

“Complementi di Fisica”
Lectures 14, 15



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Course Outline - Reminder

- The physics of semiconductor devices: an introduction
- Quantum Mechanics: an introduction
 - Reminder on waves
 - Waves as particles and particles as waves (the crisis of classical physics); atoms and the Bohr model
 - The Schrödinger equation and its interpretation
 - (1-d) free and confined (infinite well) electron; wave packets, uncertainty relations; barriers and wells
 - (3-d) Hydrogen atom, angular momentum, spin
 - Systems with many particles
- Advanced semiconductor fundamentals (bands, etc...)



Lectures 14, 15 - outline

- 1-d applications of Wave Mechanics:
 - Plane wave-function for free electrons
 - Electron confined in an infinite potential well
 - Physical meaning of eigenfunctions and eigenvalues
 - More realistic free particle, partially localized in space: wave packet, uncertainty relations
- For details on some of the calculations:
 - Blackboard and exercises
 - R.F.Pierret, Advanced Semiconductor Fundamentals, section 2.3 (p.33-46)
 - J.Bernstein et al., Modern Physics, sections 6-5, 7-1, 7-2, 7-3, 7-4, 7-5, 8-1, 8-2, 8-3, 8-4, 8-5
 - D.J.Griffiths, Introduction to Quantum Mechanics



“free particles”

General solution: plane waves

Wave number, phase velocity

Normalization

Momentum and Energy

Summary: problems...

“free particle” – general solution

Free particle (constant potential $V(x)=0$): the simplest possible case?
Not really! Surprisingly subtle and tricky...

free particle : constant potential $V(x)=0. \Rightarrow$

$$-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi(x) = E \psi(x) \Rightarrow \frac{\partial^2}{\partial x^2} \psi(x) + \frac{2mE}{\hbar^2} \psi(x) = 0$$

$$\Rightarrow \boxed{\frac{d^2 \psi}{dx^2} + k^2 \psi = 0} \quad \text{with} \quad \boxed{k \equiv \sqrt{2mE/\hbar^2}} \quad E = \frac{\hbar^2 k^2}{2m}$$

general (separable) solution :

$$\boxed{\psi(x) = A_+ e^{ikx} + A_- e^{-ikx}}$$

$$\Psi(x,t) = \psi(x)T(t) = \psi(x)e^{-iEt/\hbar} = A_+ e^{i(kx - Et/\hbar)} + A_- e^{-i(kx + Et/\hbar)}$$

The general solution looks like a “plane wave”.

All energy values E are allowed



“free particle” – plane wave

General solution including time dependence:

$$\Psi(x, t) = A_+ e^{i(kx - Et/\hbar)} + A_- e^{-i(kx + Et/\hbar)} = A_+ e^{i\left(kx - \frac{\hbar k^2}{2m}t\right)} + A_- e^{-i\left(kx + \frac{\hbar k^2}{2m}t\right)}$$

Interpretation: compare with classical harmonic waves.

travelling in the $\pm x$ direction with phase velocity $v_f = \omega/k$

$$e^{i(kx - \omega t)} = e^{ik\left(x - \frac{\omega}{k}t\right)} = e^{ik(x - v_f t)} \qquad e^{-i(kx - \omega t)} = e^{-ik\left(x + \frac{\omega}{k}t\right)} = e^{-ik(x + v_f t)}$$

Wave number k , angular frequency ω and phase velocity v_f :

$$k = \sqrt{2mE/\hbar^2} \qquad \leftrightarrow \qquad k \equiv 2\pi/\lambda$$

$$E/\hbar = \hbar k^2/2m \qquad \leftrightarrow \qquad \omega \equiv 2\pi\nu \equiv 2\pi/T$$

$$v_f = \frac{E}{\hbar} \frac{\hbar}{\sqrt{2mE}} = \sqrt{\frac{E}{2m}} \qquad \leftrightarrow \qquad v_f \equiv \omega/k = \lambda\nu$$

$$E = \frac{1}{2} m v_{\text{classical}}^2$$
$$\Rightarrow v_{\text{classical}} = \sqrt{\frac{2E}{m}} = 2v_f$$

Classical velocity is different from v_f !?!



“free particle” - normalization

- Strictly speaking, the “plane wave” wave function is not normalizable! (postulate P.4)
 - Take a plane wave propagating to +x (coefficients: $A_+ \neq 0$, $A_- = 0$): extended to $\pm\infty$, it is impossible to normalize: one must restrict the available space (for instance to within $\pm L$, with L arbitrarily large) to have a finite, although small, value for the coefficient A_+ .

$$\Psi(x, t) = A_+ e^{i(kx - Et/\hbar)}$$

$$\int_{-\infty}^{+\infty} |\Psi(x, t)|^2 dx = |A_+|^2 \int_{-\infty}^{+\infty} dx \rightarrow \infty \quad \text{unless} \quad |A_+|^2 \rightarrow 0$$

$$\int_{-L}^{+L} |\Psi(x, t)|^2 dx = 1 \quad \Rightarrow \quad |A_+|^2 = \frac{1}{2L}$$

$|\Psi(x, t)|^2 dx = \text{const.} \Rightarrow$ particle position completely undetermined



“free particle” – momentum and energy

- Momentum expectation value?

$$\Psi(x, t) = A_+ e^{i(kx - Et/\hbar)}$$

$$\langle p_x \rangle = \int_{-\infty}^{+\infty} \Psi^*(x, t) (-i\hbar) \frac{\partial}{\partial x} \Psi(x, t) dx = (-i\hbar) ik \int_{-\infty}^{+\infty} \Psi^*(x, t) \Psi(x, t) dx =$$

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

DeBroglie wavelength!

