دانشگاه آزاد اسلامی

Optoelectronic 2

فقط مرور کلی

Quantum Mechanics Applied to Semiconductor Devices

E. F. Schubert

hamiltonian equations of motion:

$$\frac{dx}{dt} = \frac{\partial}{\partial p} H(x, p)$$

$$\frac{dp}{dt} = -\frac{\partial}{\partial x} H(x, p).$$

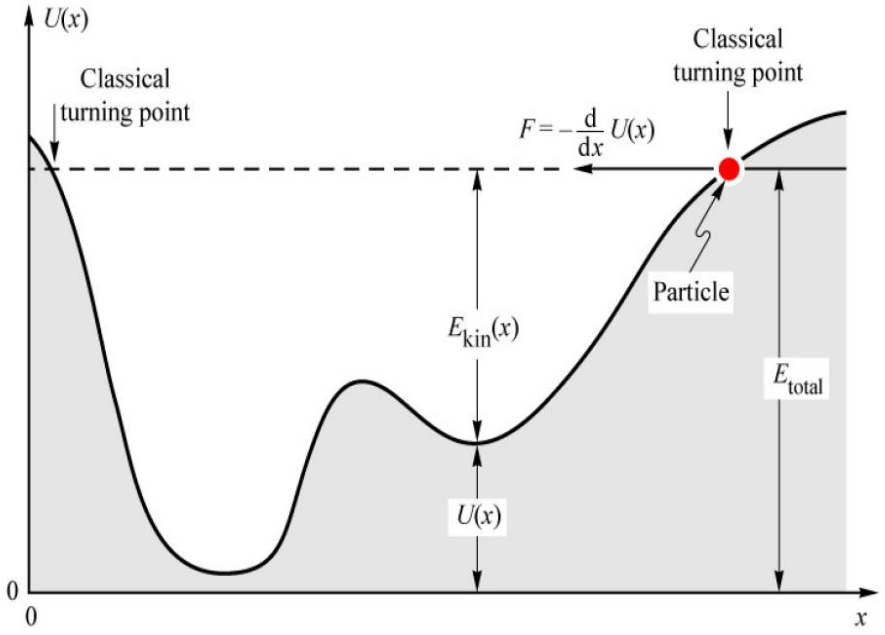

Fig. 1.1. Potential energy as a function of spatial coordinate x. The total energy of the particle shown is the sum of kinetic and potential energies. The force F acting on the particle is the negative derivative of the potential energy with respect to x.

$$H(x, p) = \frac{p^2}{2m} + U(x).$$

$$\frac{\partial}{\partial x} H(x, p) = \frac{d}{dx} U(x)$$

$$\frac{\partial}{\partial p} H(x, p) = \frac{p}{m}.$$

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The postulates of quantum mechanics

2.1 The five postulates of quantum mechanics

Postulate 1

The wave function $\Psi(x, y, z, t)$ describes the temporal and spatial evolution of a quantum-mechanical particle. The wave function $\Psi(x, t)$ describes a particle with one degree of freedom of motion.

Postulate 2

The product $\Psi^*(x, t)\,\Psi(x, t)$ is the probability density function of a quantum-mechanical particle. $\Psi^*(x, t)\Psi(x, t)\,dx$ is the probability to find the particle in the interval between x and $x + dx$. Therefore,

$$\int_{-\infty}^{\infty} \Psi^*(x, t)\ \Psi(x, t)\,dx = 1 \qquad (2.1)$$

Postulate 3

The wave function $\Psi(x, t)$ and its derivative $(\partial / \partial x)\,\Psi(x, t)$ are continuous in an isotropic medium.

$$\lim_{x \to x_0} \Psi(x, t) = \Psi(x_0, t) \qquad (2.2)$$

$$\lim_{x \to x_0} \frac{\partial}{\partial x} \Psi(x, t) = \frac{\partial}{\partial x} \Psi(x, t)\bigg|_{x=x_0}. \qquad (2.3)$$

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Postulate 4

Dynamical variable in classical mechanics	*Quantum-mechanical operator*
x	x
$\mathrm{f}(x)$	$\mathrm{f}(x)$
p	$\frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial x}$
$\mathrm{f}(p)$	$\mathrm{f}\left(\frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial x}\right)$
E_{total}	$-\frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial t}$

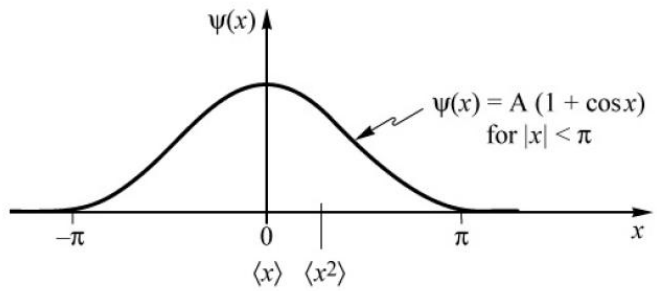
$$\frac{p^2}{2m} + U(x) = E_{\text{total}} \cdot \quad \Rightarrow \quad -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi(x,t) + U(x)\,\Psi(x,t) = -\frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial t}\Psi(x,t)\,.$$

Postulate 5

The expectation value, $\langle\xi\rangle$, of any dynamical variable ξ, is calculated from the wave function according to

$$\langle\xi\rangle = \int_{-\infty}^{\infty} \Psi^*(x,t)\,\xi_{\text{op}}\,\Psi(x,t)\,\mathrm{d}x \qquad (2.11)$$

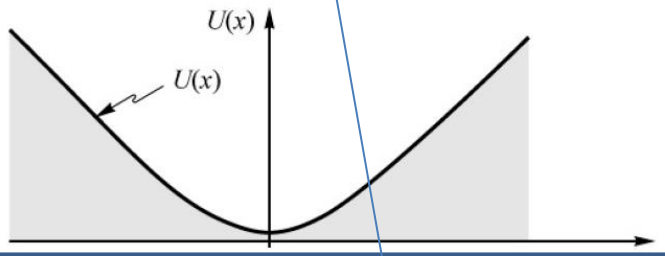
An example of a stationary wave function



$$\Psi(x,t) = \psi(x)\, e^{i\omega t}$$

$$\int_{-\infty}^{\infty} \psi^*(x)\,\psi(x)\,dx = 1 .$$

$$A = 1/\sqrt{3\pi}$$



expectation value of a particle $\langle x \rangle = \int_{-\infty}^{\infty} \psi^*(x)\, x\, \psi(x)\, dx$. $\Rightarrow$ $\langle x \rangle = 0$.

the standard deviation of any quantity, *e. g.* ξ, is defined as

$$\left(\langle \xi^2 \rangle - \langle \xi \rangle^2 \right)^{1/2}.$$

the spatial standard deviation of the particle on the *x* axis is given by

$$\sigma = \left(\langle x^2 \rangle - \langle x \rangle^2 \right)^{1/2}.$$

$$\langle x^2 \rangle = \int_{-\pi}^{\pi} \psi^*(x)\, x^2\, \psi(x)\, dx = \frac{\pi^2}{3} - \frac{5}{2}.$$

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Position and momentum space

plane wave is propagating along the x axis without any distortion

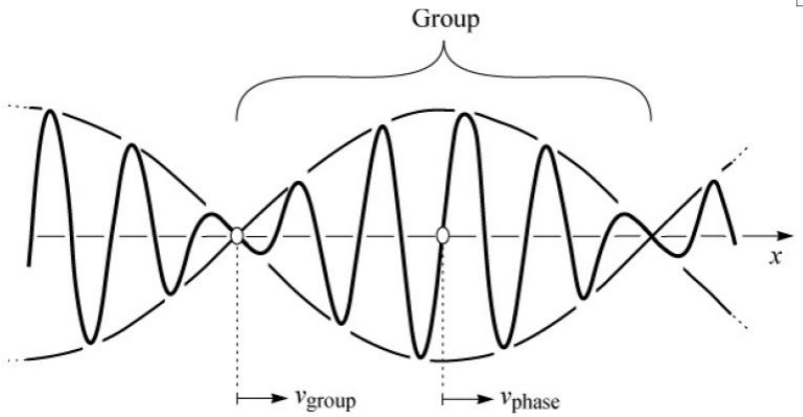
$$\Psi(x,t) = \Psi(x - v_{ph}\, t) \qquad \Psi(x,t) = A\cos(k\,x - \omega\,t).$$

constant phase are given by

$$k\,x - \omega\,t = \text{const.}$$

$$v_{ph} = \frac{dx}{dt} = \frac{\omega}{k}$$

$$v_{gr} = \frac{d\omega}{dk}$$



nondispersive media. $v_{ph} = v_{gr} = \frac{\omega}{k} = \frac{d\omega}{dk}.$

dispersive media $v_{gr} = v_{ph} + k\frac{dv_{ph}}{dk}$

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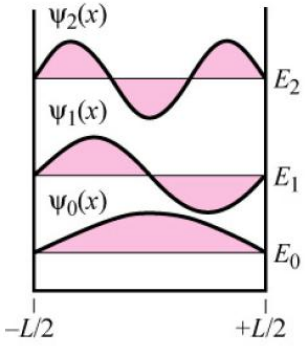
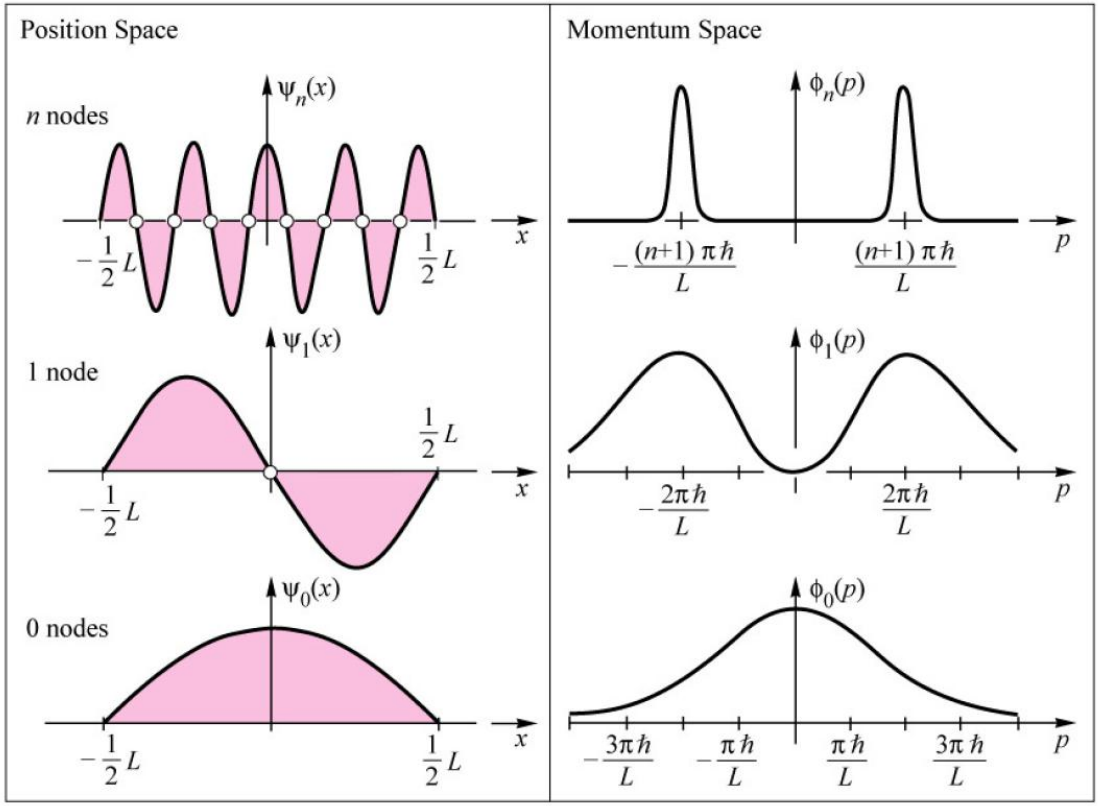
Position-space and momentum-space representation, and Fourier transform

$$\int_{-\infty}^{\infty} \psi^*(x)\,\psi(x)\,dx = \int_{-\infty}^{\infty} \Phi^*(p)\,\Phi(p)\,dp = 1$$





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Illustrative example: Position and momentum in the infinite square well

$$\psi_0(x) = \sqrt{\frac{2}{L}}\cos\left(\frac{\pi}{L}x\right) \qquad \left(|x| < \frac{1}{2}L\right)$$

$$\psi_n(x) = \sqrt{\frac{2}{L}}\cos\left(\frac{(n+1)\pi}{L}x + \frac{n\pi}{2}\right) \qquad \left(|x| < \frac{1}{2}L\right)$$

$$\Phi_0(p) = \int_{-\infty}^{\infty}\psi_0(x)\,e^{-ipx/\hbar}\,dx$$

$$= \sqrt{\frac{L}{\pi\hbar}}\left[\left(\frac{1}{\pi - pL/\hbar}\right)\cos\left(\frac{L}{2\hbar}p\right) + \left(\frac{1}{\pi + pL/\hbar}\right)\cos\left(\frac{L}{2\hbar}p\right)\right]$$

$$\Phi_n(p) = \int_{-\infty}^{\infty}\psi_n(x)\,e^{-ipx/\hbar}\,dx$$

$$= \frac{1/2}{\sqrt{\pi L\hbar}}\left[\frac{1}{i\alpha}\left(i^{n+1}\,e^{-i\frac{pL}{2\hbar}} - i^{-(n+1)}\,e^{i\frac{pL}{2\hbar}}\right) + \frac{1}{i\beta}\left(i^{-(n+1)}\,e^{-i\frac{pL}{2\hbar}} - i^{(n+1)}\,e^{i\frac{pL}{2\hbar}}\right)\right]$$

$$\alpha = (n+1)(\pi/L) - (p/\hbar) \quad \text{and} \quad \beta = -(n+1)(\pi/L) - (p/\hbar)$$

$$\langle p\rangle = \int_{-\infty}^{\infty}\psi^*(x)\,\frac{\hbar}{i}\,\frac{d}{dx}\,\psi(x)\,dx \qquad \langle p\rangle = 0.$$

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Operators

DYNAMICAL VARIABLE		OPERATOR REPRESENTATION	
Variable		Position space	Momentum space
Position	x	x	$-\frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial p_x}$
Potential energy	$U(x)$	$U(x)$	$U\left(-\frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial p_x}\right)$
	$f(x)$	$f(x)$	$\mathrm{f}\left(-\frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial p_x}\right)$
Momentum	p_x	$\frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial x}$	p_x
Kinetic energy	$\frac{p_x^2}{2m}$	$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$	$\frac{p_x^2}{2m}$
	$f(p_x)$	$\mathrm{f}\left(\frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial x}\right)$	$f(p_x)$
Total energy	E_{total}	$-\frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial t}$	$-\frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial t}$
Total energy	E_{total}	$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+U(x)$	$\frac{p_x^2}{2m}+U\left(-\frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial p_x}\right)$

$$H\,\psi(x) = -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\,\psi(x) + U(x)\,\psi(x)$$

$$H\,\Phi(p) = \frac{p^2}{2m}\Phi(p) + U\left(-\frac{\hbar}{\mathrm{i}}\frac{\mathrm{d}}{\mathrm{d}p}\right)\Phi(p)\ .$$

