Quantum Confinement in one Direction

- Confinement by effective potential $V(z)$ in z (growth) direction, free motion in x-y plane.
- Single particle states described by Schrödinger equation

$$-\frac{\hbar^2}{2m}\left[\frac{d^2}{dx^2}+\frac{d^2}{dy^2}+\frac{d^2}{dz^2}\right]\Psi(x,y,z)+V(z)\Psi(x,y,z)=E\Psi(x,y,z) \qquad (1)$$

(isotropic band-mass m).

- Solutions: plane waves with momentum $\mathbf{k}_\parallel$ in x-y direction, $\mathbf{x}_\parallel=(x,y)$, normalised to total area A. 'Standing waves' $\phi_l(z)$ in z-direction,

$$\Psi_{l,\mathbf{k}_\parallel}(\mathbf{x}_\parallel,z)=\frac{1}{\sqrt{A}}e^{i\mathbf{k}_\parallel\mathbf{x}_\parallel}\phi_l(z), \qquad (2)$$

where $\phi_l(z)$ fulfills

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dz^2}+V(z)-E_l\right]\phi_l(z)=0 \qquad (3)$$

with some given boundary conditions, e.g. $\phi_l(z=0) = \phi_l(z=L) = 0$.
Examples:

– Infinitely high quantum well: $\phi_l(z) = \sqrt{2/L}\sin(l\pi z/L), l = 1, 2, 3, ...$

– Triangular quantum well.

– *Fang-Howard* wave function $\phi_0(z) = 2a^{3/2} z \exp(-az), a > 0$ for more complicated $V(z)$ [F. F. Fang and W. E. Howard, Phys. Rev. Lett. **16**, 797 (1966).]

– Detailed form of $\phi_l(z)$ can be important when it comes to calculating scattering rates for electrons etc.

- Quantum number l labels different quantum well *subbands*.

- Parabolic *dispersion relation* in each subband l, two-dimensional wave vector $\mathbf{k}_\|$,

$$E_{l,\mathbf{k}_\|} = E_l + \frac{\hbar^2 \mathbf{k}_\|^2}{2m} \quad (4)$$

- Note: so far this only describes free, non-interacting electrons.

Additional Literature: D. K. Ferry, S. M. Goodnick, *'Transport in Nanostructures'*, Cambridge University Press, Cambridge (UK), 1997; **Chapter 2** on 'Quantum confined systems'.

Quantum Confinement in two Directions

- Confinement by effective potential $V(z)$ in z (growth) direction and effective *lateral* potential $W(y)$ in y direction, free motion in x-direction.

- Single particle states described by Schrödinger equation

$$-\frac{\hbar^2}{2m}\left[\frac{d^2}{dx^2}+\frac{d^2}{dy^2}+\frac{d^2}{dz^2}\right]\Psi(x,y,z)+\left[W(y)+V(z)\right]\Psi(x,y,z)=E\Psi(x,y,z) \quad (5)$$

(isotropic band-mass m).

- Solutions: plane waves with momentum k in x-direction, normalised to total length L. Standing waves in z- and y-direction

$$\Psi_{l,n,\mathbf{k}_{\|}}(\mathbf{x}_{\|},z)=\frac{1}{\sqrt{L}}e^{ikx}\psi_n(y)\phi_l(z). \quad (6)$$

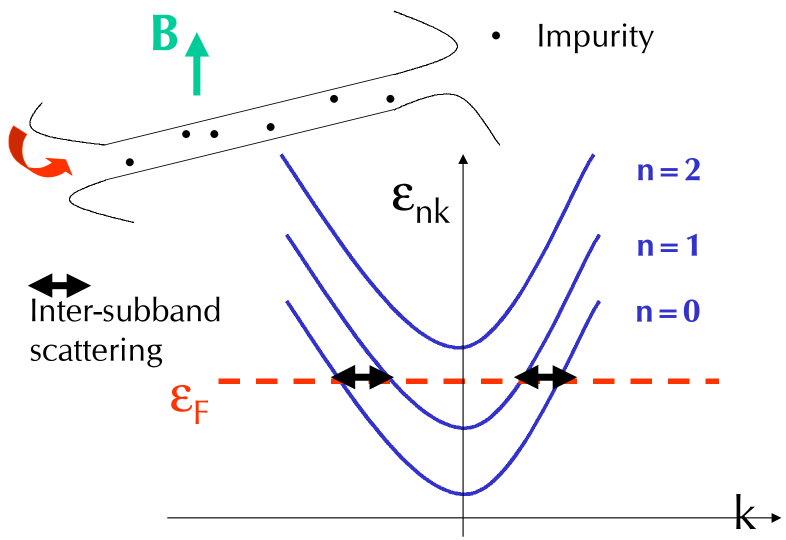
- Quantum number l labels different quantum well subbands. Quantum number n labels different *quantum wire* subbands.

- Parabolic *dispersion relation* in each subband n,

$$E_{l,n,k} \equiv E_l + \varepsilon_{nk}; \quad \varepsilon_{nk} \equiv \varepsilon_n + \frac{\hbar^2 k^2}{2m}. \tag{7}$$

- The resulting system of electrons is called a 'quasi-one-dimensional system' (quantum wire).