“forcing” the normalization to 1

- Energy eigenvalues

$$E = \frac{\hbar^2 k^2}{2m} = \frac{\langle p_x \rangle^2}{2m} \quad \text{OK!}$$

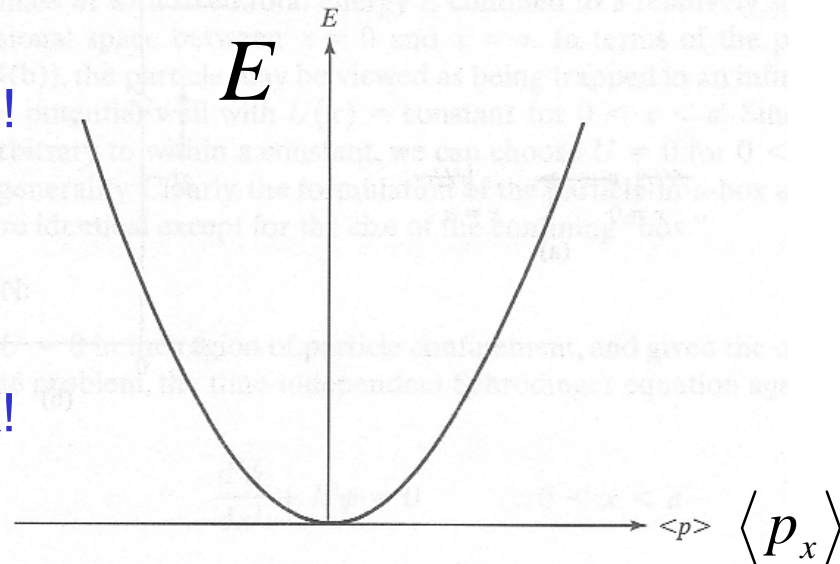


Figure 2.3 Energy-momentum relationship for a free particle.

“free particle” – plane wave, summary

- At a first look the plane wave is OK:
 - Well defined momentum expectation value
 - Well defined energy eigenvalue
 - Momentum-wavelength relationship \equiv DeBroglie!
- But:
 - Not normalizable: probability interpretation?
 - Particle position completely undetermined?
 - Wave-function phase velocity different from classical particle velocity by factor 2 ?!?
- All 3 problems will be solved by “wave packets”



Particle in an infinite 1-d potential well

“Standing wave” solutions

Energy quantization!

Normalization

Some expectation values

Energy “eigenfunctions” and “eigenvalues”

“composite” wavefunctions?

“particle in a box” – general solution

Particle in a 1-d “non-leaking” box (from $x = 0$ to $x = a$):
potential $V(x)=0$ inside, ∞ outside \Rightarrow boundary conditions for $\psi(x)$

$$V(x)=0 \quad 0 < x < a \quad \boxed{\psi(0) = \psi(a) = 0}$$
$$-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi(x) = E \psi(x) \quad \Rightarrow \quad \frac{\partial^2}{\partial x^2} \psi(x) + \frac{2mE}{\hbar^2} \psi(x) = 0$$
$$\Rightarrow \quad \boxed{\frac{d^2 \psi}{dx^2} + k^2 \psi = 0} \quad \text{with} \quad \boxed{k \equiv \sqrt{2mE/\hbar^2}} \quad E = \frac{\hbar^2 k^2}{2m}$$

(separable) solution :

$$\boxed{\psi_n(x) = A_n \sin(k_n x)} = A_n 2i(e^{ik_n x} - e^{-ik_n x}) \quad \boxed{k_n = n\pi/a \quad E_n = \frac{\hbar^2 k_n^2}{2m}}$$

$$\Psi_n(x, t) = \psi_n(x) T(t) = \psi_n(x) e^{-iE_n t/\hbar} = A_n \sin(n\pi x/a) e^{-iE_n t/\hbar}$$



“particle in a box”: standing wave

- The solution is a “standing wave”:
 - superposition of two opposite-going plane waves of equal amplitude

$$\psi_n(x) = A_n \sin(k_n x) = A_n 2i(e^{ik_n x} - e^{-ik_n x})$$

$$k_n = n\pi/a \quad (n = \pm 1, \pm 2, \pm 3, \dots) \quad E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{\pi^2 \hbar^2}{2m} n^2$$

$$\Psi(x, t) = \psi_n(x)T(t) = \psi(x)e^{-iE_n t/\hbar} = A_n \sin(n\pi x/a)e^{-iE_n t/\hbar}$$

- The energy E can only assume discrete values E_n : it is “quantized”! This is a general property of bound states in wave mechanics!
- Normalization A_n , energy, momentum? See next



“standing wave”: normalization

- Easy:

$$\begin{aligned}\int_0^a |\Psi_n(x, t)|^2 dx &= \int_0^a |\psi_n(x)|^2 dx = \int_0^a |A_n|^2 \sin^2 x dx = \\ &= |A_n|^2 \frac{a}{2} = 1 \quad \Rightarrow \quad A_n = \sqrt{\frac{2}{a}}\end{aligned}$$

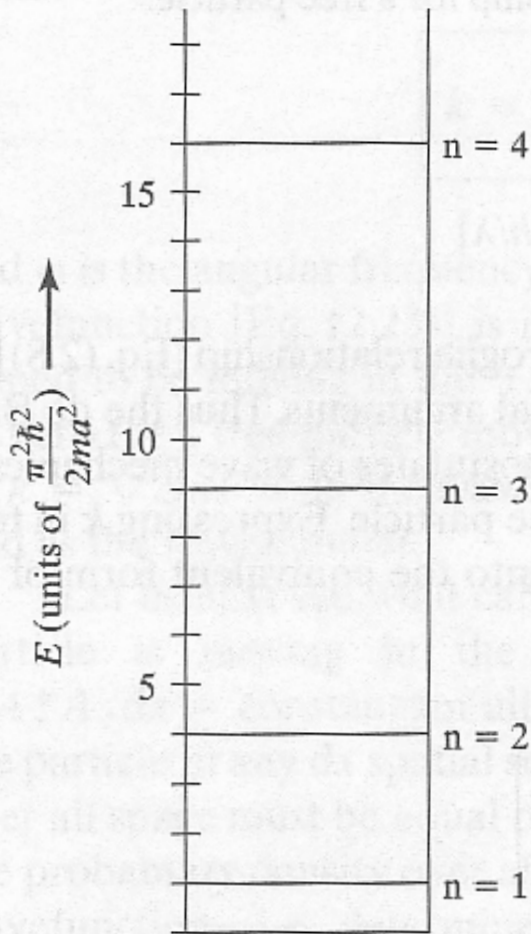
$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a} x\right)$$

$$\Psi_n(x, t) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a} x\right) e^{-i\frac{E_n t}{\hbar}}$$