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Eigenfunctions and eigenvalues $\xi_{op}\, f(x) = \lambda_s\, f(x)$

For example $\frac{d}{dx} e^{\lambda_s x} = \lambda_s\, e^{\lambda_s x}$

Linear operators $\xi_{op}\, c\, \psi(x) = c\, \xi_{op}\, \psi(x)$

commutation law $x\, p = p\, x$

Hermitian operators

hermitian operators satisfy the condition

$\lambda = \lambda^*$ eigenvalue λ

$$\int_{-\infty}^{\infty} \psi_1^*(x)\, \xi_{op}\, \psi_2(x)\, dx = \int_{-\infty}^{\infty} \psi_2(x)\, \xi_{op}^*\, \psi_1^*(x)\, dx$$

The Dirac bracket notation

$$\langle \Psi | \xi_{op} | \Psi \rangle = \int_{-\infty}^{\infty} \Phi^*(p,t)\, \xi_{op}\, \Phi(p,t)\, dp$$

$$\langle \Psi | \xi_{op} | \Psi \rangle = \int_{-\infty}^{\infty} \Psi^*(x,t)\, \xi_{op}\, \Psi(x,t)\, dx$$

$$\langle \Psi_1 | \xi_{op} | \Psi_2 \rangle = \langle \Psi_1 | \xi_{op}\, \Psi_2 \rangle$$

$$\langle \xi_{op}\, \Psi_1 | \Psi_2 \rangle = \int_{-\infty}^{\infty} \psi_2(x)\, \xi_{op}^*\, \psi_1^*(x)\, dx$$

$$\langle \Psi_1 | \xi_{op}\, \Psi_2 \rangle = \langle \xi_{op}\, \Psi_1 | \Psi_2 \rangle$$

$$\langle \Psi_1 | \xi_{op} | \Psi_2 \rangle = \langle \Psi_2 | \xi_{op} | \Psi_1 \rangle^*$$

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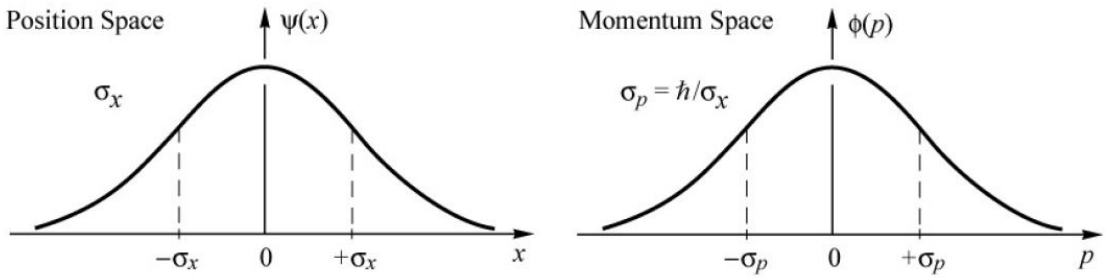
The Heisenberg uncertainty principle

$$(\Delta\xi)^2 = \left\langle \left(\xi - \langle\xi\rangle\right)^2 \right\rangle$$

Position–momentum uncertainty

$$\Delta x\, \Delta p \geq \hbar$$



Energy – time uncertainty

$$\Delta E\, \Delta t \geq \hbar$$

The Schrödinger equation

The time-dependent Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi(x,t) + U(x)\Psi(x,t) = -\frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial t}\Psi(x,t)$$

$$H\Psi(x,t) = -\frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial t}\Psi(x,t)$$

partial differential equation

با جداسازی متغیرها داریم:

$$\Psi(x,t) = \psi(x)\, \mathrm{e}^{-\mathrm{i}Et/\hbar}$$

$$\Psi(x,t) = \psi(x)\, \mathrm{f}(t)$$

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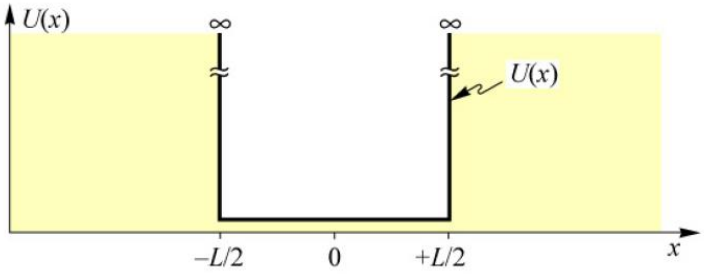
The time-independent Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) + U(x)\psi(x) = E\psi(x) \qquad H\psi(x) = E\psi(x).$$

$$\langle \psi_n | \psi_m \rangle = 0. \qquad \int_{-\infty}^{\infty} \psi_m^* \psi_n \, dx = 0$$

Applications of the Schrödinger equation in nonperiodic semiconductor structures

(a)



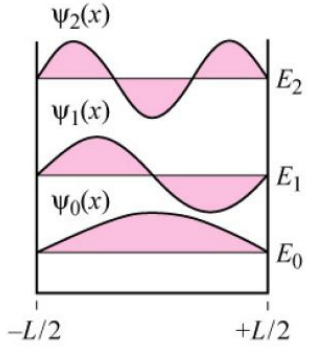
even

$$\psi_n(x) = A\cos\frac{(n+1)\pi x}{L} \qquad \left(n = 0, 2, 4, \cdots \text{ and } |x| \le \frac{L}{2}\right)$$

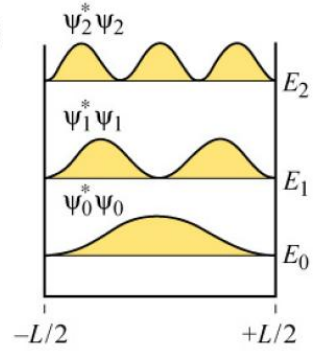
and for odd-symmetry states

$$\psi_n(x) = A\sin\frac{(n+1)\pi x}{L} \qquad \left(n = 1, 3, 5, \cdots \text{ and } |x| \le \frac{L}{2}\right).$$

(b)



(c)



$$\langle \psi | \psi \rangle = 1 \Rightarrow A = \sqrt{2/L}.$$

ground-state $$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\sqrt{\frac{2}{L}}\cos\left(\frac{\pi x}{L}\right) = E_0\sqrt{\frac{2}{L}}\cos\left(\frac{\pi x}{L}\right)$$

$$E_0 = \frac{\hbar^2}{2m}\left(\frac{\pi}{L}\right)^2 \qquad E_n = \frac{\hbar^2}{2m}\left[\frac{(n+1)\pi}{L}\right]^2$$

$$\langle E_{\text{kin},0} \rangle = \left\langle \psi_0 \left| \frac{p^2}{2m} \right| \psi_0 \right\rangle \Rightarrow \langle E_{\text{kin},n} \rangle = \frac{\hbar^2}{2m}\left[\frac{(n+1)\pi}{L}\right]^2$$

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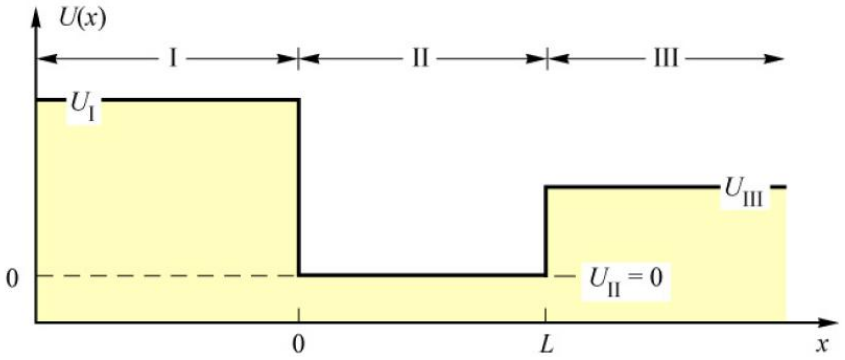
The asymmetric and symmetric finite square-shaped quantum well



first case $(E > U)$

$$\psi(x) = A\cos kx + B\sin kx$$

$$k = \sqrt{2mE/\hbar^2}$$

second case $(E < U)$

$$\psi(x) = C\,e^{\kappa x} + D\,e^{-\kappa x}$$

$$\kappa = \sqrt{2m(U - E)/\hbar^2}$$

$$= \sqrt{\frac{2mU}{\hbar^2} - k^2}\,.$$

$$\psi_I(x) = A\,e^{\kappa_I x}$$

$$\psi_{II}(x) = A\cos kx + B\sin kx$$

$$\psi_{III}(x) = (A\cos kL + B\sin kL)\,e^{-\kappa_{III}(x-L)}$$

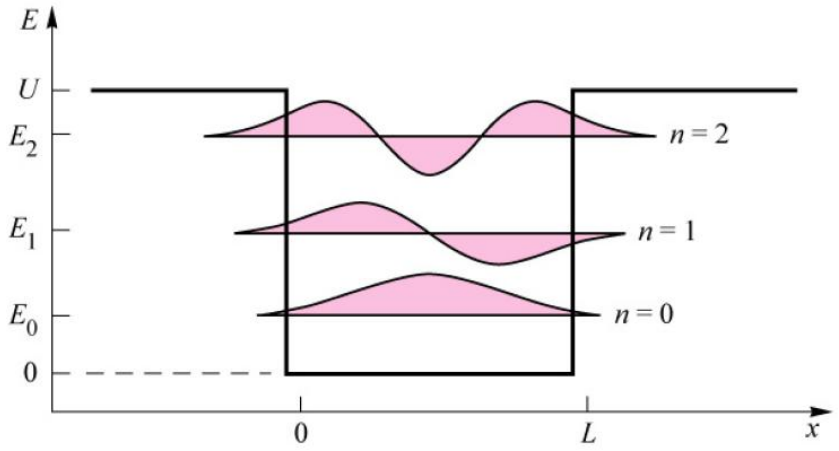


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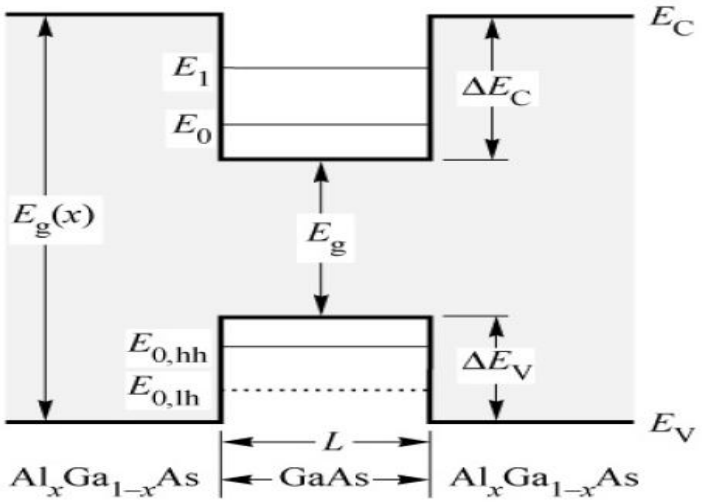
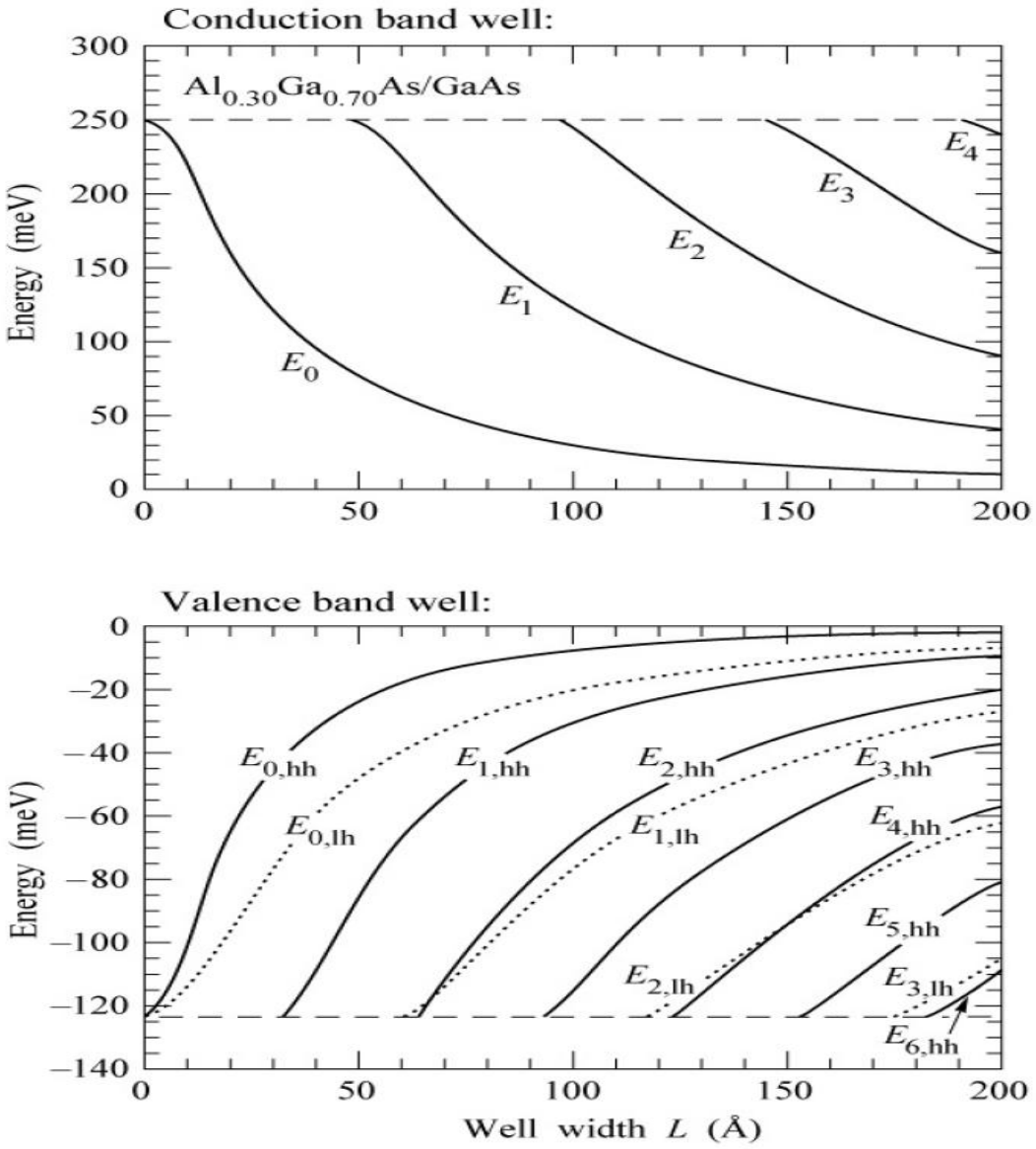
Figure 7.5 shows the numerical solutions for bound states in the conduction band and valence band of an $Al_{0.30}Ga_{0.70}As$ / GaAs square-shaped quantum well. The graph reveals that there is only one bound state in the conduction band well for well widths smaller than approximately 50 Å. Does this agree with the analytic result of Eq. (7.36)?



$$E_{g,\,Al_xGa_{1-x}As} = (1.424 + 1.247 \times x)\ \text{eV}$$
$$\Delta E_c = (2/3)\,\Delta E_g$$
$$\Delta E_v = (1/3)\,\Delta E_g$$
$$m^*_{e,\,Al_xGa_{1-x}As} = (0.067 + 0.083 \times x)\,m_0$$
$$m^*_{hh,\,Al_xGa_{1-x}As} = (0.45 + 0.30 \times x)\,m_0$$
$$m^*_{lh,\,Al_xGa_{1-x}As} = (0.08 + 0.057 \times x)\,m_0$$

Fig. 7.5. Quantized energies of subbands in the conduction band and valence band of an $Al_xGa_{1-x}As$ / GaAs single quantum well structure at room temperature. There are different subbands for heavy holes (hh) and light holes (lh) in the valence band.



