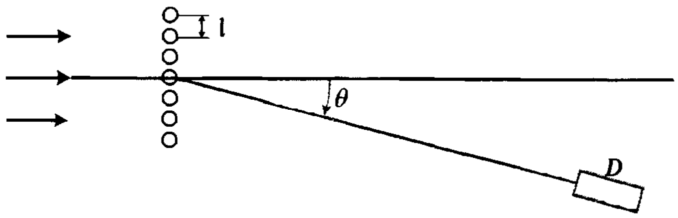
Complement K_I

EXERCISES

1. A beam of neutrons of constant velocity, mass M_n ($M_n \simeq 1.67 \times 10^{-27}$ kg) 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?

2. Bound state of a particle in a "delta function potential"

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:

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

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

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) Trace these wave functions graphically. Give an order of magnitude for their width Δx.

d) What is the probability $\overline{d\mathscr{P}(p)}$ 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 $p + dp$? 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 $\Delta x \,.\, \Delta p$.

3. Transmission of a "delta function" potential barrier

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:

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

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 $-E_L = -m\alpha^2/2\hbar^2$ (bound state energy of the particle). Calculate, in terms of the dimensionless parameter 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 $E \longrightarrow \infty$? How can this be interpreted? Show that, if the expression of T is extended for negative values of E, it diverges when $E \longrightarrow -E_L$, and discuss this result.

4. 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):

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

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

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

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 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.

5. Well consisting of two delta functions

Consider a particle of mass m whose potential energy is

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

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 $x = l/2$), 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 which you are to specify, 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 $l \longrightarrow 0$ and at the limit where $l \longrightarrow \infty$? If the repulsion of the two nuclei is taken into account, what is the total energy of the system? Show that the curve which 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. In this way we obtain 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?

6. 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). 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 $\left(\text{we find } E \simeq -\dfrac{mV_0^2a^2}{2\hbar^2}\text{, that is, an energy which varies with the square of the area } aV_0 \text{ of the well}\right)$.

b) Show that $\rho \longrightarrow 0$ and that $A'_2 = A_2 \simeq B_1/2$. 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 $V(x) = -\alpha\delta(x)$?

7. Consider a particle placed in the potential

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

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?

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

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

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 $V_0 \longrightarrow +\infty$, the quantum trajectory becomes asymptotic to the classical trajectory.