]_{p=-i\sqrt{-2mE}} = \frac{1}{8mE}\end{aligned}$$

hence,

$$\begin{aligned}\frac{1}{(p^2-2mE)^2} &= \frac{i}{4(-2mE)^{3/2}}\left(\frac{1}{p+i\sqrt{-2mE}} - \frac{1}{p-i\sqrt{-2mE}}\right)\\ &\quad + \frac{1}{8mE}\left(\frac{1}{(p+i\sqrt{-2mE})^2} + \frac{1}{(p-i\sqrt{-2mE})^2}\right)\\ &= \frac{1}{2(-2mE)}\frac{1}{p^2-2mE} + \frac{1}{8mE}\left(\frac{1}{(p+i\sqrt{-2mE})^2}\right.\\ &\quad \left. + \frac{1}{(p-i\sqrt{-2mE})^2}\right)\end{aligned}$$

An antiderivative of this rational fraction is thus

$$\begin{aligned}\int \frac{\mathrm{d}p}{(p^2-2mE)^2} &= \frac{1}{2(-2mE)^{3/2}}\arctan\left(\frac{p}{\sqrt{-2mE}}\right)\\ &\quad - \frac{1}{8mE}\left(\frac{1}{p+i\sqrt{-2mE}} + \frac{1}{p-i\sqrt{-2mE}}\right)\end{aligned}$$

$$\int \frac{\mathrm{d}p}{(p^2 - 2mE)^2} = \frac{1}{2(-2mE)^{3/2}} \arctan\left(\frac{p}{\sqrt{-2mE}}\right) - \frac{1}{4mE}\frac{p}{p^2 - 2mE}$$

This means that necessarily $E < 0$ and:

$$\begin{aligned}\int_{-\infty}^{+\infty} |\overline{\varphi}(p)|^2 \mathrm{d}p = 1 &\Leftrightarrow \frac{2m^2\alpha^2\varphi^2(0)}{\pi\hbar}\frac{\pi}{2(-2mE)^{3/2}} = 1\\ &\Leftrightarrow (-2mE)^{3/2} = \frac{m^2\alpha^2\varphi^2(0)}{\hbar}\\ &\Leftrightarrow -mE = \frac{m^{4/3}\alpha^{4/3}\varphi^{4/3}(0)}{2\hbar^{2/3}} \Leftrightarrow E = -\frac{m^{1/3}\alpha^{4/3}\varphi^{4/3}(0)}{2\hbar^{2/3}}\end{aligned}$$

because

$$\begin{aligned}\int_{-\infty}^{+\infty} \frac{\mathrm{d}p}{(p^2 - 2mE)^2} &= \left[\frac{1}{2(-2mE)^{3/2}} \arctan\left(\frac{p}{\sqrt{-2mE}}\right) - \frac{1}{4mE}\frac{p}{p^2 - 2mE}\right]_{-\infty}^{+\infty}\\ &= \frac{\pi}{2(-2mE)^{3/2}}\end{aligned}$$

By using the expression of $\varphi(x)$ found in exercise 2, we get $\varphi(0) = \sqrt{\frac{m\alpha}{\hbar^2}}$, from which we deduce:

$$\varphi^{4/3}(0) = \frac{m^{2/3}\alpha^{2/3}}{\hbar^{4/3}} \Rightarrow E = -\frac{m\alpha^2}{2\hbar^2}$$

which is the energy of the bound state of the particle. We do not find excited states of the particle when it propagates because the functions $\overline{\varphi}(p)$, that are eigenfunctions of H, are not square-integrable when $E > 0$ and hence are not defined. Let us now calculate $\varphi(x)$ by inverse Fourier transform:

$$\varphi(x) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} \overline{\varphi}(p) e^{ipx/\hbar} \mathrm{d}p = \frac{m\alpha\varphi(0)}{\pi\hbar} \int_{-\infty}^{+\infty} \frac{e^{ipx/\hbar}}{p^2 - 2mE} \mathrm{d}p$$

It is not possible to calculate $\varphi(x)$ using this expression simply because the wave function $\varphi(x)$ does not have a unique expression over all $\mathbb{R}$, but two distinct expressions, one for $x < 0$ and one for $x > 0$. We proved, in question d exercise 2, that the Fourier transform of the wave function defined as:

$$\begin{cases} \text{if} \quad x < 0 \quad \varphi(x) = Ae^{\rho x} \\ \text{if} \quad x > 0 \quad \varphi(x) = Ae^{-\rho x} \end{cases}$$

was actually:

$$\overline{\varphi}(p) = \frac{1}{\sqrt{2\pi\hbar}} \frac{2\rho A\hbar^2}{p^2 + \rho^2\hbar^2}$$

Comparing to the expression

$$\overline{\varphi}(p) = \frac{1}{\sqrt{2\pi\hbar}} \frac{2m\alpha\varphi(0)}{p^2 - 2mE}$$

we can deduce that

$$\rho = \sqrt{\frac{-2mE}{\hbar^2}} = \frac{m\alpha}{\hbar^2} \text{ and } A = \varphi(0) = \sqrt{\frac{m\alpha}{\hbar^2}}$$

We, therefore, find the same wave function as in exercise 2 and so we can once more deduce the same results as in exercise 2.

b. The average kinetic energy of the particle can be written (*cf*. Chap. III):

$$E_k = \frac{1}{2m}\int_{-\infty}^{+\infty} p^2|\overline{\varphi}(p)|^2 \mathrm{d}p$$

Show that, when $\overline{\varphi}(p)$ is a "sufficiently smooth" function, we also have:

$$E_k = -\frac{\hbar^2}{2m}\int_{-\infty}^{+\infty} \varphi^*(x)\frac{\mathrm{d}^2\varphi}{\mathrm{d}x^2}\mathrm{d}x$$

These formulas enable us to obtain, in two different ways, the energy E_k for a particle in the bound state calculated in a. What result is obtained? Note that, in this case, $\varphi(x)$ is not "regular" at $x = 0$, where its derivative is discontinuous. It is then necessary to differentiate $\varphi(x)$ in the sense of distributions, which introduces a contribution of the point $x = 0$ to the mean value we are looking for. Interpret this contribution physically: consider a square well, centered at $x = 0$, whose width a approaches 0 and whose depth V_0 approaches infinity (so that $aV_0 = \alpha$), and study the behavior of the wave function in this well.

We start by writing:

$$\begin{aligned} E_k &= \frac{1}{2m}\int_{-\infty}^{+\infty} p^2|\overline{\varphi}(p)|^2\mathrm{d}p = \frac{1}{2m}\int_{-\infty}^{+\infty} p^2\overline{\varphi}^*(p)\overline{\varphi}(p)\mathrm{d}p \\ &= \frac{\hbar^2}{2m}\int_{-\infty}^{+\infty}\left(\frac{ip}{\hbar}\right)^*\overline{\varphi}^*(p)\left(\frac{ip}{\hbar}\right)\overline{\varphi}(p)\mathrm{d}p = \frac{\hbar^2}{2m}\int_{-\infty}^{+\infty}\left|\mathscr{F}\left[\frac{\mathrm{d}\varphi(x)}{\mathrm{d}x}\right]\right|^2\mathrm{d}p \\ &= \frac{\hbar^2}{2m}\int_{-\infty}^{+\infty}\left|\frac{\mathrm{d}\varphi(x)}{\mathrm{d}x}\right|^2\mathrm{d}x \end{aligned}$$

using the norm conservation property of Fourier transforms, namely the Parseval-Plancherel formula (45) of Appendix I. The last line can also be written:

$$E_k = \frac{\hbar^2}{2m}\int_{-\infty}^{+\infty}\frac{\mathrm{d}\varphi^*(x)}{\mathrm{d}x}\frac{\mathrm{d}\varphi(x)}{\mathrm{d}x}\mathrm{d}x$$

This integral can be rewritten using an integration by parts, setting:

$$\begin{cases} u' = \dfrac{\mathrm{d}\varphi^*(x)}{\mathrm{d}x} \\ v = \dfrac{\mathrm{d}\varphi(x)}{\mathrm{d}x} \end{cases} \quad\text{and}\quad \begin{cases} u = \varphi^*(x) \\ v' = \dfrac{\mathrm{d}^2\varphi(x)}{\mathrm{d}x^2} \end{cases}$$

Thus:

$$E_k = \frac{\hbar^2}{2m}\left[\varphi^*(x)\frac{\mathrm{d}\varphi(x)}{\mathrm{d}x}\right]_{-\infty}^{+\infty} - \frac{\hbar^2}{2m}\int_{-\infty}^{+\infty}\varphi^*(x)\frac{\mathrm{d}^2\varphi(x)}{\mathrm{d}x^2}\mathrm{d}x$$

However, $\varphi^*(x)$ should vanish at $\pm\infty$ in order to be square-integrable, which indeed yields the sought result:

$$E_k = \frac{1}{2m}\int_{-\infty}^{+\infty} p^2|\overline{\varphi}(p)|^2 \mathrm{d}p = -\frac{\hbar^2}{2m}\int_{-\infty}^{+\infty} \varphi^*(x)\frac{\mathrm{d}^2\varphi(x)}{\mathrm{d}x^2}\mathrm{d}x$$

For a particle in the bound state calculated in a, we find $\varphi(x) = \sqrt{\frac{m\alpha}{\hbar^2}}e^{-\frac{m\alpha}{\hbar^2}|x|}$ according to the results of exercise 2 and

$$\overline{\varphi}(p) = \frac{1}{\sqrt{2\pi\hbar}}\frac{2m\alpha\varphi(0)}{p^2 - 2mE} = \frac{1}{\sqrt{2\pi\hbar^3}}\frac{2m^{3/2}\alpha^{3/2}}{p^2 - 2mE}$$

according to the results of question a. Using these results as the basis for a first line of reasoning:

$$\begin{aligned} E_k &= \frac{1}{2m}\int_{-\infty}^{+\infty} p^2|\overline{\varphi}(p)|^2 \mathrm{d}p = \frac{1}{2m}\frac{2m^3\alpha^3}{\pi\hbar^3}\int_{-\infty}^{+\infty}\frac{p^2}{(p^2-2mE)^2}\mathrm{d}p \\ &= \frac{m^2\alpha^3}{\pi\hbar^3}\int_{-\infty}^{+\infty}\frac{p^2}{(p^2-2mE)^2}\mathrm{d}p \end{aligned}$$

A partial fraction decomposition of $\frac{p^2}{(p^2-2mE)^2}$ yields:

$$\begin{aligned} \frac{p^2}{(p^2-2mE)^2} &= \frac{p^2}{(p^2-(i\sqrt{-2mE})^2)^2} = \frac{p^2}{(p+i\sqrt{-2mE})^2(p-i\sqrt{-2mE})^2} \\ &= \frac{\gamma}{p+i\sqrt{-2mE}} + \frac{\delta}{(p+i\sqrt{-2mE})^2} \\ &\quad + \frac{\gamma^*}{p-i\sqrt{-2mE}} + \frac{\delta^*}{(p-i\sqrt{-2mE})^2} \end{aligned}$$

Then, we write:

$$\begin{aligned} \gamma &= \left[\frac{\mathrm{d}}{\mathrm{d}p}\left(\frac{p^2}{(p-i\sqrt{-2mE})^2}\right)\right]_{p=-i\sqrt{-2mE}} \\ &= \left[\frac{2p(p-i\sqrt{-2mE})^2 - 2(p-i\sqrt{-2mE})p^2}{(p-i\sqrt{-2mE})^4}\right]_{p=-i\sqrt{-2mE}} \\ &= \left[\frac{2p(p-i\sqrt{-2mE}) - 2p^2}{(p-i\sqrt{-2mE})^3}\right]_{p=-i\sqrt{-2mE}} \\ &= \left[-\frac{2pi\sqrt{-2mE}}{(p-i\sqrt{-2mE})^3}\right]_{p=-i\sqrt{-2mE}} \\ &= \frac{4mE}{8i(-2mE)^{3/2}} = \frac{i}{4\sqrt{-2mE}} \end{aligned}$$

$$\delta = \left[\frac{p^2}{(p-i\sqrt{-2mE})^2}\right]_{p=-i\sqrt{-2mE}} = \frac{2mE}{8mE} = \frac{1}{4}$$

hence

$$\frac{p^2}{(p^2-2mE)^2} = \frac{i}{4\sqrt{-2mE}}\left(\frac{1}{p+i\sqrt{-2mE}} - \frac{1}{p-i\sqrt{-2mE}}\right)$$
$$+\frac{1}{4}\left(\frac{1}{(p+i\sqrt{-2mE})^2} + \frac{1}{(p-i\sqrt{-2mE})^2}\right)$$
$$= \frac{1}{2}\frac{1}{p^2-2mE} + \frac{1}{4}\left(\frac{1}{(p+i\sqrt{-2mE})^2} + \frac{1}{(p-i\sqrt{-2mE})^2}\right)$$

An antiderivative of this rational fraction is thus,

$$\int \frac{p^2}{(p^2-2mE)^2}\mathrm{d}p = \frac{1}{2\sqrt{-2mE}}\arctan\left(\frac{p}{\sqrt{-2mE}}\right)$$
$$-\frac{1}{4}\left(\frac{1}{p+i\sqrt{-2mE}} + \frac{1}{p-i\sqrt{-2mE}}\right)$$
$$= \frac{1}{2\sqrt{-2mE}}\arctan\left(\frac{p}{\sqrt{-2mE}}\right) - \frac{1}{2}\frac{p}{p^2-2mE}$$

which gives

$$\int_{-\infty}^{+\infty} \frac{p^2}{(p^2-2mE)^2}\mathrm{d}p = \left[\frac{1}{2\sqrt{-2mE}}\arctan\left(\frac{p}{\sqrt{-2mE}}\right) - \frac{1}{2}\frac{p}{p^2-2mE}\right]_{-\infty}^{+\infty}$$
$$= \frac{\pi}{2\sqrt{-2mE}}$$

and therefore:

$$E_k = \frac{m^2\alpha^3}{\pi\hbar^3}\frac{\pi}{2\sqrt{-2mE}} = \frac{m^2\alpha^3}{2\hbar^3\sqrt{-2mE}} = \frac{m\alpha^2}{2\hbar^2} = -E$$

since $E = -\dfrac{m\alpha^2}{2\hbar^2} \Leftrightarrow \sqrt{-2mE} = \dfrac{m\alpha}{\hbar}$ according to the results of question a.

