# "Complementi di Fisica" Lectures 7-10

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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 Schrὸdinger 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 12, 13 - outline

- 1-d applications of Wave Mechanics:
  - Plane wave-function for free electrons
  - 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"

"separable" solution: plane waves

Wave number, phase velocity

Normalization

Momentum and Energy

Summary: problems…

# "free particle" – separable solution

**Free particle (constant potential energy *U(x)=0*): the simplest possible case? Not really! Surprisingly subtle and tricky…**

$$\text{free particle: constant potential energy} \quad U(x)=0. \quad \Rightarrow$$

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

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

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**

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# "free particle" – plane wave

**Separable 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 ± *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 $\omega$ and phase velocity $v_f$ :**

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

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

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

$$\boxed{E = \frac{1}{2}mv^2_{classical} \quad \Rightarrow \quad v_{classical} = \sqrt{\frac{2E}{m}} = 2v_f}$$

**Classical velocity is different from $v_f$ ?!?**

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## "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 $A_+$ .

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

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

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

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



## "free particle" – momentum and energy

- Momentum expectation value?

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

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

"forcing" the normalization to 1

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

**DeBroglie wavelength!**

- Energy eigenvalues

$$E = \frac{\hbar^2 k^2}{2m} = \frac{\langle p_x \rangle^2}{2m}$$

OK!

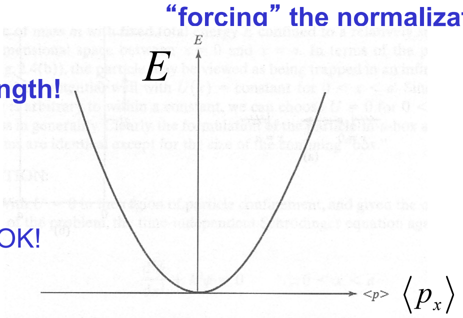


Figure 2.3 Energy–momentum relationship for a free particle.

## “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 ≡ 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”

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# 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:

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

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



# 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 $\phi(k)$

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

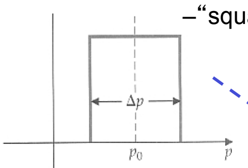
at later times, the wavefunction $\Psi(x,t)$ evolves according to the S.eq., that is:

- Let's see
  - –Two examples of "weights"
  - –Group velocity and uncertainties in x and $p_x$ ; (time evolution…)

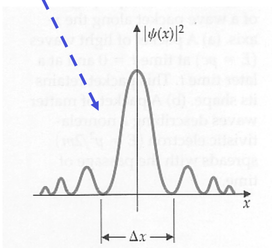
$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty}\phi(k)e^{i\left(kx-\frac{\hbar k^2}{2m}t\right)}dk$$

# Wave packets: Fourier transform pairs

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




$$\phi(k) = \begin{cases} 1 & |k-k_0| < \Delta k/2 \\ 0 & |k-k_0| > \Delta k/2 \end{cases} \quad \Leftrightarrow \quad \Psi(x,0) = \frac{\Delta k}{\sqrt{2\pi}} \frac{\sin(x \cdot \Delta k/2)}{x \cdot \Delta k/2} e^{ik_0 x}$$




  - –the “spreads” in x and k are inversely proportional!



# Wave packets: Gaussian

- Another example: at *t=0* the space part of the wave function is a gaussian, representing the uncertainty in the knowledge of the position appropriately by the “standard deviation” *a*

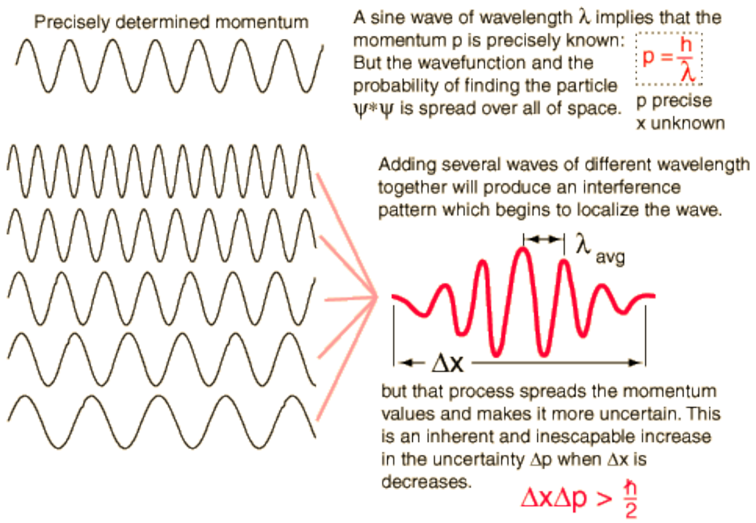
$$\Psi(x,0) = \frac{A}{a\sqrt{2}} e^{-\frac{x^2}{4a^2}} e^{ik_0 x}$$

