Outline

- First Middle Term Examination.
- Additional Comments

A. Natural unit
↓
will cover it again in 5 minuate

B. Degeracy
definition
one dimensional problem → no degenercy.

C. Spread of the wave function
will cover it again in 5 minuates
↓
related to path integral
Green's function, transformation function.

D. Hesinberg's equation of motion
↓
covered well
↓
will mention it only briefly
↓
two minuates

E. Wave function in momentum space.
↓
after the discussion of Fourier transform and the δ-function.

This section will be covered in the second middle term examination.

F. Sudden expansion.

G. Classical limit of harmonic oscillator

A. Natural Unit

Show that

in S.I. unit $\quad \frac{e^2}{4\pi\epsilon_0 \hbar c} \cong \frac{1}{137}$

in C.g.s unit $\quad \frac{e^2}{\hbar c} \simeq \frac{1}{137}$

$\hbar c = 197.33$ Mev fm

$m_e c^2 = 0.511$ Mev ~ 0.5 Mev

$M_p c^2 = 938$ Mev ~ 1 Gev

In Bohr model

$$r = \frac{n^2 \hbar^2}{e^2 m_e}$$

we can put in the number $\longrightarrow$ get the answer.

In the atomic unit $\quad \hbar = c = m_e = 1$

(actually, we use $\hbar, c, m_e$ as units)

$$r = \frac{n^2}{e^2} = 137 n^2 \quad \text{in atomic unit}$$

The r is a length

In atomic unit, the length unit is

$$\frac{\hbar}{m_e c} = \frac{\hbar c}{m_e c^2} = \frac{197.33 \text{ Mev fm}}{0.511 \text{ Mev}}$$

$$= \frac{197.33}{0.511} \text{ fm}$$

$$\Rightarrow \quad r = 137 n^2 \cdot \frac{197.33}{0.511} \text{ fm}$$

↓

easily calculated.

Examination question

$\lambda \sim a$ $\qquad a = 0.2\,fm$

↕

length unit of the natural unit with

$\hbar = c = M_p = 1$

$$\lambda = \frac{h}{p} = \frac{2\pi\hbar}{p}$$

$$1 = \frac{2\pi}{p}$$

$p = 2\pi$ $\qquad \boxed{E^2 = p^2 + m^2}$ $\qquad m = \frac{.511}{938}$

↓

in natural unit $\qquad E \sim 2\pi\,GeV$

p unit $\quad M_p c = 938\ MeV/c$

A. Natural Unit

In weak interaction, we sometime encounter the following type of equation.

$$\sigma = \frac{4G^2}{\pi} p^2$$

G → weak coupling constant

p → momentum

σ → cross section

Want to find the cross section at $p = 5\ GeV/c$

In high energy, we usually use the natural unit $\hbar = c = M_p = 1$

In this unit $G = 10^{-5} \left(\frac{1}{M_p^2}\right) = 10^{-5}$

$$\sigma = \frac{4}{\pi}(10^{-5})^2 p^2$$

p^2 → 5^2

$$= \frac{4}{\pi} 10^{-10} \cdot 25 = \frac{10^{-8}}{\pi}$$

↓ in this unit

σ has dimension of $(\text{length})^2$

In that unit, dimension of length is

$$\frac{\hbar c}{M_p c^2} = \frac{197.33\ Mev\ fm}{938\ Mev}$$

$$= 0.21\ fm$$

$$\Rightarrow \quad \sigma = \frac{10^{-8}}{\pi} \cdot (0.21\ fm)^2$$

$$= \frac{(0.21)^2}{\pi} \cdot 10^{-8} \cdot (10^{-15} m)^2$$

$$= 0.014 \cdot 10^{-38}\ m^2$$

$$= 0.014 \cdot 10^{-38} \cdot 10^4\ cm^2$$

$$= 0.014 \cdot 10^{-34}\ cm^2 = 14 \cdot 10^{-37}\ cm^2$$

cross sections are usually express in barns

$$1\ barn = 10^{-24}\ cm^2$$

B. Degeneracy

Show that, in one-dimensional problems, the energy spectrum of the bound states is always non-degenerate.

For the sake of argument let us suppose that the opposite is true. Let $\psi_1(x)$ and $\psi_2(x)$ then be two linearly independent eigenfunctions with the same energy eigenvalue E. From the equations

$$\psi_1'' + \frac{2m}{\hbar^2}(E-V)\psi_1 = 0, \quad \psi_2'' + \frac{2m}{\hbar^2}(E-V)\psi_2 = 0,$$

we obtain

$$\frac{\psi_1''}{\psi_1} = \frac{\psi_2''}{\psi_2} = \frac{2m}{\hbar^2}(V-E),$$

i.e.

$$\psi_1''\psi_2 - \psi_2''\psi_1 = (\psi_1'\psi_2)' - (\psi_2'\psi_1)' = 0.$$

After integrating this equation we find that

$$\psi_1'\psi_2 - \psi_2'\psi_1 = \text{a constant}.$$

Since, at infinity, $\psi_1 = \psi_2 = 0$ (bound states), we must have the constant $= 0$ and hence

$$\frac{\psi_1'}{\psi_1} = \frac{\psi_2'}{\psi_2}.$$

Integrating once more we have $\ln \psi_1 = \ln \psi_2 + \ln c$, i.e. $\psi_1 = c\psi_2$, which contradicts the assumed linear independence of the two functions.

C.4 Spread of the Wave Function

Assume that, at time $t = 0$, the wavefunction $\psi(x, t)$ of a particle is of the form (cf. problem 16, Chapter III):

$$\psi(x, 0) = \frac{1}{(2\pi\delta^2)^{1/4}} \exp\left(-\frac{x^2}{4\delta^2}\right), \quad \delta^2 = (\Delta x)^2.$$

Investigate the change in time of this wave-packet if, for $t > 0$, no forces act on the particle.