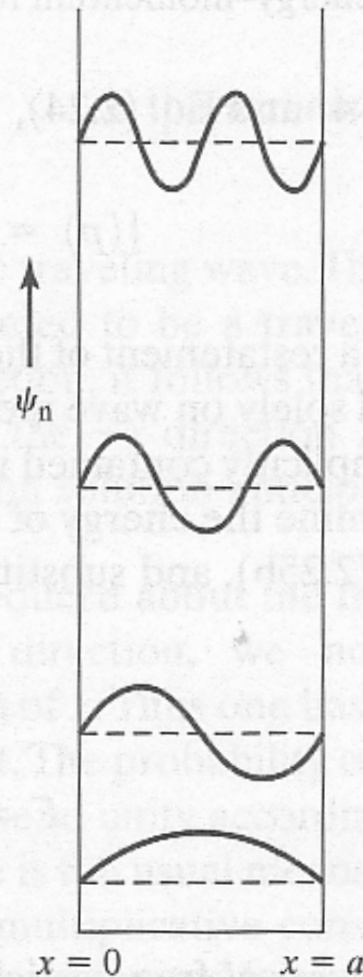


Infinite well: energy quantization

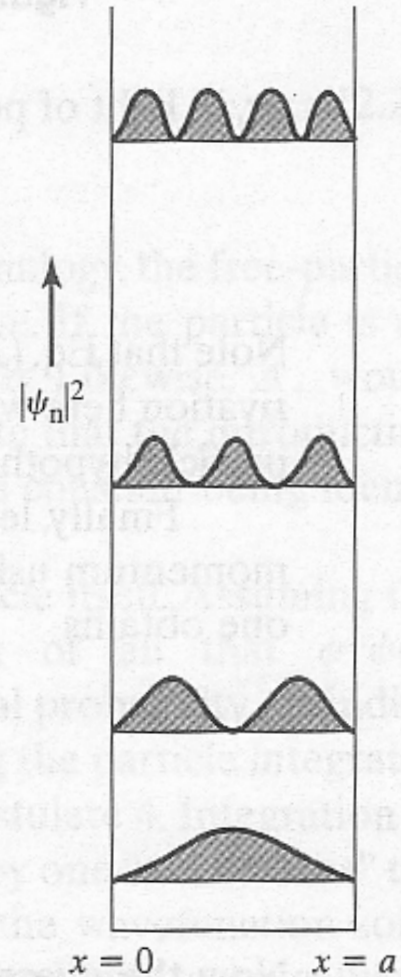
Energy
"eigenvalues"



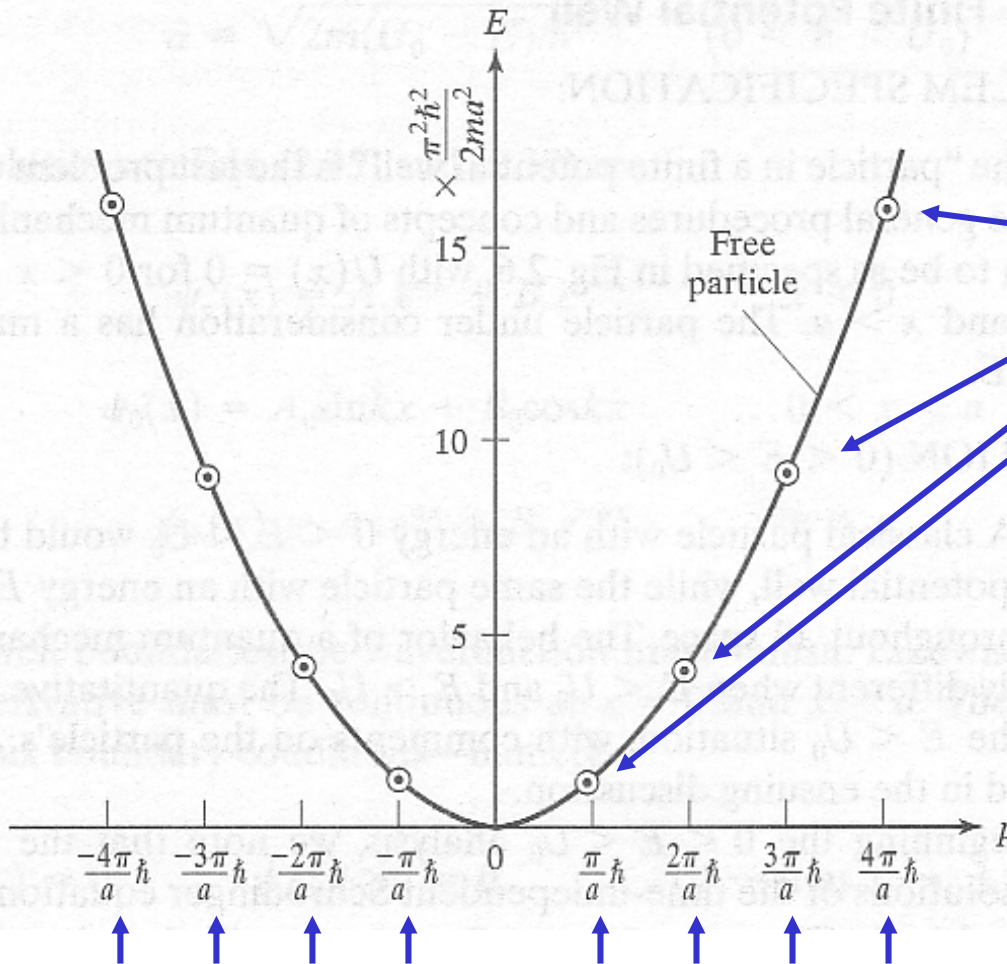
Wavefunctions
(eigenfunctions)