- Note: so far this only describes free, non-interacting electrons.



Density of States

- *'States'* refers to stationary, single particle eigenstates $|\Psi_\alpha\rangle$ of a given quantum system. States are characterised by a quantum number α (single or multiple/vector index) and the corresponding eigenenergy E_α.
- The set $\{E_\alpha\}$ of all the eigenenergies is called the single-particle spectrum.
- The density of states $\rho(E)$ is defined as

$$\rho(E) \equiv \frac{1}{V} \sum_\alpha \delta(E - E_\alpha) \tag{8}$$

  and represents the number of eigenstates per volume $V = L^d$ and per energy E. Here, d is the dimension of the system: L^3 is a cube, L^2 is an area, and L a line. This is always understood in the limit of $L \to \infty$ where it is assumed that the shape of the volume (e.g., sphere or cube in $d = 3$) does not play any role any longer.

Example 1: harmonic oscillator of angular frequency ω, *discrete* spectrum

$E_\alpha \equiv E_n = \hbar\omega(n+\frac{1}{2})$,

$$\rho_{\rm osc}(E) = V^{-1}\sum_{n=0}^{\infty}\delta\left(E-\hbar\omega(n+\frac{1}{2})\right). \quad (9)$$

Example 2: spinless particle of mass m in three dimensions, *continuous* spectrum $E_\alpha \equiv E_{\mathbf{k}} = \hbar^2|\mathbf{k}|^2/2m$ for $V = L^3 \to \infty$,

$$\begin{aligned}
\rho_{\rm 3d}(E) &= \lim_{L\to\infty} L^{-3}\sum_{\mathbf{k}} \quad \delta(E-E_{\mathbf{k}}) && (10)\\
&= \frac{1}{(2\pi)^3}\int d^3\mathbf{k} \quad \delta(E-E_{\mathbf{k}}) && (11)\\
&= \frac{1}{(2\pi)^3}\int_0^\infty dk k^2 \int_0^{2\pi} d\phi \int_0^\pi \sin\theta d\theta \quad \delta(E-E_{\mathbf{k}}) && (12)\\
&= \frac{1}{(2\pi)^3}4\pi\int_0^\infty dk k^2 \delta(E-\hbar^2k^2/2m) && (13)
\end{aligned}$$

In order to calculate the integral over the Dirac Delta function, we need the property

$$\delta(f(x)) = \sum_{\mathrm{x_i}} \frac{\delta(x - x_i)}{|f'(x_i)|}, \tag{14}$$

for functions $f(x)$ with simple real zeroes x_i.

Here, $x = k$ and

$$0 = f(k) = E - \hbar^2 k^2/2m, \quad k_1 = \sqrt{2mE/\hbar^2}, \quad k_2 = -\sqrt{2mE/\hbar^2} \tag{15}$$

if $E > 0$. For $E < 0$ there is no real solution to $E - \hbar^2 k^2/2m = 0$. In that case, $\delta(f(k)) = 0$. We indicate these two cases by the *step-function* $\theta(E)$, where $\theta(E > 0) = 1$ and $\theta(E < 0) = 0$:

$$\rho_{3\mathrm{d}}(E) \quad = \quad \frac{1}{(2\pi)^3} 4\pi \int_0^\infty dk k^2 \left[\frac{\delta(k - \sqrt{2mE/\hbar^2})}{|\hbar^2 k/m|} + \frac{\delta(k + \sqrt{2mE/\hbar^2})}{|\hbar^2 k/m|} \right] \theta(E)$$

$$= \frac{1}{(2\pi)^3} 4\pi \int_0^\infty dk k^2 \frac{\delta(k - \sqrt{2mE/\hbar^2})}{|\hbar^2 k/m|} \theta(E) \quad (16)$$

$$= \frac{1}{(2\pi)^3} 4\pi \frac{\sqrt{2mE/\hbar^2}}{\hbar^2/m} \theta(E) = \underline{\underline{\frac{m^{3/2}}{\sqrt{2}\pi^2\hbar^3} \sqrt{E}\theta(E).}} \quad (17)$$

Exercise: We consider the density of states $\rho_{\mathrm{QW}}(E)$ of a quantum well system with $E_{l,\mathbf{k}_\parallel} = E_l + \frac{\hbar^2 \mathbf{k}_\parallel^2}{2m}$, Eq. (4). Here, the quantum number $\alpha = (l, \mathbf{k}_\parallel)$ consists of the subband index $l = 0, 1, 2, ...$ and the in-plane, two-dimensional wave vector $\mathbf{k}_\parallel$.

a) Show how to write the $\sum_\alpha ... = \sum_{(l,\mathbf{k}_\parallel)} ...$ in Eq. (8) as a sum over l and a two-dimensional integral over the wave vector.

b) Calculate $\rho_{\mathrm{QW}}(E)$ explicitly. Take care to properly take into account the role of the step functions $\theta(..)$ when you evaluate Eq. (8).