It is necessary to determine the wavefunction $\psi(x, t)$ which satisfies the Schrödinger equation

$$i\hbar \frac{\partial \psi(x, t)}{\partial t} = H\psi(x, t),$$

and which, at time $t = 0$, is the given function $\psi(x, 0)$. With that end in view we expand $\psi(x, 0)$ in terms of the set of orthonormal time-independent eigenfunctions $\psi_n(x)$, $(H\psi_n(x) = E_n\psi_n(x))$ (see p. 204, footnote), thus:

$$\psi(x, 0) = \sum_n a_n \psi_n(x), \qquad a_n = \int \psi_n^*(x)\, \psi(x, 0)\, dx.$$

The function $\sum_n a_n \psi_n(x) \exp\left(-\frac{i}{\hbar} E_n t\right)$ then satisfies the Schrödinger equation, and, at time $t = 0$, coincides with $\psi(x, 0)$. Hence

$$\psi(x, t) = \sum_n a_n \psi_n(x) e^{-\frac{i}{\hbar} E_n t},$$

i.e.

$$\psi(x, t) = \int G(\xi, x, t)\psi(\xi, 0)\, d\xi$$

where

$$G(\xi, x, t) = \sum_n \psi_n^*(\xi)\, \psi_n(x)\, e^{-\frac{i}{\hbar} E_n t}$$ (Green's function)

Since, in the case of free motion, the eigenfunctions are

$$\psi_p(x) = \frac{1}{(2\pi\hbar)^{1/2}} \exp\left(\frac{i}{\hbar} p x\right);$$

the Green's function (8.4) becomes (with p continuous)

$$G(\xi, x, t) = \int \frac{1}{2\pi\hbar} \exp\left\{\frac{i}{\hbar}\left[p(x-\xi) - \frac{p^2 t}{2m}\right]\right\} dp$$
$$= \left(\frac{m}{2\pi i\hbar t}\right)^{1/2} e^{\frac{im}{2\hbar t}(x-\xi)^2}.$$

From (8.3) and (8a) it follows that

$$\psi(x, t) = \int \left(\frac{m}{2\pi i\hbar t}\right)^{1/2} \frac{1}{(2\pi\delta^2)^{1/4}} \exp\left\{-\frac{\xi^2}{4\delta^2} + \frac{im}{2\hbar t}(x-\xi)^2\right\} d\xi,$$

whence we obtain finally, for the wave function,

$$\psi(x, t) = \frac{1}{(2\pi\delta^2)^{1/4}\left(1+\frac{\hbar^2 t^2}{4m^2\delta^4}\right)^{1/4}} \exp\left\{-\frac{x^2}{4\delta^2\left(1+\frac{\hbar^2 t^2}{4m^2\delta^4}\right)}\left(1-\frac{i\hbar t}{2m\delta^2}\right)\right\},$$

and for the probability density

$$|\psi(x, t)|^2 = \left[2\pi\delta^2\left(1+\frac{\hbar^2 t^2}{4m^2\delta^4}\right)\right]^{-1/2} \exp\left\{-\frac{x^2}{2\delta^2\left(1+\frac{\hbar^2 t^2}{4m^2\delta^4}\right)}\right\}.$$

This expression has the same form as the initial probability density

$$|\psi(x, 0)|^2 = \frac{1}{(2\pi\delta^2)^{1/2}} \exp\left\{-\frac{x^2}{2\delta^2}\right\},$$

D. 6. Commutator, Heisenberg's Equation of Motion.

$$\langle Q \rangle_t = \int \psi^*(x,t)\, \hat{Q}\, \psi(x,t)\, dx$$

$$\hat{H}\psi = i\hbar \frac{\partial}{\partial t}\psi \qquad \text{Schrodinger equation}$$

$$\frac{d\langle Q\rangle_t}{dt} = \int \frac{\partial \psi^*}{\partial t}\hat{Q}\,\psi\, dx + \int \psi^* \hat{Q}\frac{\partial \psi}{\partial t} dx + \int \psi^* \frac{\partial \hat{Q}}{\partial t}\psi\, dx$$

$$H\psi = i\hbar \frac{\partial}{\partial t}\psi \Rightarrow \frac{\partial \psi}{\partial t} = \frac{1}{i\hbar}\hat{H}\psi$$

$$(H\psi)^* = -i\hbar \frac{\partial \psi^*}{\partial t} \Rightarrow \frac{\partial \psi^*}{\partial t} = \frac{1}{-i\hbar}(H\psi)^*$$

$$\frac{d\langle \hat{Q}\rangle}{dt} = \int \frac{\partial \psi^*}{\partial t}\hat{Q}\,\psi\, dx + \int \psi^* \hat{Q}\frac{\partial \psi}{\partial t} dx + \int \psi^* \frac{\partial \hat{Q}}{\partial t}\psi\, dx$$

$$= \frac{1}{-i\hbar}\int (\hat{H}\psi)^* \hat{Q}\psi\, dx + \frac{1}{i\hbar}\int \psi^* \hat{Q}\hat{H}\psi\, dx + \int \psi^* \frac{\partial Q}{\partial t}\psi\, dx$$

Look at

$$\int (\hat{H}\psi)^* \hat{Q}\psi\, dx$$

Definition of Hermitian adjoint $\hat{A}^+$

$$\int (\hat{A}\psi_2)^* \psi_1\, dx = \int \psi_2^* \hat{A}^+ \psi_1\, dx$$

$\hat{H} \leftrightarrow A \qquad \psi_2 \to \psi$

$(\hat{Q}\psi) \to \psi_1$

$$\int (\hat{H}\psi)^* \hat{Q}\psi\, dx = \int \psi^* \hat{H}^+ \hat{Q}\psi\, dx$$

$\hat{H} \to$ Hamiltonian operator

Energy operator $\longleftrightarrow$ physical observerable

$\downarrow$

$\hat{H}$ is Hermitian, i.e., $\hat{H} = \hat{H}^+$

$$\int (H\psi)^* \hat{Q}\psi\, dx = \int \psi^* H Q \psi\, dx$$

Put it all together

$$\frac{d\langle \hat{Q}\rangle}{dt} = \frac{1}{i\hbar}\int \psi^*(\hat{Q}\hat{H} - \hat{H}\hat{Q})\psi \, dx + \left\langle \frac{\partial \hat{Q}}{\partial t}\right\rangle$$

$$= \frac{1}{i\hbar}\int \psi^* [\hat{Q}, \hat{H}]\psi \, dx + \left\langle \frac{\partial \hat{Q}}{\partial t}\right\rangle$$

$$\frac{d\langle \hat{Q}\rangle}{dt} = \frac{i}{\hbar}\langle [\hat{H}, \hat{Q}]\rangle + \left\langle \frac{\partial \hat{Q}}{\partial t}\right\rangle$$

This is one of the most useful equation in quantum mechanics

(1) Example: $\hat{H} = \frac{\hat{p}^2}{2m} + \hat{V}(x)$, $\hat{Q} \to \hat{x}$ does not explicitly depend on t

$$[\hat{H}, x] = [\frac{\hat{p}^2}{2m} + \hat{V}(x), \hat{x}]$$

$[\hat{V}(x), \hat{x}] = 0$; commutes

$$= [\frac{\hat{p}^2}{2m}, \hat{x}]$$

↓

examination problem

$$\Rightarrow \frac{d\langle \hat{x}\rangle}{dt} = \frac{\langle \hat{p}\rangle}{m}.$$