Corresponding
probability distributions



Infinite well: energy quantization



Energy
“eigenvalues”

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

To understand better,
Let's compute some
expectation values !

$$p_n = \hbar k_n = \pm \hbar n \frac{\pi}{a} \quad (n = 1, 2, 3, \dots) \quad ? \text{ What are these exactly ?}$$



Expectation values and uncertainties - 1

- We found the energy “eigenfunctions” and “eigenvalues”: what happens if the particle state is described by such an eigenfunction?

$$\hat{H}\psi_n(x) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi_n(x) = E_n \psi_n(x)$$

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a} x\right) \quad E_n = \frac{\pi^2 \hbar^2}{2ma^2} n^2$$

- Rather easy to compute: energy “expectation values” and “uncertainty”

$$\langle \hat{H} \rangle = \int_0^a \Psi_n^* (\hat{H} \Psi_n) dx = \int_0^a \Psi_n^* (E_n \Psi_n) dx = E_n$$

$$\langle \hat{H}^2 \rangle = \int_0^a \Psi_n^* (\hat{H} (\hat{H} \Psi_n)) dx = \int_0^a \Psi_n^* (E_n^2 \Psi_n) dx = E_n^2$$

- No uncertainty!
 E_n is “certain”

$$\sigma_H^2 = \langle \hat{H}^2 \rangle - \langle \hat{H} \rangle^2 = E_n^2 - E_n^2 = 0$$



Expectation values and uncertainties - 2

- What about momentum, in the same state? compute similarly the momentum “expectation values” and “uncertainty”

$$\begin{aligned}\langle \hat{p}_x \rangle &= \int_0^a \Psi_n^* (\hat{p}_x \Psi_n) dx = \int_0^a \Psi_n^* \left(-i\hbar \frac{\partial}{\partial x} \Psi_n \right) dx = \\ &= \frac{2}{a} \left(-i\hbar \frac{n\pi}{a} \right) \int_0^a \sin\left(\frac{n\pi}{a} x\right) \cos\left(\frac{n\pi}{a} x\right) dx = \\ &= 0\end{aligned}$$

- Result: the uncertainty on p_x is not zero!

$$\begin{aligned}\langle \hat{p}_x^2 \rangle &= \int_0^a \Psi_n^* (\hat{p}_x (\hat{p}_x \Psi_n)) dx = \dots \\ &= \frac{\pi^2 \hbar^2 n^2}{a^2} = 2mE_n = 2m \langle \hat{H} \rangle \neq 0\end{aligned}$$

- We should have expected it: superposition of two plane wave states, with opposite momenta: a measurement can give one of two opposite values for p_x

$$\sigma_{p_x}^2 = \langle \hat{p}_x^2 \rangle - \langle \hat{p}_x \rangle^2 = \frac{\pi^2 \hbar^2 n^2}{a^2} \neq 0$$



“Standing wave” and other solutions - 1

- For a given n , the corresponding standing wave solution Ψ_n
 - Corresponds to a “certain”, well defined value of energy E_n , since it is an eigenfunction of the energy operator
 - Has also a well defined
 - absolute value of momentum $|p_x|$
 - square of momentum p_x^2
 - But the momentum p_x is “uncertain”: we understand this! This happens because the “standing waves” are not eigenfunctions of the operator corresponding to p_x , but rather superpositions of two plane waves with opposite values of p_x
- Can the particle be in other states, described by different wave functions? What happens of energy in these cases? Can one generalize?



“Standing wave” and other solutions - 2

- Can the particle be in other (non-standing wave) states, described by different wave functions? Yes!
 - Any normalized linear combination of solutions is still a solution of the time-dependent Schrödinger equation,
 - even if it will no longer be a solution of the time-independent equation... For instance

Standing wave (ground state, $n = 1$)

$$\psi_1 = \frac{2}{a} \sin \frac{\pi x}{a} e^{j\omega_1 t}; \quad \text{where} \quad \omega_1 = \frac{\hbar \pi^2}{2ma^2}$$

Superposition of two standing waves ($n = 1$ and $n = 2$)

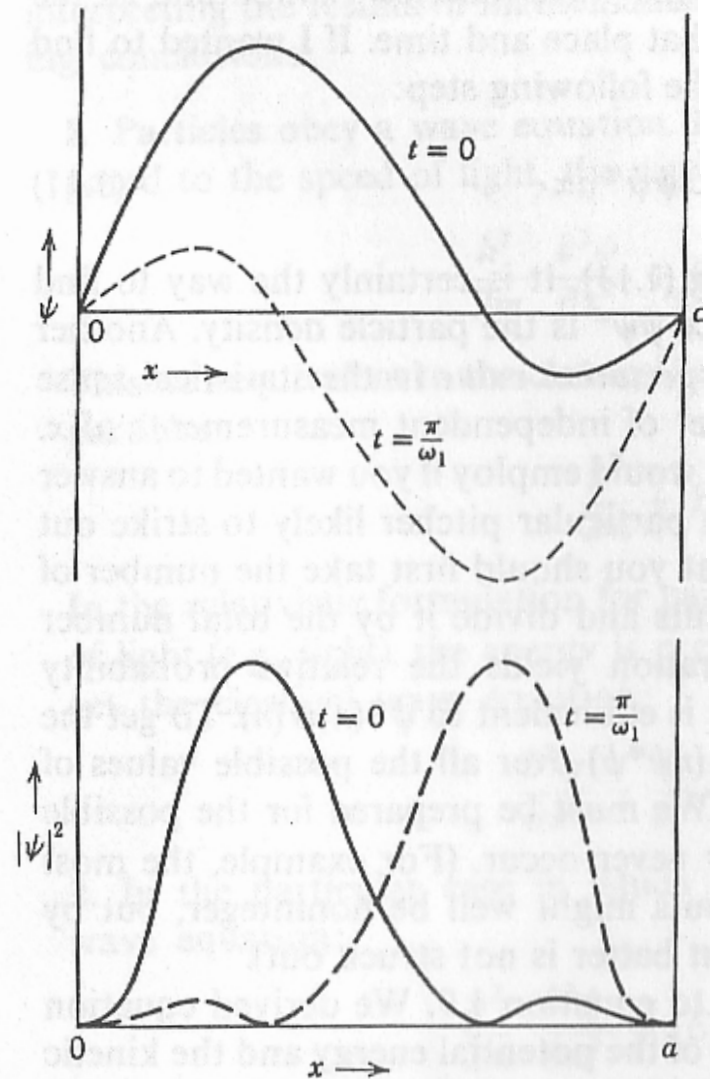
$$\psi_2 = \left(\frac{1}{a} \right)^{1/2} \left[\sin \frac{\pi x}{a} e^{j\omega_1 t} + \sin \frac{2\pi x}{a} e^{j\omega_2 t} \right] \quad \omega_2 = 4\omega_1$$