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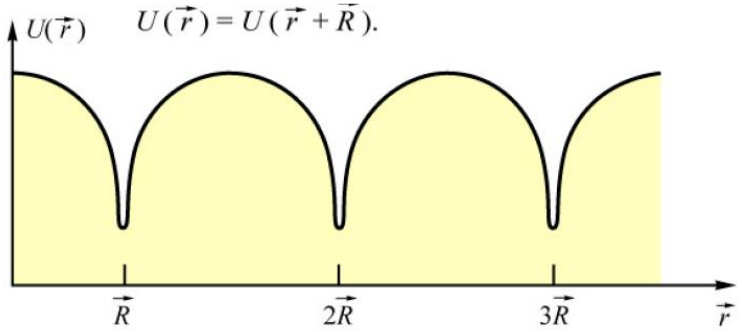
Applications of the Schrödinger equation in periodic semiconductor structures

Free electrons

$$-\frac{\hbar^2}{2m}\nabla^2\psi + U\psi = E\psi \qquad E = \frac{\hbar^2}{2m}\left(k_x^2 + k_y^2 + k_z^2\right).$$

$$\psi(\vec{r}) = A\,e^{i\vec{k}\cdot\vec{r}}$$

The Bloch theorem



$$U(\vec{r}) = U(\vec{r} + n\vec{R}) \qquad \text{for} \qquad n = 1, 2, 3, \ldots$$

$$\psi_{nk}(\vec{r}) = u_{nk}\,e^{i\vec{k}\cdot\vec{r}}$$

$$u_{nk}(\vec{r}) = u_{nk}(\vec{r} + \vec{R}) = u_{nk}(\vec{r} + 2\vec{R}) = \cdots$$

$$\psi_{nk}(\vec{r} + \vec{R}) = \psi_{nk}(r)\,e^{i\vec{k}\cdot\vec{R}}$$

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The Kronig–Penney model

energy band structure or ***band structure*** of the lattice

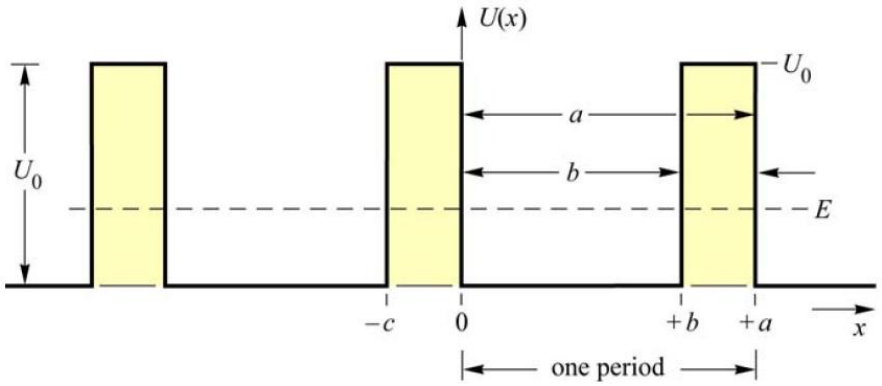

Fig. 8.2. Periodic square well potential used for the Kronig-Penney calculation. The height of the barriers is U_0 and the electron energy is denoted as E.

Introducing the abbreviations

$$\alpha^2 = 2mE/\hbar^2$$

$$\beta^2 = 2m(U_0 - E)/\hbar^2$$

time-independent Schrödinger equation can be written

$$\frac{d^2\psi}{dx^2} + \alpha^2\psi = 0 \qquad \text{for} \quad 0 \le x \le b$$

$$\frac{d^2\psi}{dx^2} + \beta^2\psi = 0 \qquad \text{for} \quad -c < x < 0 .$$

Insertion of the Bloch wave function into the Schrödinger equation

$$\frac{d^2u_{nk}}{dx^2} + 2ik\frac{du_{nk}}{dx} - k^2u_{nk} + \alpha^2u_{nk} = 0 \qquad \text{for} \quad 0 \le x \le b$$

and

$$\frac{d^2u_{nk}}{dx^2} + 2ik\frac{du_{nk}}{dx} + k^2u_{nk} + \beta^2u_{nk} = 0 \qquad \text{for} \quad -c < x < 0$$

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با حل این معادله و اعمال شرایط مرزی خواهیم داشت:

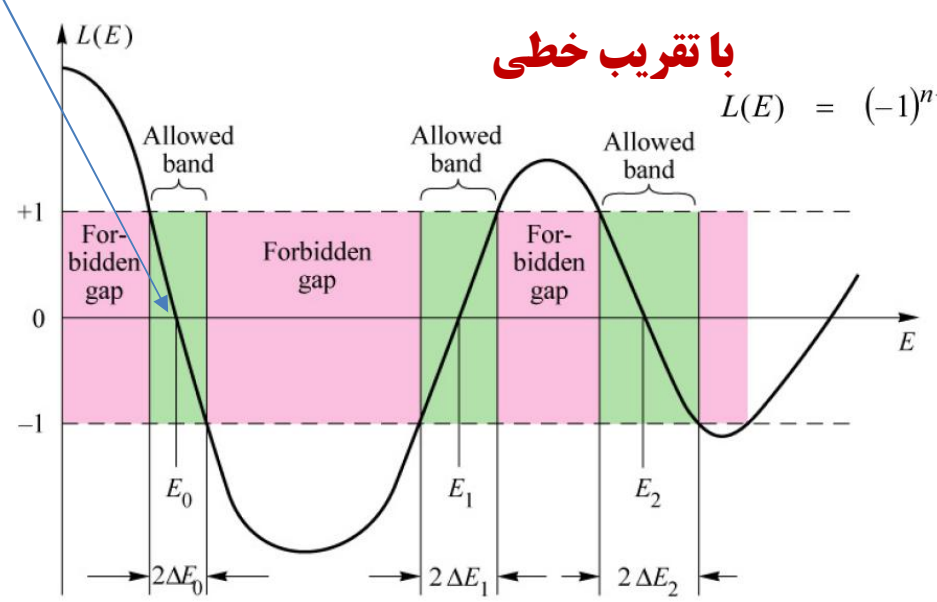
$$L(E) = \frac{\beta^2 - \alpha^2}{2\alpha\beta}\sinh(\beta c)\sin(\alpha b) + \cosh(\beta c)\cos(\alpha b)$$

$$= \frac{U_0 - 2E}{2\sqrt{E U_0 - E^2}}\sinh\left(\sqrt{\frac{2m}{\hbar^2}(U_0 - E)}\, c\right)\sin\left(\sqrt{\frac{2m}{\hbar^2}E}\, b\right)$$

$$+ \cosh\left(\sqrt{\frac{2m}{\hbar^2}(U_0 - E)}\, c\right)\cos\left(\sqrt{\frac{2m}{\hbar^2}E}\, b\right)$$

$$L(E) = \cos(k a)$$

$$L(E) = -\frac{1}{\Delta E_0}(E - E_0)$$



با تقریب خطی

$$L(E) = (-1)^{n+1}\frac{1}{\Delta E_n}(E - E_n)$$

$$L(E) = \cos(k a)$$

$$E = E_0 - \Delta E_0 \cos ka$$

$$E = E_n + (-1)^{n+1}\Delta E_n \cos ka$$

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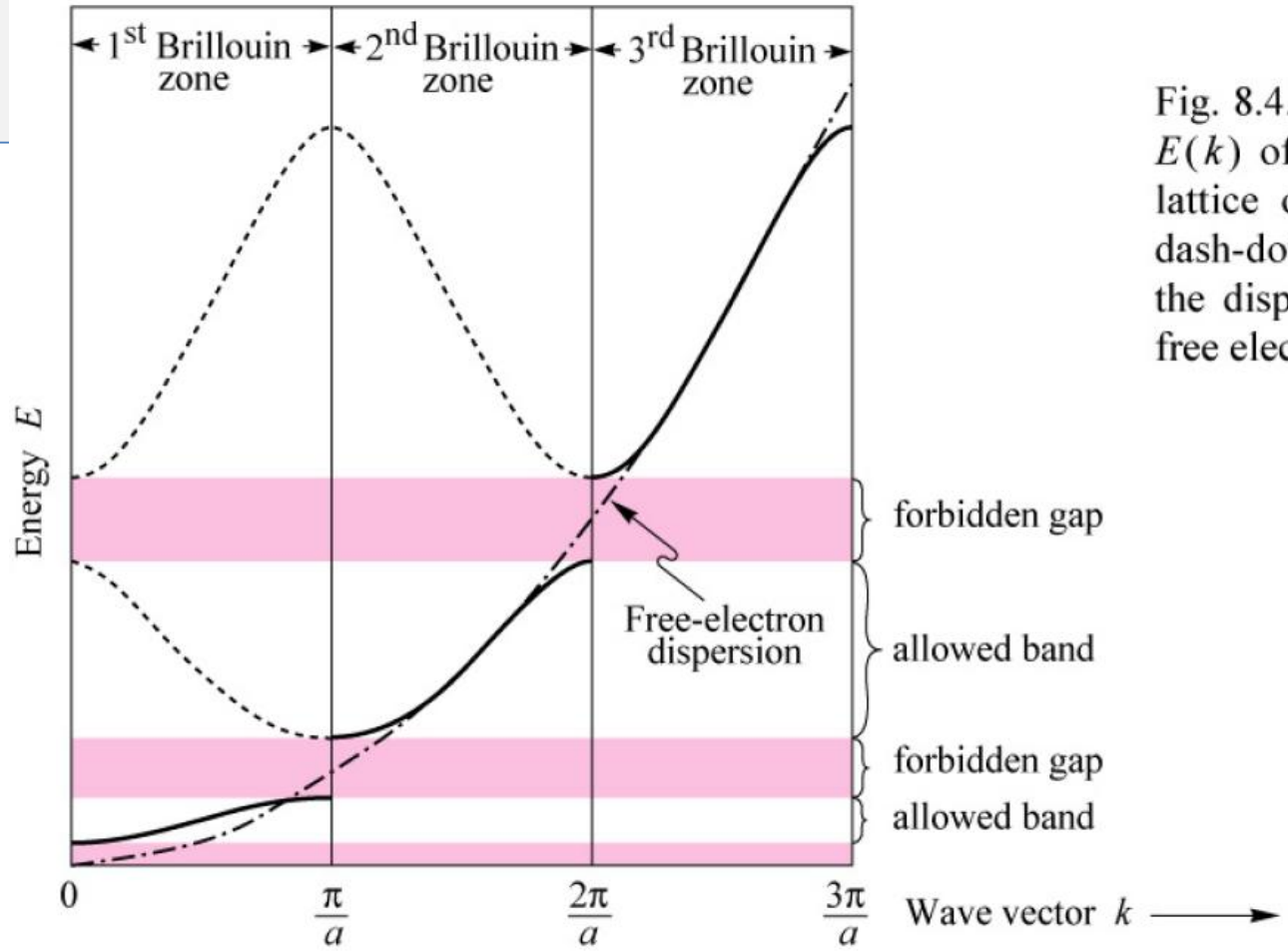

Fig. 8.4. Dispersion relation $E(k)$ of a one-dimensional lattice of a period a. The dash-dotted line represents the dispersion relation of a free electron.

Bragg reflection condition

$$n\lambda = 2a$$

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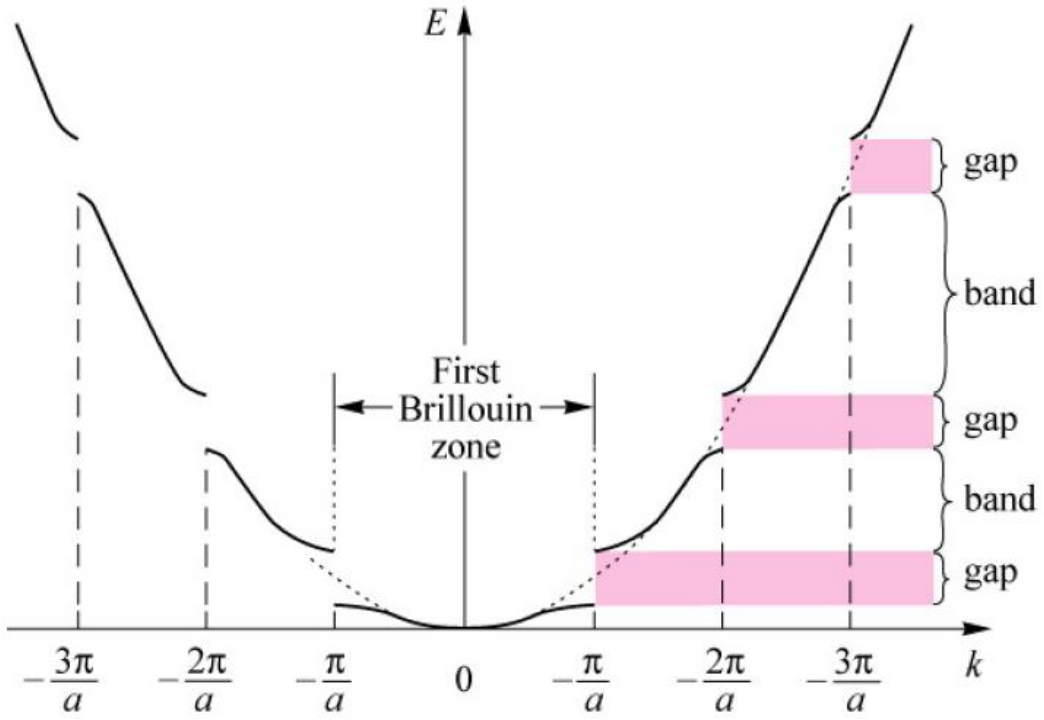

Fig. 8.5. The energy of an electron as a function of its wave vector (*i. e.* dispersion relation) in a one-dimensional periodic potential.

