Complement A_{III}

PARTICLE IN AN INFINITE POTENTIAL WELL

In complement H_I (§2-c-β), we studied the stationary states of a particle in a one-dimensional infinite potential well. Here we intend to re-examine this subject from a physical point of view. This will allow us to apply some of the postulates of chapter III to a concrete case. We shall be particularly interested in the results that can be obtained when the position or momentum of the particle is measured.

1. Distribution of the momentum values in a stationary state

a. CALCULATION OF THE FUNCTION $\bar{\varphi}_n(p)$, OF $\langle P \rangle$ AND OF ΔP

We have seen that the stationary states of the particle correspond to the energies★:

$$E_n = \frac{n^2\pi^2\hbar^2}{2ma^2} \tag{1}$$

and to the wave functions:

$$\varphi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right) \tag{2}$$

(where a is the width of the well and n is any positive integer).

Consider a particle in the state $|\varphi_n\rangle$, with energy E_n. The probability of a measurement of the momentum P of the particle yielding a result between p and $p + dp$ is:

$$\bar{\mathscr{P}}_n(p)\, dp = |\bar{\varphi}_n(p)|^2\, dp \tag{3}$$

with:

$$\bar{\varphi}_n(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_0^a \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right) e^{-ipx/\hbar}\, dx \tag{4}$$

★ We shall use the notation of complement H_I.

This integral is easy to calculate; it is equal to:

$$\bar{\varphi}_n(p) = \frac{1}{2i\sqrt{\pi\hbar a}} \int_0^a \left[e^{i\left(\frac{n\pi}{a} - \frac{p}{\hbar}\right)x} - e^{-i\left(\frac{n\pi}{a} + \frac{p}{\hbar}\right)x} \right] dx$$

$$= \frac{1}{2i\sqrt{\pi\hbar a}} \left[\frac{e^{i\left(\frac{n\pi}{a} - \frac{p}{\hbar}\right)a} - 1}{i\left(\frac{n\pi}{a} - \frac{p}{\hbar}\right)} - \frac{e^{-i\left(\frac{n\pi}{a} + \frac{p}{\hbar}\right)a} - 1}{-i\left(\frac{n\pi}{a} + \frac{p}{\hbar}\right)} \right] \tag{5}$$

that is:

$$\bar{\varphi}_n(p) = \frac{1}{2i}\sqrt{\frac{a}{\pi\hbar}}\, e^{i\left(\frac{n\pi}{2} - \frac{pa}{2\hbar}\right)} \left[F\left(p - \frac{n\pi\hbar}{a}\right) + (-1)^{n+1} F\left(p + \frac{n\pi\hbar}{a}\right) \right] \tag{6}$$

with:

$$F(p) = \frac{\sin(pa/2\hbar)}{pa/2\hbar} \tag{7}$$

To within a proportionality factor, the function $\bar{\varphi}_n(p)$ is the sum (or the difference) of two "diffraction functions" $F\left(p \pm \frac{n\pi\hbar}{a}\right)$, centered at $p = \mp \frac{n\pi\hbar}{a}$. The "width" of these functions (the distance between the first two zeros, symmetrical with respect to the central value) does not depend on n and is equal to $\frac{4\pi\hbar}{a}$. Their "amplitude" does not depend on n either.

The function inside brackets in expression (6) is even if n is odd, and odd if n is even. The probability density $\bar{\mathscr{P}}_n(p)$ given in (3) is therefore an even function of p in all cases, so that :

$$\langle P \rangle_n = \int_{-\infty}^{+\infty} \bar{\mathscr{P}}_n(p)\, p\, dp = 0 \tag{8}$$

The mean value of the momentum of the particle in the energy state E_n is therefore zero.

Let us calculate, in the same way, the mean value $\langle P^2 \rangle_n$ of the square of the momentum. Using the fact that in the $\{ | x \rangle \}$ representation P acts like $\frac{\hbar}{i}\frac{d}{dx}$, and performing an integration by parts, we obtain*:

$$\langle P^2 \rangle_n = \hbar^2 \int_0^a \left| \frac{d\varphi_n}{dx} \right|^2 dx$$

$$= \hbar^2 \int_0^a \frac{2}{a}\left(\frac{n\pi}{a}\right)^2 \cos^2\left(\frac{n\pi x}{a}\right) dx$$

$$= \left(\frac{n\pi\hbar}{a}\right)^2 \tag{9}$$

* Result (9) could also be derived from (6) by performing the integral $\langle P^2 \rangle_n = \int_{-\infty}^{+\infty} |\bar{\varphi}_n(p)|^2\, p^2\, dp$. This calculation, which presents no theoretical difficulties, is nevertheless not as direct as the one which is given here.

