Digital Computer Laboratory
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SUBJECT: GROUP 63 SEMINAR ON MAGNETISM, XXIII

To: Group 63 Staff

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During the previous meeting we studied the problem of a particle in an infinite potential well. We arrived at the equations

$$\psi_n = 2\, iA_n \sin \sqrt{\frac{2m E_n}{\hbar^2}}\, x \qquad \text{XXII-3}$$

and

$$E_n = \frac{n^2 \pi^2 \hbar^2}{2ma^2} \qquad \text{XXII-5}$$

Therefore,

$$\psi_n = 2\, iA_n \sin \frac{n\pi x}{a}$$

and

$$\Psi = \sum C_n \sin \frac{n\pi x}{a}\, e^{-\frac{iE_n}{\hbar} t} \qquad \text{XXIII-1}$$

where the 2 iA_n is included in the C_n.

Since the momentum $p_n = \sqrt{2mE_n}$,

$$p_n = \frac{n\pi\hbar}{a} \qquad \text{XXIII-2}$$

The separation of momentum levels is therefore $\frac{\pi\hbar}{a}$, and may be thought of as the minimum uncertainty of the momentum (Δp). Furthermore, since the extent of our knowledge of the location of the particle is only that it is somewhere within the potential well, the positional uncertainty is a.

Therefore $a\Delta p = \pi\hbar \sim h$, in agreement with the uncertainty principle.

In general, the system described need not be in a stationary state. If it is not, we must find $\Psi(t)$ using the steps A to E listed in figure 43.

A. Knowledge at $t = o$

We will set our starting conditions such that when $t \leq o$, the particle is travelling on the wire with constant momentum $\underline{p}$. At time $t = o$ obstructions are clamped on the wire at $x = o$ and $x = a$, entrapping the particle within this region.

B. Find $\Psi(t = o)$

When $t \leq o$

$$-i\hbar \frac{\partial}{\partial x} \Psi_o = px$$

$$\Psi_o = K' e^{i\frac{p}{\hbar}x} \qquad \text{XXIII-3}$$

We are not interested in Ψ when $t < o$; when $t = o$ the above equation holds. Immediately afterward ($t > o$) this equation will no longer satisfy Schroedinger's equation subject to the new boundary conditions.

C. Solve $\mathcal{H}\psi_n = E_n \psi_n$

This equation was solved at the last meeting, and we obtained

$$\psi_n = 2iA_n \sin \frac{n\pi x}{a}$$

D. Find C_n

Since, in general, $C_n = \int \psi_n^* \Psi_o \, dt$, we have for this case

$$C_n = K_n \int_o^a \sin \frac{n\pi x}{a} \, e^{\frac{ip}{\hbar}x} \, dx \qquad \text{XXIII-4}$$

where $K_n = 2iA_n K'$

$$C_n = K_n \left[\frac{e^{\frac{ip}{\hbar}x}\left(\frac{ip}{\hbar} \sin \frac{n\pi x}{a} - \frac{n\pi}{a} \cos \frac{n\pi x}{a}\right)}{\left(\frac{n\pi}{a}\right)^2 - \frac{p^2}{\hbar^2}} \right]_o^a$$

$$C_n = \frac{K_n}{(\frac{n\pi}{a})^2 - \frac{p^2}{\hbar^2}} \left[e^{\frac{ipa}{\hbar}} (\frac{n\pi}{a}) (-1)^{n+1} + \frac{n\pi}{a} \right]$$

$$C_n = \frac{nK_n \frac{\pi}{a}}{(\frac{n\pi}{a})^2 - \frac{p^2}{\hbar^2}} \left[e^{\frac{ipa}{\hbar}} (-1)^{n+1} + 1 \right]$$