Now identify $\hat{Q} \to \hat{p}$

$$[\frac{\hat{p}^2}{2m} + V(x), \hat{p}]$$

$$= [\frac{\hat{p}^2}{2m}, \hat{p}] + [V(x), \hat{p}]$$

$[\frac{\hat{p}^2}{2m}, \hat{p}]$ ↓ 0 ; $[V(x), \hat{p}]$ ↓ examination problem

$$\Rightarrow \quad \frac{d\langle p\rangle}{dt} = -\left\langle \frac{\partial V}{\partial x} \right\rangle$$

(ii) If $[\hat{H}, \hat{Q}] = 0$ and $\frac{\partial \langle \hat{Q} \rangle}{\partial t} = 0$

then $\frac{d}{dt} \langle Q \rangle_t = 0$

$\langle Q \rangle_t$ is independent of time, i.e., it is constant of motion, it is conserved.

Example. For a central force problem

$\hat{V}(r)$, it can be shown that

↓ independent of θ, ϕ.

$[\hat{H}, \hat{\vec{L}}] = 0$

↳ angular momentum operator

then $\frac{d\langle \hat{\vec{L}} \rangle}{dt} = 0$

$\langle \hat{\vec{L}} \rangle$ is conserved.

Next topics

Angular momentum

Spherical coordinate

Angular momentum operator in spherical coordinates

Hydrogen atom.

E. Wave Function in Momentum Space

Normalization of wavefunctions in free space

The momentum eigenstates in the position representation, $u_p(x)$ defined by

$$\hat{p}u_p(x) = \frac{\hbar}{i}\frac{\partial}{\partial x}u_p(x) = pu_p(x), \tag{14-1}$$

and given by

$$u_p(x) = \frac{1}{\sqrt{2\pi\hbar}}e^{ipx/\hbar} \tag{14-2}$$

cannot be normalized in free space to be interpreted as a probability density since $|u_p(x)|^2 = \frac{1}{2\pi\hbar}$, and $\int_{-\infty}^{\infty} dx|u_p(x)|^2$ diverges. However, they do satisfy the **continuum orthonormality condition**

$$\boxed{\int_{-\infty}^{\infty} dx u_p{}^*(x)u_{p'}(x) = \delta(p-p')}. \tag{14-3}$$

This normalization corresponds to a uniform particle density (particle per meter) given by $|u_p(x)|^2 = \frac{1}{2\pi\hbar}$. Let us calculate the **probability current** (particles moving past a point x per second), defined by

$$\boxed{j(x) = \frac{\hbar}{2im}\left[\psi^*(x)\frac{\partial\psi}{\partial x}(x) - \left(\frac{\partial\psi^*}{\partial x}(x)\right)\psi(x)\right]} \rightarrow \text{see PS} \tag{14-4}$$

For $\psi(x) = u_p(x)$ we find

$$j(x) = \frac{\hbar}{2im}\frac{1}{2\pi\hbar}\left[\frac{ip}{\hbar} - \left(-\frac{ip}{\hbar}\right)\right] \tag{14-5}$$

$$= \frac{1}{2\pi\hbar}\frac{p}{m}, \tag{14-6}$$

which is exactly what we expect for a uniform particle density $|u_p(x)|^2 = \frac{1}{2\pi\hbar}$ moving at velocity $v = \frac{p}{m}$.

In general, choosing a wavefunction $\psi(x) = Ce^{ipx}$ corresponds to particles moving at velocity $\frac{p}{m}$, a particle density $|psi(x)|^2 = |C|^2$, and a particle current $j(x) = |C|^2\frac{p}{m}$. Alternatives to deal with the normalization problem (wavefunction not square-integrable) for momentum states are:

1. Wavepackets
   A superposition of a finite number of momentum eigenstates is not normalizable, but a wavepacket consisting of an infinite number of momentum eigenstates (Fourier components) is.

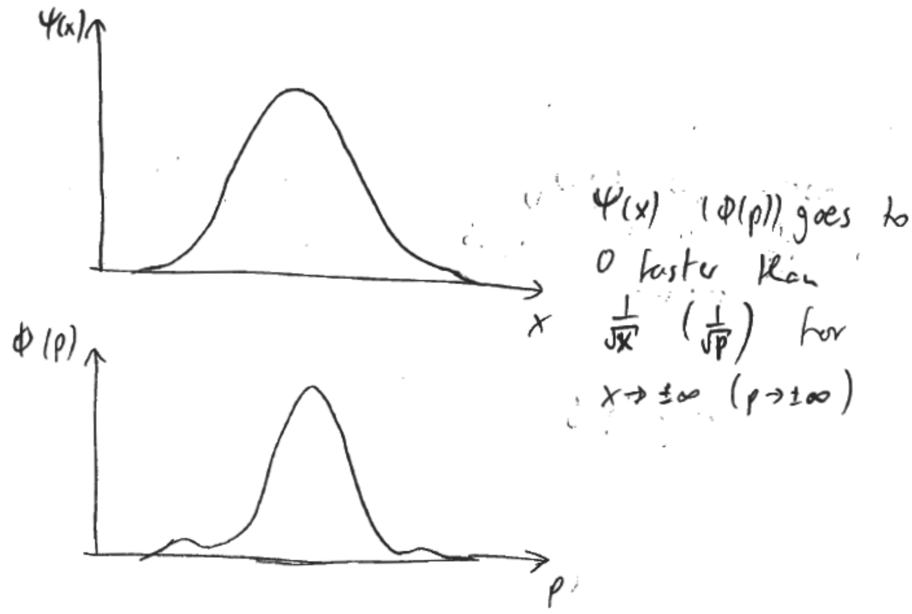

Figure I: A wavepacket $\psi(x)$ in position space or $\phi(k)$ in momentum space whose wavefunction for large x (or k) falls off faster than $x^{-1/2}$ ($k^{-1/2}$) can be directly normalized.