From (8) and (9), we get:

$$\Delta P_n = \sqrt{\langle P^2 \rangle_n - \langle P \rangle_n^2} = \frac{n\pi\hbar}{a} \tag{10}$$

The root-mean-square deviation therefore increases linearly with n.

b. DISCUSSION

Let us trace, for different values of n, the curves which give the probability density $\overline{\mathscr{P}}_n(p)$. To do this, let us begin by studying the function inside brackets in expression (6). For the ground state ($n = 1$), it is the sum of two functions F, the centers of these two diffraction curves being separated by half their width (fig. 1-a). For the first excited level ($n = 2$), the distance between these centers is twice as large, and in this case, moreover, the difference of two functions F must be taken (fig. 2-a). Finally, for an excited level corresponding to a large value of n, the centers of the two diffraction curves are separated by a distance much greater than their width.

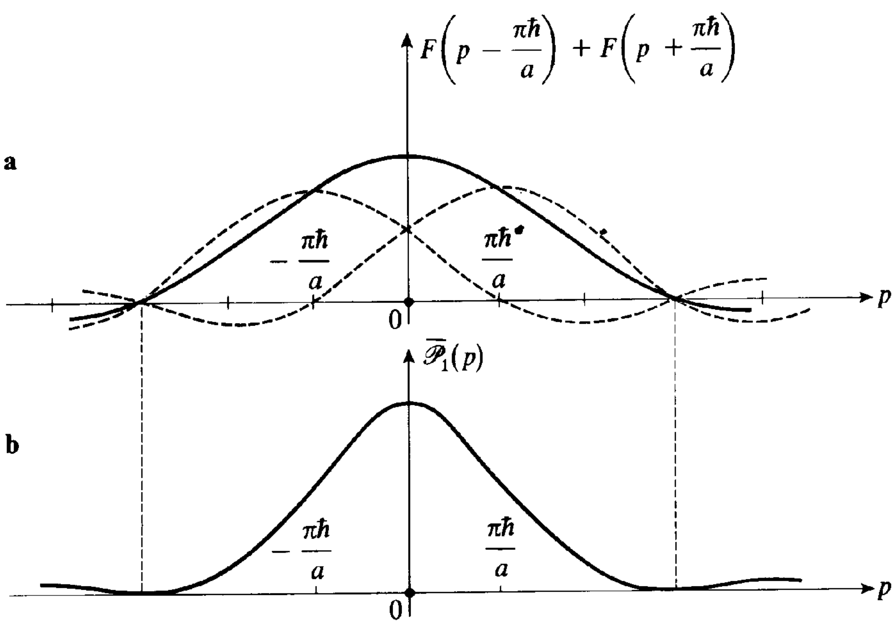

FIGURE 1

The wave function $\overline{\varphi}_1(p)$, associated in the $\{ | p \rangle \}$ representation with the ground state of a particle in a infinite well, is obtained by adding two diffraction functions F (curves in dashed lines in figure a). Since the centers of these two functions F are separated by half their width, their sum has the shape represented by the solid-line curve in figure a. Squaring this sum, one obtains the probability density $\overline{\mathscr{P}}_1(p)$ associated with a measurement of the momentum of the particle (fig. b).

Squaring these functions, one obtains the probability density $\overline{\mathscr{P}}_n(p)$ (*cf.* fig. 1-b and 2-b). Note that for large n the interference term between $F\left(p - \dfrac{n\pi\hbar}{a}\right)$ and