Let us set $p = \frac{(m + \delta)\, \pi\hbar}{a}$

where m = an integer
and $0 < \delta < 1$

Then $e^{\frac{ipa}{\hbar}} = e^{i(m+\delta)\pi} = (-1)^m e^{i\delta\pi}$

$$C_n = \frac{nK_n \frac{\pi}{a}}{(\frac{n\pi}{a})^2 - (\frac{(m+\delta)\pi}{a})^2} \left[e^{i\delta\pi} (-1)^{m+n+1} + 1 \right]$$

$$C_n = \frac{nK_n \frac{a}{\pi}}{n^2 - (m+\delta)^2} \left[e^{i\delta\pi} (-1)^{m+n+1} + 1 \right]$$

$$= \frac{nK_n \frac{a}{\pi}}{(n-m-\delta)\,(n+m+\delta)} \left[e^{i\delta\pi} (-1)^{m+n+1} + 1 \right] \qquad \text{XXIII-5}$$

For the special case $n = m$

$$C_m = \frac{mK_m \frac{a}{\pi}}{\delta\,(2m+\delta)} \left[e^{i\delta\pi} - 1 \right]$$

If we further let $\delta \to 0$

$$\lim_{\delta \to 0} C_m = \frac{mK_m \frac{a}{\pi}}{2m} \lim_{\delta \to 0} \frac{(e^{i\delta\pi} - 1)}{\delta} = \frac{K_m a}{2\pi} \lim_{\delta \to 0} (i\pi e^{i\delta\pi})$$

$$= \frac{i K_m a}{2} \qquad \text{XXIII-6}$$

E. **Find $\Psi(t)$**

$$\Psi = \sum_n c_n \psi_n e^{-\frac{iE_n t}{\hbar}}$$

$$\Psi = \frac{Ka}{\pi} \sum_n \frac{n}{(n-m-\delta)(n+m+\delta)} \left[e^{i\delta\pi} (-1)^{m+n+1} + 1 \right] \sin \frac{n\pi x}{a} \, e^{-i\left[\frac{n^2\pi^2\hbar}{2ma^2}\right]t} \qquad \text{XXIII-7}$$

Thus we see that the system is not in a stationary state. The system is described by various states with relative probabilities dependent upon the coefficients. The energy of the system is constantly changing, with energy given off in the form of heat or radiation. To consider the equilibrium set up between the system and the evolved radiation, we can no longer consider the particle on the wire as an isolated system. Interaction between matter and radiation will be discussed later.

F. **Find F**

As an example, let us determine the average value of momentum.

$$\bar{p} = \int_0^a \Psi^* \left(-i\hbar \frac{\partial}{\partial x}\right) \Psi \, dx$$

$$= \sum_n \sum_m f(n) f^*(m) \int_0^a \sin \frac{n\pi x}{a} \cos \frac{m\pi x}{a} \, dx$$

where $f(n)$ represents the entire coefficient of $\sin \frac{n\pi x}{a}$ in equation XXIII-7 and $f^*(m)$ represents the coefficient of $\cos \frac{m\pi x}{a}$.

$$\bar{p} = \sum_n \sum_m f(n) f(\overset{*}{m}) \left[\frac{\cos (m-n) \frac{\pi}{a} x}{2(m-n)\frac{\pi}{a}} - \frac{\cos (m+n) \frac{\pi}{a} x}{2(m+n)\frac{\pi}{a}} \right]_0^a$$

Considering the bracket term only

$$\left[\quad\right] = \frac{\cos (m-n)\pi}{2(m-n)\frac{\pi}{a}} - \frac{\cos (m+n)\pi}{2(m+n)\frac{\pi}{a}} - \frac{1}{2(m-n)\frac{\pi}{a}} + \frac{1}{2(m+n)\frac{\pi}{a}}$$

$$= 0 \qquad\qquad \text{for } m + n \text{ even}$$

$$\left.\begin{aligned} &= \frac{a}{(m+n)\pi} - \frac{a}{(m-n)\pi} \\ &= \frac{(m-n)a - (m+n)a}{(m^2-n^2)\pi} = -\frac{2na}{(m^2-n^2)\pi} \end{aligned}\right\} \qquad \text{for } m + n \text{ odd}$$

$$\bar{p} = \sum_{\substack{n \\ n \neq m \\ n + m \text{ odd}}} \sum_{m} - f(n)\, f(\overset{*}{m}) \frac{2na}{(m^2-n^2)\pi} \qquad \text{XXIII-8}$$