“Standing wave” and other solutions - 2

Playing with these “combined” solutions, one can see that:

- Energy is no longer “certain”
- The expectation values and “uncertainties” in position and momentum change
- One can build solutions “bouncing back and forth between the two walls”, etc.
- See here the wave function defined in the previous page and its square at two different times
- One can compute expectation values at different times and follow their evolution...



The Physical Meaning of Eigenfunctions and Eigenvalues

Generalizing
from this specific example...

The Physical Meaning of Eigenfunctions and Eigenvalues - 1

- If a particle state Ψ_α is the eigenfunction of the operator corresponding to a dynamical variable, the outcome of a measurement of that variable is “certain” and is equal to the corresponding eigenvalue α

$$\hat{\alpha} \Psi_\alpha = \alpha \Psi_\alpha$$

$$\Psi = \Psi_\alpha \Rightarrow \sigma_\alpha^2 = \langle \hat{\alpha}^2 \rangle - \langle \hat{\alpha} \rangle^2 = \alpha^2 - \alpha^2 = 0$$

- One can show that two different dynamical variables can have simultaneously “certain” measured values only if their operators share the same eigenfunctions; this happens only when the corresponding operators commute. If they don’t, we call them “incompatible observables” (for instance, x and p_x)



The Physical Meaning of Eigenfunctions and Eigenvalues - 2

One can also show that a generic state can be represented by a linear combination of eigenfunctions of a given observable, and deduce useful relations based on the coefficients of the combination (probabilities and expectation values)

The quantum theory of measurement says also that:

immediately after a measurement, the wave function is “collapsed” to the eigenfunction corresponding to the measured eigenvalue

immediate repetition of the measurement gives the “same” value

Waiting long enough, the wave function evolves according to the Schrödinger equation and will in general change to a different superposition of eigenfunctions; the result of the same measurement will no longer be “certain”



Wave Packets and the Uncertainty Relations

Plane wave: problems

Wave packets

examples

Expectation values, uncertainties

Uncertainty relations

Wave packets (1-d)

- Plane-wave problems:

- Not normalizable: probability interpretation?
- Particle position completely undetermined?
- Wave-function phase velocity different from classical particle velocity by factor 2 ?!?

- Solution: wave-packets

- “superposition” of plane waves, with “weights” depending on k:

"weights": $\frac{1}{\sqrt{2\pi}} \phi(k) dk$

$$\Psi(x, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(k) e^{i\left(kx - \frac{\hbar k^2}{2m} t\right)} dk, \quad k = \pm \frac{\sqrt{2mE}}{\hbar}$$



Wave packets (1-d)

- We recognize a Fourier transform and an inverse transform:

at $t = 0$, given the wavefunction $\Psi(x,0)$ one can find $\phi(k)$

$$\Psi(x,0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(k) e^{ikx} dk \quad \Leftrightarrow \quad \phi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \Psi(x,0) e^{-ikx} dx$$

at later times, the wavefunction $\Psi(x,t)$ evolves according to the S.eq., that is :

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(k) e^{i\left(kx - \frac{\hbar k^2}{2m}t\right)} dk$$

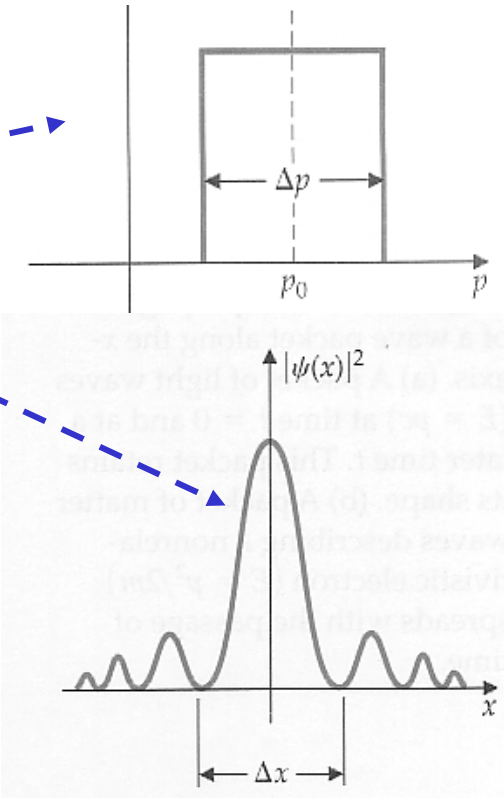
- Let's see
 - Two examples of “weights”
 - Group velocity and uncertainties in x and p_x ; (time evolution...)