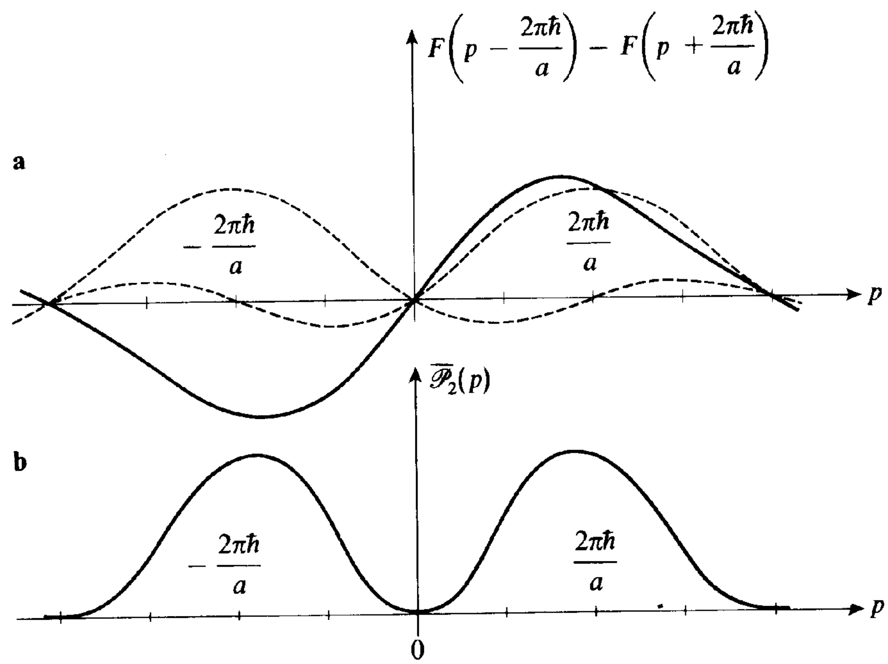

FIGURE 2

For the first excited level, the function $\overline{\varphi}_2(p)$ is obtained by taking the difference between two functions F, which have the same width as in figure 1-a but are now more widely separated (dashed-line curve in figure a). The curve obtained is the solid line in figure a. The probability density $\overline{\mathscr{P}}_2(p)$ then has two maxima located in the neighborhood of $p = \pm 2\pi\hbar/a$ (fig. b).

$F\left(p + \frac{n\pi\hbar}{a}\right)$ is negligible (because of the separation of the centers of the two curves):

$$\begin{aligned}\overline{\mathscr{P}}_n(p) &= \frac{a}{4\pi\hbar}\left[F\left(p - \frac{n\pi\hbar}{a}\right) + (-1)^{n+1}F\left(p + \frac{n\pi\hbar}{a}\right)\right]^2 \\ &\simeq \frac{a}{4\pi\hbar}\left[F^2\left(p - \frac{n\pi\hbar}{a}\right) + F^2\left(p + \frac{n\pi\hbar}{a}\right)\right] \end{aligned} \qquad (11)$$

The function $\overline{\mathscr{P}}_n(p)$ then has the shape shown in figure 3.

It can be seen that when n is large, the probability density has two symmetrical peaks, of width $\frac{4\pi\hbar}{a}$, centered at $p = \pm\frac{n\pi\hbar}{a}$. It is then possible to predict with almost complete certainty the results of a measurement of the momentum of the particle in the state $|\varphi_n\rangle$: the value found will be nearly equal to $+\frac{n\pi\hbar}{a}$ or $-\frac{n\pi\hbar}{a}$, the relative accuracy* improving as n increases (the two opposite

* The absolute accuracy is independent of n, since the width of the curves is always $\frac{4\pi\hbar}{a}$.

values $\pm \frac{n\pi\hbar}{a}$ being equally probable). This is simple to understand: for large n, the function $\varphi_n(x)$, which varies sinusoidally, performs numerous oscillations inside the well; it can then be considered to be practically the sum of two progressive waves corresponding to opposite momenta $p = \pm \frac{n\pi\hbar}{a}$.

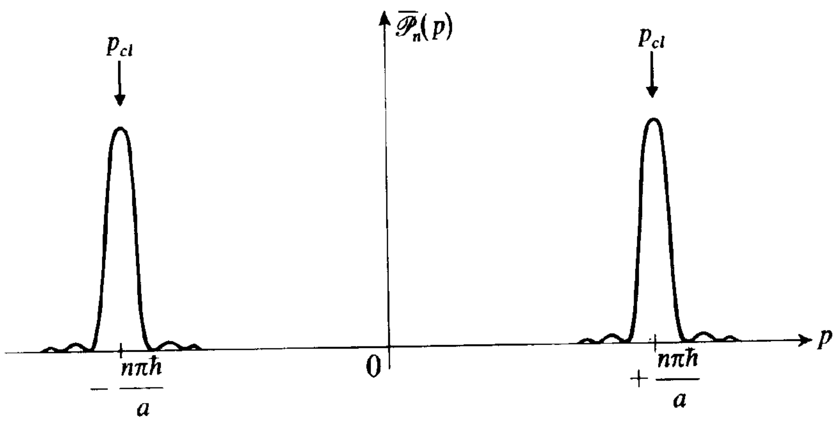

FIGURE 3

When n is large (a very excited level), the probability density has two pronounced peaks, centered at the values $p = \pm n\pi\hbar/a$, which are the momenta associated with the classical motion at the same energy.