- From Fourier transform tables:
  - –“gaussian” weights: both gaussian!
  - –In all cases the “spreads” in x and k are inversely proportional!

$$\Psi(x,0) = \frac{A}{a\sqrt{2}} e^{-\frac{x^2}{4a^2}} e^{ik_0 x} \quad \Leftrightarrow \quad \phi(k) = A e^{-a^2 (k-k_0)^2}$$

# Wave packet qualitative illustrations - 1

From: HyperPhysics (©C.R. Nave, 2003)

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# Wave packet qualitative illustrations - 2

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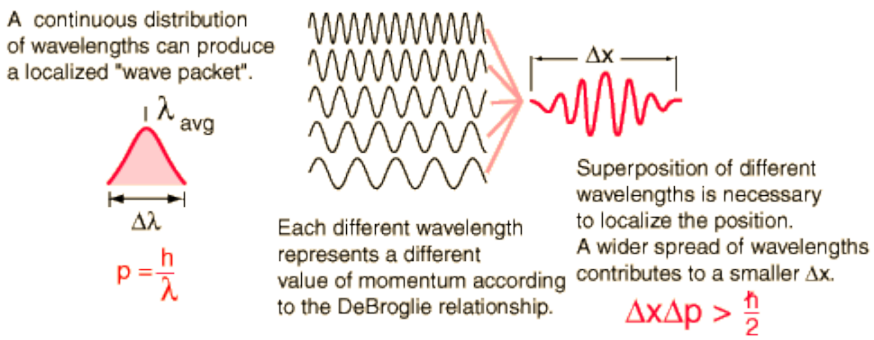


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# Gaussian wave packet: time evolution?

**For the given wave function at t=0, find the Fourier "weights" (Fourier transform)**

$$\Psi(x,0)=\frac{A}{a\sqrt{2}}e^{-\frac{x^2}{4a^2}}e^{ik_0x} \Leftrightarrow \phi(k)=Ae^{-a^2(k-k_0)^2}$$

**Then "plug in" the time dependent term**

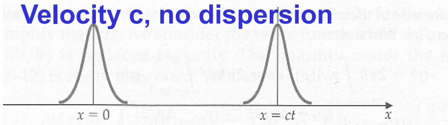
$$\Psi(x,t)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty}\phi(k)e^{ikx}e^{-i\frac{\hbar k^2}{2m}t}dk$$



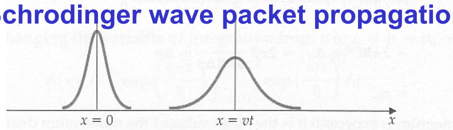
# Wave packet: time evolution

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

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




**Schrodinger wave packet propagation**




**(explicit derivation in the back-up slides")**

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

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

**Velocity $v_{group}$ =dω/dk, dispersion ω(k)**

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

# 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:

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

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

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

- 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):

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

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# The Physical Meaning of Eigenfunctions and Eigenvalues

Generalizing
from the specific example
of the Hamiltonian operator
and its "eigenvalues" and "eigenstates"

## The Physical Meaning of Eigenfunctions and Eigenvalues - 1

- If a particle state $\Psi_\alpha$ is the eigenfunction of the operator corresponding to a dynamical variable, the outcome of a measurement of that variable is "certain" (uncertainty = 0) and is equal to the corresponding eigenvalue $\alpha$

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

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

- 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 $p_x$)

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## 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"

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# Lectures 10, 11, 12 - 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 examples of 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"

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# Lecture 12, 13 - exercises

- **Exercise 12.1:** 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 $\Delta x$ and momentum $\Delta p_x$. (Hint: this problem is discussed in Bernstein, example 6-4, p.166-167)
- **Exercise 12.2:** Consider a gaussian wave packet specified at $t=0$ by $\phi(k)=C\exp(-a^2x^2)$ , 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 $\Delta x$ and momentum $\Delta p_x$. (Hint: this problem is discussed in Bernstein, example 7-3, 7-5).
- **Exercise 12.3:** 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)

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# Back-up slides

## Wavefunction normalization

- A detail: finding normalization factors

**Example 6–2** Consider the pulselike wave function $\psi(x) = A\exp(-x^2/2a^2)$, where $a$ is a constant with the dimensions of length. What value of $A$ is needed to normalize this wave function?