Wave packets: Fourier transform pairs

- From Fourier transform tables:
 - “square” k “weights”:

$$\phi(k) = \begin{cases} 1 & |k - k_0| < a \\ 0 & |k - k_0| > a \end{cases} \Leftrightarrow \Psi(x,0) = \sqrt{\frac{2}{\pi}} \frac{\sin ax}{x}$$



- “gaussian” weights: both gaussian!

$$\phi(k) = e^{-a^2 k^2} \Leftrightarrow \Psi(x,0) = \frac{1}{a\sqrt{2}} e^{-\frac{x^2}{4a^2}}$$

- In all cases the “spreads” in x and k are inversely proportional!

Wave packet qualitative illustrations - 1

From: HyperPhysics (©C.R. Nave, 2003)

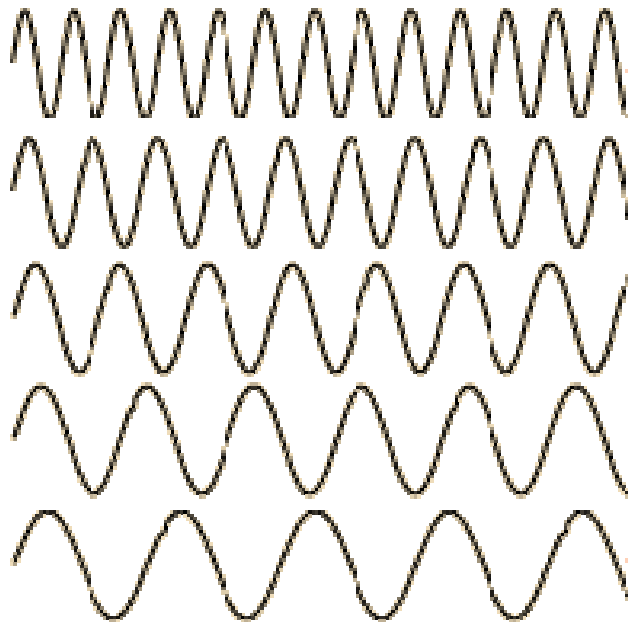
Precisely determined momentum



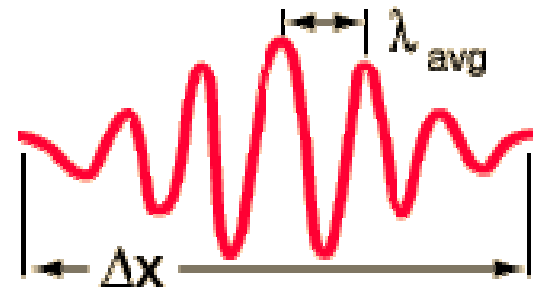
A sine wave of wavelength λ implies that the momentum p is precisely known: But the wavefunction and the probability of finding the particle $\psi^*\psi$ is spread over all of space.

$$p = \frac{h}{\lambda}$$

p precise
 x unknown



Adding several waves of different wavelength together will produce an interference pattern which begins to localize the wave.



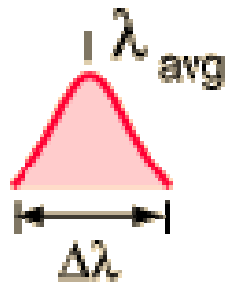
but that process spreads the momentum values and makes it more uncertain. This is an inherent and inescapable increase in the uncertainty Δp when Δx is decreases.

$$\Delta x \Delta p > \frac{\hbar}{2}$$

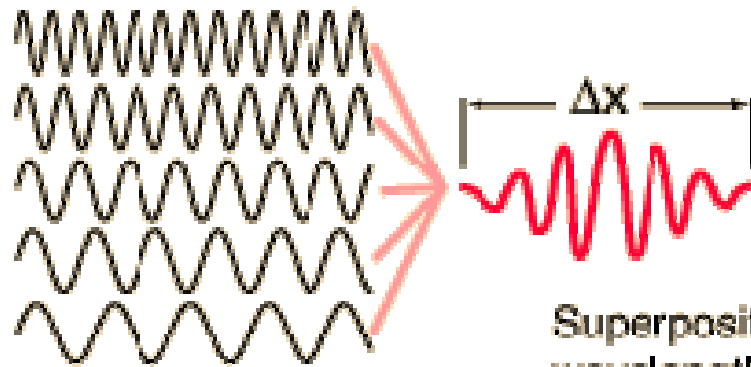
Wave packet qualitative illustrations - 2

From: HyperPhysics (©C.R. Nave, 2003)

A continuous distribution of wavelengths can produce a localized "wave packet".



$$p = \frac{h}{\lambda}$$



Each different wavelength represents a different value of momentum according to the DeBroglie relationship.

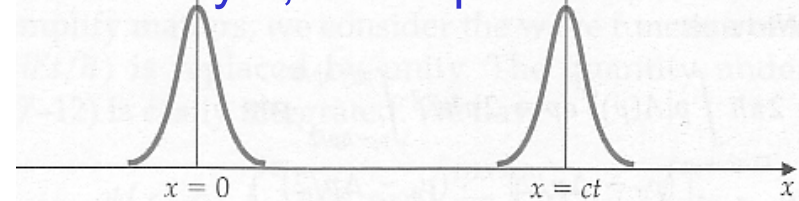
Superposition of different wavelengths is necessary to localize the position. A wider spread of wavelengths contributes to a smaller Δx .