The second line of reasoning is as follows:

$$E_k = -\frac{\hbar^2}{2m}\int_{-\infty}^{+\infty} \varphi^*(x)\frac{\mathrm{d}^2\varphi(x)}{\mathrm{d}x^2}\mathrm{d}x$$

However, $\dfrac{\mathrm{d}^2\varphi(x)}{\mathrm{d}x^2}$ presents a discontinuity at $x = 0$, and this integral must be rewritten as:

$$E_k = -\frac{\hbar^2}{2m}\left[\int_{-\infty}^{0^-} \varphi(x)\frac{\mathrm{d}^2\varphi(x)}{\mathrm{d}x^2}\mathrm{d}x + \int_{0^-}^{0^+} \varphi(x)\frac{\mathrm{d}^2\varphi(x)}{\mathrm{d}x^2}\mathrm{d}x + \int_{0^+}^{+\infty} \varphi(x)\frac{\mathrm{d}^2\varphi(x)}{\mathrm{d}x^2}\mathrm{d}x\right]$$

with $\varphi^*(x) = \varphi(x)$ since the wave function $\varphi(x) = \sqrt{\dfrac{m\alpha}{\hbar^2}}e^{-\frac{m\alpha}{\hbar^2}|x|}$ is real. We can now apply a similar method to what was used in exercise 2 to determine the value of the discontinuity of $\frac{\mathrm{d}\varphi(x)}{\mathrm{d}x}$ at $x = 0$. The eigenvalue equation of H is:

$$H\varphi(x) = E\varphi(x) \Leftrightarrow -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\varphi(x)}{\mathrm{d}x^2} - \alpha\delta(x)\varphi(x) = E\varphi(x)$$

By multiplying by $\varphi(x)$ on either side of the equation, we find:

$$-\frac{\hbar^2}{2m}\varphi(x)\frac{\mathrm{d}^2\varphi(x)}{\mathrm{d}x^2} - \alpha\delta(x)\varphi^2(x) = E\varphi^2(x)$$

Integrating this equation between $-\varepsilon$ and $+\varepsilon$ yields:

$$-\frac{\hbar^2}{2m}\int_{-\varepsilon}^{+\varepsilon}\varphi(x)\frac{\mathrm{d}^2\varphi(x)}{\mathrm{d}x^2}\mathrm{d}x - \alpha\int_{-\varepsilon}^{+\varepsilon}\delta(x)\varphi^2(x)\mathrm{d}x = E\int_{-\varepsilon}^{+\varepsilon}\varphi^2(x)\mathrm{d}x$$
$$\Leftrightarrow -\frac{\hbar^2}{2m}\int_{-\varepsilon}^{+\varepsilon}\varphi(x)\frac{\mathrm{d}^2\varphi(x)}{\mathrm{d}x^2}\mathrm{d}x - \alpha\varphi^2(0) = E\int_{-\varepsilon}^{+\varepsilon}\varphi^2(x)\mathrm{d}x$$

Letting ε approach 0 yields:

$$-\frac{\hbar^2}{2m}\int_{0^-}^{0^+}\varphi(x)\frac{\mathrm{d}^2\varphi(x)}{\mathrm{d}x^2}\mathrm{d}x = \alpha\varphi^2(0) = \frac{m\alpha^2}{\hbar^2} \Leftrightarrow \int_{0^-}^{0^+}\varphi(x)\frac{\mathrm{d}^2\varphi(x)}{\mathrm{d}x^2}\mathrm{d}x = -\frac{2m^2\alpha^2}{\hbar^4}$$

We thus deduce:

$$\begin{aligned}
E_k &= -\frac{\hbar^2}{2m}\left[\int_{-\infty}^{0^-}\varphi(x)\frac{\mathrm{d}^2\varphi(x)}{\mathrm{d}x^2}\mathrm{d}x + \int_{0^-}^{0^+}\varphi(x)\frac{\mathrm{d}^2\varphi(x)}{\mathrm{d}x^2}\mathrm{d}x + \int_{0^+}^{+\infty}\varphi(x)\frac{\mathrm{d}^2\varphi(x)}{\mathrm{d}x^2}\mathrm{d}x\right] \\
&= -\frac{\hbar^2}{2m}\left[\frac{m\alpha}{\hbar^2}\left(\frac{m\alpha}{\hbar^2}\right)^2\int_{-\infty}^{0^-} e^{\frac{2m\alpha}{\hbar^2}x}\mathrm{d}x - \frac{2m^2\alpha^2}{\hbar^4} + \frac{m\alpha}{\hbar^2}\left(\frac{m\alpha}{\hbar^2}\right)^2\int_{0^+}^{+\infty} e^{-\frac{2m\alpha}{\hbar^2}x}\mathrm{d}x\right] \\
&= -\frac{\hbar^2}{2m}\left(\frac{m\alpha}{\hbar^2}\right)^2\left(\frac{m\alpha}{\hbar^2}\left[\frac{\hbar^2}{2m\alpha}e^{\frac{2m\alpha}{\hbar^2}x}\right]_{-\infty}^{0^-} - 2 - \frac{m\alpha}{\hbar^2}\left[\frac{\hbar^2}{2m\alpha}e^{-\frac{2m\alpha}{\hbar^2}x}\right]_{0^+}^{+\infty}\right) \\
&= -\frac{m\alpha^2}{2\hbar^2}\left(\frac{1}{2} - 2 + \frac{1}{2}\right) = \frac{m\alpha^2}{2\hbar^2} = -E
\end{aligned}$$

and we find the same result as previously but using another method, namely that the average kinetic energy of the particle equals the opposite of the bound state energy. Note that the contribution of point $x = 0$ to the average kinetic energy of the particle amounts to:

$$-\frac{\hbar^2}{2m}\int_{0^-}^{0^+}\varphi(x)\frac{\mathrm{d}^2\varphi(x)}{\mathrm{d}x^2}\mathrm{d}x = \frac{m\alpha^2}{\hbar^2}$$

That is twice the average kinetic energy of the particle computed just above. To rationalize this finding, let us now consider a square potential well centered at $x = 0$, whose width is a and depth is V_0 such that $aV_0 = \alpha$. We know from § 2-c-α of Complement $\mathrm{H_I}$ that the expression of the wave function of a stationary state whose energy is between $-V_0$ and 0 is:

$$\varphi(x) = \begin{cases} B_1 e^{\rho x} & \text{if} \quad x < -\frac{a}{2} \\ A_2 e^{ikx} + A_2' e^{-ikx} & \text{if} \quad -\frac{a}{2} \leqslant x \leqslant \frac{a}{2} \\ B_3' e^{-\rho x} & \text{if} \quad x > \frac{a}{2} \end{cases}$$

with $\rho = \sqrt{-\frac{2mE}{\hbar^2}}$ and $k = \sqrt{\frac{2m(E+V_0)}{\hbar^2}}$. We find, according to § 2-c-α of complement $\mathrm{H_I}$:

$$\begin{cases} A_2 = e^{(-\rho+ik)a/2} \dfrac{\rho + ik}{2ik} B_1 \\ A_2' = -e^{-(\rho+ik)a/2} \dfrac{\rho - ik}{2ik} B_1 \\ B_3' = \dfrac{\rho^2 + k^2}{2k\rho} \sin ka \; B_1 \end{cases}$$

We can determine an additional equation verified by B_1, A_2, A_2', and B_3' since the wave function is normalized:

$$\int_{-\infty}^{+\infty} |\varphi(x)|^2 \mathrm{d}x = 1$$

$$\Leftrightarrow \int_{-\infty}^{-\frac{a}{2}} |B_1|^2 e^{2\rho x} \mathrm{d}x + \int_{-\frac{a}{2}}^{\frac{a}{2}} (A_2^* e^{-ikx} + A_2'^* e^{ikx})(A_2 e^{ikx} + A_2' e^{-ikx}) \mathrm{d}x$$

$$+ \int_{\frac{a}{2}}^{+\infty} |B_3'|^2 e^{-2\rho x} \mathrm{d}x = 1$$

$$\Leftrightarrow \int_{-\infty}^{-\frac{a}{2}} |B_1|^2 e^{2\rho x} \mathrm{d}x + \int_{-\frac{a}{2}}^{\frac{a}{2}} (|A_2|^2 + |A_2'|^2 + A_2 A_2'^* e^{2ikx} + A_2^* A_2' e^{-2ikx}) \mathrm{d}x$$

$$+ \int_{\frac{a}{2}}^{+\infty} |B_3'|^2 e^{-2\rho x} \mathrm{d}x = 1$$

$$\Leftrightarrow |B_1|^2 \left[\frac{e^{2\rho x}}{2\rho} \right]_{-\infty}^{-\frac{a}{2}} + (|A_2|^2 + |A_2'|^2) a + A_2 A_2'^* \left[\frac{e^{2ikx}}{2ik} \right]_{-\frac{a}{2}}^{\frac{a}{2}}$$

$$-A_2^* A_2' \left[\frac{e^{-2ikx}}{2ik} \right]_{-\frac{a}{2}}^{\frac{a}{2}} - |B_3'|^2 \left[\frac{e^{-2\rho x}}{2\rho} \right]_{\frac{a}{2}}^{+\infty} = 1$$

$$\Leftrightarrow (|B_1|^2 + |B_3'|^2) \frac{e^{-\rho a}}{2\rho} + (|A_2|^2 + |A_2'|^2) a + (A_2 A_2'^* + A_2^* A_2') \frac{e^{ika} - e^{-ika}}{2ik} = 1$$

$$\Leftrightarrow (|B_1|^2 + |B_3'|^2) \frac{e^{-\rho a}}{2\rho} + (|A_2|^2 + |A_2'|^2) a + (A_2 A_2'^* + A_2^* A_2') \frac{\sin ka}{k} = 1$$

Using the expressions of A_2, A_2', and B_3' and replacing ρ and k by their expressions, we find:

$$A_2 = e^{(-\rho+ik)a/2}\frac{\rho+ik}{2ik}B_1$$

$$= e^{-\rho a/2}\exp\left(\frac{ia}{2}\sqrt{\frac{2m(E+V_0)}{\hbar^2}}\right)\frac{\sqrt{-\frac{2mE}{\hbar^2}}+i\sqrt{\frac{2m(E+V_0)}{\hbar^2}}}{2i\sqrt{\frac{2m(E+V_0)}{\hbar^2}}}B_1$$

$$= e^{-\rho a/2}\exp\left(\frac{iaV_0}{2}\sqrt{\frac{2m}{\hbar^2 V_0}}\sqrt{1+\frac{E}{V_0}}\right)\left(\frac{1}{2}+\frac{1}{2i}\sqrt{-\frac{E}{E+V_0}}\right)B_1$$

$$= e^{-\rho a/2}\exp\left(\frac{i\alpha}{2}\sqrt{\frac{2m}{\hbar^2 V_0}}\sqrt{1+\frac{E}{V_0}}\right)\left(\frac{1}{2}+\frac{1}{2i}\sqrt{-\frac{E}{E+V_0}}\right)B_1$$

$$A_2' = -e^{-(\rho+ik)a/2}\frac{\rho-ik}{2ik}B_1$$

$$= -e^{-\rho a/2}\exp\left(-\frac{ia}{2}\sqrt{\frac{2m(E+V_0)}{\hbar^2}}\right)\frac{\sqrt{-\frac{2mE}{\hbar^2}}-i\sqrt{\frac{2m(E+V_0)}{\hbar^2}}}{2i\sqrt{\frac{2m(E+V_0)}{\hbar^2}}}B_1$$

$$= -e^{-\rho a/2}\exp\left(-\frac{iaV_0}{2}\sqrt{\frac{2m}{\hbar^2 V_0}}\sqrt{1+\frac{E}{V_0}}\right)\left(-\frac{1}{2}+\frac{1}{2i}\sqrt{-\frac{E}{E+V_0}}\right)B_1$$

$$= -e^{-\rho a/2}\exp\left(-\frac{i\alpha}{2}\sqrt{\frac{2m}{\hbar^2 V_0}}\sqrt{1+\frac{E}{V_0}}\right)\left(-\frac{1}{2}+\frac{1}{2i}\sqrt{-\frac{E}{E+V_0}}\right)B_1$$

$$B_3' = \frac{\rho^2+k^2}{2k\rho}\sin kaB_1$$

$$= \frac{-\frac{2mE}{\hbar^2}+\frac{2m\left(E+V_0\right)}{\hbar^2}}{2\sqrt{\frac{2m\left(E+V_0\right)}{\hbar^2}}\sqrt{-\frac{2mE}{\hbar^2}}}\sin\left(\sqrt{\frac{2m(E+V_0)}{\hbar^2}}a\right)B_1$$

$$= \frac{V_0}{2\sqrt{-E(E+V_0)}}\sin\left(aV_0\sqrt{\frac{2m}{\hbar^2 V_0}}\sqrt{1+\frac{E}{V_0}}\right)B_1$$

$$= \sqrt{-\frac{V_0}{E}}\frac{1}{2\sqrt{1+\frac{E}{V_0}}}\sin\left(\alpha\sqrt{\frac{2m}{\hbar^2 V_0}}\sqrt{1+\frac{E}{V_0}}\right)B_1$$

Letting a approach 0 and V_0 approach infinity yields:

$$\begin{cases} A_2 \simeq \frac{B_1}{2}\left(1+\frac{i\alpha}{2}\sqrt{\frac{2m}{\hbar^2 V_0}}\left(1+\frac{E}{2V_0}\right)\right) \simeq \frac{B_1}{2}\left(1+\frac{i\alpha}{2}\sqrt{\frac{2m}{\hbar^2 V_0}}\right) \\ A_2' \simeq \frac{B_1}{2}\left(1-\frac{i\alpha}{2}\sqrt{\frac{2m}{\hbar^2 V_0}}\left(1+\frac{E}{2V_0}\right)\right) \simeq \frac{B_1}{2}\left(1-\frac{i\alpha}{2}\sqrt{\frac{2m}{\hbar^2 V_0}}\right) \\ B_3' \simeq \frac{B_1}{2}\sqrt{-\frac{V_0}{E}}\left(1-\frac{E}{2V_0}\right)\alpha\sqrt{\frac{2m}{\hbar^2 V_0}}\left(1+\frac{E}{2V_0}\right) \simeq \frac{B_1}{2}\alpha\sqrt{-\frac{2m}{\hbar^2 E}} \end{cases}$$

and we deduce:

$$|B_3'|^2 \simeq -|B_1|^2 \frac{m\alpha^2}{2\hbar^2 E}$$

On top of this, according to our previous findings:

$$\sin ka \simeq \alpha\sqrt{\frac{2m}{\hbar^2 V_0}} \Rightarrow \frac{\sin ka}{k} \simeq \frac{\alpha}{\sqrt{V_0(E+V_0)}} = \frac{\alpha}{V_0\sqrt{1+\frac{E}{V_0}}} \simeq \frac{\alpha}{V_0} = a$$

The wave function normalization condition therefore becomes:

$$\begin{aligned} &\frac{(|B_1|^2+|B_3'|^2)}{2\rho} + (|A_2|^2+|A_2'|^2)a + (A_2A_2'^* + A_2^*A_2')a \simeq 1 \\ \Leftrightarrow\ &\frac{|B_1|^2}{2}\left(1-\frac{m\alpha^2}{2\hbar^2E}\right)\sqrt{-\frac{\hbar^2}{2mE}} \simeq 1 \\ \Leftrightarrow\ &|B_1|^2 \simeq 2\left[\left(1-\frac{m\alpha^2}{2\hbar^2E}\right)\sqrt{-\frac{\hbar^2}{2mE}}\right]^{-1} \end{aligned}$$

The kinetic energy of the particle in the well, according to the previous results, is:

$$\begin{aligned} E_k &= -\frac{\hbar^2}{2m}\int_{-\frac{a}{2}}^{\frac{a}{2}} \varphi^*(x)\frac{\mathrm{d}^2\varphi(x)}{\mathrm{d}x^2}\mathrm{d}x \\ &= \frac{\hbar^2k^2}{2m}\int_{-\frac{a}{2}}^{\frac{a}{2}} (A_2^*e^{-ikx} + A_2'^*e^{ikx})(A_2e^{ikx} + A_2'e^{-ikx})\mathrm{d}x \\ &= (E+V_0)\int_{-\frac{a}{2}}^{\frac{a}{2}} (|A_2|^2 + |A_2'|^2 + A_2A_2'^*e^{2ikx} + A_2^*A_2'e^{-2ikx})\mathrm{d}x \\ &= (E+V_0)\left[(|A_2|^2+|A_2'|^2)a + (A_2A_2'^* + A_2^*A_2')\frac{\sin ka}{k}\right] \end{aligned}$$

Letting a approach 0 and V_0 approach infinity, we find:

$$E_k \simeq (E + V_0)(A_2 + A_2')(A_2^* + A_2'^*)a \simeq |B_1|^2(E + V_0)a \simeq \alpha|B_1|^2$$
$$\simeq 2\alpha\left[\left(1 - \frac{m\alpha^2}{2\hbar^2 E}\right)\sqrt{-\frac{\hbar^2}{2mE}}\right]^{-1}$$

Finally, as a approaches 0 and V_0 approaches infinity with $\alpha = aV_0$, the square potential well approaches a delta function well whose area equals α, and the energy E, therefore, approaches the energy of the particle in the bound state as studied in question a, namely $E = -\dfrac{m\alpha^2}{2\hbar^2}$. We can replace E by this value in the expression for the kinetic energy of the particle in the well which yields:

$$E_k \simeq 2\alpha\left[\left(1 - \frac{m\alpha^2}{2\hbar^2 E}\right)\sqrt{-\frac{\hbar^2}{2mE}}\right]^{-1} = 2\alpha\left[2\frac{\hbar^2}{m\alpha}\right]^{-1} = \frac{m\alpha^2}{\hbar^2}$$

The contribution of the point $x = 0$ to the average kinetic energy of the particle in a square potential well does indeed correspond to that of the same particle in a delta function well when the square potential approches a delta potential.