**Solution** The constant $A$ is determined by the requirement that

$$1 = \int_{-\infty}^{+\infty} |\psi(x)|^2\, dx = A^2 \int_{-\infty}^{+\infty} \exp\left(\frac{-x^2}{a^2}\right) dx.$$

The integral is a standard integral found in Appendix B.2:

$$\int_{-\infty}^{+\infty} \exp\left(\frac{-x^2}{a^2}\right) dx = a\sqrt{\pi}.$$

With this result, our first equation reads

$$1 = A^2 a(\pi)^{1/2},$$

an equation easily solved for $A$:

$$A = (a)^{-1/2}(\pi)^{-1/4}.$$

normalized Gaussian
centered at x = 0
standard deviation
σ = a
At the given time

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# Exercise 10.3 - 1

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

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

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 $\alpha$ and $\beta$ such that $-\pi/4 < \arg(\alpha) < \pi/4$,

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

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

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

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

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

$$= -\left(\frac{a^2}{4}+\frac{i\hbar t}{2m}\right)\left[k - \frac{\frac{a^2}{2}k_0 + ix}{2\left(\frac{a^2}{4}+\frac{i\hbar t}{2m}\right)}\right]^2 + \frac{\left(\frac{a^2}{2}k_0 + ix\right)^2}{4\left(\frac{a^2}{4}+\frac{i\hbar t}{2m}\right)} - \frac{a^2}{4}k_0^2 \qquad (3.13.4)$$



# Exercise 10.3 - 2

Substituting in (*3.13.4*) and using (*3.13.2*) yields

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

The conjugate complex of (*3.13.5*) is

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

Hence,

$$|\psi(x,t)|^2 = \frac{a}{2^{3/2}\sqrt{\pi}} \frac{\exp\left(-\frac{a^2k_0^2}{2}\right)}{\sqrt{\left(\frac{a^2}{4}+\frac{i\hbar t}{2m}\right)\left(\frac{a^2}{4}-\frac{i\hbar t}{2m}\right)}} \exp\left[\frac{\left(\frac{a^2k_0}{2}\right)^2 - x^2 + ia^2k_0x}{a^2+2i\hbar t/m} + \frac{\left(\frac{a^2k_0}{2}\right)^2 - x^2 - ia^2k_0x}{a^2-2i\hbar t/m}\right]$$

$$= \sqrt{\frac{2}{\pi a^2}} \frac{1}{\sqrt{1+4\hbar^2t^2/m^2a^4}} \exp\left[-\frac{\frac{a^2k_0^2}{2}\left(a^4+\frac{4\hbar^2t^2}{m^2}\right) + 2a^2\left(\frac{a^4k_0^2}{2} - x^2\right) + \frac{4\hbar k_0 a^2}{m}xt}{a^4 + 4\hbar^2t^2/m^2}\right]$$

$$= \sqrt{\frac{2}{\pi a^2}} \frac{1}{\sqrt{1+4\hbar^2t^2/m^2a^4}} \exp\left[-\frac{2a^2(x-\hbar k_0 t/m)^2}{a^4+4\hbar^2t^2/m^2}\right] \qquad (3.13.7)$$

# Exercise 10.3 - 3

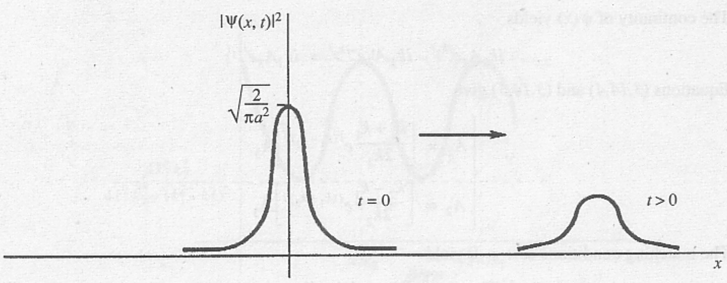


**Fig. 3-4**

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 $t \to \infty$. The width of the wave-packet is minimal for $t = 0$ and tends to $\infty$ when $t \to \infty$; see Fig. 3-4.