Potential Well with finite wall

We have considered a region of potential $V = 0$ bounded by infinite potential barriers at $x = 0$ and $x = a$. Let us now consider a modification of this system. We will maintain a region of zero potential from 0 to a, bounded by an infinite potential barrier at $x = 0$. However, the potential barrier at $x = a$ will be finite. As shown in figure 45, the potential is:

$$V = V_o \text{ for } x > a$$

$$V = V_o \text{ for } 0 < x < a$$

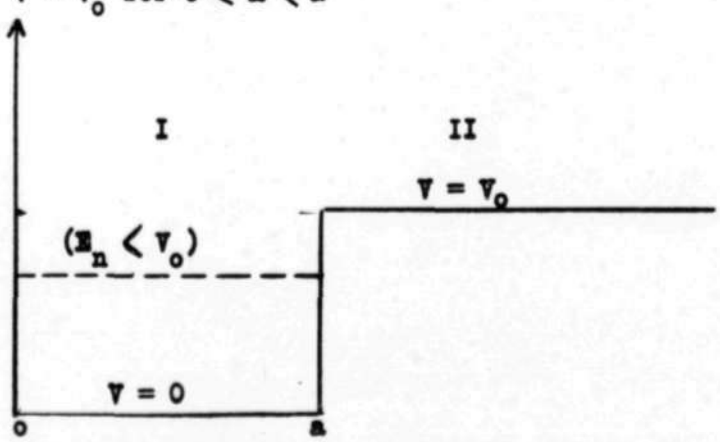

FIGURE 45

In this case there are two distinct regions of interest, as shown in figure 45. Region I extends from $X = 0$ to $X = a$; and Region II is that in which $X > a$.

In region I we can use the solution obtained in our previous meeting (equ XXII-3)

$$\psi_{nI} = C_I \sin \sqrt{\frac{2m E_n}{\hbar^2}}\, x \qquad \text{XXIII-9}$$

In region II:

$$H \psi_{nII} = E_n \psi_{nII}$$

$$\frac{d^2 \psi_{nII}}{dx^2} + \frac{2m}{\hbar^2} (E_n - V_o) \psi_{nII} = 0$$

$$\psi_{nII} = C_{II}\, e^{i\sqrt{\frac{2m (E_n - V_o)}{\hbar^2}}\, x} \qquad \text{XXIII-10}$$

There is no negative exponential term since the wave is being propagated in the positive x-direction, and ψ_{nII} must go to zero properly at infinity.

Since a properly behaved wave function is continuous,

$$\psi_{nI} (a) = \psi_{nII} (a).$$

Thus

$$C_I \sin\sqrt{\frac{2m E_n}{\hbar^2}}\, a = C_{II}\, e^{i\sqrt{\frac{2m (E_n-V_o)}{\hbar^2}}\, a}$$

$$C_I = C_{II} \frac{e^{i\sqrt{\frac{2m (E_n - V_o)}{\hbar^2}}\, a}}{\text{Sin} \sqrt{\frac{2m E_n}{\hbar^2}}\, a}$$

Thus:

$$\psi_{nI} = C_{II} \frac{e^{i\sqrt{\frac{2m(E_n - V_o)}{\hbar^2}}\, a}}{\sin\sqrt{\frac{2m E_n}{\hbar^2}}\, a} \sin\sqrt{\frac{2m E_n}{\hbar^2}}\, x$$

XXIII - 11

$$\psi_{nII} = C_{II}\, e^{i\sqrt{\frac{2m(E_n - V_o)}{\hbar^2}}\, x}$$

C_{II} is generally found by the normalization condition

$$\int_{\tau} \psi_{nII}^{*}\, \psi_{nII}\, d\tau = 1$$

For the case of unlimited space over which to integrate, the integral does not converge. This difficulty is usually avoided by limiting the region of interest to a large but finite region. In the problem we are considering, this situation would apply if $E_n > V_o$.