2. Periodic boundary conditions
   Assume box of finite length L, require periodic boundary conditions

$$\psi(0) = \psi(L) \tag{14-7}$$

For plane waves $e^{ipx/\hbar}$ this implies that $e^{ipL/\hbar} = 1$ or $\frac{pL}{\hbar} = kL = n2\pi$, n integer, i.e. momentum is quantized, $p_n = n\hbar k_o$ with $k_0 = \frac{2\pi}{L}$. The corresponding momentum states are normalizable in the interval $[0, L]$,

$$\int_0^L dx|Ce^{ipx/\hbar}|^2 = L|C|^2 = 1 \tag{14-8}$$

$$\boxed{u_{p_n}(x) = \frac{1}{\sqrt{L}}e^{ip_nx/\hbar}} \tag{14-9}$$

→ **normalized momentum eigenstates** in box of size L with $p_n = n\hbar k_o$

$$\int_0^L dx u_{p_n}{}^*(x)u_{p_m}(x) = \delta_{nm} \quad \rightarrow \quad \text{orthonormality condition in box} \tag{14-10}$$

We perform all calculations for fixed size box, then take the limit $L \to \infty$ (i.e. $k_0 \to 0$, momentum spectrum becomes continuous). All physically sensible

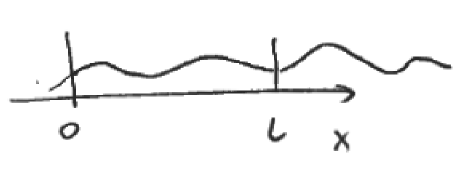

Figure II: Wavefunction in box of length L with periodic boundary conditions.

results will be independent of the initially chosen box size L as long as L is large compared to distances of interest.

Time evolution of free-particle wavepackets

In free space we often work with **normalized Gaussian wavepackets**

$$\Psi(x, t = 0) = \frac{1}{(2\pi)^{1/4} {w_0}^{1/2}} e^{-\frac{x^2}{4{w_0}^2}} \tag{14-11}$$

Written in this form we have

- $|\Psi(x, 0)|^2 = \frac{1}{(2\pi)^{1/2} w_0} e^{-\frac{x^2}{2{w_0}^2}}$
- $\int dx |\Psi(x, 0)|^2 = 1$
- $\langle x \rangle = 0$
- $\langle x^2 \rangle = {w_0}^2$
- $(\delta x)^2 = \langle x^2 \rangle - \langle x \rangle^2 = {w_0}^2$

$\Delta x = w_0$ is the uncertainty or rms width (root-mean-square width) of the wavepacket. Why do we prefer this Gaussian form of wavepacket?

1. Particularly simple and symmetric, the **Fourier transform is also a Gaussian** wavepacket:

   $$\phi(k) = \frac{1}{(2\pi)^{1/4} {k_0}^{1/2}} e^{-\frac{k^2}{4{k_0}^2}} \tag{14-12}$$

   with $k_0 = \frac{1}{2w_0}$. $(\Delta k)^2 = \langle k^2 \rangle - \langle k \rangle = {k_0}^2$

2. This is a wavepacket with the **minimum uncertainty** $\Delta x \Delta k = \frac{1}{2}$ $(\Delta x \Delta p = \frac{\hbar}{2})$ allowed by **QM**

3. Physical system after give rise to Gaussian broadening in momentum or position, e.g., thermal distribution of atomic momenta in a gas is a Gaussian distribution.

How do we make a wavepacket move at velocity v_1?

We displace the distribution in momentum space from $\langle p\rangle = \langle \hbar k\rangle = 0$ to $\langle p\rangle = \langle \hbar k\rangle = \hbar k_1 = mv_1$ (see Fig. III).

$$\phi(k) = \frac{1}{(2\pi)^{1/4}{k_0}^{1/2}} e^{-\frac{(k-k_1)^2}{4{k_0}^2}}. \tag{14-13}$$

The inverse Fourier transform, i.e., the spatial wavefunction

$$\Psi(x, t = 0) = \frac{1}{(2\pi)^{1/4}{w_0}^{1/2}} e^{-\frac{x^2}{4{w_o}^2}} e^{ik_1 x} \tag{14-14}$$

is still a Gaussian, but now with a phase variation e^{ik_1x}, rather than a constant phase over the wavepacket (compare Eq. (14-11). This phase variation e^{ik_1x} in position

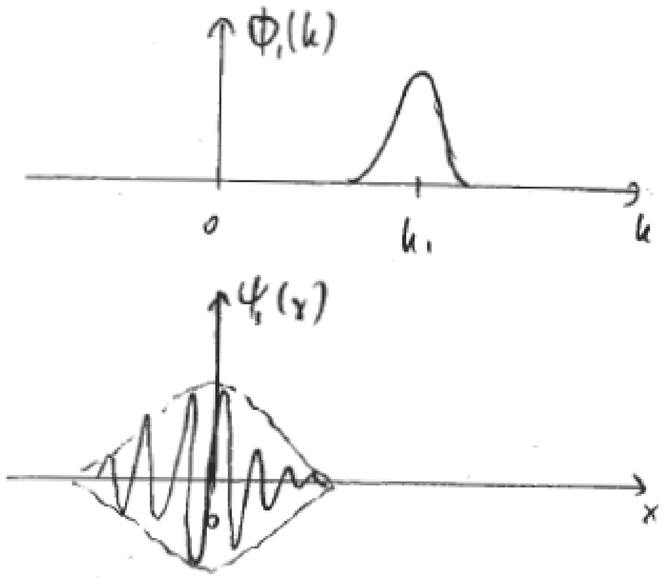

Figure III: Moving Gaussian wavepacket with average velocity $v_1 = \hbar k_1/m$ and spatial wavefunction $\psi_1(x) = \frac{1}{(2\pi)^{1/4}w_0^{1/2}} e^{-\frac{x^2}{4w_0^2}e^{ik_1x}}$.

space "encodes" the motion of the wavepacket at velocity $v_1 = \frac{\hbar k_1}{m}$: The dominant de Broglie wavelength in the wavepacket corresponds to a wavevector k_1, or a momentum $\hbar k_1$.

How does a free-space Gaussian wave packet evolve in time?

In general, we expand a wavefunction $\Psi(x,0)$ into energy eigenfunctions $u_E(x)$, and then evolve the energy eigenfunctions as $e^{-iEt/\hbar}$.