1.5 Well Consisting of Two Delta Functions

Statement

Consider a particle of mass m whose potential energy is

$$V(x) = -\alpha\delta(x) - \alpha\delta(x - l) \quad \alpha > 0$$

where l is a constant length.

a. Calculate the bound states of the particle, setting $E = -\dfrac{\hbar^2\rho^2}{2m}$. Show that the possible energies are given by the relation:

$$e^{-\rho l} = \pm\left(1 - \frac{2\rho}{\mu}\right)$$

where μ is defined by $\mu = \dfrac{2m\alpha}{\hbar^2}$. Give a graphic solution of this equation.

(i) *Ground state*. Show that this state is even (invariant with respect to reflection about the point $x = \dfrac{l}{2}$), and that its energy E_S is less than the energy $-E_L$ introduced in problem 3. Interpret this result physically. Represent graphically the corresponding wave function.

(ii) *Excited state*. Show that, when l is greater than a value to be specified, there exists an odd excited state, of energy E_A greater than $-E_L$. Find the corresponding wave function.

(iii) Explain how the preceding calculations enable us to construct a model which represents an ionized diatomic molecule (H_2^+, for example) whose nuclei are separated by a distance l. How do the energies of the two levels vary with respect to l? What happens at the limit where $l \to 0$ and at the limit where $l \to \infty$? If the repulsion of the two nuclei is taken into account, what is the total energy of the system? Show that the curve that gives the variation with respect to l of the energies thus obtained enables us to predict in certain cases the existence of bound states of H_2^+ and to determine the value of l at equilibrium. The calculation provides a very elementary model of the chemical bond.

b. Calculate the reflection and transmission coefficients of the system of two delta function barriers. Study their variations with respect to l. Do the resonances thus obtained occur when l is an integral multiple of the de Broglie wavelength of the particle? Why?

Comments

This exercise requires the completion of exercise 2, but not that of exercise 4. In classical mechanics, for $E < 0$, the particle is either in the well at $x = 0$ or in the well at $x = l$ and cannot escape.

It is now possible to use our quantum intuition, which has recently been acquired through the resolution of the previous exercises. In quantum mechanics, the strict confinement of the particle is not possible due to the Heisenberg uncertainty principle. The particle can and will explore the classically forbidden zones, outside both wells, over a characteristic distance denoted $\frac{1}{\rho}$ in exercise 2. If l is not too large with respect to the distance $\frac{1}{\rho}$, then the influence of the well at $x = l$ is felt on the well at $x = 0$ (and *vice versa*). Thanks to quantum tunneling, the particle can pass from one well to the other. This passing, hence coupling between wells, allows a stabilization of quantum states as studied in this exercise. This situation constitutes a simple model describing the NH_3 molecule studied in Complement G_{IV}.

Given the symmetry about $x = \frac{l}{2}$ of the problem (because the potential is symmetric), we expect the ground state to correspond to a symmetric state and the excited state to an antisymmetric state (as for a particle trapped in an infinite potential well). More generally, wave functions will alternatively be symmetric and antisymmetric.

The approach to this problem is standard. As in the previous exercises, the stationary spatial wave functions must be written for the various spatial zones using real exponentials in the classically forbidden zones, before establishing relations between the amplitudes of these waves and deducing the conditions on the energy of the particle (*i.e.* its quantization) in order for this system of constants to yield nontrivial solutions.

Solution

Consider a particle of mass m whose potential energy is

$$V(x) = -\alpha\delta(x) - \alpha\delta(x - l) \quad \alpha > 0$$

where l is a constant length.

a. Calculate the bound states of the particle, setting $E = -\dfrac{\hbar^2\rho^2}{2m}$. Show that the possible energies are given by the relation:

$$e^{-\rho l} = \pm\left(1 - \frac{2\rho}{\mu}\right)$$

where μ is defined by $\mu = \dfrac{2m\alpha}{\hbar^2}$. Give a graphic solution of this equation.

The resolution of this exercise is similar to that of exercise 2. The eigenvalue equation of H is the same, except at $x = l$; however, care must be taken when considering the continuity conditions of $\varphi(x)$ at $x = 0$ and $x = l$ (note that the first derivative is discontinuous at these points given the divergence of $V(x)$). We know $V(x) = 0$ far from the delta functions, and the eigenvalue equation of H is

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\varphi(x)}{\mathrm{d}x^2} - E\varphi(x) = 0 \Leftrightarrow \frac{\mathrm{d}^2\varphi(x)}{\mathrm{d}x^2} - \frac{-2mE}{\hbar^2}\varphi(x) = 0$$

$$\Leftrightarrow \frac{\mathrm{d}^2\varphi(x)}{\mathrm{d}x^2} - \rho^2\varphi(x) = 0$$

with $\rho = \sqrt{\dfrac{-2mE}{\hbar^2}} \Leftrightarrow E = -\dfrac{\hbar^2\rho^2}{2m}$. Note that $E < 0$ since we are considering bound states, so ρ is well defined. The eigenfunctions are thus as follows:

$$\begin{aligned} &x < 0 && \varphi_{\mathrm{I}}(x) = A_1 e^{\rho x} + A_1' e^{-\rho x} \\ &0 < x < l && \varphi_{\mathrm{II}}(x) = A_2 e^{\rho x} + A_2' e^{-\rho x} \\ &x > l && \varphi_{\mathrm{III}}(x) = A_3 e^{\rho x} + A_3' e^{-\rho x} \end{aligned}$$

$\varphi(x)$ should be bounded when $x \to \pm\infty$, so $A_1' = A_3 = 0$, which yields

$$\begin{aligned} &x < 0 && \varphi_{\mathrm{I}}(x) = A_1 e^{\rho x} \\ &0 < x < l && \varphi_{\mathrm{II}}(x) = A_2 e^{\rho x} + A_2' e^{-\rho x} \\ &x > l && \varphi_{\mathrm{III}}(x) = A_3' e^{-\rho x} \end{aligned}$$

The eigenfunction $\varphi(x)$ is continuous at $x = 0$ and $x = l$, so

$$\begin{cases} \varphi_{\mathrm{I}}(0) = \varphi_{\mathrm{II}}(0) \\ \varphi_{\mathrm{II}}(l) = \varphi_{\mathrm{III}}(l) \end{cases} \Leftrightarrow \begin{cases} A_1 = A_2 + A_2' \\ A_2 e^{\rho l} + A_2' e^{-\rho l} = A_3' e^{-\rho l} \end{cases} \Leftrightarrow \begin{cases} A_1 = A_2 + A_2' \\ A_3' = A_2 e^{2\rho l} + A_2' \end{cases}$$

Moreover, according to the solution of exercise 2, $\dfrac{\mathrm{d}\varphi(x)}{\mathrm{d}x}$ presents discontinuities at $x = 0$ and $x = l$ whose values are $-\mu\varphi(0)$ and $-\mu\varphi(l)$, respectively, setting $\mu = \dfrac{2m\alpha}{\hbar^2}$. This means that:

$$\begin{cases} \dfrac{\mathrm{d}\varphi_{\mathrm{II}}(0)}{\mathrm{d}x} - \dfrac{\mathrm{d}\varphi_{\mathrm{I}}(0)}{\mathrm{d}x} = -\mu\varphi(0) \\ \dfrac{\mathrm{d}\varphi_{\mathrm{III}}(l)}{\mathrm{d}x} - \dfrac{\mathrm{d}\varphi_{\mathrm{II}}(l)}{\mathrm{d}x} = -\mu\varphi(l) \end{cases} \Leftrightarrow \begin{cases} \rho(A_2 - A_2' - A_1) = -\mu A_1 \\ \rho(-A_3' e^{-\rho l} - A_2 e^{\rho l} + A_2' e^{-\rho l}) = -\mu A_3' e^{-\rho l} \end{cases}$$

$$\Leftrightarrow \begin{cases} \rho(A_2 - A_2' - A_1) = -\mu A_1 \\ \rho(-A_3' - A_2 e^{2\rho l} + A_2') = -\mu A_3' \end{cases}$$

Substituting A_1 and A_3' by their expressions stemming from continuity conditions, we find:

$$\begin{cases} -2\rho A_2' = -\mu(A_2 + A_2') \\ -2\rho A_2 e^{2\rho l} = -\mu(A_2 e^{2\rho l} + A_2') \end{cases}$$

The first of these two equations yields:

$$\frac{2\rho}{\mu} A_2' = A_2 + A_2' \Leftrightarrow A_2 = \left(\frac{2\rho}{\mu} - 1\right) A_2'$$

and, substituting A_2 by this expression in the second equation, we find:

$$-2\rho\left(\frac{2\rho}{\mu} - 1\right) e^{2\rho l} = -\mu\left[\left(\frac{2\rho}{\mu} - 1\right) e^{2\rho l} + 1\right]$$

$$\Leftrightarrow \frac{2\rho}{\mu}\left(\frac{2\rho}{\mu} - 1\right) e^{2\rho l} = \left(\frac{2\rho}{\mu} - 1\right) e^{2\rho l} + 1$$

$$\Leftrightarrow \left(\frac{2\rho}{\mu} - 1\right)^2 e^{2\rho l} = 1 \Leftrightarrow e^{-2\rho l} = \left(1 - \frac{2\rho}{\mu}\right)^2$$

i.e.

$$e^{-\rho l} = \pm\left(1 - \frac{2\rho}{\mu}\right)$$

The representative curves of $\pm\left(1 - \dfrac{2\rho}{\mu}\right)$ are represented in solid lines in Figure 1.3, whereas the representative curve of $e^{-\rho l}$ is represented in dashed line. We notice graphically that the previous equation has one or two solutions depending on the value of l. We exclude the solution $\rho = 0$ since it corresponds to a particle whose energy is vanishing and is, moreover, at rest.

(i) *Ground state*. Show that this state is even (invariant with respect to reflection about the point $x = \dfrac{l}{2}$), and that its energy E_S is less than the energy $-E_L$ introduced in problem 3. Interpret this result physically. Represent graphically the corresponding wave function.

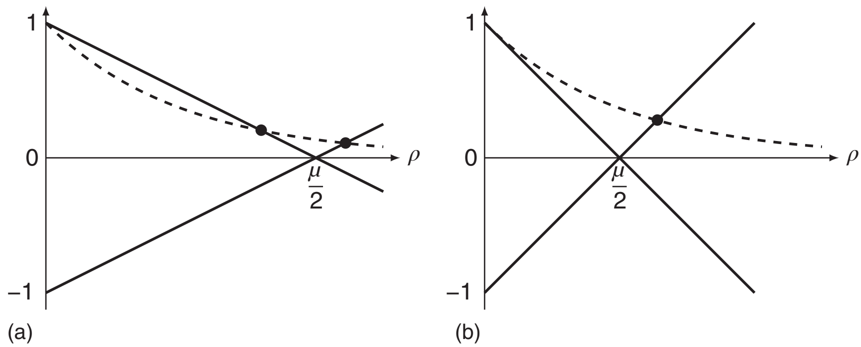


Figure 1.3 Illustration of the number of solutions (*i.e.* the number of points of intersection between the solid-line and dashed-line curves) to the equation $e^{-\rho l} = \pm\left(1 - \frac{2\rho}{\mu}\right)$ depending on the value of l : $l > \frac{2}{\mu}$ on (a) and $0 < l < \frac{2}{\mu}$ on (b).

The ground state is the state of lowest energy, in other words of highest $\rho = \sqrt{\frac{-2mE}{\hbar^2}}$ value, which is the unique solution to equation:

$$e^{-\rho l} = -\left(1 - \frac{2\rho}{\mu}\right)$$

according to Figure 1.3, in which it is represented by a dot. In this case, according to the results of question a, we can write:

$$A_2 = \left(\frac{2\rho}{\mu} - 1\right) A_2' = A_2' e^{-\rho l}$$

hence

$$\begin{cases} A_1 = A_2 + A_2' = (1 + e^{-\rho l})A_2' \\ A_3' = A_2 e^{2\rho l} + A_2' = (1 + e^{\rho l})A_2' \end{cases}$$

Setting $A_2' = A$, we find:

$$\begin{array}{ll} x < 0 & \varphi_{\rm I}(x) = (1 + e^{-\rho l})Ae^{\rho x} = Ae^{\rho(x-l)} + Ae^{\rho x} \\ 0 < x < l & \varphi_{\rm II}(x) = Ae^{\rho(x-l)} + Ae^{-\rho x} \\ x > l & \varphi_{\rm III}(x) = (1 + e^{\rho l})Ae^{-\rho x} = Ae^{-\rho(x-l)} + Ae^{-\rho x} \end{array}$$

and the constant A could be calculated given that the eigenfunction $\varphi(x)$ is normalized. The points at x and $l - x$ are symmetric with respect to the point at $\frac{l}{2}$, hence

$$\varphi(l-x) = \begin{cases} \varphi_{\rm III}(l-x) = Ae^{\rho x} + Ae^{\rho(x-l)} = \varphi_{\rm I}(x) = \varphi(x) & \text{if} \quad x < 0 \\ \varphi_{\rm II}(l-x) = Ae^{-\rho x} + Ae^{\rho(x-l)} = \varphi_{\rm II}(x) = \varphi(x) & \text{if} \quad 0 < x < l \\ \varphi_{\rm I}(l-x) = Ae^{-\rho x} + Ae^{-\rho(x-l)} = \varphi_{\rm III}(x) = \varphi(x) & \text{if} \quad x > l \end{cases}$$

The ground state is therefore even. The energy $-E_L$ introduced in problem 3 obeys the equation:

$$-E_L = -\frac{m\alpha^2}{2\hbar^2} = -\frac{\hbar^2\rho_L^2}{2m} \Leftrightarrow \rho_L = \frac{m\alpha}{\hbar^2} = \frac{\mu}{2}$$

This value of ρ corresponds to the common point of intersection of the two lines whose equations are $\pm\left(1-\frac{2\rho}{\mu}\right)$ with the horizontal axis. However, we remark graphically in Figure 1.3 that the ground state corresponds to a value of ρ such that $\rho > \rho_L$. Hence:

$$\rho > \rho_L \Leftrightarrow \rho^2 > \rho_L^2 \Leftrightarrow \frac{\hbar^2\rho^2}{2m} > \frac{\hbar^2\rho_L^2}{2m} \Leftrightarrow E_S < -E_L$$

and the energy E_S of the ground state is indeed less than the energy $-E_L$ introduced in problem 3, which means that the particle is more strongly bound in a well consisting of two delta functions than in a potential barrier of just one delta function. The corresponding wave function is represented in Figure 1.4, and its probability density is represented in Figure 1.5.