When n decreases, the relative accuracy with which one can predict the possible values of the momentum diminishes. We see, for example, in figure 2-b, that when $n = 2$, the function $\overline{\mathscr{P}}_n(p)$ has two peaks whose widths are comparable to their distance from the origin. In this case, the wave function undergoes only one oscillation inside the well. It is not surprising that, for this sinusoid "truncated" at $x = 0$ and $x = a$, the wavelength (and therefore, the momentum of the particle) is poorly defined. Finally, for the ground state, the wave function is represented by half a sinusoidal arc: the relative values of the wavelength and momentum of the particle are then very poorly known (fig. 1-b).

COMMENTS:

(*i*) Let us calculate the momentum of a classical particle of energy E_n given in (1); we have:

$$\frac{p_{cl}^2}{2m} = \frac{n^2\pi^2\hbar^2}{2ma^2} \tag{12}$$

that is:

$$p_{cl} = \pm \frac{n\pi\hbar}{a} \tag{13}$$

When n is large, the two peaks of $\overline{\mathscr{P}}_n(p)$ therefore correspond to the classical values of the momentum.

(*ii*) We see that, for large n, although the absolute value of the momentum is well-defined, its sign is not. This is why ΔP_n is large: for probability distributions with two maxima like that of figure 3, the root-mean-square deviation reflects the distance between the two peaks; it is no longer related to their widths.

2. Evolution of the particle's wave function

Each of the states $| \varphi_n \rangle$, with its wave function $\varphi_n(x)$, describes a stationary state, which leads to time-independent physical predictions. Time evolution appears only when the state vector is a linear combination of several kets $| \varphi_n \rangle$. We shall consider here a very simple case, for which at time $t = 0$ the state vector $| \psi(0) \rangle$ is:

$$| \psi(0) \rangle = \frac{1}{\sqrt{2}} [| \varphi_1 \rangle + | \varphi_2 \rangle] \tag{14}$$

a. WAVE FUNCTION AT THE INSTANT *t*

Apply formula (D-54) of chapter III; we immediately obtain:

$$| \psi(t) \rangle = \frac{1}{\sqrt{2}} [e^{-i\frac{\pi^2\hbar}{2ma^2}t} | \varphi_1 \rangle + e^{-2i\frac{\pi^2\hbar}{ma^2}t} | \varphi_2 \rangle] \tag{15}$$

or, omitting a *global* phase factor of $| \psi(t) \rangle$:

$$| \psi(t) \rangle \propto \frac{1}{\sqrt{2}} [| \varphi_1 \rangle + e^{-i\omega_{21}t} | \varphi_2 \rangle] \tag{16}$$

with:

$$\omega_{21} = \frac{E_2 - E_1}{\hbar} = \frac{3\pi^2\hbar}{2ma^2} \tag{17}$$

b. EVOLUTION OF THE SHAPE OF THE WAVE PACKET

The shape of the wave packet is given by the probability density:

$$|\psi(x, t)|^2 = \frac{1}{2} \varphi_1^2(x) + \frac{1}{2} \varphi_2^2(x) + \varphi_1(x) \varphi_2(x) \cos \omega_{21}t \tag{18}$$

We see that the time variation of the probability density is due to the interference term in $\varphi_1\varphi_2$. Only one Bohr frequency appears, $\nu_{21} = (E_2 - E_1)/h$, since the initial state (14) is composed only of the two states $| \varphi_1 \rangle$ and $| \varphi_2 \rangle$. The curves corresponding to the variation of the functions φ_1^2, φ_2^2 and $\varphi_1\varphi_2$ are traced in figures 4-a, b and c.