$$\Delta x \Delta p > \frac{\hbar}{2}$$

Wave packet: time variation

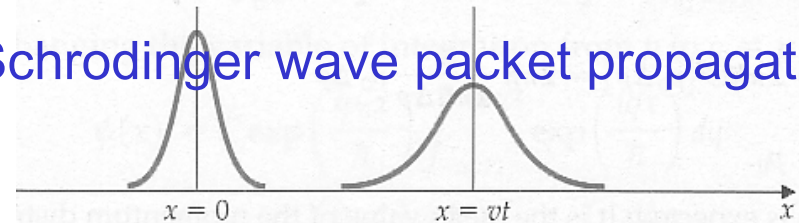
- Detailed calculation is rather lengthy: result, for the “gaussian envelope”:

e.m. wave packet in vacuum:
Velocity c , no dispersion



Schrodinger wave packet propagation

Velocity $v_{\text{group}} = d\omega/dk$,
dispersion $\omega(k)$



- In general: the group velocity is OK, and corresponds to the classical velocity

$$v_f = \frac{\omega}{k} = \frac{E}{\hbar} \frac{1}{k} = \frac{\hbar k^2}{2m} \frac{1}{k} = \frac{\hbar k}{2m} = \frac{1}{2} v_{\text{classical}}$$

$$v_g = \frac{d\omega}{dk} = \frac{d}{dk} \left(\frac{\hbar k^2}{2m} \right) = \frac{\hbar k}{m} = 2v_f = v_{\text{classical}}$$

Uncertainty Relations

- For the gaussian wave packet, the product of the spreads (“uncertainties”) of position and momentum is minimal: taking the usual definitions, one can show that, for any packet:

$$\Delta x \equiv \sigma_x \quad \sigma_x^2 = \langle x^2 \rangle - \langle x \rangle^2$$

$$\Delta p_x \equiv \sigma_{p_x} \quad \sigma_{p_x}^2 = \langle \hat{p}_x^2 \rangle - \langle \hat{p}_x \rangle^2$$

$$\Delta x \Delta p_x \geq \frac{\hbar}{2}$$

- In general, for non-commuting (“incompatible”) observables, one can show similar “Heisenberg Uncertainty Relations”.
- The well known energy-time uncertainty relation has an entirely different origin ! (see discussion in Griffiths, section 3.4.3):

$$\Delta t \Delta E \geq \frac{\hbar}{2}$$



Lectures 14, 15 - summary

- We discussed some 1-d problems that can be solved with Wave Mechanics, in particular:
 - “free” particles (electrons)
 - “bound” particles (electrons)
- This allowed us to investigate two fundamental properties of q.m. related to the measurement process:
 - The meaning of the eigenfunctions and eigenvalues of an observable dynamical variable
 - Uncertainty Relations for “non-commuting” observables
- To become familiar with the method, you can complete the study of some special cases on your own. Several interesting variations of these problems have applications in advanced semiconductor devices! Our next steps: potential barriers, tunneling and then “periodic potential” and “energy bands”



Lecture 14, 15 - exercises

- **Exercise 14.1:** Consider a particle of mass m , bound in a one-dimensional “infinite potential well” of width a , and assume that its wave function is the ground energy eigenfunction, with $n=1$. Compute the corresponding uncertainties in position Δx and momentum Δp_x . (Hint: this problem is discussed in Bernstein, example 6-4, p.166-167)
- **Exercise 15.1:** Consider a gaussian wave packet specified at $t=0$ by $\phi(k)=Cexp(-a^2k^2)$, where C is a suitable normalization constant, k is the wave number and a is a parameter with dimensions $[a]=[L]$. Write the wave function $\Psi(x,0)$ at $t=0$ and find the corresponding uncertainties in position Δx and momentum Δp_x . (Hint: this problem is discussed in Bernstein, example 7-3, 7-5).
- **Exercise 15.2:** Study the time evolution of a gaussian wave packet, and in particular (a) the velocity and (b) show that the width of the packet increases with time. (Hint: see the next “back-up” slides)



Back-up slides

Exercise 14.2 - 1

3.13. Consider a free particle of mass m whose wave function at time $t = 0$ is given by

$$\psi(x, 0) = \frac{\sqrt{a}}{(2\pi)^{3/4}} \int_{-\infty}^{\infty} e^{-a^2(k-k_0)^2/4} e^{ikx} dk \quad (3.13.1)$$

Calculate the time-evolution of the wave-packet $\psi(x, t)$ and the probability density $|\psi(x, t)|^2$. Sketch qualitatively the probability density for $t < 0$, $t = 0$, and $t > 0$. You may use the following identity: For any complex number α and β such that $-\pi/4 < \arg(\alpha) < \pi/4$,

$$\int_{-\infty}^{\infty} e^{-\alpha^2(y+\beta)^2} dy = \frac{\sqrt{\pi}}{\alpha} \quad (3.13.2)$$

The wave-packet at $t = 0$ is a superposition of plane waves e^{ikx} with coefficients $\frac{\sqrt{a}}{(2\pi)^{3/4}} e^{-a^2(k-k_0)^2/4}$; this is a Gaussian curve centered at $k = k_0$. The time-evolution of a plane wave e^{ikx} has the form $e^{ikx} e^{-iE(k)t/\hbar} = e^{ikx} e^{-i\hbar k^2 t/2m}$. We set $\omega(k) = \hbar k^2/2m$, so using the superposition principle, the time-evolution of the wave-packet $\psi(x, 0)$ is

$$\psi(x, t) = \frac{\sqrt{a}}{(2\pi)^{3/4}} \int_{-\infty}^{\infty} e^{-a^2(k-k_0)^2/4} e^{i[kx - \omega(k)t]} dk \quad (3.13.3)$$

Our aim is to transform this integral into the form of (3.13.2). Therefore, we rearrange the terms in the exponent:

$$\begin{aligned} -\frac{a^2}{4}(k-k_0)^2 + i[kx - \omega(k)t] &= -\left(\frac{a^2}{4} + \frac{i\hbar t}{2m}\right)k^2 + \left(\frac{a^2}{2}k_0 + ix\right)k - \frac{a^2}{4}k_0^2 \\ &= -\left(\frac{a^2}{4} + \frac{i\hbar t}{2m}\right) \left[k - \frac{\frac{a^2}{2}k_0 + ix}{2\left(\frac{a^2}{4} + \frac{i\hbar t}{2m}\right)} \right]^2 + \frac{\left(\frac{a^2}{2}k_0 + ix\right)^2}{4\left(\frac{a^2}{4} + \frac{i\hbar t}{2m}\right)} - \frac{a^2}{4}k_0^2 \end{aligned} \quad (3.13.4)$$