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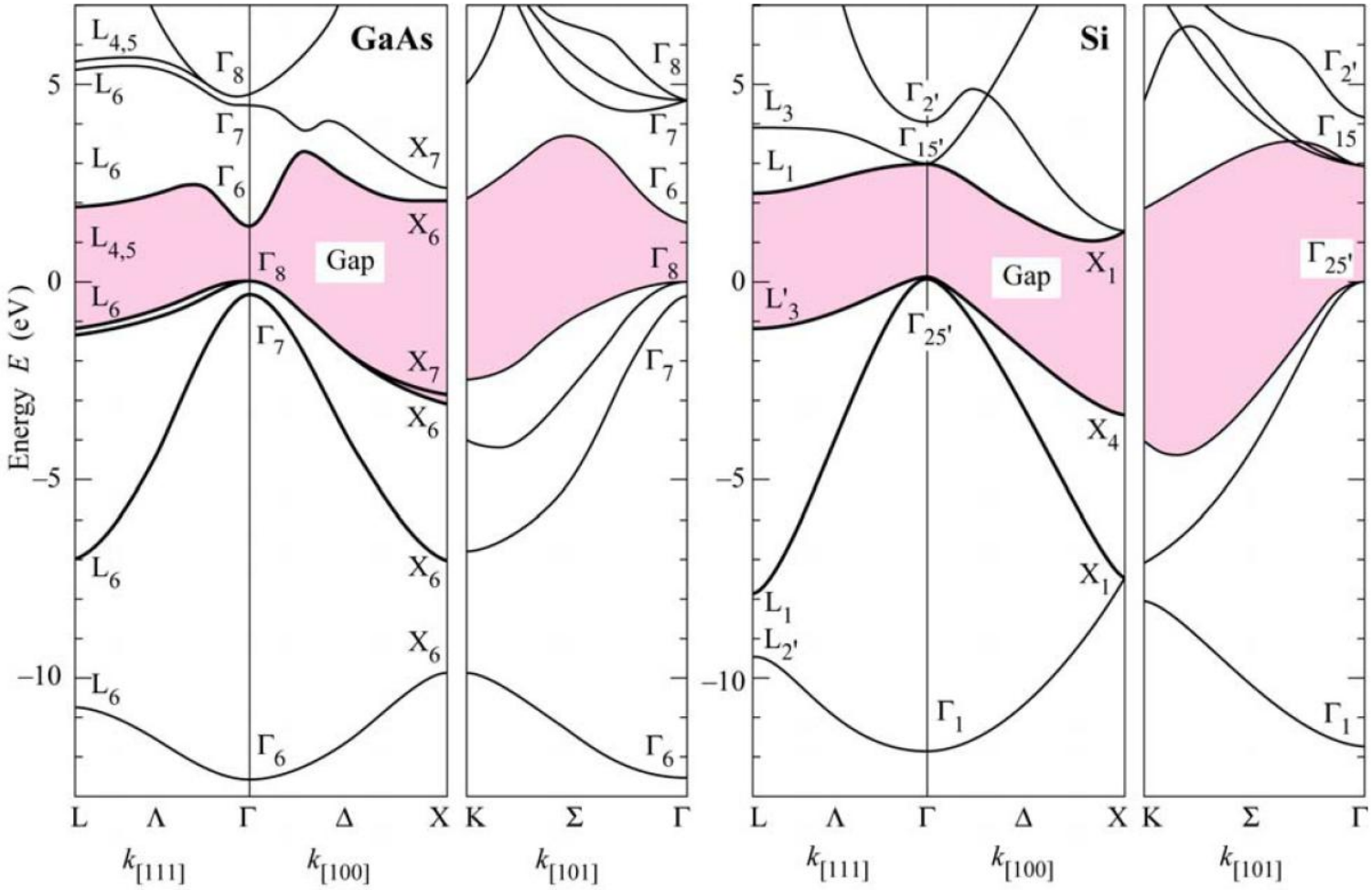

Fig. 8.6 Dispersion relation (band structure) for electrons and holes in the conduction and valence band within the first Brillouin zone for GaAs and Si.

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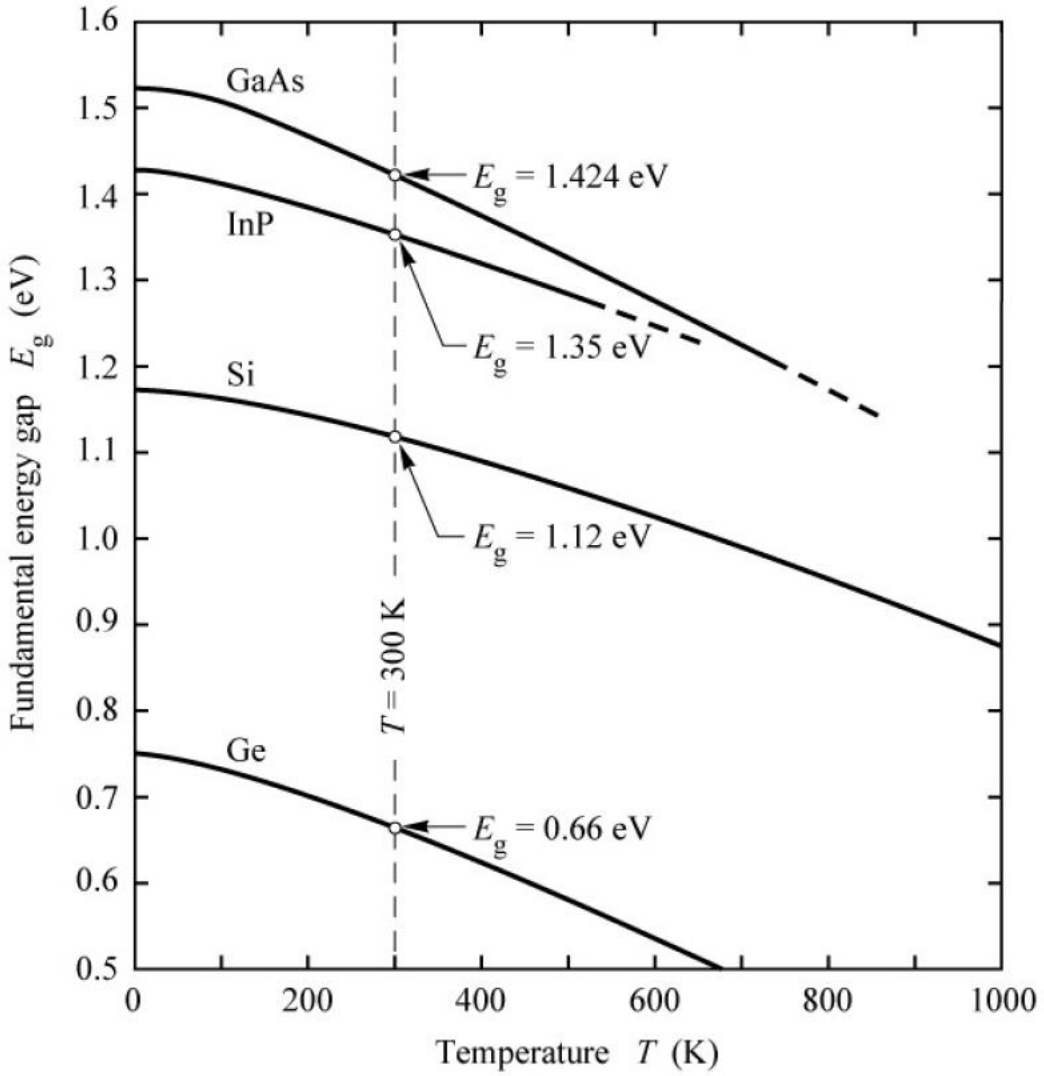

$$E_g = E_g(0\text{K}) - \frac{\alpha T^2}{T + \beta}$$

	E_g(0K)	α (10^{-4} eV/K)	β (K)
GaAs	1.519	5.41	204
InP	1.425	4.50	327
Si	1.170	4.73	636
Ge	0.744	4.77	235

Fig. 8.7. Fundamental energy gap of GaAs, InP, Si, and Ge as a function of temperature. The energy gap can be approximated by a parabolic equation with the fitting parameters α and β.

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The effective mass

$m_0 = 9.11 \times 10^{-31}$ kg ⇒ m^* due to the influence of the periodic potential

$F = ma$

$a = (\mathrm{d}/\mathrm{d}t)\, v_{gr} = (\mathrm{d}/\mathrm{d}t)\, \mathrm{d}\omega/\mathrm{d}k,$

$E = \hbar\omega.$

$$a = \frac{1}{\hbar}\frac{\mathrm{d}^2E}{\mathrm{d}t\,\mathrm{d}k} = \frac{1}{\hbar}\frac{\mathrm{d}^2E}{\mathrm{d}k^2}\frac{\mathrm{d}k}{\mathrm{d}t}$$

$$F = \frac{\mathrm{d}p}{\mathrm{d}t} = \hbar\frac{\mathrm{d}k}{\mathrm{d}t}$$

$$m^* = \frac{\hbar^2}{\mathrm{d}^2E/\mathrm{d}k^2}$$

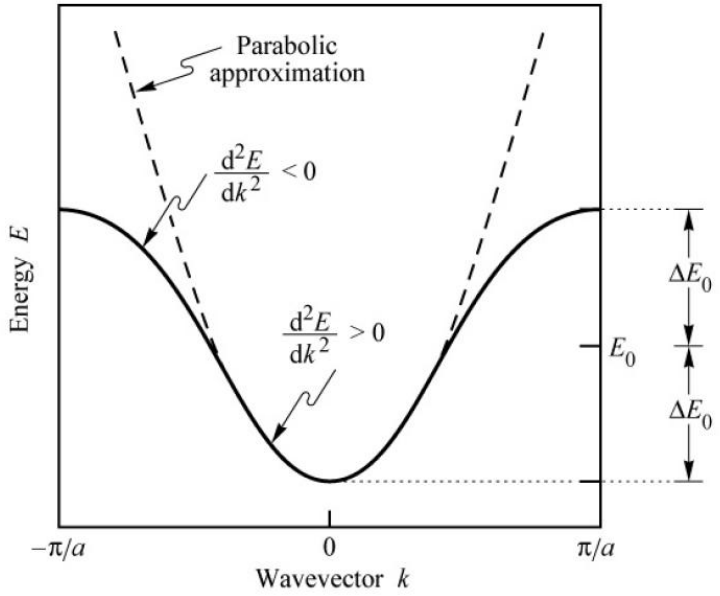

Fig. 8.8. Dispersion relation of a one-dimensional lattice with positive effective mass ($\mathrm{d}^2E/\mathrm{d}k^2 > 0$) near the zone-center, and negative effective mass ($\mathrm{d}^2E/\mathrm{d}k^2 < 0$) near the zone-boundary. close to the zone-center, the dispersion relation can be approximated by a parabola.

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Generally, the effective mass is a tensor and not just a scalar

$$\begin{pmatrix} F_x \\ F_y \\ F_z \end{pmatrix} = \begin{pmatrix} m^*_{xx} & m^*_{xy} & m^*_{xz} \\ m^*_{yx} & m^*_{yy} & m^*_{yz} \\ m^*_{zx} & m^*_{zy} & m^*_{zz} \end{pmatrix} \begin{pmatrix} a_x \\ a_y \\ a_z \end{pmatrix}$$

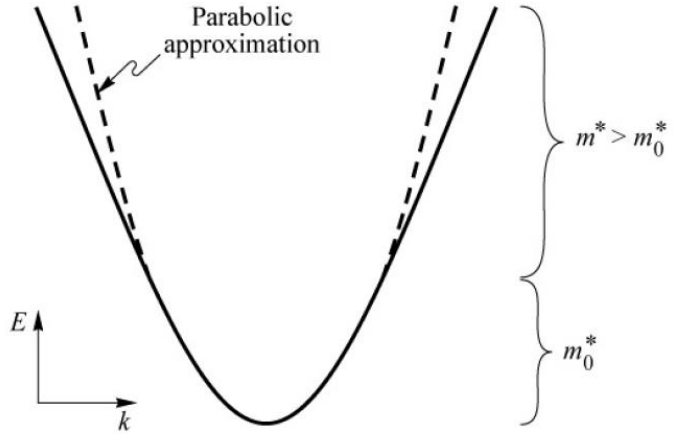
$$a_y = \frac{1}{\hbar}\frac{\partial^2 E}{\partial k_y\,\partial t} = \frac{1}{\hbar}\frac{\partial^2 E}{\partial k_y\,\partial k_x}\frac{\partial k_x}{\partial t} \qquad F_x = \frac{dp_x}{dt} = \hbar\frac{dk_x}{dt}$$

$$m^*_{xy} = \hbar^2\left(\frac{\partial^2 E}{\partial k_x\,\partial k_y}\right)^{-1}$$

direction of the force — direction of the acceleration

with an isotropic dispersion relation with a band minimum at $k = 0$

In the case of an isotropic semiconductor it is $m_{xx}^* = m_{yy}^* = m_{zz}^*$



$$m^* = m_0^*\left(1 + \frac{E - (E_0 - \Delta E_0)}{\Delta E_0}\right)$$

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Approximate solutions of the Schrödinger equation

The WKB method

Wentzel, Kramers Brillouin (1926)

The WKB approximation can be used, if the potential energy $U(x)$ varies *slowly*. Specifically, changes in $U(x)$ should be small on the length scale of the de Broglie wavelength.

$$\psi(x) = e^{i\phi(x)}$$

$\phi(x)$ represents the *phase* of the wave

In a constant potential $\phi(x) = \pm k\,x$

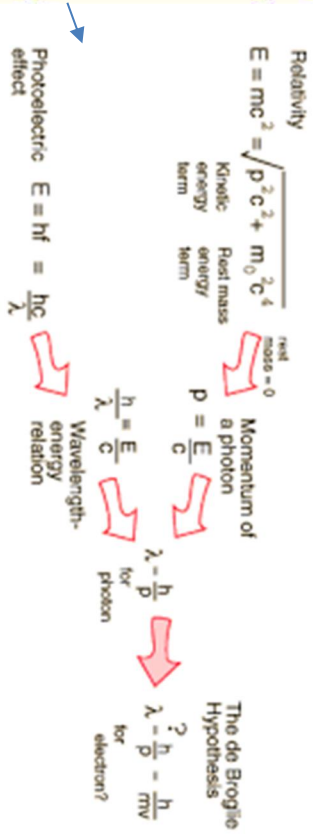
$$k(x) = \frac{1}{\hbar}\sqrt{2\,m\,[E - U(x)]} \qquad \text{for} \quad E \geq U(x)$$

$$k(x) = \frac{-i}{\hbar}\sqrt{2\,m\,[U(x) - E]} = -i\,\kappa(x) \qquad \text{for} \quad E \leq U(x).$$

بعد از محاسباتی

$$\psi(x) \approx \exp\left(\pm i \int_x k(x)\,dx\right) \qquad \text{(zero-order WKB)}$$

$$\psi(x) \approx \frac{1}{\sqrt{k(x)}} \exp\left(\pm i \int_x k(x)\,dx\right) \qquad \text{(first-order WKB)}$$



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$$\psi_{III}(x) = \psi_{III}(0)\exp\left[-\int_0^x \kappa(x)\,dx\right] = \psi_{III}(0)\exp\left\{-\int_0^x \frac{1}{\hbar}\sqrt{2m\left[U(x)-E\right]}\,dx\right\}$$