In free space, there is only KE. Then the momentum eigenstates $u_p(x)$ are **simultaneous eigenstates of energy**:

$$\hat{H}u_p(x) = \frac{\hat{p}^2}{2m}u_p(x) \tag{14-15}$$

$$= \frac{1}{2m}\left(\hbar i\frac{\partial}{\partial x}\right)^2 \frac{1}{\sqrt{2\pi\hbar}}e^{ipx/\hbar} \tag{14-16}$$

$$= \frac{p^2}{2m}u_p(x) \tag{14-17}$$

or

$$\hat{H}u_p(x) = \frac{p^2}{2m}u_p(x) \tag{14-18}$$

$$= E_p u_p(x) \tag{14-19}$$

in free space. The energy eigenstates are said to be **doubly degenerate**: For each eigenvalue of energy $E > 0$ there are two different momentum states (namely $u_{\pm p}(x)$ with $p = \sqrt{2m\hbar}$) that have the same energy. It follows that a momentum eigenstate with eigenvalue p evolves in time as $e^{-iE_pt/\hbar}$, so that the wavefunction in momentum space evolves in time as

$$\Phi(p,t) = \Phi(p,0)e^{-i\frac{p^2}{2m}t/\hbar} \tag{14-20}$$

$\rightarrow$ **time evolution of momentum eigenfunctions in free space**. The wavefunction in real space is given by the inverse Fourier transform $\Psi(x,t)$, or equivalently, as the superposition of energy eigenfunctions with their corresponding phase evolution factors $e^{-iE_pt/\hbar}$:

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}}\int dp\Phi(p,t)e^{ipx/\hbar} \tag{14-21}$$

$$\left(= \int dp\Phi(p,t)u_p(x)\right) \tag{14-22}$$

$$= \frac{1}{\sqrt{2\pi\hbar}}\int dp\Phi(p,0)e^{ipx/\hbar}e^{-\frac{p^2}{2m}t/\hbar} \tag{14-23}$$

$$= \int dp\Phi(p,0)U_p(x,t) \tag{14-24}$$

$$= \int dp\Phi(p,t)u_p(x) \tag{14-25}$$

where $U_p(x,t) = u_p(x)e^{-\frac{p^2}{2m}t/\hbar} = \frac{1}{\sqrt{2\pi\hbar}}e^{ipx/\hbar}e^{-i\frac{p^2}{2m}t/\hbar}$ are the time-dependent momentum eigenfunctions in free space. The above equation shows that the phases of different Fourier components $u_p(x) = \frac{1}{\sqrt{2\pi\hbar}}e^{ipx/\hbar}$ evolve in time at different speeds, the "running out of phase" of different Fourier components leads to a spreading of the wavepacket in position space. In the problem sets you will show that the rms width $\Delta x(t) = w(t)$ of the wavepacket grows in time as

$$w(t) = w_0\sqrt{1 + \frac{\hbar^2 k^2}{m^2 {w_0}^2}} \tag{14-26}$$

Since a wavepacket contains different momentum components, it changes in time in free space even though there are non external forces acting. For long times $t \gg t_0 = \frac{m{w_o}^2}{\hbar}$ the wavepacket spreads as $w(t) \approx \frac{\hbar}{mw_0}t$, i.e. at a speed $v_0 = \frac{\hbar}{mw_0}$ that is inversely proportional to its initial size. That speed is negligible for macroscopic wavepacket size, but can be appreciable for initially well-localized microscopic objects. The spreading of a wavepacket in free space was early evidence that the wavepacket size cannot be identified with the particle size. The spreading is due to the quadratic (i.e. not linear) dependence of the energy, and hence the phase evolution rate, on momentum. Note that the wavepacket of a massless particle, e.g. a photon, with $E = pc$ would not spread. (The SE is non-relativistic and does not apply to photons.)

Motion of wave packets, group velocity, and stationary phase

Why is it that a wavefunction

$$\Psi(x,0) = \frac{1}{(2\pi)^{1/4}{w_0}^{1/2}}e^{-\frac{x^2}{4{w_0}^2}}e^{ik_1x} \tag{14-27}$$

represents a particle moving at velocity $v_1 = \frac{\hbar k_1}{m}$? Since a crest of a single momentum component $u_{k_1}(x,t) = \frac{1}{\sqrt{2\pi}}e^{-k_1x}e^{-i\frac{\hbar k^2}{2m}t}$ moves forward a distance $\lambda = \frac{2\pi}{k_1}$ in a time $T = \frac{2\pi}{\omega_1}$ (remember that $\omega_1 = \frac{\hbar {k_1}^2}{2m}$ and $e^{-iE_1t/\hbar} = e^{-i\omega_1 t}$), the velocity of the crest is $v_{\rm ph} = \frac{\lambda}{T} = \frac{2\pi}{k_1}\frac{\omega}{2\pi} = \frac{\omega_1}{k_1} = \frac{\hbar k_1}{2m}$

$$\boxed{v_{\rm ph} = \frac{\omega_1}{k_1} = \frac{\hbar k_1}{2m} = \frac{p_1}{2m}} \tag{14-28}$$

This is the **phase velocity of a momentum component**.

The particle does **not** move at the phase velocity $v_{\rm ph} = \frac{\omega_1}{k_1}$ at which the plane wave associated with a single momentum moves forward. At what velocity then?

- Look at exponent and write:
  $E_1 = E_1(k_1) = \hbar\omega_1 = \hbar\omega(k_1) = \frac{\hbar {k_1}^2}{2m}$
- $e^{\left(-\frac{x^2}{4{w_0}^2}+ik_1x-i\omega(k_1)t\right)}$

Remember Fermat's principle of stationary phase: path is defined by region of space where phasors point mostly in one direction, i.e. where the phase $\phi(k) = -\frac{x^2}{4{w_o}^2} + ikx + i\omega(k_1)t$ does not vary between different momentum components k to lowest order

$$0 = \frac{\partial\phi}{\partial k} = ix - i\left(\frac{\partial\omega}{\partial k}\right)t = i\left(x - \left(\frac{\partial\omega}{\partial x}t\right)\right), \tag{14-29}$$

or

$$x(t) = \left(\frac{\partial\omega}{\partial k}\right)t. \tag{14-30}$$

Fermat's principle leads us to the concept of group velocity

$$\boxed{v_{\text{gr}} = \frac{\partial\omega}{\partial k}(k_1) = \frac{\hbar k_1}{m} = \frac{p_1}{m}} \tag{14-31}$$

Group velocity of the wavepacket at which the wavepacket, i.e. the region of constructive interference, propagates. The difference between group and phase velocity is due to the fact the $\frac{\partial\omega}{\partial k} \neq \frac{\omega}{k}$, or $\frac{\partial E}{\partial p} = \frac{\partial(\hbar\omega)}{\partial(\hbar k)} \neq \frac{E}{p}$, i.e. the quadratic dependence of KE on momentum in free space. This is in contrast to photons with a linear dispersion relation $\frac{\partial\omega}{\partial k} = \frac{\omega}{k} = c$ in vacuum, where group and phase velocity are the same.