(ii) *Excited state*. Show that, when l is greater than a value to be specified, there exists an odd excited state, of energy E_A greater than $-E_L$. Find the corresponding wave function.

We previously showed that the possible energies are given by equation:

$$e^{-\rho l} = \pm\left(1-\frac{2\rho}{\mu}\right)$$

The slope in origin of the exponential function $\rho \mapsto e^{-\rho l}$ is $-l$, whereas the slope of the line whose equation is $\rho \mapsto +\left(1-\frac{2\rho}{\mu}\right)$ is $-\frac{2}{\mu}$.

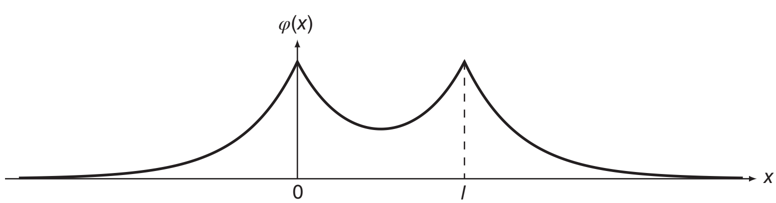


Figure 1.4 Graphic representation of the ground state wave function. It is a symmetric state. The fact that the probability density is nonzero between the two wells leads to a coupling between them.

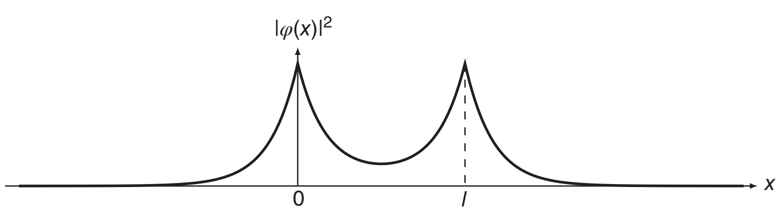


Figure 1.5 Graphic representation of the ground state probability density.

If $-l > -\frac{2}{\mu} \Leftrightarrow l < \frac{2}{\mu}$ (Figure 1.3b), the previous equation has only one nonzero solution and there is no excited state. In order for an excited state to exist, it is necessary for $-l < -\frac{2}{\mu} \Leftrightarrow l > \frac{2}{\mu}$ (Figure 1.3a). This excited state corresponds to the only nonzero solution to equation:

$$e^{-\rho l} = 1 - \frac{2\rho}{\mu}$$

according to Figure 1.3, in which it is represented by a dot. In this case, according to the results of question a:

$$A_2 = \left(\frac{2\rho}{\mu} - 1\right) A_2' = -A_2' e^{-\rho l}$$

Therefore,

$$\begin{cases} A_1 = A_2 + A_2' = (1 - e^{-\rho l})A_2' \\ A_3' = A_2 e^{2\rho l} + A_2' = (1 - e^{\rho l})A_2' \end{cases}$$

Setting $A_2' = A$, we can write:

$$\begin{array}{ll} x < 0 & \varphi_{\mathrm{I}}(x) = (1 - e^{-\rho l})Ae^{\rho x} = Ae^{\rho x} - Ae^{\rho(x-l)} \\ 0 < x < l & \varphi_{\mathrm{II}}(x) = Ae^{-\rho x} - Ae^{\rho(x-l)} \\ x > l & \varphi_{\mathrm{III}}(x) = (1 - e^{\rho l})Ae^{-\rho x} = Ae^{-\rho x} - Ae^{-\rho(x-l)} \end{array}$$

and the constant A could be calculated given that the eigenfunction $\varphi(x)$ is normalized. The points at x and $l - x$ are symmetric with respect to the point at $\frac{l}{2}$, hence

$$\varphi(l-x) = \begin{cases} \varphi_{\mathrm{III}}(l-x) = Ae^{\rho(x-l)} - Ae^{\rho x} = -\varphi_{\mathrm{I}}(x) = -\varphi(x) & \text{if} \quad x < 0 \\ \varphi_{\mathrm{II}}(l-x) = Ae^{\rho(x-l)} - Ae^{-\rho x} = -\varphi_{\mathrm{II}}(x) = -\varphi(x) & \text{if} \quad 0 < x < l \\ \varphi_{\mathrm{I}}(l-x) = Ae^{-\rho(x-l)} - Ae^{-\rho x} = -\varphi_{\mathrm{III}}(x) = -\varphi(x) & \text{if} \quad x > l \end{cases}$$

Therefore, the excited state is indeed odd. The energy $-E_L$ introduced in problem 3 obeys

$$-E_L = -\frac{m\alpha^2}{2\hbar^2} = -\frac{\hbar^2 \rho_L^2}{2m} \Leftrightarrow \rho_L = \frac{m\alpha}{\hbar^2} = \frac{\mu}{2}$$

This value of ρ corresponds to the common point of intersection of the two lines whose equations are $\pm\left(1 - \frac{2\rho}{\mu}\right)$ with the horizontal axis. However, we notice graphically in Figure 1.3 that the excited state corresponds to a value of ρ such that $\rho < \rho_L$. Hence:

$$\rho < \rho_L \Leftrightarrow \rho^2 < \rho_L^2 \Leftrightarrow \frac{\hbar^2 \rho^2}{2m} < \frac{\hbar^2 \rho_L^2}{2m} \Leftrightarrow E_A > -E_L$$

and the energy E_A of the excited state is indeed greater than the energy $-E_L$ introduced in problem 3. The corresponding wave function is represented in Figure 1.6, and its probability density is represented in Figure 1.7.

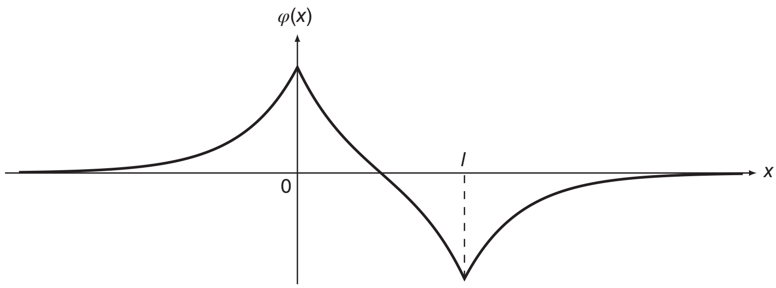


Figure 1.6 Graphic representation of the wave function of the excited state. The excited state is an antisymmetric state. The probability density vanishes at $\frac{l}{2}$. The particle cannot pass between wells.

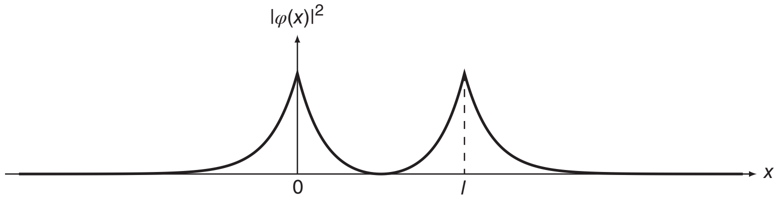


Figure 1.7 Graphic representation of the probability density of the excited state. Note that the probability of finding the particle in the middle between the potential wells while in the excited state is vanishing ($|\varphi(l/2)|^2 = 0$).

(iii) Explain how the preceding calculations enable us to construct a model which represents an ionized diatomic molecule (H_2^+, for example) whose nuclei are separated by a distance l. How do the energies of the two levels vary with respect to l? What happens at the limit where $l \to 0$ and at the limit where $l \to \infty$? If the repulsion of the two nuclei is taken into account, what is the total energy of the system? Show that the curve that gives the variation with respect to l of the energies thus obtained enables us to predict in certain cases the existence of bound states of H_2^+ and to determine the value of l at equilibrium. The calculation provides a very elementary model of the chemical bond.

Let us consider an ionized diatomic molecule such as H_2^+ whose nuclei are separated by a distance l. Each hydrogen atom contributes one electron to the molecule, so the ionized molecule only has one electron. By defining the Ox axis as the axis of symmetry of the molecule, the potential felt by the electron far from the nuclei is practically vanishing, but is very intense and attractive in the vicinity of the two nuclei, that is at $x = 0$ and $x = l$. The preceding calculations, therefore, enable us to construct a model which represents such an ionized diatomic molecule, in which the attractive potential created by the two nuclei is modeled by the two delta functions. For small values of l, *i.e.* when the two nuclei are close together, only the ground state exists. The energy $E_S < -E_L$ of this ground state increases with l (since ρ decreases as l increases, as shown in Figure 1.3) approaching $-E_L$ for large values of l, *i.e.* when the nuclei are far apart. The excited state appears when $l > \frac{2}{\mu}$ and its energy $E_A > -E_L$ decreases when l increases (since ρ increases with l) approaching $-E_L$ for large values of l. When $l \to 0$, only the ground state exists and the only possible energy is given by:

$$e^{-\rho l} = -\left(1 - \frac{2\rho}{\mu}\right) \Leftrightarrow 1 = -1 + \frac{2\rho}{\mu} \Leftrightarrow \rho = \mu$$

which corresponds to an energy E_s of the ground state:

$$E_S = -\frac{\hbar^2\rho^2}{2m} = -\frac{\hbar^2\mu^2}{2m} = -\frac{4\hbar^2\left(\frac{\mu}{2}\right)^2}{2m} = 4(-E_L)$$

When $l \to \infty$, the possible energies are solutions to equation:

$$e^{-\rho l} = \pm\left(1 - \frac{2\rho}{\mu}\right) \Leftrightarrow 1 - \frac{2\rho}{\mu} = 0 \Leftrightarrow \rho = \frac{\mu}{2}$$

which once more shows that the energies of the ground and excited states, E_S and E_A, respectively, both approach $-E_L$ as the nuclei move further and further apart. If we now account for the repulsion of the two nuclei, the total energy of the system becomes

$$E(l) = E_e + \frac{1}{4\pi\varepsilon_0}\frac{(Ze)^2}{l} = E_e + \frac{1}{4\pi\varepsilon_0}\frac{e^2}{l}$$

in the case of H_2^+, where E_e represents the electron energy and the second term represents the repulsion energy between nuclei:

- The electron can be in its ground state, in which case the total energy is

  $$E_0(l) = E_S + \frac{1}{4\pi\varepsilon_0}\frac{e^2}{l}$$

  with E_S an increasing function of l. The repulsion energy between the two nuclei is a rapidly decreasing function of l, so we can expect variations of E_S and the repulsion energy as represented in Figure 1.8 in dashed and dotted lines, respectively, in order for the total energy E_0, represented in solid line, to display a minimum corresponding to an equilibrium: the H_2^+ molecule is thus stable in its ground state. The corresponding value of l ($l = l_{eq}$) represents the length of the chemical bond of H_2^+ at equilibrium. The fact that the energy (E_{min}) of the ground state of H_2^+ at equilibrium is lower than the energy ($-E_L$) of $H + H^+$ taken separately, *i.e.* the products of dissociation, leads to the stability of the molecule and the strength of the chemical bond between the two nuclei. In fact, this difference in energy corresponds to the energy contained within the chemical bond; that is the energy required to dissociate the molecule, or the energy released when

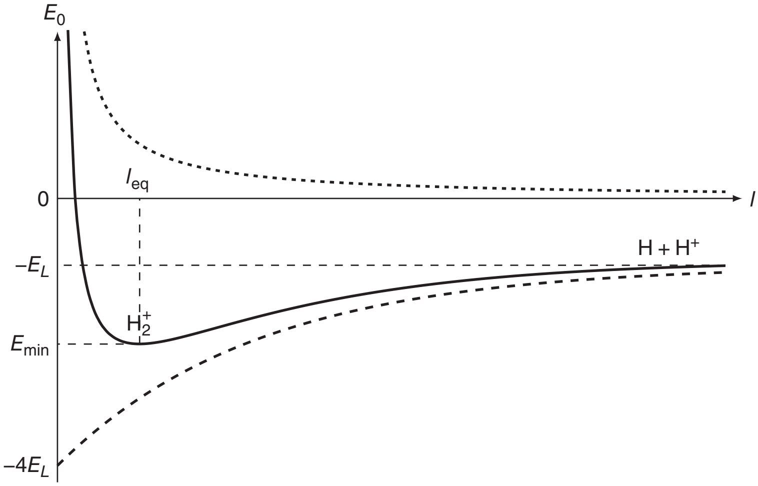


Figure 1.8 Variations of total energy with respect to l for an electron in its ground state. The distance l_{eq} at equilibrium represents the length of the chemical bond at rest between the two hydrogen atoms of the H_2^+ molecule. $H + H^+$ represents the products of dissociation, obtained when $l \to \infty$.

the molecule is formed, and we can thus define the dissociation energy as follows: $E_{disso} = -E_L - E_{min}$.

- If $l > \frac{2}{\mu}$, the electron can also be in its excited state, in which case the total energy is

$$E_1(l) = E_A + \frac{1}{4\pi\varepsilon_0}\frac{e^2}{l}$$

E_A is a decreasing function of l, as is the repulsion energy, which implies that the total energy E_1 is also decreasing with l. Therefore, there is no state of equilibrium and the molecule is unstable in its excited state.

So there are bound states of H_2^+ if the internuclear distance is greater than the value of l for which the representative curves of E_0 and E_1 intercept the horizontal axis. To summarize, by defining l_0 and l_1 such that $E_0(l_0) = E_1(l_1) = 0$:

- there is no bound state if $l \leqslant l_0$;
- there is only one bound state (corresponding to the ground state) if $l_0 < l \leqslant l_1$;
- there are two bound states (corresponding to the ground and excited states) if $l > l_1$.

In the literature, in both experimental and theoretical works, only one bound state is reported (the ground state) for which the internuclear distance is determined to be around 1.052 Å. All identified excited states are repulsive and lead to the dissociation of the molecule. H_2^+ therefore falls into the second category of the model ($l_0 < l \leqslant l_1$).

b. Calculate the reflection and transmission coefficients of the system of two delta function barriers. Study their variations with respect to l. Do the resonances thus obtained occur when l is an integral multiple of the de Broglie wavelength of the particle? Why?