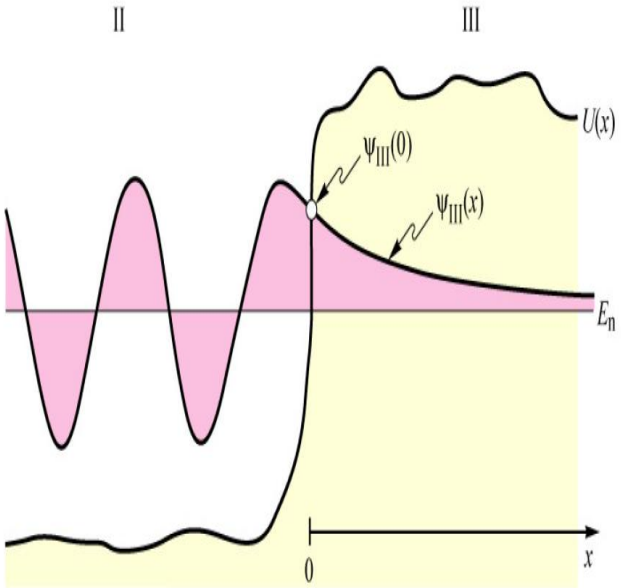
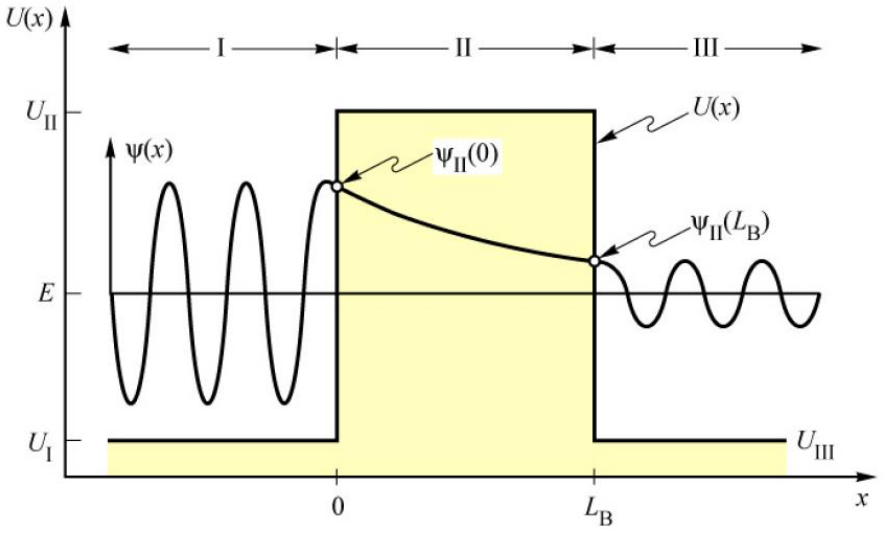


Fig. 9.1 Oscillating and exponentially decaying wavefunction in the classically allowed region II and disallowed region III, respectively. The decaying wave function in region III can be calculated by the WKB approximation.



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4. Numerical Solution of the Schrödinger Equation

For a complex $V(x)$, the time-independent Schrödinger equation describing may need to be solved numerically

$$H\psi_n(\mathbf{r}) = \left(\frac{-\hbar^2}{2m}\nabla^2 + V(\mathbf{r})\right)\psi_n(\mathbf{r}) = E_n\psi_n(\mathbf{r}) \qquad (38)$$

1st should discretize the functions, to a set of $N+1$ equally-spaced points, $x_j = \mathrm{j}\times h_0$ and $x_{j+1} \equiv x_j + h_0$ where $j = 0, 1, 2, \ldots, N$.

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We wish to solve the Schrödinger equation in a region of length $L = Nh_0$.

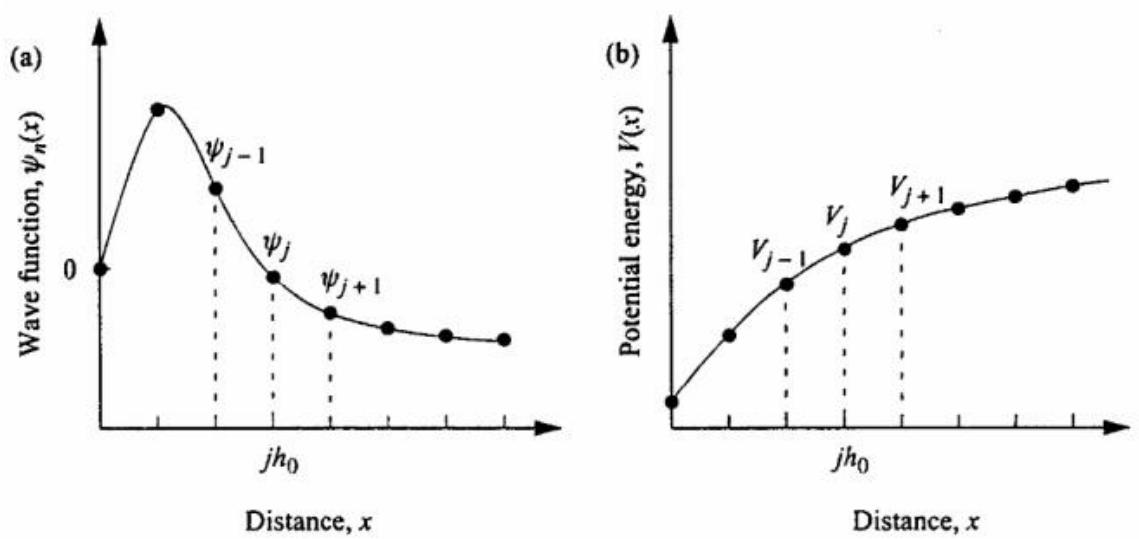

Fig. 5: (a) Sampling $\psi(x)$ (b) $V(x)$ at equally-spaced intervals of h_0.

At each sampling point, j, $\psi_j = \psi(x_j)$ and $V_j = V(x_j)$.

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In the finite- difference approximation:

$$d\psi(x_j)/dx = [\psi(x_j) - \psi(x_{j-1})]/h_0 \qquad (39)$$

and $$d^2\psi(x_j)/dx^2 = [\psi(x_{j-1}) - 2\psi(x_j) + \psi(x_{j+1})]/h_0^2 \qquad (40)$$

Eqn (40) into Eqn (38) results in the matrix equation,

$$H\psi(x_j) = -u_j\psi(x_{j-1}) + d_j\psi(x_j) - u_{j+1}\psi(x_{j+1}) = E\psi(x_j) \qquad (41)$$

The Hamiltonian is a symmetric tri-diagonal matrix, with

diagonal matrix $$d_j = \hbar^2/mh_0^2 + V_j \qquad (42)$$

and off-diagonal matrix $$u_j = \hbar^2/2mh_0^2 \qquad (43)$$

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As discussed for a particle of mass m in an infinite 1-D, rectangular potential well, at boundaries $\psi_0(x_0) = \psi_N(x_N) = 0$.

Because the boundary conditions force the wave function to zero at positions $x = 0$ and $x = L$, Eqn (41) may be written as

$$(\mathbf{H} - E\mathbf{I})\psi =$$

$$= \begin{bmatrix} (d_1 - E) & -u_2 & 0 & 0 & \cdots \\ -u_2 & (d_2 - E) & -u_3 & 0 & \cdots \\ 0 & -u_3 & (d_3 - E) & -u_4 & \cdots \\ \vdots & \vdots & \vdots & \ddots & \\ & & & -u_{N-1} & (d_{N-1} - E) \end{bmatrix} \begin{bmatrix} \psi_1 \\ \psi_2 \\ \\ \\ \psi_{N-1} \end{bmatrix} = 0 \qquad (44)$$

H = The Hamiltonian matrix and **I** = The identity matrix.

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Because the particle is not transmitted beyond the boundaries $x = 0$ and $x = L$ (quantum nontransmitting boundary problem).

When there are transmitting boundaries at positions $x = 0$ and $x = L$, then $\psi_0(x_0) \neq 0$ and $\psi_N(x_N) \neq 0$.

In this case there is the possibility of unbound particle states as well as sources and sinks of particle flux to consider.

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Perturbation theory

Perturbation theory is one of the most important methods for obtaining approximate solutions to Schrödinger's equation.

First-order time-independent perturbation theory

$$H^0 \psi_n^0 = E_n^0 \psi_n^0 .$$ *unperturbed*

$$H = H^0 + \lambda H'$$ perturbation on ($\lambda = 1$) and off ($\lambda = 0$)

$$H \psi_n = \left(H^0 + \lambda H'\right)\psi_n = E_n \psi_n$$

an expansion of E_n and ψ_n in a power series in λ

$$\lim_{\lambda \to 0} E_n = E_n^0$$

$$\lim_{\lambda \to 0} \psi_n = \psi_n^0 .$$

$$E_n = E_n^0 + \lambda E_n' + \lambda^2 E_n'' + \cdots$$

$$\psi_n = \psi_n^0 + \lambda \psi_n' + \lambda^2 \psi_n'' + \cdots$$

$$E_n' = dE_n / d\lambda \quad \text{and} \quad \psi_n' = d\psi_n / d\lambda$$

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$$\lambda^0 \left(H^0 \psi_n^0 - E_n^0 \psi_n^0 \right)$$

$$+ \lambda^1 \left(H^0 \psi_n' + H' \psi_n^0 - E_n^0 \psi_n' - E_n' \psi_n^0 \right)$$

$$+ \lambda^2 \left(H^0 \psi_n'' + H' \psi_n' - E_n^0 \psi_n'' - E_n' \psi_n' - E_n'' \psi_n^0 \right)$$

$$+ \lambda^3 (\cdots)$$

$$+ \lambda^4 (\cdots)$$

$$+ \cdots = 0 .$$

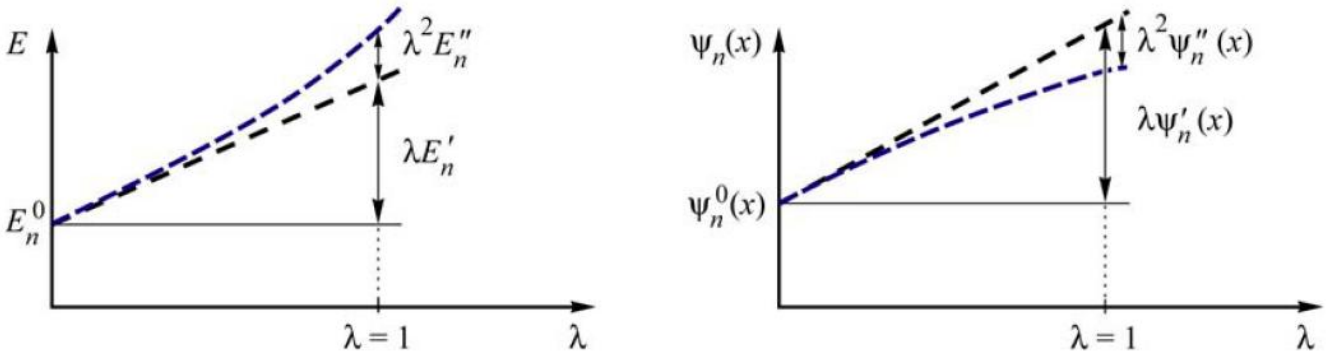

Fig. 10.1. Illustration of first-order and second-order corrections terms to the unperturbed energy E_n^0 and to the amplitude of the unperturbed wavefunction ψ_n^0 at a particular position x. The parameter λ is a parameter that controls the magnitude of the perturbation; $\lambda = 0$ corresponds to "no perturbation".

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0th order terms: $$H^0 \psi_n^0 = E_n^0 \psi_n^0$$

1st order terms: $$H^0 \psi_n' + H' \psi_n^0 = E_n^0 \psi_n' + E_n' \psi_n^0$$

2nd order terms: $$H^0 \psi_n'' + H' \psi_n' = E_n^0 \psi_n'' + E_n' \psi_n' + E_n'' \psi_n^0$$

. Note that in the above three equations, H^0, ψ_n^0, E_n^0, and H' are known.

It is the purpose of first-order perturbation theory to find solutions for E_n' and ψ_n'

برای شروع داریم:

$$\psi_n' = \sum_j a_j \psi_j^0$$

$$H^0 \sum_j a_j \psi_j^0 + H' \psi_n^0 = E_n^0 \sum_j a_j \psi_j^0 + E_n' \psi_n^0 .$$

Using

$$H^0 \sum_j a_j \psi_j^0 = \sum_j a_j E_j^0 \psi_j^0$$

one obtains

$$\sum_j a_j E_j^0 \psi_j^0 + H' \psi_n^0 = E_n^0 \sum_j a_j \psi_j^0 + E_n' \psi_n^0 .$$

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$$\sum_j a_j E_j^0 \psi_j^0 + H' \psi_n^0 = E_n^0 \sum_j a_j \psi_j^0 + E_n' \psi_n^0$$

Pre-multiplication of Eq. (10.15) with ψ_m^{0*}, and integration over position space yields

$$a_m E_m^0 + \langle \psi_m^0 | H' | \psi_n^0 \rangle = a_m E_n^0 + E_n' \delta_{mn}$$

$\langle \psi_m^0 | \psi_j^0 \rangle = 0$ for $m \neq j$

$\langle \psi_m^0 | \psi_j^0 \rangle = \delta_{mj}$

$\langle \psi_m^0 | \psi_j^0 \rangle = 1$ for $m = j$

$\langle \psi_m^0 | \psi_n^0 \rangle = \delta_{mn}$

$m = n$:

$$E_n' = \langle \psi_n^0 | H' | \psi_n^0 \rangle$$

$$E_n = E_n^0 + \lambda \langle \psi_n^0 | H' | \psi_n^0 \rangle$$

Furthermore, one obtains for

$m \neq n$:

$$a_m = \frac{\langle \psi_m^0 | H' | \psi_n^0 \rangle}{E_n^0 - E_m^0}$$

except the value of $a_{m=n}$

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value of $a_{m=n}$ $\Rightarrow$ $\left\langle \psi_n^0 + \lambda\psi'_n \,|\, \psi_n^0 + \lambda\psi'_n \right\rangle = 1$

$m = n$:

$$\int_{-\infty}^{\infty} \left(\psi_n^0 + \lambda \sum_m a_m \psi_m^0 \right)^* \left(\psi_n^0 + \lambda \sum_m a_m \psi_m^0 \right) dx = 1 + \lambda a_m + \lambda a_m^* + \lambda^2 \sum_m a_m a_m^* = 1$$

$$\psi_n = \psi_n^0 + \lambda \sum_{m \neq n} \frac{\left\langle \psi_m^0 \,|\, H' \,|\, \psi_n^0 \right\rangle}{E_n^0 - E_m^0} \psi_m^0$$

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Example for first-order perturbation calculation