Supplement 2-A

The Fourier Integral and Delta Functions

Consider a function $f(x)$ that is periodic, with period $2L$, so that

$$f(x) = f(x + 2L) \tag{2A-1}$$

Such a function can be expanded in a Fourier series in the interval $(-L, L)$, and the series has the form

$$f(x) = \sum_{n=0}^{\infty} A_n \cos\frac{n\pi x}{L} + \sum_{n=1}^{\infty} B_n \sin\frac{n\pi x}{L} \tag{2A-2}$$

We can rewrite the series in the form

$$f(x) = \sum_{n=-\infty}^{\infty} a_n e^{in\pi x/L} \tag{2A-3}$$

which is certainly possible, since

$$\cos\frac{n\pi x}{L} = \frac{1}{2}\left(e^{in\pi x/L} + e^{-in\pi x/L}\right)$$

$$\sin\frac{n\pi x}{L} = \frac{1}{2i}\left(e^{in\pi x/L} - e^{-in\pi x/L}\right)$$

The coefficients can be determined with the help of the orthonormality relation

$$\frac{1}{2L}\int_{-L}^{L} dx\, e^{in\pi x/L} e^{-im\pi x/L} = \delta_{mn} = \begin{cases} 1 & m = n \\ 0 & m \neq n \end{cases} \tag{2A-4}$$

Thus

$$a_n = \frac{1}{2L}\int_{-L}^{L} dx\, f(x) e^{-in\pi x/L} \tag{2A-5}$$

Let us now rewrite (2A-3) by introducing Δn, the difference between two successive integers. Since this is unity, we have

$$\begin{aligned} f(x) &= \sum_n a_n e^{in\pi x/L}\, \Delta n \\ &= \frac{L}{\pi}\sum_n a_n e^{in\pi x/L} \frac{\pi\, \Delta n}{L} \end{aligned} \tag{2A-6}$$

Let us change the notation by writing

$$\frac{\pi n}{L} = k \tag{2A-7}$$

and

$$\frac{\pi \Delta n}{L} = \Delta k \tag{2A-8}$$

We also write

$$\frac{La_n}{\pi} = \frac{A(k)}{\sqrt{2\pi}} \tag{2A-9}$$

Hence (2A-6) becomes

$$f(x) = \sum \frac{A(k)}{\sqrt{2\pi}} e^{ikx} \Delta k \tag{2A-10}$$

If we now let $L \to \infty$, then k approaches a continuous variable, since Δk becomes infinitesimally small. If we recall the Riemann definition of an integral, we see that in the limit (2A-10) can be written in the form

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk\, A(k) e^{ikx} \tag{2A-11}$$

The coefficient $A(k)$ is given by

$$\begin{aligned} A(k) &= \sqrt{2\pi} \frac{L}{\pi} \cdot \frac{1}{2L} \int_{-L}^{L} dx\, f(x) e^{-in\pi x/L} \\ &\to \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx\, f(x) e^{-ikx} \end{aligned} \tag{2A-12}$$

Equations (2A-11) and (2A-12) define the Fourier integral transformations. If we insert the second equation into the first we get

$$f(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dk\, e^{ikx} \int_{-\infty}^{\infty} dy\, f(y) e^{-iky} \tag{2A-13}$$

Suppose now that we interchange, without question, the order of integrations. We then get

$$f(x) = \int_{-\infty}^{\infty} dy\, f(y) \left[\frac{1}{2\pi} \int_{-\infty}^{\infty} dk\, e^{ik(x-y)} \right] \tag{2A-14}$$

For this to be true, the quantity $\delta(x - y)$ defined by

$$\delta(x-y) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dk\, e^{ik(x-y)} \tag{2A-15}$$

and called the *Dirac delta function* must be a very peculiar kind of function; it must vanish when $x \neq y$, and it must tend to infinity in an appropriate way when $x - y = 0$, since the range of integration is infinitesimally small. It is therefore not a function of the usual mathematical sense, but it is rather a "generalized function" or a "distribution."[1] It does not have any meaning by itself, but it can be defined provided it always appears in the form

$$\int dx\, f(x)\, \delta(x-a)$$

with the function $f(x)$ sufficiently smooth in the range of values that the argument of the delta function takes. We will take that for granted and manipulate the delta function by itself, with the understanding that at the end all the relations that we write down only occur under the integral sign.

The following properties of the delta function can be demonstrated:

(i)

$$\delta(ax) = \frac{1}{|a|}\delta(x) \tag{2A-16}$$

This can be seen to follow from

$$f(x) = \int dy\, f(y)\, \delta(x-y) \tag{2A-17}$$

If we write $x = a\xi$ and y and $a\eta$, then this reads

$$f(a\xi) = |a| \int d\eta\, f(a\eta)\, \delta[a(\xi - \eta)]$$

On the other hand,

$$f(a\xi) = \int d\eta\, f(a\eta)\, \delta(\xi - \eta)$$

which implies our result.

(ii) A relation that follows from (2A-16) is

$$\delta(x^2 - a^2) = \frac{1}{2|a|}[\delta(x-a) + \delta(x+a)] \tag{2A-18}$$

This follows from the fact that the argument of the delta function vanishes at $x = a$ and $x = -a$. Thus there are two contributions:

$$\begin{aligned}\delta(x^2 - a^2) &= \delta[(x-a)(x+a)] \\ &= \frac{1}{|x+a|}\delta(x-a) + \frac{1}{|x-a|}\delta(x+a) \\ &= \frac{1}{2|a|}[\delta(x-a) + \delta(x+a)]\end{aligned}$$

More generally, one can show that

$$\delta[f(x)] = \sum_i \frac{\delta(x - x_i)}{|df/dx|_{x=x_i}} \tag{2A-19}$$

where the x_i are the roots of $f(x)$ in the interval of integration.

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[1]The theory of distributions was developed by the mathematician Laurent Schwartz. An introductory treatment may be found in M. J. Lighthill, *Introduction to Fourier Analysis and Generalized Functions*, Cambridge University Press, Cambridge, England, 1958.

In addition to the representation (2A-15) of the delta function, there are other representations that may prove useful. We discuss several of them.