Let us now assume $E > 0$. We know that $V(x) = 0$ away from the two delta functions, and the eigenvalue equation of H is

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\varphi(x)}{\mathrm{d}x^2} - E\varphi(x) = 0 \Leftrightarrow \frac{\mathrm{d}^2\varphi(x)}{\mathrm{d}x^2} + \frac{2mE}{\hbar^2}\varphi(x) = 0 \Leftrightarrow \frac{\mathrm{d}^2\varphi(x)}{\mathrm{d}x^2} + k^2\varphi(x) = 0$$

with $k = \sqrt{\dfrac{2mE}{\hbar^2}}$. The eigenfunctions can thus be written:

$$\begin{array}{ll} x < 0 & \varphi_{\mathrm{I}}(x) = A_1 e^{ikx} + A_1' e^{-ikx} \\ 0 < x < l & \varphi_{\mathrm{II}}(x) = A_2 e^{ikx} + A_2' e^{-ikx} \\ x > l & \varphi_{\mathrm{III}}(x) = A_3 e^{ikx} + A_3' e^{-ikx} \end{array}$$

Assuming that the particle is propagating from left to right we can set $A_3' = 0$, hence

$$\begin{array}{ll} x < 0 & \varphi_{\mathrm{I}}(x) = A_1 e^{ikx} + A_1' e^{-ikx} \\ 0 < x < l & \varphi_{\mathrm{II}}(x) = A_2 e^{ikx} + A_2' e^{-ikx} \\ x > l & \varphi_{\mathrm{III}}(x) = A_3 e^{ikx} \end{array}$$

The eigenfunction $\varphi(x)$ is continuous at $x = 0$ and $x = l$, so

$$\begin{cases} \varphi_{\mathrm{I}}(0) = \varphi_{\mathrm{II}}(0) \\ \varphi_{\mathrm{II}}(l) = \varphi_{\mathrm{III}}(l) \end{cases} \Leftrightarrow \begin{cases} A_1 + A_1' = A_2 + A_2' \\ A_2 e^{ikl} + A_2' e^{-ikl} = A_3 e^{ikl} \end{cases}$$

$$\Leftrightarrow \begin{cases} A_1 + A_1' = A_2 + A_2' \\ A_2 + A_2' e^{-2ikl} = A_3 \end{cases}$$

Moreover, according to our findings in exercise 2, $\dfrac{\mathrm{d}\varphi(x)}{\mathrm{d}x}$ is discontinuous at $x = 0$ and $x = l$, its discontinuity equalling $-\mu\varphi(0)$ and $-\mu\varphi(l)$, respectively, with $\mu = \dfrac{2m\alpha}{\hbar^2}$. This means that:

$$\begin{cases} \dfrac{\mathrm{d}\varphi_{\mathrm{II}}(0)}{\mathrm{d}x} - \dfrac{\mathrm{d}\varphi_{\mathrm{I}}(0)}{\mathrm{d}x} = -\mu\varphi(0) \\ \dfrac{\mathrm{d}\varphi_{\mathrm{III}}(l)}{\mathrm{d}x} - \dfrac{\mathrm{d}\varphi_{\mathrm{II}}(l)}{\mathrm{d}x} = -\mu\varphi(l) \end{cases}$$

$$\Leftrightarrow \begin{cases} ik(A_2 - A_2' - A_1 + A_1') = -\mu(A_1 + A_1') \\ ik(A_3 e^{ikl} - A_2 e^{ikl} + A_2' e^{-ikl}) = -\mu A_3 e^{ikl} \end{cases}$$

$$\Leftrightarrow \begin{cases} ik(A_2 - A_2' - A_1 + A_1') = -\mu(A_1 + A_1') \\ ik(A_3 - A_2 + A_2' e^{-2ikl}) = -\mu A_3 \end{cases}$$

hence the following four equations:

$$\begin{cases} A_1' - A_2 - A_2' = -A_1 \\ A_2 + e^{-2ikl}A_2' - A_3 = 0 \\ (ik+\mu)A_1' + ikA_2 - ikA_2' = (ik-\mu)A_1 \\ -ikA_2 + ike^{-2ikl}A_2' + (ik+\mu)A_3 = 0 \end{cases}$$

Considering A_1', A_2, A_2', and A_3 as the only unknowns in order to express them as functions of A_1, the corresponding determinant is

$$D = \begin{vmatrix} 1 & -1 & -1 & 0 \\ 0 & 1 & e^{-2ikl} & -1 \\ ik+\mu & ik & -ik & 0 \\ 0 & -ik & ike^{-2ikl} & ik+\mu \end{vmatrix}$$

We then simplify this determinant by performing operations on the lines:

$$\begin{aligned} D &= \begin{vmatrix} 1 & -1 & -1 & 0 \\ 0 & 1 & e^{-2ikl} & -1 \\ 0 & 2ik+\mu & \mu & 0 \\ 0 & -ik & ike^{-2ikl} & ik+\mu \end{vmatrix} = \begin{vmatrix} 1 & e^{-2ikl} & -1 \\ 2ik+\mu & \mu & 0 \\ -ik & ike^{-2ikl} & ik+\mu \end{vmatrix} \\ &= \begin{vmatrix} 1 & e^{-2ikl} & -1 \\ 0 & \mu-(2ik+\mu)e^{-2ikl} & 2ik+\mu \\ 0 & 2ike^{-2ikl} & \mu \end{vmatrix} = \begin{vmatrix} \mu-(2ik+\mu)e^{-2ikl} & 2ik+\mu \\ 2ike^{-2ikl} & \mu \end{vmatrix} \\ &= \mu\left[\mu-(2ik+\mu)e^{-2ikl}\right] - (2ik+\mu)2ike^{-2ikl} \\ &= \mu^2 - (\mu+2ik)^2e^{-2ikl} \end{aligned}$$

We are now able to calculate A_1' and A_3 as functions of A_1, as these are the only necessary variables for calculating the transmission and reflection coefficients:

$$\begin{aligned} A_1' &= \frac{1}{D}\begin{vmatrix} -A_1 & -1 & -1 & 0 \\ 0 & 1 & e^{-2ikl} & -1 \\ (ik-\mu)A_1 & ik & -ik & 0 \\ 0 & -ik & ike^{-2ikl} & ik+\mu \end{vmatrix} \\ &= \frac{A_1}{D}\begin{vmatrix} -1 & -1 & -1 & 0 \\ 0 & 1 & e^{-2ikl} & -1 \\ ik-\mu & ik & -ik & 0 \\ 0 & -ik & ike^{-2ikl} & ik+\mu \end{vmatrix} \end{aligned}$$

$$A_1' = \frac{A_1}{D}\begin{vmatrix} -1 & -1 & -1 & 0 \\ 0 & 1 & e^{-2ikl} & -1 \\ 0 & \mu & \mu - 2ik & 0 \\ 0 & -ik & ike^{-2ikl} & ik+\mu \end{vmatrix} = -\frac{A_1}{D}\begin{vmatrix} 1 & e^{-2ikl} & -1 \\ \mu & \mu - 2ik & 0 \\ -ik & ike^{-2ikl} & ik+\mu \end{vmatrix}$$

$$= -\frac{A_1}{D}\begin{vmatrix} 1 & e^{-2ikl} & -1 \\ 0 & \mu - 2ik - \mu e^{-2ikl} & \mu \\ 0 & 2ike^{-2ikl} & \mu \end{vmatrix} = -\frac{A_1}{D}\begin{vmatrix} \mu - 2ik - \mu e^{-2ikl} & \mu \\ 2ike^{-2ikl} & \mu \end{vmatrix}$$

$$= \frac{(2ik-\mu)\mu + (2ik+\mu)\mu e^{-2ikl}}{\mu^2 - (\mu+2ik)^2 e^{-2ikl}} A_1$$

$$A_3 = \frac{1}{D}\begin{vmatrix} 1 & -1 & -1 & -A_1 \\ 0 & 1 & e^{-2ikl} & 0 \\ ik+\mu & ik & -ik & (ik-\mu)A_1 \\ 0 & -ik & ike^{-2ikl} & 0 \end{vmatrix}$$

$$= \frac{A_1}{D}\begin{vmatrix} 1 & -1 & -1 & -1 \\ 0 & 1 & e^{-2ikl} & 0 \\ ik+\mu & ik & -ik & ik-\mu \\ 0 & -ik & ike^{-2ikl} & 0 \end{vmatrix}$$

$$= \frac{A_1}{D}\begin{vmatrix} 0 & -1 & -1 & -1 \\ 0 & 1 & e^{-2ikl} & 0 \\ 2ik & ik & -ik & ik-\mu \\ 0 & -ik & ike^{-2ikl} & 0 \end{vmatrix} = 2ik\frac{A_1}{D}\begin{vmatrix} -1 & -1 & -1 \\ 1 & e^{-2ikl} & 0 \\ -ik & ike^{-2ikl} & 0 \end{vmatrix}$$

$$= -2ik\frac{A_1}{D}\begin{vmatrix} 1 & e^{-2ikl} \\ -ik & ike^{-2ikl} \end{vmatrix} = 4k^2 e^{-2ikl}\frac{A_1}{D} = \frac{4k^2 e^{-2ikl}}{\mu^2 - (\mu+2ik)^2 e^{-2ikl}} A_1$$

Hence:

$$R = \left|\frac{A_1'}{A_1}\right|^2 = \left|\frac{(2ik-\mu)\mu + (2ik+\mu)\mu e^{-2ikl}}{\mu^2 - (\mu+2ik)^2 e^{-2ikl}}\right|^2$$

$$= \left|\frac{(2ik-\mu)\mu e^{ikl} + (2ik+\mu)\mu e^{-ikl}}{\mu^2 e^{ikl} - (\mu+2ik)^2 e^{-ikl}}\right|^2$$

$$= \left|\frac{(2ik-\mu)\mu(\cos kl + i\sin kl) + (2ik+\mu)\mu(\cos kl - i\sin kl)}{\mu^2(\cos kl + i\sin kl) - (\mu+2ik)^2(\cos kl - i\sin kl)}\right|^2$$

$$= \left|\frac{4ik\mu\cos kl - 2i\mu^2\sin kl}{(4k^2 - 4ik\mu)\cos kl + (-4k\mu + i(2\mu^2 - 4k^2))\sin kl}\right|^2$$

i.e.

$$R = \frac{(4k\mu\cos kl - 2\mu^2\sin kl)^2}{(4k^2\cos kl - 4k\mu\sin kl)^2 + (-4k\mu\cos kl + (2\mu^2 - 4k^2)\sin kl)^2}$$

and

$$T = \left|\frac{A_3}{A_1}\right|^2 = \left|\frac{4k^2 e^{-2ikl}}{\mu^2 - (\mu + 2ik)^2 e^{-2ikl}}\right|^2 = \left|\frac{4k^2}{\mu^2 e^{ikl} - (\mu + 2ik)^2 e^{-ikl}}\right|^2$$

$$= \left|\frac{4k^2}{(4k^2 - 4ik\mu)\cos kl + (-4k\mu + i(2\mu^2 - 4k^2))\sin kl}\right|^2$$

i.e.

$$T = \frac{16k^4}{(4k^2\cos kl - 4k\mu\sin kl)^2 + (-4k\mu\cos kl + (2\mu^2 - 4k^2)\sin kl)^2}$$

The variations of R and T as functions of l are depicted in Figure 1.9 for $k = \mu$.

The de Broglie wavelength of the particle can be computed using $\lambda = \frac{2\pi}{k}$, which is also the period of R and T. When $l = n\lambda = n\frac{2\pi}{k}$ with $n \in \mathbb{N}$, we find

$$T = \frac{16k^4}{(4k^2)^2 + (-4k\mu)^2} = \frac{16k^4}{16k^4 + 16k^2\mu^2} = \frac{k^2}{k^2 + \mu^2} < 1$$

so there is no resonance when l is a multiple of the de Broglie wavelength of the particle. Resonances occur when $T = 1 \Leftrightarrow R = 0$, if and only if

$$4k\mu\cos kl - 2\mu^2\sin kl = 0 \Leftrightarrow \tan kl = \frac{2k}{\mu}$$

A resonance will thus be observed if

$$kl = \arctan\frac{2k}{\mu} + n\pi \Leftrightarrow l = \frac{1}{k}\arctan\frac{2k}{\mu} + n\frac{\pi}{k} = \frac{1}{k}\arctan\frac{2k}{\mu} + n\frac{\lambda}{2}$$

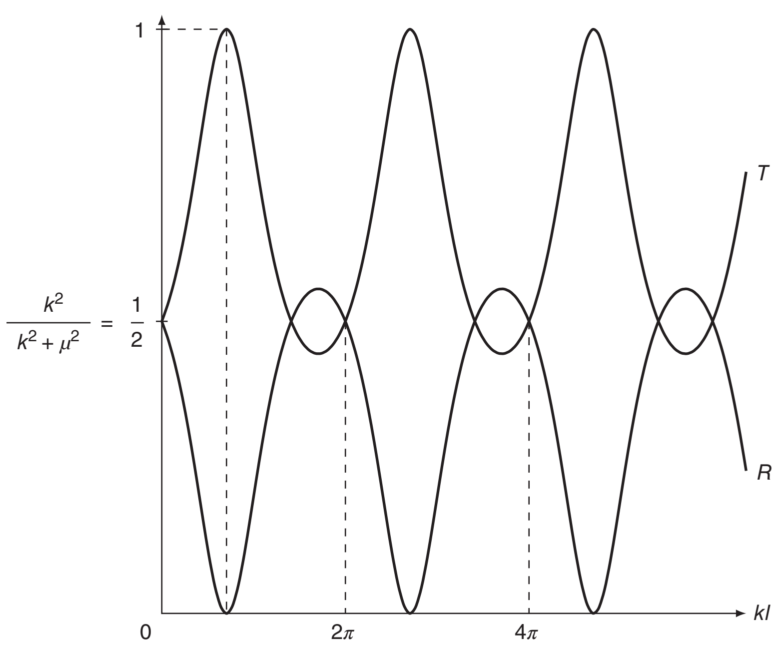


Figure 1.9 Variations of R and T as functions of l for $k = \mu$.

with

$$\frac{2k}{\mu} = 2\sqrt{\frac{2mE}{\hbar^2}\frac{\hbar^2}{2m\alpha}} = \sqrt{\frac{2E\hbar^2}{m\alpha^2}} = \sqrt{\frac{E}{E_L}}$$

The resonance can also be understood in terms of constructive and destructive interferences, owing to wave–particle duality. On a round trip, *i.e.* for a path length of $2l$, the wave can interfere constructively with itself, which creates this periodic resonance.

The distance between the two barriers must at least reach a minimal value, function of the particle energy, for a first resonance to occur, and the following resonances can be observed with a periodicity equal to the half-wavelength of the particle, as in the case of a classical potential barrier studied in § 2-b-α of Complement H_I. This difference in behavior "at the origin" is due to the fact that the barriers here are of infinite height and is thus due to the discontinuity of the derivative of the wave function in the vicinity of the barriers.

1.6 Bound State in a Square Potential

Statement

Consider a square well potential of width a and depth V_0 (in this exercise, we will use systematically the notation of § 2-c-α of Complement H_I). We intend to study the properties of the bound state of a particle in this well when its width a approaches zero.

a. Show that there indeed exists only one bound state and calculate its energy E (we find $E \simeq -\dfrac{mV_0^2a^2}{2\hbar^2}$, that is an energy which varies with the square of the area aV_0 of the well).

b. Show that $\rho \to 0$ and that $A_2 = A_2' \simeq \dfrac{B_1}{2}$. Deduce from this that, in the bound state, the probability of finding the particle outside the well approaches 1.

c. How can the preceding considerations be applied to a particle placed, as in exercise 2, in the potential $V(x) = -\alpha\delta(x)$?

Comments

This is a very standard exercise. The energy E is assumed to be such that $-V_0 < E < 0$ to produce a bound state.

The problem should be clearly laid out, with an emphasis on distinguishing the three spatial zones and adapting the form of the spatial wave function to each zone through the introduction of various constants. The boundary or continuity conditions guarantee that in the case of a finite discontinuity of the potential, as is the case here, the spatial wave function and its first derivative remain continuous at the discontinuity, which constrains the various constants. However, in order to compute a nontrivial wave function, these continuity conditions impose constraints on the energy.

Once again, we encounter a fundamental idea in quantum mechanics, namely that accounting for boundary conditions imposes the quantization of the particle energy. The precise study of this quantization (of the eigenmodes) is undertaken here graphically.

In addition to the constraints set by the boundary conditions, the final constraint is fixed by the normalization condition of the total wave function.

Solution

Consider a square well potential of width a and depth V_0 (in this exercise, we shall use systematically the notation of § 2-c-α of Complement H_I, which is recalled in Figure 1.10). We intend to study the properties of the bound state of a particle in this well when its width a approaches zero.

a. Show that there indeed exists only one bound state and calculate its energy E (we find $E \simeq -\dfrac{mV_0^2a^2}{2\hbar^2}$, that is an energy which varies with the square of the area aV_0 of the well).