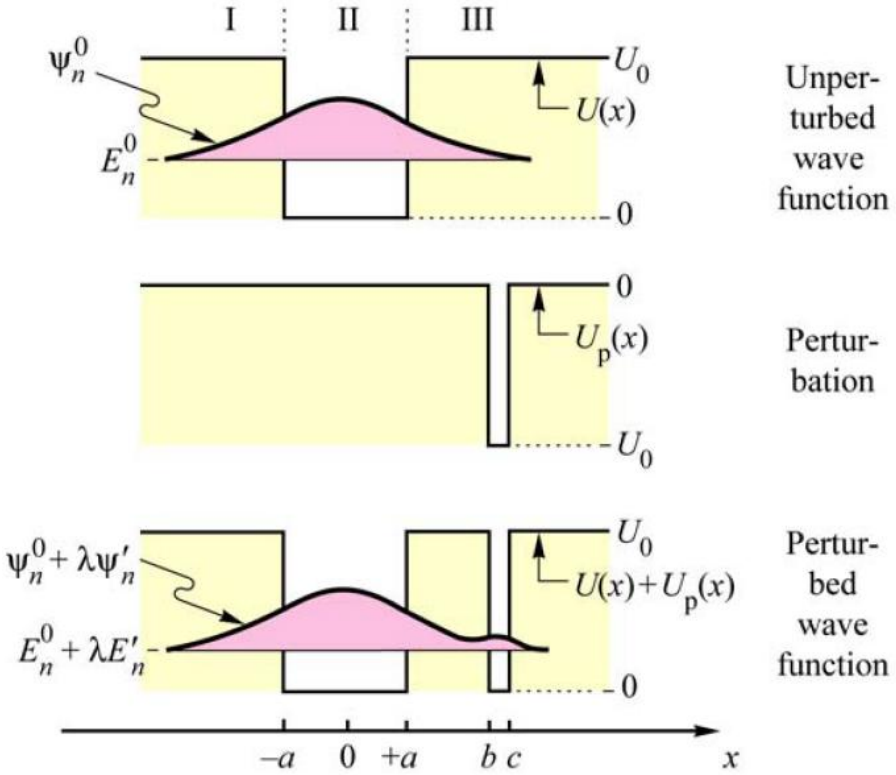

Fig. 10.2. Simple example of an (*i*) unperturbed wave function, (*ii*) a small perturbation, and (*iii*) and resulting perturbed wave function. The first-order correction to the energy due to the perturbation is $\lambda E'_n$. The correction to the wavefunction is $\lambda\psi'_n$.

$$H = H^0 + H' = H^0 + U_p(x).$$

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$$\psi_I(x) = A_1 e^{\kappa x}$$

$$\psi_{II}(x) = A_1 \left(\frac{e^{-\kappa a}}{\cos ka} \right) \cos kx$$

$$\psi_{III}(x) = A_1 e^{-\kappa x}$$

$$\kappa = \frac{1}{\hbar} \sqrt{2m\left(U_0 - E_0^0\right)}$$

$$k = \frac{1}{\hbar} \sqrt{2m E_0^0}$$

$$E_n = E_n^0 + \lambda \left\langle \psi_n^0 \middle| H' \middle| \psi_n^0 \right\rangle \Longrightarrow E_0 = E_0^0 + \int_{-\infty}^{\infty} \psi_0^0 U_p(x) \psi_0^0 \, dx .$$

$$E_0 = E_0^0 + \int_b^c (-U_0) A_1^2 e^{-2\kappa} \, dx = E_0^0 - \frac{U_0 A_1^2}{2\kappa} \left(e^{-2\kappa b} - e^{-2\kappa c} \right) .$$

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Second-order time-independent perturbation theory

E_n'' and ψ_n''

$$\psi_n'' = \sum_j b_j \psi_j^0$$

$$H^0 \psi_n'' + H' \psi_n' = E_n^0 \psi_n'' + E_n' \psi_n' + E_n'' \psi_n^0$$

$$\sum_j b_j E_j^0 \psi_j^0 + H' \sum_j a_j \psi_j^0 = \sum_j b_j E_n^0 \psi_j^0 + \sum_j a_j E_n' \psi_j' + E_n'' \psi_n^0$$

Pre-multiplication of Eq. (10.15) with ψ_m^{0*}, and integration over position space yields

$\langle \psi_m^0 | \psi_j^0 \rangle = \delta_{mj}$

$$b_m E_m^0 + \sum_j a_j \left\langle \psi_m^0 \middle| H' \middle| \psi_j^0 \right\rangle = b_m E_n^0 + E_n' a_m + E_n'' \delta_{nm}$$

$m = n$ or $m \neq n$

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$m = n$:

$$E_n'' = \sum_j a_j \left\langle \psi_n^0 \middle| H' \middle| \psi_j^0 \right\rangle - E_n' a_n$$

$$= \sum_{j \neq n} a_j \left\langle \psi_n^0 \middle| H' \middle| \psi_j^0 \right\rangle + a_n \left\langle \psi_n^0 \middle| H' \middle| \psi_n^0 \right\rangle - E_n' a_n$$

$j = n$ ⇒

$$E_n'' = \sum_{j \neq n} \frac{\left| \left\langle \psi_n^0 \middle| H' \middle| \psi_j^0 \right\rangle \right|^2}{E_n^0 - E_j^0}$$

Perturbation can be neglected

Like the above can prove that

$m \neq n$:

$$b_m = \sum_{j \neq n} \frac{\left\langle \psi_j^0 \middle| H' \middle| \psi_n^0 \right\rangle \left\langle \psi_m^0 \middle| H' \middle| \psi_j^0 \right\rangle}{\left(E_n^0 - E_j^0\right)\left(E_n^0 - E_m^0\right)} - \frac{\left\langle \psi_n^0 \middle| H' \middle| \psi_n^0 \right\rangle \left\langle \psi_m^0 \middle| H' \middle| \psi_n^0 \right\rangle}{\left(E_n^0 - E_m^0\right)^2}$$

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Finally $b_m = b_n \ (m = n)$

normalization

$$m = n: \quad \left\langle \psi_n^0 + \lambda \sum_j a_j \psi_j^0 + \lambda^2 \sum_j b_j \psi_j^0 \middle| \psi_n^0 + \lambda \sum_j a_j \psi_j^0 + \lambda^2 \sum_j b_j \psi_j^0 \right\rangle = 1$$

$b_{m=n} = b_n$

$$b_n = -\frac{1}{2} \sum_j |a_j|^2 = -\frac{1}{2} \sum_{j \neq n} \frac{\left| \left\langle \psi_j^0 \middle| H' \middle| \psi_n^0 \right\rangle \right|^2}{\left(E_n^0 - E_j^0 \right)^2}$$

$$\psi_n'' = \sum_{m \neq n} \left\{ \left[\sum_{j \neq n} \frac{\left\langle \psi_j^0 | H' | \psi_n^0 \right\rangle \left\langle \psi_m^0 | H' | \psi_j^0 \right\rangle}{\left(E_n^0 - E_j^0 \right)\left(E_n^0 - E_m^0 \right)} - \frac{\left\langle \psi_n^0 | H' | \psi_n^0 \right\rangle \left\langle \psi_m^0 | H' | \psi_n^0 \right\rangle}{\left(E_n^0 - E_m^0 \right)^2} \right] \psi_m^0 - \frac{\left| \left\langle \psi_m^0 | H' | \psi_n^0 \right\rangle \right|^2}{2 \left(E_n^0 - E_m^0 \right)^2} \psi_n^0 \right\}$$

*First- and second-order correction to the energy of the n*th *state*:

$$E_n = E_n^0 + \lambda\left\langle\psi_n^0\right| H' \left|\psi_n^0\right\rangle + \lambda^2 \sum_{j\neq n} \frac{\left|\left\langle\psi_n^0\right| H' \left|\psi_j^0\right\rangle\right|^2}{E_n^0 - E_j^0}$$

*First- and second-order correction to the wave function of the n*th *state*:

$$\psi_n = \psi_n^0 + \lambda \sum_{m\neq n} \frac{\left\langle\psi_m^0\right| H' \left|\psi_n^0\right\rangle}{E_n^0 - E_m^0} \psi_m^0 +$$

$$\lambda^2 \sum_{m\neq n} \left\{ \left[\sum_{j\neq n} \frac{\left\langle\psi_j^0\right|H'\left|\psi_n^0\right\rangle\left\langle\psi_m^0\right|H'\left|\psi_j^0\right\rangle}{\left(E_n^0 - E_j^0\right)\left(E_n^0 - E_m^0\right)} - \frac{\left\langle\psi_n^0\right|H'\left|\psi_n^0\right\rangle\left\langle\psi_m^0\right|H'\left|\psi_n^0\right\rangle}{\left(E_n^0 - E_m^0\right)^2} \right] \psi_m^0 - \frac{\left|\left\langle\psi_m^0\right|H'\left|\psi_n^0\right\rangle\right|^2}{2\left(E_n^0 - E_m^0\right)^2} \psi_n^0 \right\}$$

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Time-dependent perturbation theory

It is important to keep in mind that in such stationary systems, nothing observable ever happens

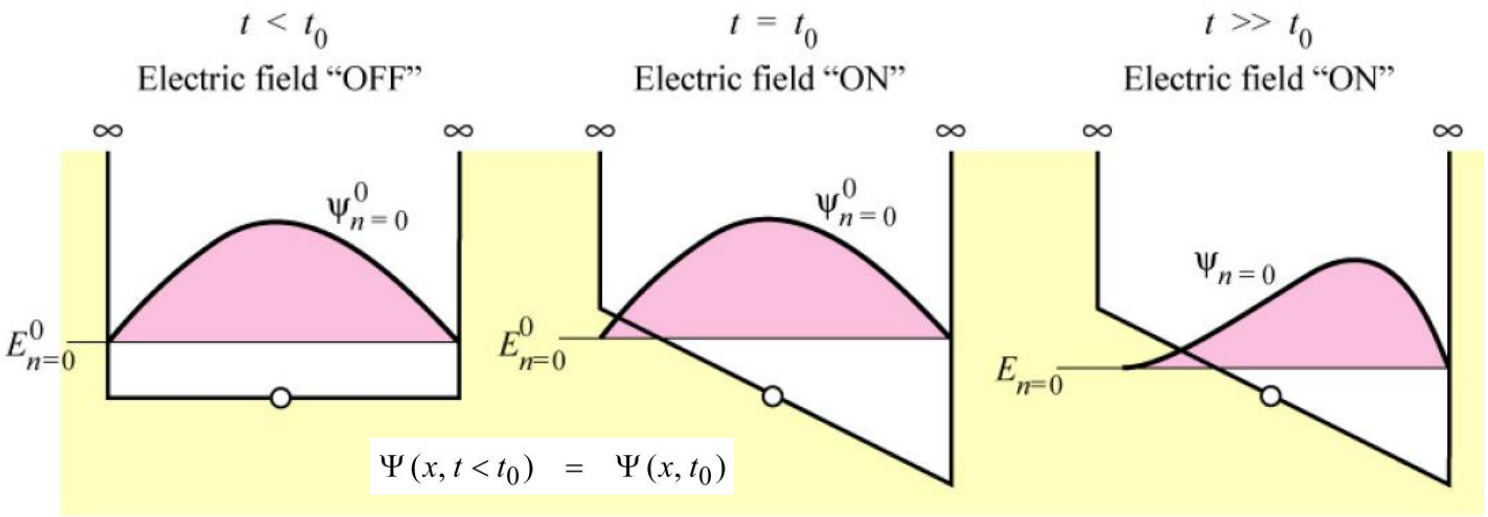

Fig. 11.1. Temporal evolution of a perturbation. The perturbation is assumed to occur instantly at the time t_0. The wavefunction at $t = t_0$ has still the shape as $\psi^0_{n=0}$ $(t < 0)$. Then, the wavefunction changes according to the perturbation, and, it is given by $\Psi_{n=0}$. The perturbation shown here is a constant electric field.

$$E_{\text{kin}}(t = t_0) = \left\langle \Psi(x, t_0) \left| \frac{p^2}{2m} \right| \Psi(x, t_0) \right\rangle \qquad E_{\text{pot}}(t = t_0) = \left\langle \Psi(x, t_0) \left| U(x) \right| \Psi(x, t_0) \right\rangle$$

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The starting point

$$\Psi = \Psi(x, t)$$

$$H\,\Psi = -\frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial t}\Psi$$

$$H = H^0 + \lambda H'(t)$$

before the perturbation

$$H^0\,\psi_n^0 = E_n^0\,\psi_n^0 \Rightarrow H^0\,\Psi_n^0 = -\frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial t}\Psi_n^0 = E_n^0\,\Psi_n^0$$

$$\Psi_n^0 = \psi_n^0\,\mathrm{e}^{-\mathrm{i}E_n^0 t/\hbar}$$

unperturbed system

$$\Psi^0 = \sum_n a_n\,\Psi_n^0$$

$$\left\langle \Psi^0 \middle| \Psi^0 \right\rangle = 1$$

$$\left[H^0 + \lambda H'(t)\right]\Psi = -\frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial t}\Psi$$

$$\Psi(x,t) = \sum_n a_n(t)\,\Psi_n^0(x,t)$$

method of *variation of parameters* (also called *variation of constants*) is quite powerful

$$\Psi(x,t) = \sum_n a_n(t)\,\Psi_n^0(x,t) \qquad \left[H^0 + \lambda H'(t)\right]\Psi = -\frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial t}\Psi$$

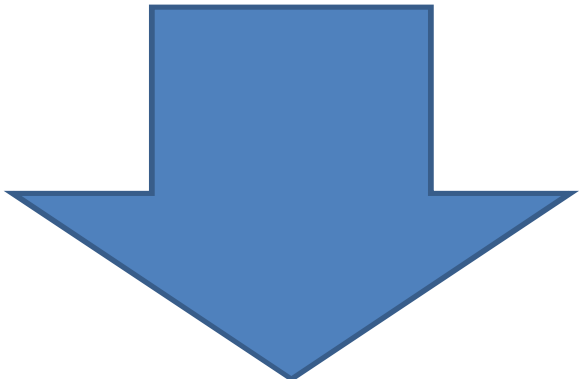
$$\sum_n a_n(t)\,H^0\,\Psi_n^0 + \sum_n a_n(t)\,\lambda\,H'\,\Psi_n^0 = -\frac{\hbar}{\mathrm{i}}\sum_n\left[\frac{\partial}{\partial t}a_n(t)\right]\Psi_n^0 - \frac{\hbar}{\mathrm{i}}\sum_n a_n(t)\frac{\partial}{\partial t}\Psi_n^0$$