For the case $E_n > V_o$, ψ_{nII} is a cisoidal function as shown above. In this case the probability of finding the particle in region II will be constant throughout the region since $\psi_{nII}^{*}\, \psi_{nII}$ is then a constant.

However, if $E_n < V_o$, we find the probability of finding the particle in region II decays exponentially with increasing x. This is in sharp contrast with the result one would expect in classical physics, since classically the particle does not have enough energy to escape from region I.

The probability of finding the particle in region I varies as the square of a sin function. The relative probabilities in the two regions for $E_n < V_o$ and $E_n > V_o$ are shown in figure 46.

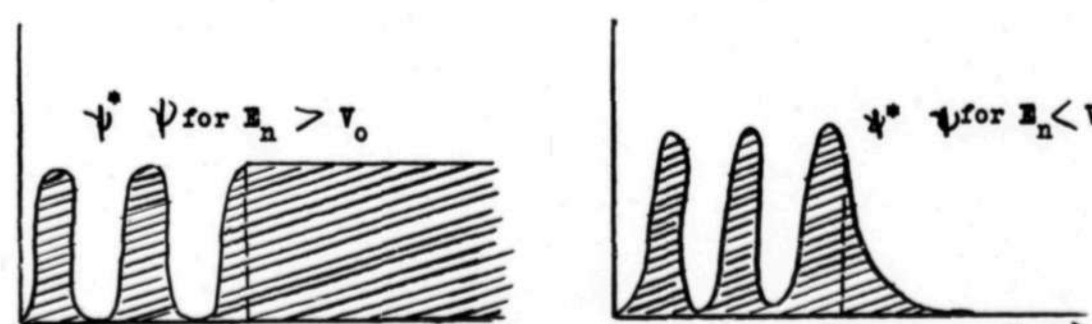

FIGURE 46

Under certain conditions Schroedinger's hypothesis leads to an additional property for the wave function, namely that it has a continuous derivative.

Schroedinger's time independent equation tells us that

$$\frac{d^2\psi}{dx^2} \propto -(E - V)\psi \qquad \text{XXIII-12}$$

Suppose that we consider the boundaries of regions I and II in figure 45 as separated by a narrow region as shown in figure 47.

FIGURE 47

We will then investigate the derivative of ψ at the boundaries of this narrow region. If the derivative is continuous, the derivatives at both boundaries of the narrow region will approach each other as the width of the region is reduced to zero.

From XXIII-12 we see that

$$\lim_{(x_{II} - x_I) \to 0} \left[\left(\frac{d\psi}{dx}\right)_{II} - \left(\frac{d\psi}{dx}\right)_I\right] \propto \lim_{(x_{II} - x_I) \to 0} \left[-(x_{II} - x_I)(E - V)\psi\right]$$

In the limit, as $(x_{II} - x_I) \to 0$, we see that the right hand side of the above equation goes to zero if $(E - V)$ and ψ are finite quantities. Since a well behaved wave function is always finite, the derivative of the function is always continuous across a finite potential barrier. However, it is not necessarily continuous across an infinite barrier, and we have seen that the derivative is not continuous across the boundary of an infinite potential well.

Physically, the derivative corresponds to the momentum, since

$$p = -i\hbar \frac{\partial}{\partial x}.$$

At an infinite boundary (rigid membrane), all particles are reflected elastically. At a finite potential boundary some particles escape while others are reflected with a decreased speed. The average momentum is continuous across the break.