   The potential in this well is given by:

$$V(x) = \begin{cases} 0 & \text{if } x < -\dfrac{a}{2} \\ -V_0 & \text{if } -\dfrac{a}{2} < x < \dfrac{a}{2} \\ 0 & \text{if } x > \dfrac{a}{2} \end{cases}$$

   and we are looking for bound states, whose energies verify $-V_0 < E < 0$. The eigenvalue equation of H can be written:

$$-\frac{\hbar^2}{2m}\frac{d^2\varphi(x)}{dx^2} - E\varphi(x) = 0 \Leftrightarrow \frac{d^2\varphi(x)}{dx^2} - \frac{-2mE}{\hbar^2}\varphi(x) = 0$$

$$\Leftrightarrow \frac{d^2\varphi(x)}{dx^2} - \rho^2\varphi(x) = 0$$

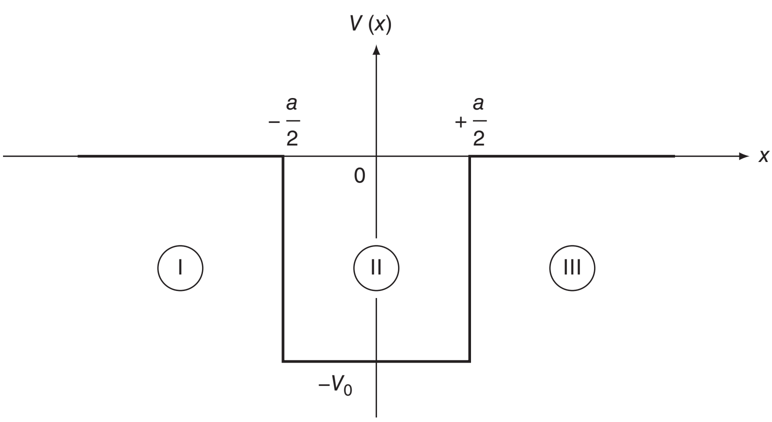


Figure 1.10 Notation of § 2-c-α of Complement H_I.

with $\rho = \sqrt{\frac{-2mE}{\hbar^2}}$ in zones I $\left(x < -\frac{a}{2}\right)$ and III $\left(x > \frac{a}{2}\right)$, and

$$-\frac{\hbar^2}{2m}\frac{d^2\varphi(x)}{dx^2} - (E+V_0)\varphi(x) = 0 \Leftrightarrow \frac{d^2\varphi(x)}{dx^2} + \frac{2m(E+V_0)}{\hbar^2}\varphi(x) = 0$$
$$\Leftrightarrow \frac{d^2\varphi(x)}{dx^2} + k^2\varphi(x) = 0$$

with $k = \sqrt{\frac{2m(E+V_0)}{\hbar^2}}$ in zone II $\left(-\frac{a}{2} < x < \frac{a}{2}\right)$. The expressions of the eigenfunctions in the three zones are as follows:

$$\begin{cases} \varphi_{I}(x) = B_1 e^{\rho x} + B_1' e^{-\rho x} \\ \varphi_{II}(x) = A_2 e^{ikx} + A_2' e^{-ikx} \\ \varphi_{III}(x) = B_3 e^{\rho x} + B_3' e^{-\rho x} \end{cases}$$

$\varphi(x)$ should be bounded when $x \to \pm\infty$, so $B_1' = B_3 = 0$, yielding

$$\begin{cases} \varphi_{I}(x) = B_1 e^{\rho x} \\ \varphi_{II}(x) = A_2 e^{ikx} + A_2' e^{-ikx} \\ \varphi_{III}(x) = B_3' e^{-\rho x} \end{cases}$$

Firstly, $\varphi(x)$ is continuous at $x = -\frac{a}{2}$ and $x = +\frac{a}{2}$, so:

$$\begin{cases} \varphi_I\left(-\frac{a}{2}\right) = \varphi_{II}\left(-\frac{a}{2}\right) \\ \varphi_{II}\left(+\frac{a}{2}\right) = \varphi_{III}\left(+\frac{a}{2}\right) \end{cases} \Leftrightarrow \begin{cases} B_1 e^{-\rho\frac{a}{2}} = A_2 e^{-ik\frac{a}{2}} + A_2' e^{ik\frac{a}{2}} \\ A_2 e^{ik\frac{a}{2}} + A_2' e^{-ik\frac{a}{2}} = B_3' e^{-\rho\frac{a}{2}} \end{cases}$$

Secondly, $\frac{d\varphi(x)}{dx}$ is continuous at $x = -\frac{a}{2}$ and $x = +\frac{a}{2}$ since the well is of finite depth (V_0), so:

$$\begin{cases} \frac{d\varphi_I}{dx}\left(-\frac{a}{2}\right) = \frac{d\varphi_{II}}{dx}\left(-\frac{a}{2}\right) \\ \frac{d\varphi_{II}}{dx}\left(+\frac{a}{2}\right) = \frac{d\varphi_{III}}{dx}\left(+\frac{a}{2}\right) \end{cases} \Leftrightarrow \begin{cases} \rho B_1 e^{-\rho\frac{a}{2}} = ikA_2 e^{-ik\frac{a}{2}} - ikA_2' e^{ik\frac{a}{2}} \\ ikA_2 e^{ik\frac{a}{2}} - ikA_2' e^{-ik\frac{a}{2}} = -\rho B_3' e^{-\rho\frac{a}{2}} \end{cases}$$

$$\Leftrightarrow \begin{cases} \frac{\rho}{ik} B_1 e^{-\rho\frac{a}{2}} = A_2 e^{-ik\frac{a}{2}} - A_2' e^{ik\frac{a}{2}} \\ A_2 e^{ik\frac{a}{2}} - A_2' e^{-ik\frac{a}{2}} = -\frac{\rho}{ik} B_3' e^{-\rho\frac{a}{2}} \end{cases}$$

We thus find:

$$A_2 = \frac{1}{2}\left(1 + \frac{\rho}{ik}\right) e^{(ik-\rho)\frac{a}{2}} B_1 = \frac{\rho + ik}{2ik} e^{(ik-\rho)\frac{a}{2}} B_1$$
$$= \frac{1}{2}\left(1 - \frac{\rho}{ik}\right) e^{-(ik+\rho)\frac{a}{2}} B_3' = \frac{ik - \rho}{2ik} e^{-(ik+\rho)\frac{a}{2}} B_3'$$

and

$$A_2' = \frac{1}{2}\left(1 - \frac{\rho}{ik}\right) e^{-(ik+\rho)\frac{a}{2}} B_1 = \frac{ik-\rho}{2ik} e^{-(ik+\rho)\frac{a}{2}} B_1$$
$$= \frac{1}{2}\left(1 + \frac{\rho}{ik}\right) e^{(ik-\rho)\frac{a}{2}} B_3' = \frac{\rho+ik}{2ik} e^{(ik-\rho)\frac{a}{2}} B_3'$$

Subsequently:

$$B_3' = \frac{\rho+ik}{ik-\rho} e^{ika} B_1 = \frac{ik-\rho}{\rho+ik} e^{-ika} B_1$$

thus

$$\frac{\rho+ik}{ik-\rho} e^{ika} = \frac{ik-\rho}{\rho+ik} e^{-ika} \Leftrightarrow \left(\frac{\rho-ik}{\rho+ik}\right)^2 = e^{2ika}$$

This equation corresponds to equation (42) of Complement H_I, whose solutions are represented graphically in Figure 1.5 of Complement H_I and recalled in Figure 1.11. Additionally here, $a \to 0$ so $\frac{\pi}{a} \to +\infty$, which implies $k_0 = \sqrt{\frac{2mV_0}{\hbar^2}} < \frac{\pi}{a}$: there indeed exists only one bound state of the particle, which is even, such that

$$\frac{\rho}{k} = \tan\left(\frac{ka}{2}\right)$$

according to equation (44) of Complement H_I. We find:

$$1 + \frac{\rho^2}{k^2} = 1 + \tan^2\left(\frac{ka}{2}\right) = \frac{1}{\cos^2\left(\frac{ka}{2}\right)} \underset{a\to 0}{\sim} \frac{1}{\left(1 - \frac{k^2a^2}{8}\right)^2} \underset{a\to 0}{\sim} 1 + \frac{k^2a^2}{4}$$

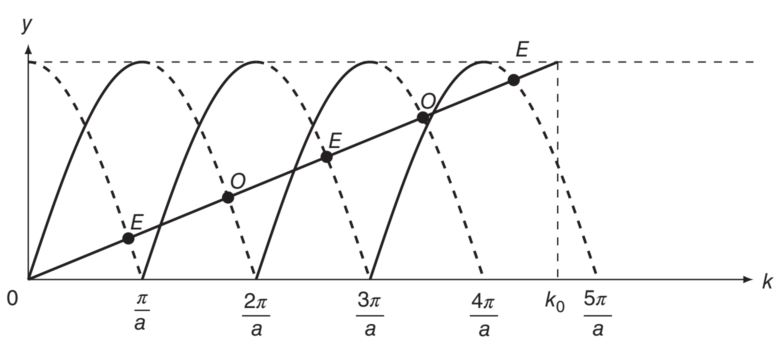


Figure 1.11 Graphic solution of equation $\left(\frac{\rho-ik}{\rho+ik}\right)^2 = e^{2ika}$, giving the energies of the bound states of a particle in a square well potential. In the case shown in the figure, there are five bound states, three even (associated with the points *E* of the figure), and two odd (points *O*).

hence

$$\frac{\rho^2}{k^4} \underset{a\to 0}{\sim} \frac{a^2}{4} \Leftrightarrow \frac{\frac{-2mE}{\hbar^2}}{\frac{4m^2(E+V_0)^2}{\hbar^4}} \underset{a\to 0}{\sim} \frac{a^2}{4} \Leftrightarrow \frac{E}{(E+V_0)^2} \underset{a\to 0}{\sim} -\frac{ma^2}{2\hbar^2}$$

Setting $\alpha = -\frac{ma^2}{2\hbar^2}$, we find

$$\alpha E^2 + (2\alpha V_0 - 1)E + \alpha V_0^2 = 0$$

We know that $2\alpha V_0 \ll 1$ since $a \to 0 \Rightarrow \alpha \to 0$. The previous equation can be simplified:

$$\alpha E^2 - E + \alpha V_0^2 = 0$$

We identify a quadratic equation with E as the unknown and whose discriminant is given by:

$$\Delta = 1 - 4\alpha^2 V_0^2 > 0$$

since $\alpha \to 0$. The possible energies are therefore

$$E = \frac{1 \pm \sqrt{1 - 4\alpha^2 V_0^2}}{2\alpha} \simeq \frac{1 \pm \left(1 - 2\alpha^2 V_0^2\right)}{2\alpha}$$

As we are searching for bound states such that $E < 0$, there is only one bound state whose energy is

$$E \simeq \alpha V_0^2 = -\frac{mV_0^2 a^2}{2\hbar^2}$$

b. Show that $\rho \to 0$ and that $A_2 = A_2' \simeq \frac{B_1}{2}$. Deduce from this that, in the bound state, the probability of finding the particle outside the well approaches 1.

As $E \simeq -\frac{mV_0^2 a^2}{2\hbar^2}$ according to the results of question a, we find

$$\rho = \sqrt{\frac{-2mE}{\hbar^2}} \simeq \frac{mV_0 a}{\hbar^2}$$

and $\rho \to 0$ when $a \to 0$. This means that:

$$A_2 = \frac{\rho + ik}{2ik} e^{(ik-\rho)\frac{a}{2}} B_1 \simeq \frac{B_1}{2} \text{ and } A_2' = \frac{ik - \rho}{2ik} e^{-(ik+\rho)\frac{a}{2}} B_1 \simeq \frac{B_1}{2}$$

and the probability for the particle to be in the well is

$$\int_{-\frac{a}{2}}^{\frac{a}{2}} |\varphi(x)|^2 \mathrm{d}x = \int_{-\frac{a}{2}}^{\frac{a}{2}} |\varphi_{\mathrm{II}}(x)|^2 \mathrm{d}x \simeq \frac{|B_1|^2}{4} \int_{-\frac{a}{2}}^{\frac{a}{2}} (e^{ikx} + e^{-ikx})^2 \mathrm{d}x$$

$$\int_{-\frac{a}{2}}^{\frac{a}{2}} |\varphi(x)|^2 \mathrm{d}x \simeq |B_1|^2 \int_{-\frac{a}{2}}^{\frac{a}{2}} \cos^2 kx \, \mathrm{d}x = \frac{|B_1|^2}{2} \int_{-\frac{a}{2}}^{\frac{a}{2}} (1 + \cos 2kx)\mathrm{d}x$$

$$\simeq \frac{|B_1|^2}{2} \left[x + \frac{\sin 2kx}{2k} \right]_{-\frac{a}{2}}^{\frac{a}{2}} = \frac{|B_1|^2}{2} \left(a + \frac{\sin ka}{k} \right) \underset{a \to 0}{\sim} a|B_1|^2$$

which approaches 0 when $a \to 0$. In the bound state, the probability to find the particle outside the well approaches 1.

c. How can the preceding considerations be applied to a particle placed, as in exercise 2, in the potential $V(x) = -\alpha\delta(x)$?

In exercise 2, the delta function potential (whose area is α) is equivalent to a square well of width a and depth V_0 (and thus whose area is $\alpha = aV_0$) when $a \to 0$. We therefore simply substitute aV_0 by α in the previous results. According to the results of question a, there is thus only one bound state whose energy is $E \simeq -\frac{m\alpha^2}{2\hbar^2}$ (which is precisely the expression found in exercise 2) and, according to the results of question b, the probability to find the particle outside the delta function well is 1, which makes sense.

1.7 The Piecewise Constant Lennard–Jones Potential

Statement
Consider a particle placed in the potential:

$$V(x) = 0 \qquad \text{if} \quad x \geqslant a$$

$$V(x) = -V_0 \qquad \text{if} \quad 0 \leqslant x < a,$$

with $V(x)$ infinite for negative x. Let $\varphi(x)$ be a wave function associated with a stationary state of the particle. Show that $\varphi(x)$ can be extended to give an odd wave function which corresponds to a stationary state for a square well of width $2a$ and depth V_0 (*cf*. Complement H_I, § 2-c-α). Discuss, with respect to a and V_0, the number of bound states of the particle. Is there always at least one such state, as for the symmetric square well?

Comments
This is a standard exercise on a wave function associated with a bound state, such that $-V_0 < E < 0$, in a potential that is highly repulsive over short distances, but attractive over long distances (as a first approximation, this potential can be likened to a Lennard–Jones potential).

In classical mechanics, the particle is trapped in the well. It cannot escape, the probability of finding the particle outside the well is zero according to a classical approach.

In quantum mechanics, the particle can exit the well and explore the classically "forbidden" zones. Exploration in the zone where the potential is infinite is impossible (the exploration distance approaches zero when the potential is infinite), but in the zone where the potential is vanishing, the particle can have a nonzero probability of presence, which limits, as we know, the number of accessible states.

For an infinite discontinuity of potential, only the spatial wave function is continuous (not its derivative). For a finite discontinuity of potential, the wave function along with its first derivative is continuous at the discontinuity of potential. All of these conditions constrain the various constants that appear in the wave function. However, for the wave function to be nontrivial, the continuity conditions also impose a constraint on the energy, which is therefore shown to be quantized as in the previous exercise.