Pre-multiplication of the remainder of the equation with Ψ_m^{0*} followed by integration (recall that $\langle\Psi_m^0 \mid \Psi_n^0\rangle = \delta_{mn}$) yields

fundamental result of time-dependent perturbation theory

$$\frac{\mathrm{d}}{\mathrm{d}t}a_m(t) = -\frac{\mathrm{i}}{\hbar}\lambda\sum_n a_n(t)\left\langle\Psi_m^0\middle|H'\middle|\Psi_n^0\right\rangle$$

matrix elements $\langle\Psi_m^0|\,H'\,|\Psi_n^0\rangle$



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$$-\frac{\hbar}{\mathrm{i}}\frac{\mathrm{d}a_0}{\mathrm{d}t} = a_0\left\langle \Psi_0^0 \middle| H' \middle| \Psi_0^0 \right\rangle + a_1\left\langle \Psi_0^0 \middle| H' \middle| \Psi_1^0 \right\rangle + \cdots + a_j\left\langle \Psi_0^0 \middle| H' \middle| \Psi_j^0 \right\rangle + \cdots$$

$$-\frac{\hbar}{\mathrm{i}}\frac{\mathrm{d}a_1}{\mathrm{d}t} = a_0\left\langle \Psi_1^0 \middle| H' \middle| \Psi_0^0 \right\rangle + a_1\left\langle \Psi_1^0 \middle| H' \middle| \Psi_1^0 \right\rangle + \cdots + a_j\left\langle \Psi_1^0 \middle| H' \middle| \Psi_j^0 \right\rangle + \cdots$$

$$\vdots \qquad \vdots \qquad \vdots \qquad \vdots \qquad (11.15)$$

$$-\frac{\hbar}{\mathrm{i}}\frac{\mathrm{d}a_j}{\mathrm{d}t} = a_0\left\langle \Psi_j^0 \middle| H' \middle| \Psi_0^0 \right\rangle + a_1\left\langle \Psi_j^0 \middle| H' \middle| \Psi_1^0 \right\rangle + \cdots + a_j\left\langle \Psi_j^0 \middle| H' \middle| \Psi_j^0 \right\rangle + \cdots$$

$$\vdots \qquad \vdots \qquad \vdots \qquad \vdots$$

To simplify the solution of the system of equations, a first-order approximation for $a_j(t)$ will be used; to do so, $a_j(t)$ is expanded into a power series of λ

$$a_j = a_j^0 + \lambda a_j' + \lambda^2 a_j'' + \cdots \qquad (11.16)$$

where $a_j' = \mathrm{d}a_j/\mathrm{d}\lambda$ and $a_j'' = \mathrm{d}^2a_j/\mathrm{d}\lambda^2$

دانشگاه آزاد
اسلامی

$$-\frac{\hbar}{\mathrm{i}}\frac{\mathrm{d}}{\mathrm{d}t}\left(a_j^0 + \lambda a_j' + \lambda^2 a_j''\right) = \left(a_0^0 + \lambda a_0' + \lambda^2 a_0''\right)\left\langle \Psi_j^0 \middle| \lambda H' \middle| \Psi_0^0 \right\rangle$$

$$+ \cdots$$

$$+ \left(a_j^0 + \lambda a_j' + \lambda^2 a_j''\right)\left\langle \Psi_j^0 \middle| \lambda H' \middle| \Psi_j^0 \right\rangle$$

$$+ \cdots$$

$\lambda = 0$ (no perturbation) $\Rightarrow$ $\frac{\mathrm{d}}{\mathrm{d}t}a_0^0 = 0;$ $\frac{\mathrm{d}}{\mathrm{d}t}a_1^0 = 0;$ $\frac{\mathrm{d}}{\mathrm{d}t}a_2^0 = 0;$ $\cdots$

first-order correction terms for λ^1

$$-\frac{\hbar}{\mathrm{i}}\frac{\mathrm{d}a_0'}{\mathrm{d}t} = a_0^0\left\langle \Psi_0^0 \middle| H' \middle| \Psi_0^0 \right\rangle + a_1^0\left\langle \Psi_0^0 \middle| H' \middle| \Psi_1^0 \right\rangle + \cdots + a_j^0\left\langle \Psi_0^0 \middle| H' \middle| \Psi_j^0 \right\rangle + \cdots$$

$$-\frac{\hbar}{\mathrm{i}}\frac{\mathrm{d}a_1'}{\mathrm{d}t} = a_0^0\left\langle \Psi_1^0 \middle| H' \middle| \Psi_0^0 \right\rangle + a_1^0\left\langle \Psi_1^0 \middle| H' \middle| \Psi_1^0 \right\rangle + \cdots + a_j^0\left\langle \Psi_1^0 \middle| H' \middle| \Psi_j^0 \right\rangle + \cdots$$

$$\vdots \qquad \vdots \qquad \vdots \qquad \vdots \qquad (11.19)$$

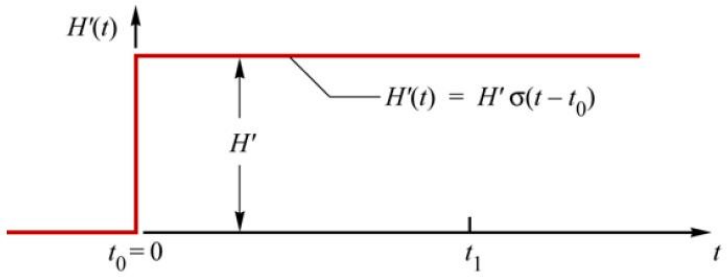
$$-\frac{\hbar}{\mathrm{i}}\frac{\mathrm{d}a_j'}{\mathrm{d}t} = a_0^0\left\langle \Psi_j^0 \middle| H' \middle| \Psi_0^0 \right\rangle + a_1^0\left\langle \Psi_j^0 \middle| H' \middle| \Psi_1^0 \right\rangle + \cdots + a_j^0\left\langle \Psi_j^0 \middle| H' \middle| \Psi_j^0 \right\rangle + \cdots$$

$$\vdots \qquad \vdots \qquad \vdots \qquad \vdots$$

دانشگاه آزاد اسلامی

Step-function-like perturbation

$$H'(t) = H'\,\sigma(t)$$



$$\Psi_n^{\,0} = \Psi_n^{\,0}\, e^{-iEnt/\hbar},$$

$$-\frac{\hbar}{i}\frac{d}{dt}a'_0 = \left\langle \psi_0^0 \middle| H' \middle| \psi_j^0 \right\rangle e^{i\omega_{0j}t} \qquad \omega_{mj} = (E_m^{\,0} - E_j^{\,0})/\hbar$$

$$-\frac{\hbar}{i}\frac{d}{dt}a'_1 = \left\langle \psi_1^0 \middle| H' \middle| \psi_j^0 \right\rangle e^{i\omega_{1j}t}$$

$a_j \approx 1$ for $t \geq 0$ due to the smallness of the perturbation → $a'_j \approx 0$

$$-\frac{\hbar}{i}\frac{d}{dt}a'_m = \left\langle \psi_m^0 \middle| H' \middle| \psi_j^0 \right\rangle e^{i\omega_{mj}t}$$

$$a'_m(t_1) = -\frac{1}{\hbar}\left\langle \psi_m^0 \middle| H' \middle| \psi_j^0 \right\rangle \frac{e^{i\omega_{mj}t_1} - 1}{\omega_{mj}} \qquad (m = 0, 1, 2, \ldots, m \neq j, \ldots)$$

دانشگاه آزاد
اسلامی

expectation values

$$a_m'^{*}\, a_m' = \frac{\left\langle \psi_m^0 \middle| H' \middle| \psi_j^0 \right\rangle^{*} \left\langle \psi_m^0 \middle| H' \middle| \psi_j^0 \right\rangle \sin^2\left(\frac{1}{2}\omega_{mj}\, t_1\right)}{\hbar^2 \left(\frac{1}{2}\omega_{mj}\right)^2} \qquad (m = 0, 1, 2, \ldots, m \neq j, \ldots)$$

This equation gives the temporal dependence of the intensity

A perturbation can result in a *very selective redistribution* of probabilities, that is, the wave functions of some states may remain completely unaffected. To illustrate this, we consider the quantity $\langle \Psi_m^0 | H' | \Psi_j^0 \rangle$, in which the wave function Ψ_j^0 (of the initially populated jth state) is connected via the perturbation hamiltonian H' to the wave function Ψ_m^0 (of the initially unpopulated state). The quantity

$$H_{mj}' = \left\langle \psi_m^0 \middle| H' \middle| \psi_j^0 \right\rangle$$

is called the ***transition matrix element*** of the two wave functions Ψ_m^0 and Ψ_j^0.

$$H_{mj}' = \int_{-\infty}^{\infty} \psi_m^{0*}(x)\, H'(x)\, \psi_j^0(x)\, dx$$

The integrand will be an odd function and the integration yields $H_{mj}' = 0$.

The matrix element H_{mj}' is the source of the ***selection rules*** of atomic, nuclear or semiconductor quantum well spectra. In such spectra some transitions are *allowed* ($H_{mj}' \neq 0$) while other transitions are *forbidden* or *disallowed* ($H_{mj}' = 0$).

دانشگاه آزاد اسلامی

Harmonic perturbation and Fermi's Golden Rule

$$H' = 0 \qquad (t < 0)$$

$$H' = A(x)\left(e^{i\omega_0 t} + e^{-i\omega_0 t}\right) \qquad (t \geq 0)$$

$$-\frac{\hbar}{i}\frac{d}{dt}a'_m = H'_{mj}\, e^{i\omega_{mj}t}\left(e^{i\omega_0 t} + e^{-i\omega_0 t}\right) \qquad (m = 0, 1, 2, \ldots, m \neq j, \ldots)$$

$$H'_{mj} = \left\langle \psi_m^0 \middle| H' \middle| \psi_j^0 \right\rangle = \int_{-\infty}^{\infty} \psi_m^{0*}(x)\, A(x)\, \psi_j^0(x)\, dx$$

If the mth state is unoccupied at $t = 0$, *i. e.*, $a_m'(t = 0) = 0$. Then $(d/dt)\, a_m'$

$$a'_m(t_1) = -\frac{H'_{mj}}{\hbar}\left[\frac{\left(e^{i(\omega_{mj}+\omega_0)t_1} - 1\right)}{\omega_{mj} + \omega_0} - \frac{\left(e^{i(\omega_{mj}-\omega_0)t_1} - 1\right)}{\omega_{mj} - \omega_0}\right].$$

By: Dr. Jabbari

دانشگاه آزاد اسلامی

We obtain for $E_m^0 \approx E_j^0 + \hbar\omega_0$:

$$a'^{*}_m(t)\, a'_m(t) \approx \frac{4\, H'^{*}_{mj}\, H'_{mj}}{\hbar^2} \frac{\sin^2\left[\frac{1}{2}\left(\omega_{mj} - \omega_0\right)t\right]}{\left(\omega_{mj} - \omega_0\right)^2}$$

And in the vicinity of $E_m^0 \approx E_j^0 - \hbar\omega_0$:

$$a'^{*}_m(t)\, a'_m(t) \approx \frac{4\, H'^{*}_{mj}\, H'_{mj}}{\hbar^2} \frac{\sin^2\left[\frac{1}{2}\left(\omega_{mj} + \omega_0\right)t\right]}{\left(\omega_{mj} + \omega_0\right)^2}$$

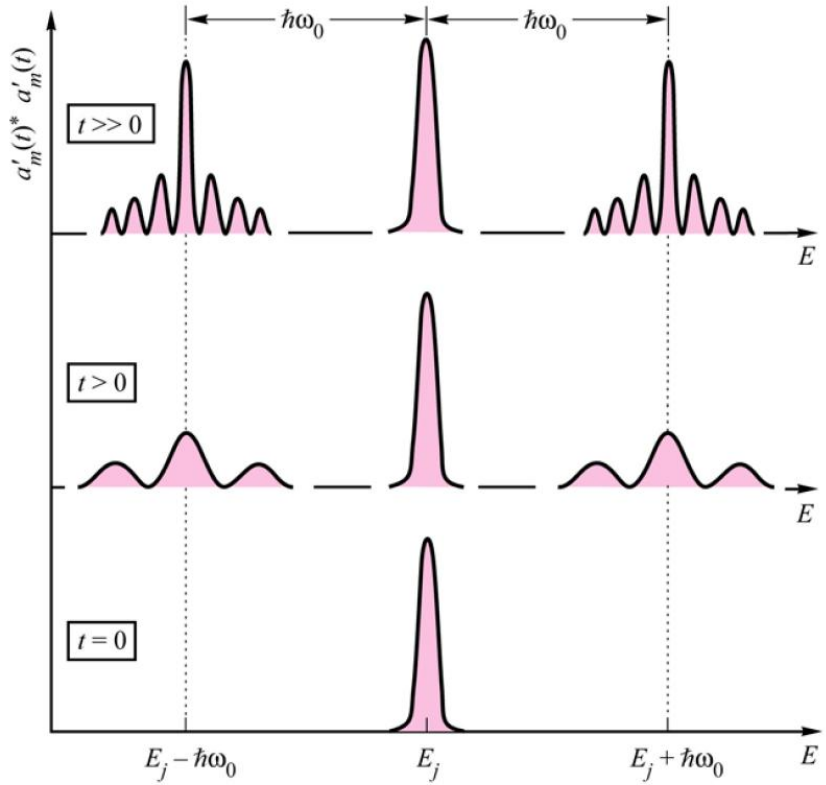


Fig. 11.3. Temporal development of intensities of wave functions. Initially the system is represented by a single occupied state with energy $E_j\,(t = 0)$. After a harmonic perturbation with energy $(h/2\pi)\,\omega_0$, states of energy $E_j \pm (h/2\pi)\,\omega_0$ become increasingly populated. A transition to the state with energy $E_j + (h/2\pi)\,\omega_0$ is a *stimulated upward* (excitation) transition or *stimulated absorption* transition. Correspondingly, a quantum mechanical transition to the state with energy $E_j - (h/2\pi)\,\omega_0$ is a *stimulated downward* (de-excitation) transition or *stimulated emission* transition.

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Frequently, a transition occurs between a single state and a *group of states* clustered about a state m with $E_m^0 > E_j^0$. Transitions between an impurity state and band states in semiconductors are an example of such a transition. Let the cluster of states be characterized by a density of states $\rho(\omega_{mj})$ per unit of ω_{mj}. Assuming that the transition is an *excitation transition* in which the final state energy is higher than the initial state energy, *i. e.*, $E_m^0 \approx E_j^0 + \hbar\omega_0$, then Eq. (11.31) becomes

$$|a'_m(t)|^2 = \frac{1}{\hbar^2} \int_{-\infty}^{\infty} |H'_{mj}|^2 \frac{\sin^2\left[\frac{1}{2}(\omega_{mj} - \omega_0)t\right]}{\left[\frac{1}{2}(\omega_{mj} - \omega_0)\right]^2} \rho(\omega_{mj})\, d\omega_{mj}$$

If $|H_{mj}'|^2$ is not a strong function of the final state m, then we can take it outside of the integral.

product of two functions, namely the density of states

$$\rho(\omega_{mj})$$

$$\frac{\sin^2\left[\frac{1}{2}(\omega_{mj} - \omega_0)t\right]}{\left[\frac{1}{2}(\omega_{mj} - \omega_0)\right]^2}$$

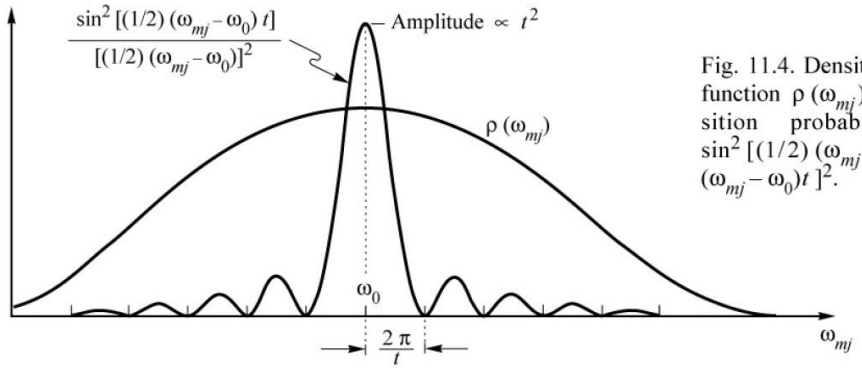

Fig. 11.4. Density of final states function $\rho(\omega_{mj})$ and the transition probability function $\sin^2[(1/2)(\omega_{mj} - \omega_0)t] / [(1/2)(\omega_{mj} - \omega_0)t]^2$.