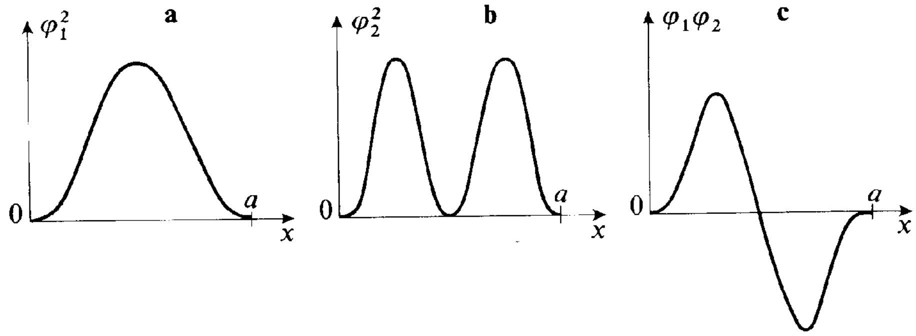

FIGURE 4

Graphical representation of the functions φ_1^2 (the probability density of the particle in the ground state), φ_2^2 (the probability density of the particle in the first excited state) and $\varphi_1\varphi_2$ (the cross term responsible for the evolution of the shape of the wave packet).

Using these figures and relation (18), it is not difficult to represent graphically the variation in time of the shape of the wave packet (*cf.* fig. 5): we see that the wave packet oscillates between the two walls of the well.

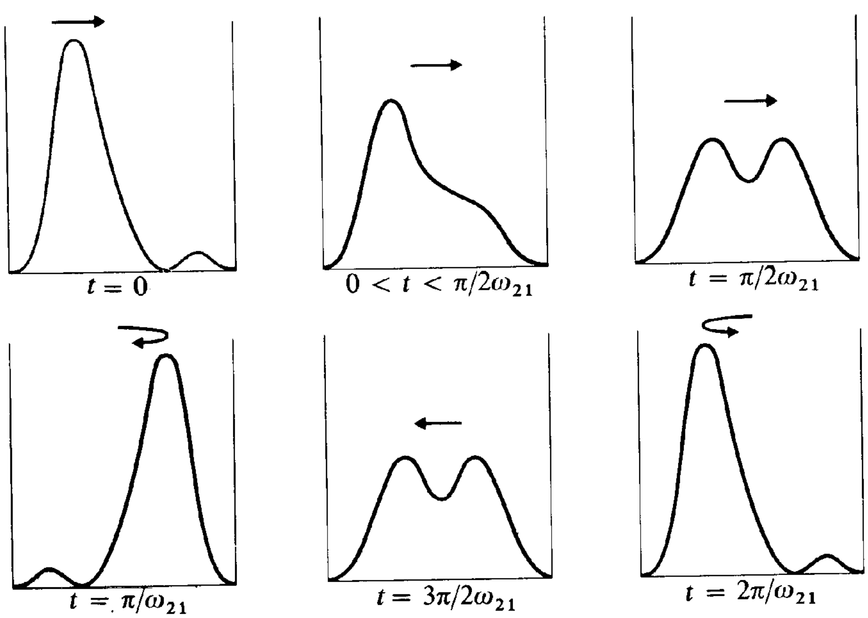

FIGURE 5

Periodic motion of a wave packet obtained by superposing the ground state and the first excited state of a particle in an infinite well. The frequency of the motion is the Bohr frequency $\omega_{21}/2\pi$.

c. MOTION OF THE CENTER OF THE WAVE PACKET

Let us calculate the mean value $\langle X \rangle(t)$ of the position of the particle at time t. It is convenient to take:

$$X' = X - a/2 \tag{19}$$

since, by symmetry, the diagonal matrix elements of X' are zero:

$$\langle \varphi_1 | X' | \varphi_1 \rangle \propto \int_0^a \left(x - \frac{a}{2}\right) \sin^2\left(\frac{\pi x}{a}\right) \mathrm{d}x = 0$$

$$\langle \varphi_2 | X' | \varphi_2 \rangle \propto \int_0^a \left(x - \frac{a}{2}\right) \sin^2\left(\frac{2\pi x}{a}\right) \mathrm{d}x = 0 \tag{20}$$