Solution
Consider a particle placed in the potential:

$$V(x) = 0 \qquad \text{if} \quad x \geqslant a$$
$$V(x) = -V_0 \quad \text{if} \quad 0 \leqslant x < a,$$

with $V(x)$ infinite for negative x. Let $\varphi(x)$ be a wave function associated with a stationary state of the particle. Show that $\varphi(x)$ can be extended to give an odd wave function which corresponds to a stationary state for a square well of width $2a$ and depth V_0 (*cf*. Complement H_I, § 2-c-α). Discuss, with respect to a and V_0, the number of bound states of the particle. Is there always at least one such state, as for the symmetric square well?

The potential is given by:

$$V(x) = \begin{cases} +\infty & \text{if } x < 0 \\ -V_0 & \text{if } 0 \leqslant x < a \\ 0 & \text{if } x \geqslant a \end{cases}$$

and represented in Figure 1.12.

The particle cannot exist in zone I ($x < 0$), and the eigenvalue equation of H is

$$-\frac{\hbar^2}{2m}\frac{d^2\varphi(x)}{dx^2} - (E + V_0)\varphi(x) = 0 \Leftrightarrow \frac{d^2\varphi(x)}{dx^2} + \frac{2m(E + V_0)}{\hbar^2}\varphi(x) = 0$$
$$\Leftrightarrow \frac{d^2\varphi(x)}{dx^2} + k^2\varphi(x) = 0$$

with $k = \sqrt{\dfrac{2m(E + V_0)}{\hbar^2}}$ in zone II ($0 \leqslant x < a$) and

$$-\frac{\hbar^2}{2m}\frac{d^2\varphi(x)}{dx^2} - E\varphi(x) = 0 \Leftrightarrow \frac{d^2\varphi(x)}{dx^2} - \frac{-2mE}{\hbar^2}\varphi(x) = 0$$
$$\Leftrightarrow \frac{d^2\varphi(x)}{dx^2} - \rho^2\varphi(x) = 0$$

with $\rho = \sqrt{\dfrac{-2mE}{\hbar^2}}$ in zone III ($x \geqslant a$) for a bound state whose energy is E such that $-V_0 < E < 0$. The expressions of the eigenfunctions for a bound state in the three

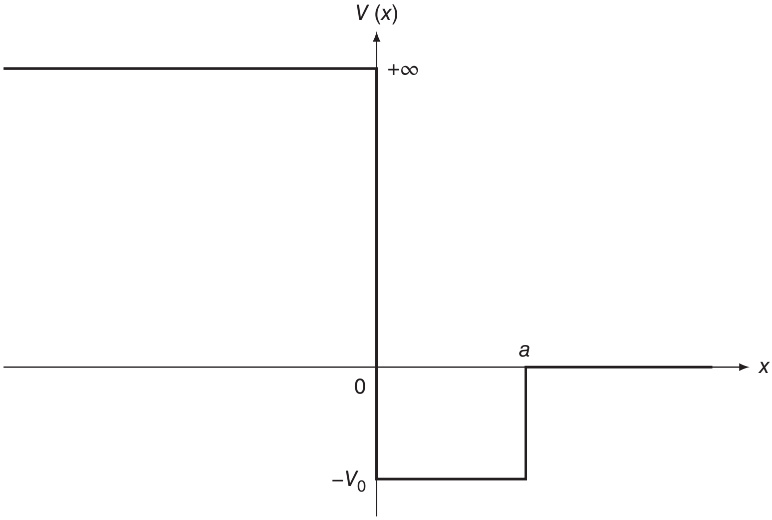


Figure 1.12 Graphic representation of the potential considered.

zones are:

$$\begin{cases} \varphi_{\mathrm{I}}(x) = 0 \\ \varphi_{\mathrm{II}}(x) = A_2 e^{ikx} + A'_2 e^{-ikx} \\ \varphi_{\mathrm{III}}(x) = B_3 e^{\rho x} + B'_3 e^{-\rho x} \end{cases}$$

$\varphi(x)$ should be bounded when $x \to +\infty$ so $B_3 = 0$, hence

$$\begin{cases} \varphi_{\mathrm{I}}(x) = 0 \\ \varphi_{\mathrm{II}}(x) = A_2 e^{ikx} + A'_2 e^{-ikx} \\ \varphi_{\mathrm{III}}(x) = B'_3 e^{-\rho x} \end{cases}$$

Firstly, $\varphi(x)$ is continuous at $x = 0$ and $x = a$, so:

$$\begin{cases} \varphi_{\mathrm{I}}(0) = \varphi_{\mathrm{II}}(0) \\ \varphi_{\mathrm{II}}(a) = \varphi_{\mathrm{III}}(a) \end{cases} \Leftrightarrow \begin{cases} A_2 + A'_2 = 0 \\ A_2 e^{ika} + A'_2 e^{-ika} = B'_3 e^{-\rho a} \end{cases}$$

Secondly, $\dfrac{\mathrm{d}\varphi(x)}{\mathrm{d}x}$ is continuous at $x = a$ since the variation of $V(x)$ at $x = a$ is finite, so

$$\frac{\mathrm{d}\varphi_{\mathrm{II}}(a)}{\mathrm{d}x} = \frac{\mathrm{d}\varphi_{\mathrm{III}}(a)}{\mathrm{d}x} \Leftrightarrow ikA_2 e^{ika} - ikA'_2 e^{-ika} = -\rho B'_3 e^{-\rho a}$$

$$\Leftrightarrow A_2 e^{ika} - A'_2 e^{-ika} = -\frac{\rho}{ik} B'_3 e^{-\rho a}$$

This means that, setting $A_2 = A$ and $B'_3 = B$:

$$\begin{cases} \varphi_{\mathrm{I}}(x) = 0 \\ \varphi_{\mathrm{II}}(x) = Ae^{ikx} - Ae^{-ikx} \\ \varphi_{\mathrm{III}}(x) = Be^{-\rho x} \end{cases}$$

$\varphi_{II}(x)$ is odd, so it can easily be extended for $-a < x \leqslant 0$, by setting $\varphi_I(x) = -Be^{\rho x}$ such that $\varphi(x)$ is odd. We find:

$$\begin{cases} \varphi_I(x) = -Be^{\rho x} & \text{if } x \leqslant -a \\ \varphi_{II}(x) = Ae^{ikx} - Ae^{-ikx} & \text{if } -a < x < a \\ \varphi_{III}(x) = Be^{-\rho x} & \text{if } x \geqslant a \end{cases}$$

and this odd wave function does indeed correspond to a stationary state for a square well of width $2a$ and depth V_0, as seen in Complement H_I. Hence:

$$\begin{cases} A_2 = \frac{1}{2}\left(1 - \frac{\rho}{ik}\right) e^{-(\rho+ik)a} B_3' = \frac{ik-\rho}{2ik} e^{-(\rho+ik)a} B_3' \\ A_2' = \frac{1}{2}\left(1 + \frac{\rho}{ik}\right) e^{(ik-\rho)a} B_3' = \frac{\rho+ik}{2ik} e^{(ik-\rho)a} B_3' \end{cases}$$

according to the results of question a in exercise 6, substituting a by $2a$. Finally, we find

$$A_2 + A_2' = 0 \Leftrightarrow (ik-\rho)e^{-ika} + (\rho+ik)e^{ika} = 0 \Leftrightarrow \frac{\rho - ik}{\rho + ik} = e^{2ika}$$

and so

$$\begin{aligned} \rho - ik = (\rho + ik)e^{2ika} &\Leftrightarrow (1 - e^{2ika})\rho = ik(1 + e^{2ika}) \\ &\Leftrightarrow \frac{\rho}{k} = i\frac{1+e^{2ika}}{1-e^{2ika}} = i\frac{e^{-ika}+e^{ika}}{e^{-ika}-e^{ika}} = -\frac{1}{\tan ka} \end{aligned}$$

Let $k_0 = \sqrt{\dfrac{2mV_0}{\hbar^2}} = \sqrt{k^2+\rho^2}$, thus

$$\cos^2 ka = \frac{1}{1+\tan^2 ka} = \frac{1}{1+\dfrac{k^2}{\rho^2}} = \frac{\rho^2}{k^2+\rho^2} \Leftrightarrow \sin^2 ka = \frac{k^2}{k^2+\rho^2} = \frac{k^2}{k_0^2}$$

and equation $\dfrac{\rho - ik}{\rho + ik} = e^{2ika}$ is equivalent to the following system of two equations:

$$\begin{cases} |\sin ka| = \dfrac{k}{k_0} \\ \tan ka < 0 \end{cases}$$

The possible energy levels are thus determined by the intersection of a line with slope $\dfrac{1}{k_0}$ (represented by a solid straight line in Figure 1.13) with sinusoidal arcs (represented by a dashed line in Figure 1.13):

- if $k_0 < \dfrac{\pi}{2a} \Leftrightarrow \sqrt{\dfrac{2mV_0}{\hbar^2}} < \dfrac{\pi}{2a} \Leftrightarrow V_0 < V_1 = \dfrac{\pi^2\hbar^2}{8ma^2}$, there is no bound state of the particle, conversely to the case of the symmetric square well;
- if $\dfrac{\pi}{2a} < k_0 < \dfrac{3\pi}{2a} \Leftrightarrow \dfrac{\pi^2\hbar^2}{8ma^2} < V_0 < \dfrac{9\pi^2\hbar^2}{8ma^2}$, there is only one bound state of the particle;

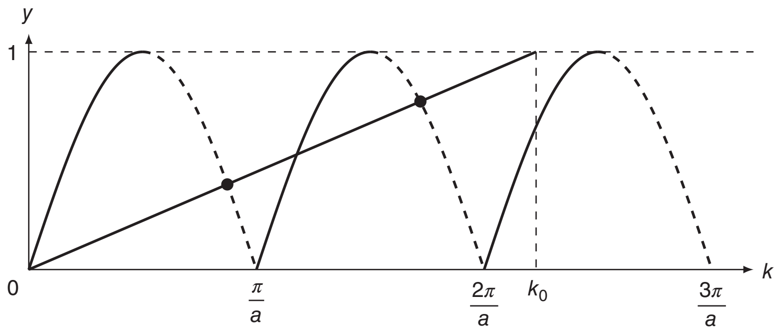


Figure 1.13 Graphic determination of bound states of the particle. In this example, only two bound states (located with dots) are possible given the value of V_0, which is directly linked to the value of k_0.

- to generalize, if

$$(2n-1)\frac{\pi}{2a} < k_0 < (2n+1)\frac{\pi}{2a} \Leftrightarrow \frac{(2n-1)^2\pi^2\hbar^2}{8ma^2} < V_0 < \frac{(2n+1)^2\pi^2\hbar^2}{8ma^2}$$

  there are $n \in \mathbb{N}^*$ bound states of the particle;

which makes sense since the wave function is odd, implying that the bound states are also necessarily odd.

1.8 Two-Dimensional Potential

Statement

Consider, in a two-dimensional problem, the oblique reflection of a particle from a potential step defined by:

$$V(x,y) = 0 \quad \text{if } x < 0$$
$$V(x,y) = V_0 \quad \text{if } x > 0$$

Study the motion of the center of the wave packet. In the case of total reflection, interpret physically the differences between the trajectory of this center and the classical trajectory (lateral shift upon reflection). Show that, when $V_0 \to +\infty$, the quantum trajectory becomes asymptotic to the classical trajectory.

Comments

This exercise deals with the total reflection on an interface, *i.e.* a change of medium, which is characterized here by a change in potential energy. As the statement mentions total reflection, the energy of the particle E is lower than V_0 in the zone where $x > 0$, in other words in the zone that is forbidden by classical mechanics.

The statement explicitly asks for a comparison with the reflection of a beam of particles on an interface.

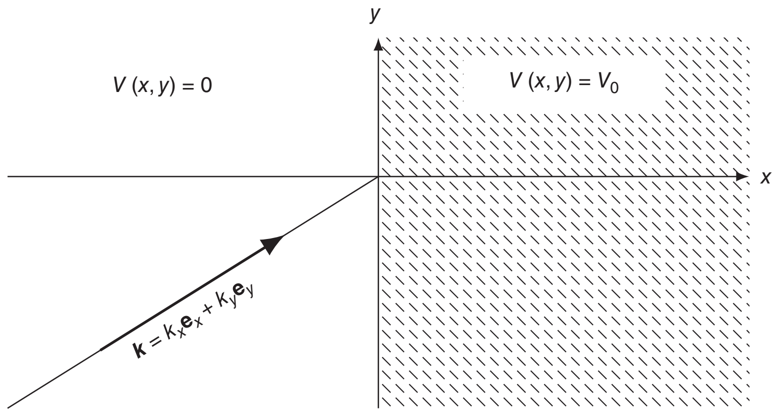


Figure 1.14 Incident wave on an interface.

Bearing in mind the wave–particle duality of the system, we must also recall the experiment of a wave totally reflecting on an interface. Indeed, even if the wave is totally reflected, there is still an "evanescent" wave on the other side of the interface.

In quantum mechanics, intuitively, the particle explores the classically "forbidden" zone: the wave function in the forbidden zone should take the form of an "evanescent" wave.

The problem, albeit two-dimensional, aims to describe particles moving along a straight path, and is therefore associated to a plane wave (or a wave packet of plane waves) whose wave vector is denoted $\mathbf{k} = k_x\mathbf{e}_x + k_y\mathbf{e}_y$. This decomposition encourages us to separate the spatial wave function $\varphi(x, y)$ of the problem as $\varphi(x, y) = \varphi_1(x)\varphi_2(y)$. The problem is depicted in Figure 1.14.

Solution

Consider, in a two-dimensional problem, the oblique reflection of a particle from a potential step defined by:

$$V(x, y) = 0 \quad \text{if } x < 0$$
$$V(x, y) = V_0 \quad \text{if } x > 0$$

Study the motion of the center of the wave packet. In the case of total reflection, interpret physically the differences between the trajectory of this center and the classical trajectory (lateral shift upon reflection). Show that, when $V_0 \to +\infty$, the quantum trajectory becomes asymptotic to the classical trajectory.