Equation XXIII-12 shows that $\frac{d^2\psi}{dx^2}$ changes sign when $(E - V)$ changes sign. And, when $E > V$, the curve for ψ has a second derivative opposite in sign to ψ ; hence the curve is concave towards the axis. Similarly, for $E < V$, the curve is concave away from the axis.

If there is a finite break in V in such a way that $(E - V)$ changes sign across the break, then the second derivative must also change sign across the break. Because of continuity requirements, this is only possible if the second derivative is zero. Thus, at the point where $(E - V)$ changes sign, ψ has a point of inflection if the break is finite.

To point up some of these features, $\psi(x)$ is drawn for potential wells with varying values of $(E - V)$ in figure 48.

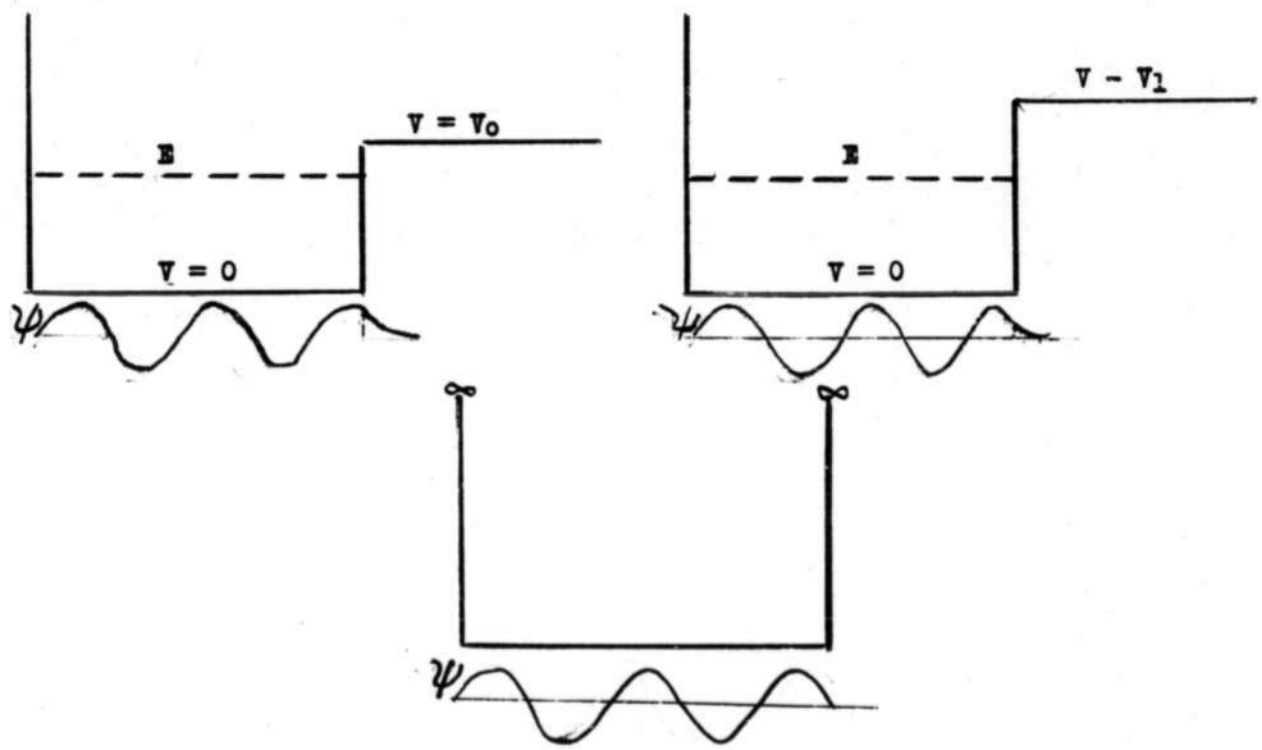

FIGURE 48

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