We then have:

$$\langle X' \rangle(t) = \mathrm{Re}\left\{ \mathrm{e}^{-i\omega_{21}t} \langle \varphi_1 | X' | \varphi_2 \rangle \right\} \tag{21}$$

with:

$$\begin{aligned} \langle \varphi_1 | X' | \varphi_2 \rangle &= \langle \varphi_1 | X | \varphi_2 \rangle - \frac{a}{2} \langle \varphi_1 | \varphi_2 \rangle \\ &= \frac{2}{a} \int_0^a x \sin\frac{\pi x}{a} \sin\frac{2\pi x}{a} \mathrm{d}x \\ &= -\frac{16a}{9\pi^2} \end{aligned} \tag{22}$$

Therefore:

$$\langle X \rangle(t) = \frac{a}{2} - \frac{16a}{9\pi^2} \cos \omega_{21} t \tag{23}$$

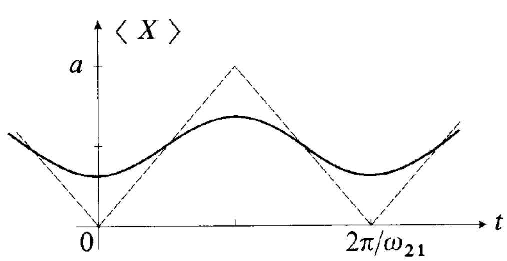

FIGURE 6

Time variation of the mean value $\langle X \rangle$ corresponding to the wave packet of figure 5. The dashed line represents the position of a classical particle moving with the same period. Quantum mechanics predicts that the center of the wave packet will turn back before reaching the wall, as explained by the action of the potential on the "edges" of the wave packet.

The variation of $\langle X \rangle(t)$ is represented in figure 6. In dashed lines, the variation of the position of a classical particle has been traced, for a particle moving to and fro in the well with an angular frequency of ω_{21} (since it is not subjected to any force except at the walls, its position varies linearly with t between 0 and a during each half-period).

We immediately notice a very clear difference between these two types of motion, classical and quantum mechanical. The center of the quantum wave packet, instead of turning back at the walls of the well, executes a movement of smaller amplitude and retraces its steps before reaching the regions where the potential is not zero. We see again here a result of §D-2 of chapter I: since the potential varies infinitely quickly at $x = 0$ and $x = a$, its variation within a domain of the order of the dimension of the wave packet is not negligible, and the motion of the center of the wave packet does not obey the laws of classical mechanics (see also chapter III, § D-1-d-γ). The physical explanation of this phenomenon is the following: before the center of the wave packet has touched the wall, the action of the potential on the "edges" of this packet is sufficient to make it turn back.

COMMENT:

The mean value of the energy of the particle in the state $|\psi(t)\rangle$ calculated in (15) is easy to obtain:

$$\langle H \rangle = \frac{1}{2}E_1 + \frac{1}{2}E_2 = \frac{5}{2}E_1 \tag{24}$$

as is:

$$\langle H^2 \rangle = \frac{1}{2}E_1^2 + \frac{1}{2}E_2^2 = \frac{17}{2}E_1^2 \tag{25}$$

which gives:

$$\Delta H = \frac{3}{2}E_1 \tag{26}$$

Note in particular that $\langle H \rangle$, $\langle H^2 \rangle$ and ΔH are not time-dependent; since H is a constant of the motion, this could have been foreseen. In addition, we see from the preceding discussion that the wave packet evolves appreciably over a time of the order of:

$$\Delta t \simeq \frac{1}{\omega_{21}} \tag{27}$$

Using (26) and (27), we find:

$$\Delta H \, . \, \Delta t \simeq \frac{3}{2}E_1 \times \frac{\hbar}{3E_1} = \frac{\hbar}{2} \tag{28}$$

We again find the time-energy uncertainty relation.

3. Perturbation created by a position measurement

Consider a particle in the state $|\varphi_1\rangle$. Assume that the position of the particle is measured at time $t = 0$, with the result $x = a/2$. What are the probabilities of the different results that can be obtained in a measurement of the energy, performed immediately after this first measurement?

One must beware of the following false argument: after the measurement, the particle is in the eigenstate of X corresponding to the result found, and its wave function is therefore proportional to $\delta(x - a/2)$; if a measurement of the energy is then performed, the various values E_n can be found, with probabilities proportional to:

$$\left| \int_0^a \mathrm{d}x\, \delta\left(x - \frac{a}{2}\right) \varphi_n^*(x) \right|^2 = \left| \varphi_n\left(\frac{a}{2}\right) \right|^2 = \begin{cases} 2/a & \text{if } n \text{ is odd} \\ 0 & \text{if } n \text{ is even} \end{cases} \tag{29}$$

Using this incorrect argument, one would find the probabilities of all values of E_n corresponding to odd n to be equal. This is absurd, since the sum of these probabilities would then be infinite.