In this case, the potential only depends on x, but it is useful, as will become clear below, to separate the spatial variables x and y to decompose it as follows:

$$V(x, y) = V_1(x) + V_2(y)$$

with

$$V_1(x) = \begin{cases} 0 & \text{if } x < 0 \\ V_0 & \text{if } x > 0 \end{cases} \quad \text{and } \forall y \in \mathbb{R}, V_2(y) = 0$$

Let us now look for solutions assuming the form $\varphi(x,y) = \varphi_1(x)\varphi_2(y)$. These functions satisfy the eigenvalue equation:

$$-\frac{\hbar^2}{2m}\frac{\partial^2\varphi(x,y)}{\partial x^2} - \frac{\hbar^2}{2m}\frac{\partial^2\varphi(x,y)}{\partial y^2} + V(x,y)\varphi(x,y) = E\varphi(x,y)$$

$$\Leftrightarrow -\frac{\hbar^2}{2m}\left(\frac{\mathrm{d}^2\varphi_1(x)}{\mathrm{d}x^2}\varphi_2(y) + \varphi_1(x)\frac{\mathrm{d}^2\varphi_2(y)}{\mathrm{d}y^2}\right)$$
$$+ (V_1(x) + V_2(y))\varphi_1(x)\varphi_2(y) = E\varphi_1(x)\varphi_2(y)$$

We then divide both sides of the equation by $\varphi_1(x)\varphi_2(y)$ yielding:

$$-\frac{\hbar^2}{2m}\frac{1}{\varphi_1(x)}\frac{\mathrm{d}^2\varphi_1(x)}{\mathrm{d}x^2} - \frac{\hbar^2}{2m}\frac{1}{\varphi_2(y)}\frac{\mathrm{d}^2\varphi_2(y)}{\mathrm{d}y^2} + V_1(x) + V_2(y) = E$$

and the x and y variables can be separated to produce two eigenvalue equations:

$$\begin{cases} -\dfrac{\hbar^2}{2m}\dfrac{\mathrm{d}^2\varphi_1(x)}{\mathrm{d}x^2} + V_1(x)\varphi_1(x) = E_1\varphi_1(x) \\ -\dfrac{\hbar^2}{2m}\dfrac{\mathrm{d}^2\varphi_2(y)}{\mathrm{d}y^2} + V_2(y)\varphi_2(y) = E_2\varphi_2(y) \end{cases}$$

with $E = E_1 + E_2$. We assume, in this case, that total reflection occurs, meaning that the particle energy E_1 satisfies $0 < E_1 < V_0$. The eigenfunctions $\varphi_1(x)$ are solutions to the eigenvalue equation:

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\varphi_1(x)}{\mathrm{d}x^2} - E_1\varphi_1(x) = 0 \Leftrightarrow \frac{\mathrm{d}^2\varphi_1(x)}{\mathrm{d}x^2} + \frac{2mE_1}{\hbar^2}\varphi_1(x) = 0$$
$$\Leftrightarrow \frac{\mathrm{d}^2\varphi_1(x)}{\mathrm{d}x^2} + k_1^2\varphi_1(x) = 0$$

with $k_1 = \sqrt{\dfrac{2mE_1}{\hbar^2}}$ in zone I ($x < 0$) and

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\varphi_1(x)}{\mathrm{d}x^2} + (V_0 - E_1)\varphi_1(x) = 0 \Leftrightarrow \frac{\mathrm{d}^2\varphi_1(x)}{\mathrm{d}x^2} - \frac{2m(V_0 - E_1)}{\hbar^2}\varphi_1(x) = 0$$
$$\Leftrightarrow \frac{\mathrm{d}^2\varphi_1(x)}{\mathrm{d}x^2} - \rho_1^2\varphi_1(x) = 0$$

with $\rho_1 = \sqrt{\dfrac{2m(V_0 - E_1)}{\hbar^2}}$ in zone II ($x > 0$). The summarized expression of the eigenfunctions $\varphi_1(x)$ in both zones is:

$$\begin{cases} \varphi_{1,\mathrm{I}}(x) = Ae^{ik_1x} + A'e^{-ik_1x} \\ \varphi_{1,\mathrm{II}}(x) = Be^{\rho_1x} + B'e^{-\rho_1x} \end{cases}$$

and $B = 0$ for $\varphi_1(x)$ to remain bounded when $x \to +\infty$, thus

$$\begin{cases} \varphi_{1,\mathrm{I}}(x) = Ae^{ik_1x} + A'e^{-ik_1x} \\ \varphi_{1,\mathrm{II}}(x) = B'e^{-\rho_1x} \end{cases}$$

Moreover, the functions $\varphi_1(x)$ are continuous at $x = 0$, the same for their derivatives, so:

$$\begin{cases} \varphi_{1,\mathrm{I}}(0) = \varphi_{1,\mathrm{II}}(0) \\ \dfrac{\mathrm{d}\varphi_{1,\mathrm{I}}(0)}{\mathrm{d}x} = \dfrac{\mathrm{d}\varphi_{1,\mathrm{II}}(0)}{\mathrm{d}x} \end{cases} \Leftrightarrow \begin{cases} A + A' = B' \\ ik_1(A - A') = -\rho_1 B' \end{cases}$$

This means that

$$ik_1(A - A') = -\rho_1(A + A') \Leftrightarrow (\rho_1 + ik_1)A = (-\rho_1 + ik_1)A' \Leftrightarrow A' = \frac{ik_1 + \rho_1}{ik_1 - \rho_1}A$$

and

$$B' = A + A' = \frac{2ik_1}{ik_1 - \rho_1}A$$

Since $V_2(y) = 0$, when $E_2 > 0$, the eigenfunctions $\varphi_2(y)$ satisfy equation

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\varphi_2(x)}{\mathrm{d}x^2} - E_2\varphi_2(x) = 0 \Leftrightarrow \frac{\mathrm{d}^2\varphi_2(x)}{\mathrm{d}x^2} + \frac{2mE_2}{\hbar^2}\varphi_2(x) = 0$$
$$\Leftrightarrow \frac{\mathrm{d}^2\varphi_2(x)}{\mathrm{d}x^2} + k_2^2\varphi_2(x) = 0$$

with $k_2 = \sqrt{\dfrac{2mE_2}{\hbar^2}}$ and therefore can be written:

$$\varphi_2(y) = Ce^{ik_2y} + C'e^{-ik_2y}$$

Assuming the incident particle originates from zone $y < 0$, we find $C' = 0$ and we can choose $C = 1$ such that

$$\varphi_2(y) = e^{ik_2y}$$

The eigenfunctions $\varphi(x, y)$ therefore satisfy equation:

$$\begin{cases} \varphi_{\mathrm{I}}(x, y) = Ae^{i(k_1x + k_2y)} + A'e^{i(-k_1x + k_2y)} \\ \varphi_{\mathrm{II}}(x, y) = B'e^{-\rho_1x + ik_2y} \end{cases}$$

Let us interpret this result in terms of waves.

In zone I, there is an incident and a reflected wave. The pre-exponential constants (complex amplitudes) of each wave are A and A', respectively, and the propagation of the reflected wave along the Oy axis is identical to that of the incident wave, but its propagation along the Ox axis is inversed because of the reflection on the interface according to Snell's law.

In zone II, there is a so-called "evanescent" wave, whose pre-exponential constant is B', that propagates along the Oy axis, as the waves in zone I, but it is exponentially damped along the Ox axis. This means that the wave remains localized around the interface and only enters "forbidden" zone II over a distance of the order of $\dfrac{1}{\rho_1}$. A few lines previously, we showed that

$$\frac{A'}{A} = \frac{ik_1 + \rho_1}{ik_1 - \rho_1} = \frac{k_1 - i\rho_1}{k_1 + i\rho_1}$$

The moduli of coefficients A and A' are thus equal, and we can write

$$\frac{A'}{A} = e^{-2i\theta(k_1)} \text{ with } \tan\theta(k_1) = \frac{\rho_1}{k_1} = \frac{\sqrt{K_0^2 - k_1^2}}{k_1}$$

setting $K_0 = \sqrt{\frac{2mV_0}{\hbar^2}}$. Let us note here that $\left|\frac{A'}{A}\right|^2 = 1$ so there is indeed total reflection. In other words, the probability for the particle to be reflected is 1 or 100%. This means that the difference between quantum (and so the influence of the "evanescent" wave) and classical results is slight. However, the exercise statement aims to go further in the analysis by studying the "trajectory" of the wave packet.

The expression of the wave packet, at $t = 0$ and for negative x, is:

$$\psi(x, y, 0) = \frac{1}{2\pi} \int_{k_1=0}^{k_1=K_0} \int_{k_2=0}^{k_2=+\infty} \mathrm{d}k_1 \mathrm{d}k_2 \; g(k_1, k_2) \left[e^{i(k_1x+k_2y)} + e^{-2i\theta(k_1)} e^{i(-k_1x+k_2y)}\right]$$

since $0 < E_1 < V_0$. Let us assume that $|g(k_1, k_2)|$ presents a large peak of width Δk_1 around the value $k_1 = k_{01} < K_0$ along x and of width Δk_2 around the value $k_2 = k_{02}$ along y. The expression of the wave function $\psi(x, y, t)$ at any time t is

$$\psi(x, y, t) = \frac{1}{2\pi} \int_{k_1=0}^{k_1=K_0} \int_{k_2=0}^{k_2=+\infty} \mathrm{d}k_1 \mathrm{d}k_2 \; g(k_1, k_2) e^{i[k_1x+k_2y-\omega(k_1,k_2)t]}$$
$$+ \frac{1}{2\pi} \int_{k_1=0}^{k_1=K_0} \int_{k_2=0}^{k_2=+\infty} \mathrm{d}k_1 \mathrm{d}k_2 \; g(k_1, k_2) e^{-i[k_1x-k_2y+\omega(k_1,k_2)t+2\theta(k_1)]}$$

with $\omega(k_1, k_2) = \frac{\hbar}{2m}(k_1^2 + k_2^2)$. The first term represents the incident wave packet, the second represents the reflected wave packet. Assuming the function $g(k_1, k_2)$ is real, the stationary phase condition allows us to compute the position (x_i, y_i) of the center of the incident wave packet using equation (11) of Complement $\mathrm{F_I}$:

$$x_i = t\left[\frac{\partial\omega(k_1, k_2)}{\partial k_1}\right]_{k_1=k_{01}} = \frac{\hbar k_{01}}{m} t \text{ and } y_i = t\left[\frac{\partial\omega(k_1, k_2)}{\partial k_2}\right]_{k_2=k_{02}} = \frac{\hbar k_{02}}{m} t$$

Likewise, the position (x_r, y_r) of the center of the reflected wave packet can be determined as follows:

$$x_r = -t\left[\frac{\partial\omega(k_1, k_2)}{\partial k_1}\right]_{k_1=k_{01}} - 2\left[\frac{\partial\theta(k_1)}{\partial k_1}\right]_{k_1=k_{01}} = -\frac{\hbar k_{01}}{m} t - 2\left[\frac{\mathrm{d}\theta(k_1)}{\mathrm{d}k_1}\right]_{k_1=k_{01}}$$
$$y_r = t\left[\frac{\partial\omega(k_1, k_2)}{\partial k_2}\right]_{k_2=k_{02}} + 2\left[\frac{\partial\theta(k_1)}{\partial k_2}\right]_{k_2=k_{02}} = \frac{\hbar k_{02}}{m} t$$

However, by differentiating

$$\tan\theta(k_1) = \frac{\sqrt{K_0^2 - k_1^2}}{k_1}$$

we find

$$(1 + \tan^2\theta(k_1))\mathrm{d}\theta = \left[1 + \frac{K_0^2 - k_1^2}{k_1^2}\right]\mathrm{d}\theta = -\frac{\sqrt{K_0^2 - k_1^2}}{k_1^2}\mathrm{d}k_1 - \frac{\mathrm{d}k_1}{\sqrt{K_0^2 - k_1^2}}$$

$$\Leftrightarrow \frac{K_0^2}{k_1^2}\mathrm{d}\theta = -\frac{K_0^2}{k_1^2\sqrt{K_0^2 - k_1^2}}\mathrm{d}k_1$$

which finally yields

$$(x_r, y_r) = \left(-\frac{\hbar k_{01}}{m}t + \frac{2}{\sqrt{K_0^2 - k_1^2}}, \frac{\hbar k_{02}}{m}t\right)$$

Let us firstly consider what happens for negative t. The center (x_i, y_i) of the incident wave packet propagates in the direction of increasing x and y at constant speeds $\frac{\hbar k_{01}}{m}$ along x and $\frac{\hbar k_{02}}{m}$ along y. Secondly, we can note that, for $t < 0$, x_r is positive and is thus located outside zone $x < 0$ where the expression $\psi(x, y, t)$ is valid; this means that, for all negative x values, the various waves of the reflected wave packet interfere destructively: for negative t, there is no reflected wave packet, only an incident wave packet.

The center of the incident wave packet reaches the potential step at time $t = 0$. During a certain amount of time around $t = 0$, the wave packet is localized in the zone $x \simeq 0$, where the barrier is located, and its form is relatively complicated. However, for sufficiently large t values, we observe that it is now the incident wave packet that has disappeared, only the reflected wave packet remains. Indeed, now x_i is positive, and x_r has become negative: the waves of the incident wave packet interfere destructively for all negative x values, whereas those of the reflected wave packet interfere constructively at $x = x_r < 0$. The reflected wave packet propagates in the direction of decreasing x at speed $-\frac{\hbar k_{01}}{m}$ which is opposite the speed of the incident wave packet before reaching the barrier, and in the direction of increasing y at speed $\frac{\hbar k_{02}}{m}$ that is the same as the speed of the incident wave packet before reaching the barrier; its form is unchanged (except for one symmetry). Moreover, the expression of x_r indicates that the reflection has introduced a delay τ such that

$$\tau = \frac{2m}{\hbar k_{01}\sqrt{K_0^2 - k_1^2}}$$

Unlike what is predicted by classical mechanics, the particle is not instantaneously reflected. We can rationalize this delay given that, for close-to-zero t, the probability of finding the particle in the classically "forbidden" zone $x > 0$ is nonzero: we can say that it is as if the particle "wastes" time of the order of τ in this zone before turning around. Note also that the particle returns to zone $x < 0$ at $t = \tau$: it "leaves" the step

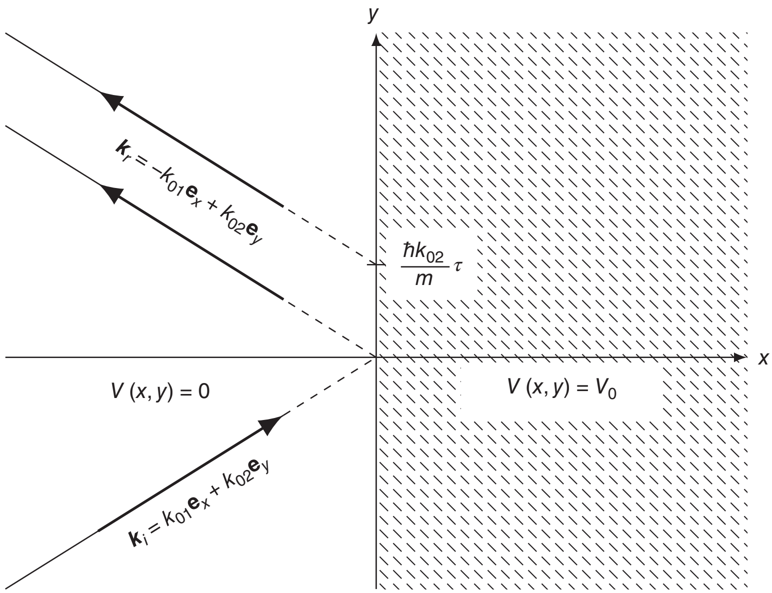


Figure 1.15 Trajectory of the center of the incident wave packet, and quantum and classical trajectories of the center of the reflected wave packet. Note that the trajectories are represented by dashed lines in the vicinity of the interface since the actual notion of trajectory no longer has much meaning. This is due to the complex form of the wave packet, which results from the interactions between incident, reflected, and transmitted waves in this region.

at $y = \frac{\hbar k_{02}}{m}\tau$ after having "entered" it at $y = 0$, which leads to a lateral offset. τ represents the characteristic time during which the incident, reflected, and transmitted wave packets interact and coexist in the vicinity of the interface. The waves of the transmitted wave packet only interfere constructively during the time τ, while the transmitted wave packet moves by a distance $v_2\tau = \frac{\hbar k_{02}}{m}\tau$ (v_2 is the group velocity here, *i.e.* the speed of the envelope of the wave packet $\left[\frac{\partial\omega(k_1,k_2)}{\partial k_2}\right]_{k_2=k_{02}}$).

When $V_0 \to +\infty$, $E_1 \ll V_0 \Leftrightarrow k_1 \ll K_0$ and the delay τ therefore approaches 0: the reflection happens instantaneously and without any lateral offset. The quantum trajectory, therefore, becomes asymptotic to the classical trajectory when $V_0 \to +\infty$. The trajectory of the center of the incident wave packet and the quantum and classical trajectories of the center of the reflected wave packet are depicted in Figure 1.15.