دانشگاه آزاد
اسلامی

$$\int_{-\infty}^{\infty} \frac{\sin^2\left[\frac{1}{2}(\omega_{mj}-\omega_0)t\right]}{\left[\frac{1}{2}(\omega_{mj}-\omega_0)\right]^2} d\omega_{mj} = 2\pi t$$

$$|a'_m(t)|^2 = \frac{2\pi}{\hbar^2} |H'_{mj}|^2 \rho(\omega_{mj}=\omega_0)\, t$$

Fermi's Golden Rule

transition probability

$$W_{j\to m} = \frac{d}{dt}|a'_m(t)|^2 = \frac{2\pi}{\hbar}|H'_{mj}|^2 \rho(E = E_j + \hbar\omega_0)$$

transition from one state to another single state

$$W_{j\to m} = \frac{d}{dt}|a'_m(t)|^2 = \frac{2\pi}{\hbar}|H'_{mj}|^2 \delta(E_m - E_j - \hbar\omega_0)$$

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Exercise: *Band-to-band transitions in semiconductors*

$\vec{E}(t) = \mathcal{E}_0 \, \vec{\mathbf{u}}_x \cos \omega t$

electromagnetic field

$$U(x) = -e \mathcal{E}_0 \, x$$

$$H'(x) = -e \mathcal{E}_0 \, x \, (1/2)\left(e^{i\omega t} + e^{-i\omega t}\right)$$

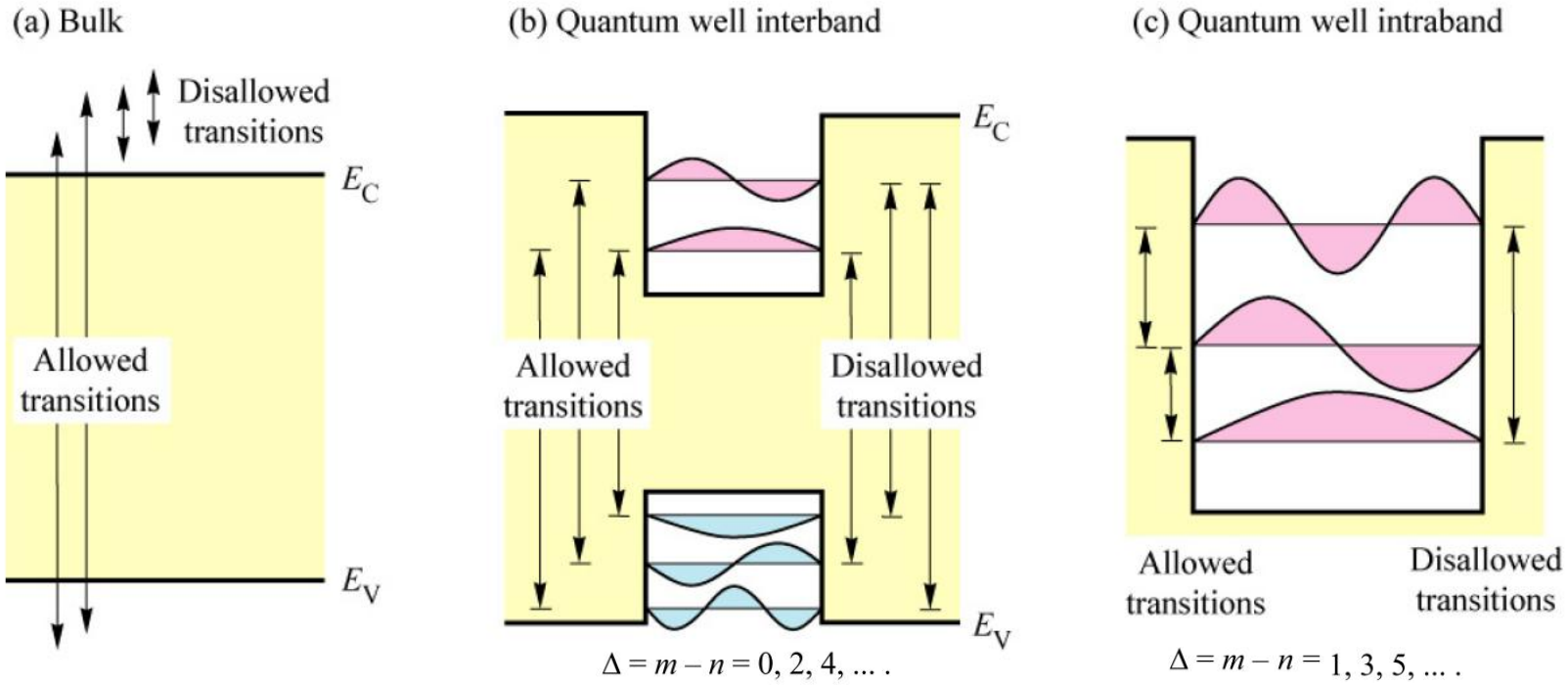

Fig. 11.5 Allowed and disallowed optical interband and intraband transitions in bulk and quantum well semiconductors.

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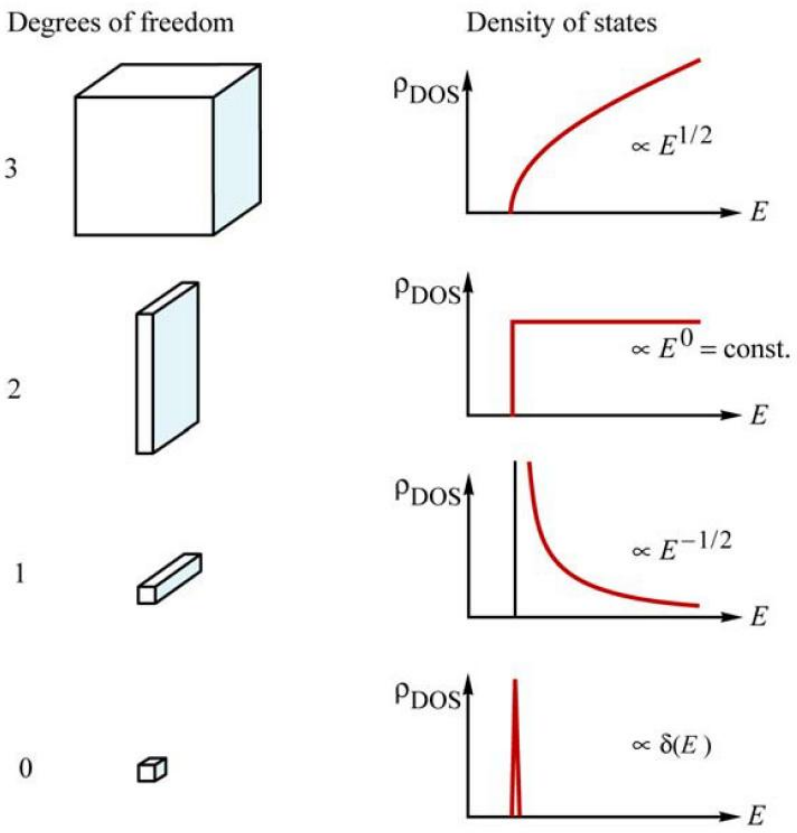
Density of states



$$\rho^{1D}_{DOS}(E) = \frac{1}{\pi\hbar}\sum_n \sqrt{\frac{m^*}{2\,(E-E_n)}}\;\sigma(E-E_n)$$

Fig. 12.7. Electronic density of states of semiconductors with 3, 2, 1, and 0 degrees of freedom for electron propagation. Systems with 2, 1, and 0 degrees of freedom are referred to as quantum wells, quantum wires, and quantum boxes, respectively.

$$\rho^{0D}_{DOS}(E) = 2\,\delta(E-E_0)$$

دانشگاه آزاد اسلامی

Degrees of freedom	Dispersion (kinetic energy)	Density of states	Effective density of states
3 (bulk)	$E = \frac{\hbar^2}{2m^*}(k_x^2 + k_y^2 + k_z^2)$	$\rho_{\mathrm{DOS}}^{3\mathrm{D}} = \frac{1}{2\pi^2}\left(\frac{2m^*}{\hbar^2}\right)^{\frac{3}{2}}\sqrt{E - E_{\mathrm{C}}}$	$N_{\mathrm{c}}^{3\mathrm{D}} = \frac{1}{\sqrt{2}}\left(\frac{m^* kT}{\pi\hbar^2}\right)^{\frac{3}{2}}$
2 (slab)	$E = \frac{\hbar^2}{2m^*}(k_x^2 + k_y^2)$	$\rho_{\mathrm{DOS}}^{2\mathrm{D}} = \frac{m^*}{\pi\hbar^2}\sigma(E - E_{\mathrm{C}})$	$N_{\mathrm{c}}^{2\mathrm{D}} = \frac{m^*}{\pi\hbar^2}kT$
1 (wire)	$E = \frac{\hbar^2}{2m^*}(k_x^2)$	$\rho_{\mathrm{DOS}}^{1\mathrm{D}} = \frac{m^*}{\pi\hbar}\sqrt{\frac{m^*}{2(E - E_{\mathrm{C}})}}$	$N_{\mathrm{c}}^{1\mathrm{D}} = \sqrt{\frac{m^* kT}{2\pi\hbar^2}}$
0 (box)	–	$\rho_{\mathrm{DOS}}^{0\mathrm{D}} = 2\delta(E - E_{\mathrm{C}})$	$N_{\mathrm{c}}^{0\mathrm{D}} = 2$

Table 12.1 Density of states for semiconductor with 3, 2, 1, and 0 degrees of freedom for propagation of electrons. The dispersion relations are assumed to be parabolic. The formulas can be applied to anisotropic semiconductors if the effective mass m^* is replaced by the density-of-states effective mass m_{DOS}^*. If the semiconductor has a number of M_{c} equivalent minima, the corresponding density of states must be multiplied by M_{c}. The bottom of the band is denoted as E_{C} and $\sigma(E)$ is the step-function.

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$$N = \int_{E_1}^{E_2} \rho_{DOS}(E)\, dE$$

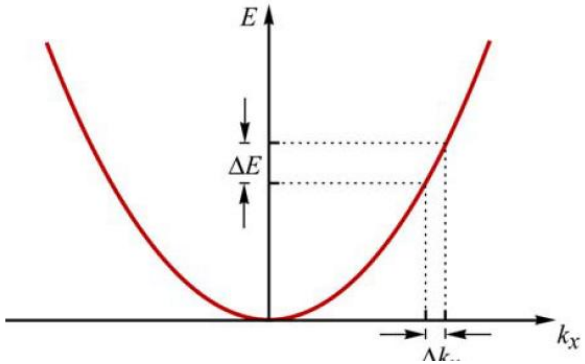

Fig. 12.1. Parabolic dispersion relation with a k-space interval Δk_x and a corresponding energy interval $\Delta E = (\partial E/\partial k_x)\,\Delta k_x$.

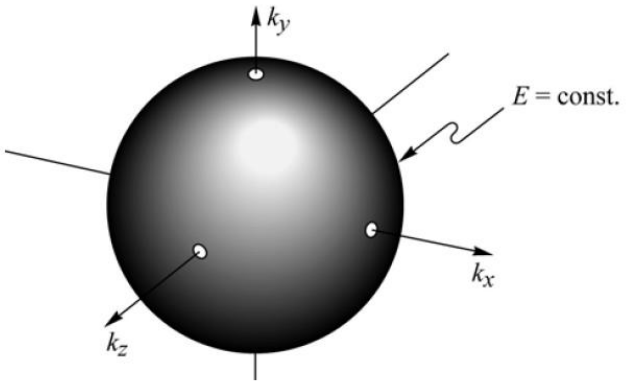

Fig. 12.2. Constant energy surface for a single-valley, isotropic band.

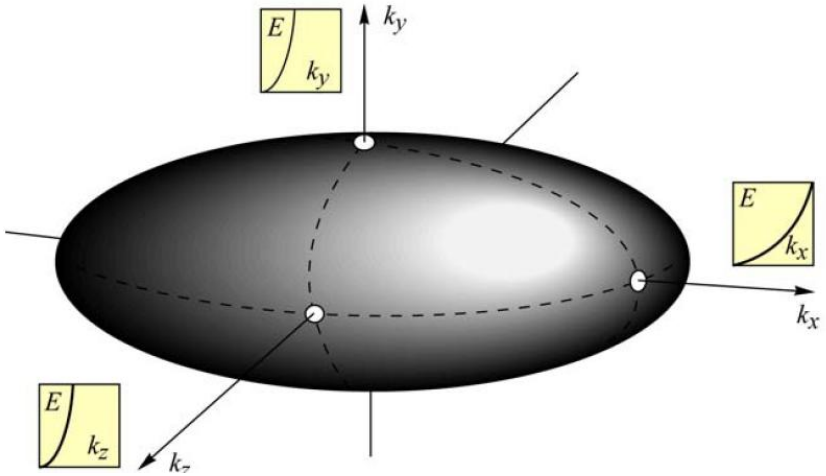

Fig. 12.4. Ellipsoidal constant energy surface with a weakly curved dispersion relation along the k_x axis and strongly curved dispersion along the k_y and k_z axis.

By: Dr. Jabbari

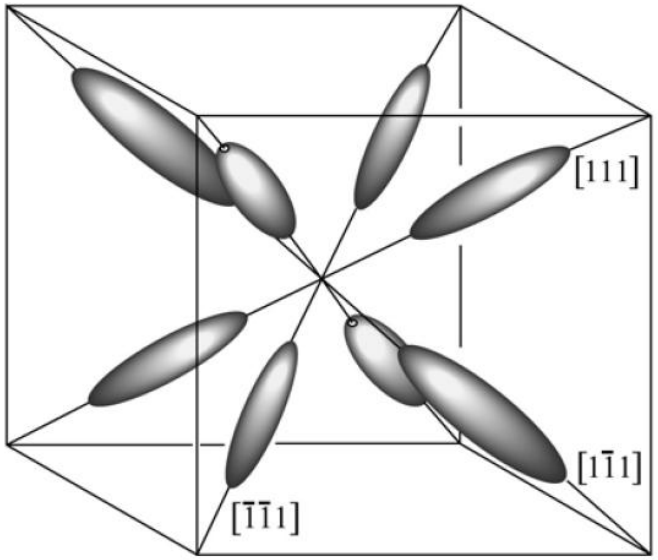

Fig. 12.5. Constant energy surface for the *L*-point of the Brillouin zone. The band structure consists of eight equivalent rotational ellipsoids.