This error results from the fact that we have not taken the norm of the wave function into account. To apply the fourth postulate of chapter III correctly, it is necessary to write the wave function as normalized just after the first measurement. However it is not possible to normalize the function $\delta(x - a/2)$*. The problem posed above must be stated more precisely.

As we saw in §E-2-b of chapter III, an experiment in which the measurement of an observable with a continuous spectrum is performed never yields any result with complete accuracy. For the case with which we are concerned, we can only say that:

$$\frac{a}{2} - \frac{\varepsilon}{2} \leqslant x \leqslant \frac{a}{2} + \frac{\varepsilon}{2} \tag{30}$$

where ε depends on the measurement device used but is never zero.

If we assume ε to be much smaller than the extension of the wave function before the measurement (here a), the wave function after the measurement will be practically $\sqrt{\varepsilon}\, \delta^{(\varepsilon)}\left(x - \frac{a}{2}\right)$ [$\delta^{(\varepsilon)}(x)$ is the null function everywhere except in the interval defined in (30), where it takes on the value $1/\varepsilon$; *cf.* appendix II, §1-a]. This wave function is indeed normalized since:

$$\int \mathrm{d}x \left| \sqrt{\varepsilon}\, \delta^{(\varepsilon)}\left(x - \frac{a}{2}\right) \right|^2 = 1 \tag{31}$$

* We see concretely in this example that a δ-function cannot represent a physically realizable state.

What happens now if the energy is measured? Each value E_n can be found with the probability:

$$\mathscr{P}(E_n) = \left| \int \varphi_n^*(x) \sqrt{\varepsilon}\, \delta^{(\varepsilon)}\left(x - \frac{a}{2}\right) \mathrm{d}x \right|^2$$

$$= \begin{cases} \dfrac{8a}{\varepsilon} \left(\dfrac{1}{n\pi}\right)^2 \sin^2 \left(\dfrac{n\pi\varepsilon}{2a}\right) & \text{if } n \text{ is odd} \\ 0 & \text{if } n \text{ is even} \end{cases} \tag{32}$$

The variation with respect to n of $\mathscr{P}(E_n)$, for fixed ε and odd n, is shown in figure 7. This figure shows that the probability $\mathscr{P}(E_n)$ becomes negligible when n is much larger than a/ε. Therefore, however small ε may be, the distribution of probabilities $\mathscr{P}(E_n)$ depends strongly on ε. This is why, in the first argument, where we set $\varepsilon = 0$ at the beginning, we could not obtain the correct result. We also see from the figure that the smaller ε is, the more the curve extends towards large values of n. The interpretation of this result is the following: according to Heisenberg's uncertainty relations (*cf.* chap. I, § C-3), if one measures the position of the particle with great accuracy, one drastically changes its momentum. Thus kinetic energy is transferred to the particle, the amount increasing as ε decreases.

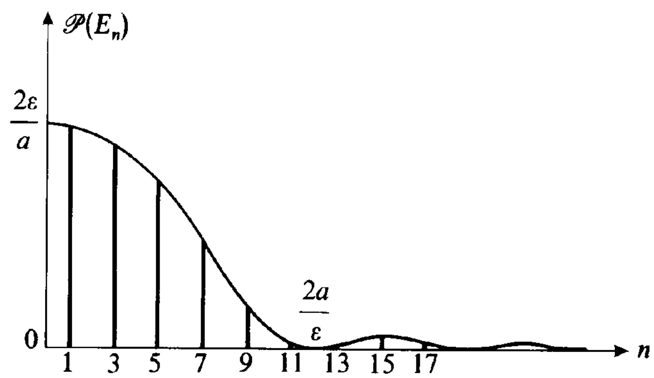

FIGURE 7

Variation with n of the probability $\mathscr{P}(E_n)$ of finding the energy E_n after a measurement of the particle's position has yielded the result $a/2$ with an accuracy of ε ($\varepsilon \ll a$). The smaller ε, the greater the probability of finding high energy values.