(a) Consider the form (2A-15), which we write in the form

$$\delta(x) = \frac{1}{2\pi} \operatorname*{Lim}_{L\to\infty} \int_{-L}^{L} dk\, e^{ikx} \tag{2A-20}$$

The integral can be done, and we get

$$\begin{aligned}\delta(x) &= \operatorname*{Lim}_{L\to\infty} \frac{1}{2\pi} \frac{e^{iLx} - e^{-iLx}}{ix} \\ &= \operatorname*{Lim}_{L\to\infty} \frac{\sin Lx}{\pi x}\end{aligned} \tag{2A-21}$$

(b) Consider the function $\Delta(x, a)$ defined by

$$\begin{aligned}\Delta(x, a) &= 0 && x < -a \\ &= \frac{1}{2a} && -a < x < a \\ &= 0 && a < x\end{aligned} \tag{2A-22}$$

Then

$$\delta(x) = \operatorname*{Lim}_{a\to 0} \Delta(x, a) \tag{2A-23}$$

It is clear that an integral of a product of $\Delta(x, a)$ and a function $f(x)$ that is smooth near the origin will pick out the value at the origin

$$\begin{aligned}\operatorname*{Lim}_{a\to 0} \int dx\, f(x)\, \Delta(x, a) &= f(0) \operatorname*{Lim}_{a\to 0} \int dx\, \Delta(x, a) \\ &= f(0)\end{aligned}$$

(c) By the same token, any peaked function, normalized to unit area under it, will approach a delta function in the limit that the width of the peak goes to zero. We will leave it to the reader to show that the following are representations of the delta function:

$$\delta(x) = \operatorname*{Lim}_{a\to 0} \frac{1}{\pi} \frac{a}{x^2 + a^2} \tag{2A-24}$$

and

$$\delta(x) = \operatorname*{Lim}_{a\to\infty} \frac{\alpha}{\sqrt{\pi}} e^{-\alpha^2 x^2} \tag{2A-25}$$

(d) We will have occasion to deal with *orthonormal polynomials*, which we denote by the general symbol $P_n(x)$. These have the property that

$$\int dx\, P_m(x) P_n(x) w(x) = \delta_{mn} \tag{2A-26}$$

where $w(x)$ may be unity or some simple function, called the weight function. For functions that may be expanded in a series of these orthogonal polynomials, we can write

$$f(x) = \sum_n a_n P_n(x) \tag{2A-27}$$

If we multiply both sides by $w(x)P_m(x)$ and integrate over x, we find that

$$a_m = \int dy\, w(y)f(y)P_m(y) \tag{2A-28}$$

We can insert this into (2A-27) and, prepared to deal with "generalized functions," we freely interchange sum and integral. We get

$$\begin{aligned} f(x) &= \sum_n P_n(x) \int dy\, w(y)f(y)P_n(y) \\ &= \int dy\, f(y)\left(\sum_n P_n(x)w(y)P_n(y)\right) \end{aligned} \tag{2A-29}$$

Thus we get still another representation of the delta function. Examples of the $P_n(x)$ are Legendre polynomials, Hermite polynomials, and Laguerre polynomials, all of which make their appearance in quantum mechanical problems.

Since the delta function always appears multiplied by a smooth function under an integral sign, we can give meaning to its derivatives. For example,

$$\begin{aligned} \int_{-\varepsilon}^{\varepsilon} dx\, f(x)\frac{d}{dx}\delta(x) &= \int_{-\varepsilon}^{\varepsilon} dx\,\frac{d}{dx}[f(x)\,\delta(x)] - \int_{-\varepsilon}^{\varepsilon} dx\,\frac{df(x)}{dx}\delta(x) \\ &= -\int_{-\varepsilon}^{\varepsilon} dx\,\frac{df(x)}{dx}\delta(x) \\ &= -\left(\frac{df}{dx}\right)_{x=0} \end{aligned} \tag{2A-30}$$

and so on. The delta function is an extremely useful tool, and the student will encounter it in every part of mathematical physics.

The integral of a delta function is

$$\begin{aligned} \int_{-\infty}^{x} dy\,\delta(y-a) &= 0 \qquad x < a \\ &= 1 \qquad x > a \\ &\equiv \theta(x-a) \end{aligned} \tag{2A-31}$$

which is the standard notation for this discontinuous function. Conversely, the derivative of the so-called *step function* is the Dirac delta function:

$$\frac{d}{dx}\theta(x-a) = \delta(x-a) \tag{2A-32}$$

F. Sudden Expansion

A particle is initially ($t < 0$) in the ground state of an infinite, one-dimensional potential well with walls at $x = 0$ and $x = a$.

(a) If the wall at $x = a$ is moved *slowly* to $x = 8a$, find the energy and wave function of the particle in the new well. Calculate the work done in this process.

(b) If the wall at $x = a$ is now *suddenly* moved (at $t = 0$) to $x = 8a$, calculate the probability of finding the particle in (i) the ground state, (ii) the first excited state, and (iii) the second excited state of the new potential well.

Solution

For $t < 0$ the particle was in a potential well with walls at $x = 0$ and $x = a$, and hence

$$E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}, \qquad \psi_n(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right) \qquad (0 \le x \le a). \tag{10.76}$$

(a) When the wall is moved slowly, the adiabatic theorem dictates that the particle will be found at time t in the ground state of the new potential well (the well with walls at $x = 0$ and $x = 8a$). Thus, we have

$$E_1(t) = \frac{\pi^2\hbar^2}{2m(8a)^2} = \frac{\pi^2\hbar^2}{128ma^2}, \qquad \psi_1'(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{\pi x}{8a}\right) \qquad (0 \le x \le a). \tag{10.77}$$

The work needed to move the wall is $\Delta W = E_1 - E_1(t) = \pi^2\hbar^2/(2ma^2) - \pi^2\hbar^2/(2m(8a)^2) = 63\pi^2\hbar^2/(128ma^2)$.