Exercise 14.2 - 2

Substituting in (3.13.4) and using (3.13.2) yields

$$\psi(x, t) = \frac{\sqrt{a}}{2^{3/4}\pi^{1/4}} \frac{\exp\left(-\frac{a^2 k_0^2}{4}\right)}{\sqrt{\frac{a^2}{4} + \frac{i\hbar t}{2m}}} \exp\left[\frac{\left(\frac{a^2}{2}k_0 + ix\right)^2}{a^2 + \frac{2i\hbar t}{m}}\right] \quad (3.13.5)$$

The conjugate complex of (3.13.5) is

$$\psi^*(x, t) = \frac{\sqrt{a}}{2^{3/4}\pi^{1/4}} \frac{\exp\left(-\frac{a^2 k_0^2}{4}\right)}{\sqrt{\frac{a^2}{4} - \frac{i\hbar t}{2m}}} \exp\left[\frac{\left(\frac{a^2}{2}k_0 - ix\right)^2}{a^2 - \frac{2i\hbar t}{m}}\right] \quad (3.13.6)$$

Hence,

$$\begin{aligned} |\psi(x, t)|^2 &= \frac{a}{2^{3/2}\sqrt{\pi}} \frac{\exp\left(-\frac{a^2 k_0^2}{2}\right)}{\sqrt{\left(\frac{a^2}{4} + \frac{i\hbar t}{2m}\right)\left(\frac{a^2}{4} - \frac{i\hbar t}{2m}\right)}} \exp\left[\frac{\left(\frac{a^2 k_0}{2}\right)^2 - x^2 + ia^2 k_0 x}{a^2 + 2i\hbar t/m} + \frac{\left(\frac{a^2 k_0}{2}\right)^2 - x^2 - ia^2 k_0 x}{a^2 - 2i\hbar t/m}\right] \\ &= \sqrt{\frac{2}{\pi a^2}} \frac{1}{\sqrt{1 + 4\hbar^2 t^2/m^2 a^4}} \exp\left[-\frac{\frac{a^2 k_0^2}{2}\left(a^4 + \frac{4\hbar^2 t^2}{m^2}\right) + 2a^2\left(\frac{a^2 k_0}{2} - x\right) + \frac{4\hbar k_0 a^2}{m} xt}{a^4 + 4\hbar^2 t^2/m^2}\right] \\ &= \sqrt{\frac{2}{\pi a^2}} \frac{1}{\sqrt{1 + 4\hbar^2 t^2/m^2 a^4}} \exp\left[-\frac{2a^2(x - \hbar k_0 t/m)^2}{a^4 + 4\hbar^2 t^2/m^2}\right] \quad (3.13.7) \end{aligned}$$



Exercise 14.2 - 3

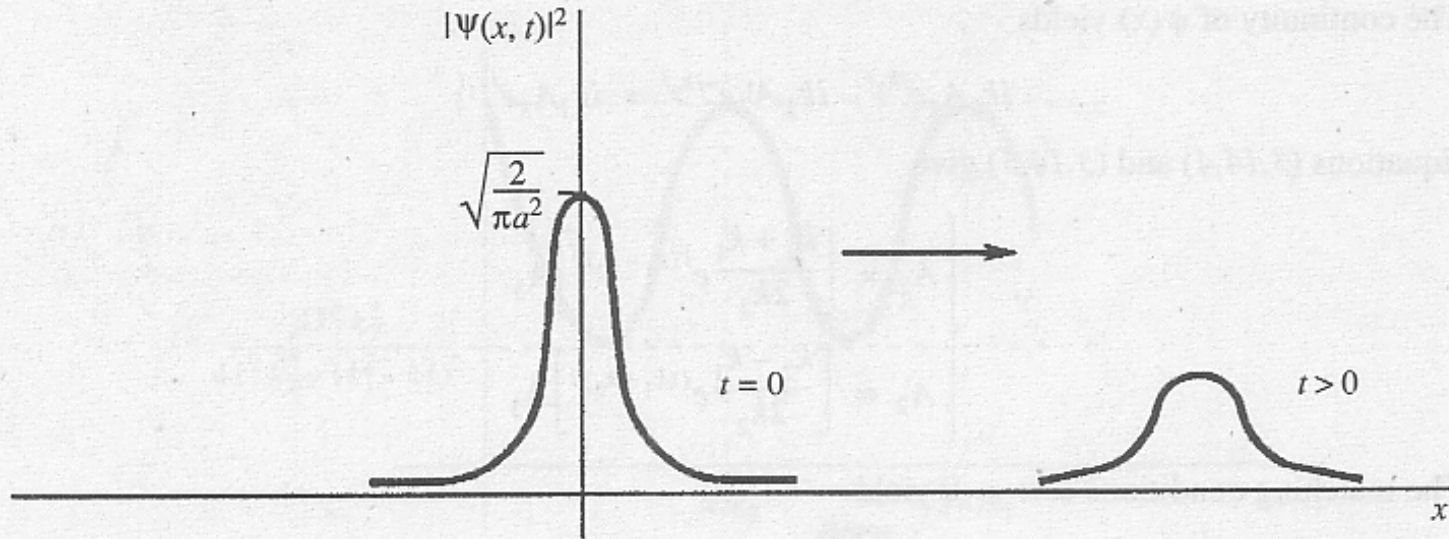


Fig. 3-4

The probability density is a Gaussian curve for every time t entered at $x_C = (\hbar k_0/m) t$. (i.e., the wave-packet moves with a velocity $V_0 = \hbar k_0/m$.) The value of $|\Psi(x, t)|^2$ is maximal for $t = 0$ and tends to zero when $t \rightarrow \infty$. The width of the wave-packet is minimal for $t = 0$ and tends to ∞ when $t \rightarrow \infty$; see Fig. 3-4.