(b) When the wall is moved rapidly, the particle will find itself instantly (at $t \ge 0$) in the new potential well; its energy levels and wave function are now given by

$$E_n' = \frac{n^2\pi^2\hbar^2}{2m(8a)^2} = \frac{n^2\pi^2\hbar^2}{128ma^2}, \qquad \psi_n'(x) = \sqrt{\frac{2}{8a}}\sin\left(\frac{n\pi x}{8a}\right) \qquad (0 \le x \le 8a). \tag{10.78}$$

The probability of finding the particle in the ground state of the new box potential can be obtained from (10.73): $P_{11} = |\langle \psi_1' \mid \psi_1\rangle|^2$ where

$$\langle \psi_1' \mid \psi_1\rangle = \int_0^a \psi_1'^*(x)\psi_1(x)\,dx = \frac{2}{\sqrt{8}a}\int_0^a \sin\left(\frac{\pi x}{8a}\right)\sin\left(\frac{\pi x}{a}\right)dx = \frac{16}{63\pi}\sqrt{4-2\sqrt{2}}, \tag{10.79}$$

hence

$$P_{11} = |\langle \psi_1' \mid \psi_1\rangle|^2 = \left(\frac{16}{63\pi}\right)^2(4-2\sqrt{2}) = 0.0077 \simeq 0.7\%. \tag{10.80}$$

The probability of finding the particle in the first excited state of the new box potential is given by $P_{12} = |\langle \psi_2' \mid \psi_1\rangle|^2$ where

$$\langle \psi_2' \mid \psi_1\rangle = \int_0^a \psi_2'^*(x)\psi_1(x)\,dx = \frac{2}{\sqrt{8}a}\int_0^a \sin\left(\frac{\pi x}{4a}\right)\sin\left(\frac{\pi x}{a}\right)dx = \frac{8}{15\pi},$$

hence

$$P_{12} = |\langle \psi_2' \mid \psi_1\rangle|^2 = \left(\frac{8}{15\pi}\right)^2 = 0.1699 \simeq 17\%.$$

A similar calculation leads to

$$P_{13} = |\langle \psi_3' \mid \psi_1\rangle|^2 = \left|\frac{2}{\sqrt{8}a}\int_0^a \sin\left(\frac{3\pi x}{8a}\right)\sin\left(\frac{\pi x}{a}\right)dx\right|^2 = \left|\frac{16}{55\pi}\sqrt{4+2\sqrt{2}}\right|^2 \simeq 24.2\%. \tag{10.83}$$

These calculations show that the particle is most likely to be found in higher excited states; the probability of finding it in the ground state is very small.

G.

Classical limit of Harmonic Oscillator

Since the general solution of the equation of motion of a classical oscillator, $\ddot{x}+\omega^2 x = 0$, is of the form $x = C \sin(\omega t+\phi)$, the total energy

$$E_1 = T+V = \frac{m\dot{x}^2}{2}+\frac{m\omega^2}{2}x^2$$

of such an oscillator is given by $E_1 = m\omega^2 c^2/2$.

Since $T \geqslant 0$, we have $E_1 \geqslant V$, which means that, classically, the particle can be found only in the range $-a \leqslant x \leqslant +a$. At the ends of this interval, where $E_1 = V$, its kinetic energy vanishes; the points $x = \pm a$ are called "turning points". Accordingly, $C^2 = a^2 = 2E_1/m\omega^2 = 3\hbar/m\omega$. The classical probability of finding the particle in the interval $(x, x+dx)$ is proportional to the time dt which it takes to pass through this interval. If the period of oscillation is $T = 2\pi/\omega$, then

$$W_{cl}(x)\,dx = 2\frac{dt}{T} = \frac{\omega}{\pi}\frac{dx}{\dot{x}} = \frac{\omega}{\pi}\frac{dx}{a\omega\cos(\omega t+\phi)} = \frac{1}{\pi a}\left(1-\frac{x^2}{a^2}\right)^{-1/2}dx,$$

which is the required expression.

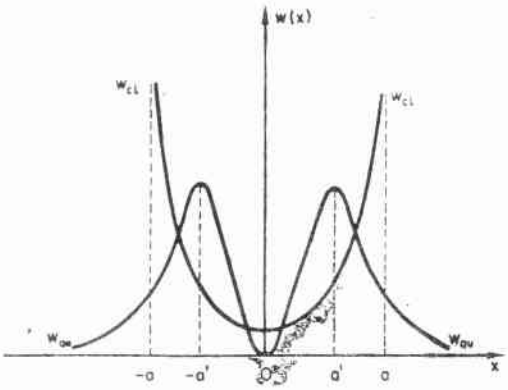

FIG. II.23.

It can be seen that this probability is greatest at the turning points $x = \pm a$ (Fig. II.23). According to quantum mechanics the probability of finding the particle in the interval $(x, x+dx)$ is

$$W_{qu}(x)\,dx = 2\pi^{-1/2}x_0^{-3}x^2 \exp\left(-\frac{x^2}{x_0^2}\right)dx.$$

It should be noted that $W_{qu}(x)$ has maxima near the classical turning points $\left(a = \sqrt{3\hbar/m\omega},\ a' = \sqrt{\hbar/m\omega}\right)$, but, in contrast with the classical case, it does not vanish beyond these points. This phenomenon, of the penetration of a particle into regions with "negative kinetic energy" $(|x| > a)$, does not lead to any contradiction because the equality $E = T+V$ in quantum mechanics is not a simple relation between numbers, but between operators; the kinetic and the potential energies cannot in fact be determined simultaneously.

For higher levels, it is found that the curve $2W_{cl}(x)$ becomes the envelope of the peaks of $W_{qu}(x)$ in the classical limit $n \to \infty$ (cf. Fig. II.24, which represents $W_{qu}(x) = |\psi_{10}(x)|^2$, $a = \sqrt{21\hbar/m\omega}$).

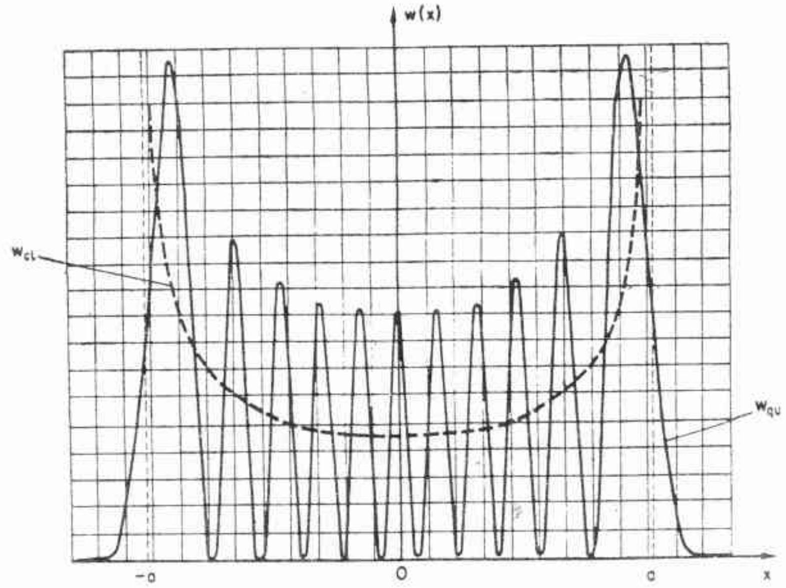

FIG. II.24.