DSE CLASS

CONDENSED MATTER PHYSICS

Lecture-11

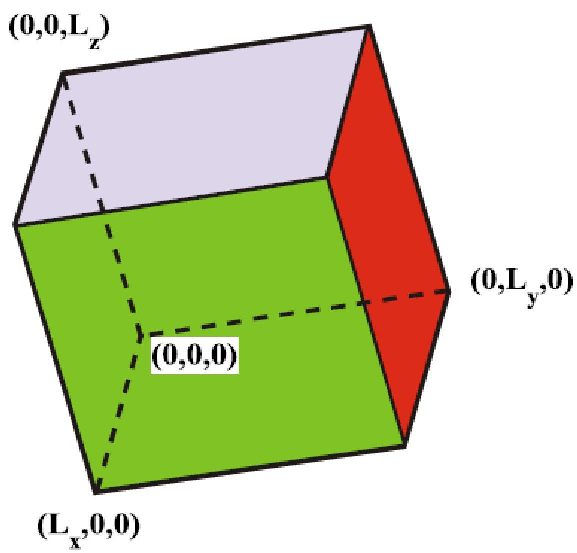
5/1/2021

Density of States

The density of states (DOS) is essentially the number of different states at a particular energy level that electrons are allowed to occupy, i.e. the number of electron states per unit volume per unit energy.

Calculation of the density of states

Assume that the semiconductor can be modeled as an infinite quantum well in which electrons with effective mass, m^*, are free to move.
The semiconductor is assumed a cube with side L.



The wavefunction solution is:

$$\psi(x,y,z) = \sin(k_x x)\sin(k_y y)\sin(k_z z)$$

k_x, k_y, k_z, and are the wavevectors for an electron in the x, y, and z directions

At the opposite boundaries of the rectangular region,

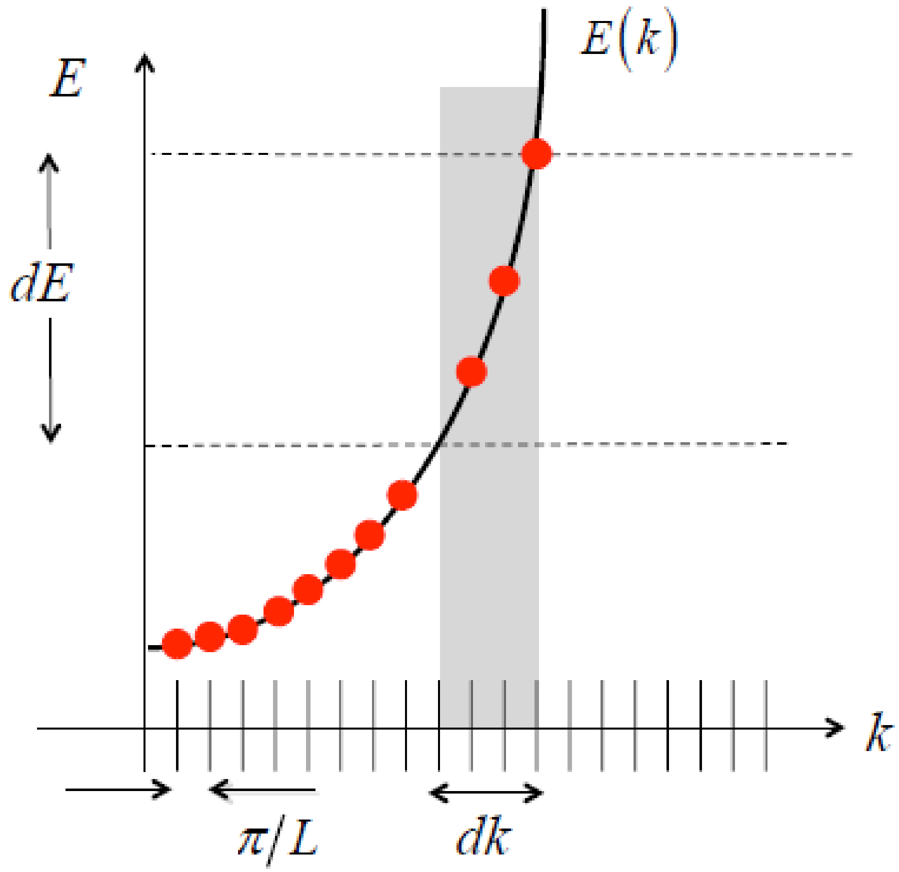
$\sin(k_x L_x) = 0$, $\sin(k_y L_y) = 0$, and $\sin(k_z L_z) = 0$

$$k_x L_x = \pi n_x, k_y L_y = \pi n_y, k_z L_z = \pi n_z, \text{ for } n_x, n_y, n_z \text{ integers}$$

The allowed states can be plotted as a grid of points in k space.

Allowed states are separated by $\pi / L_{x,y,z}$

in the 3 directions in k space

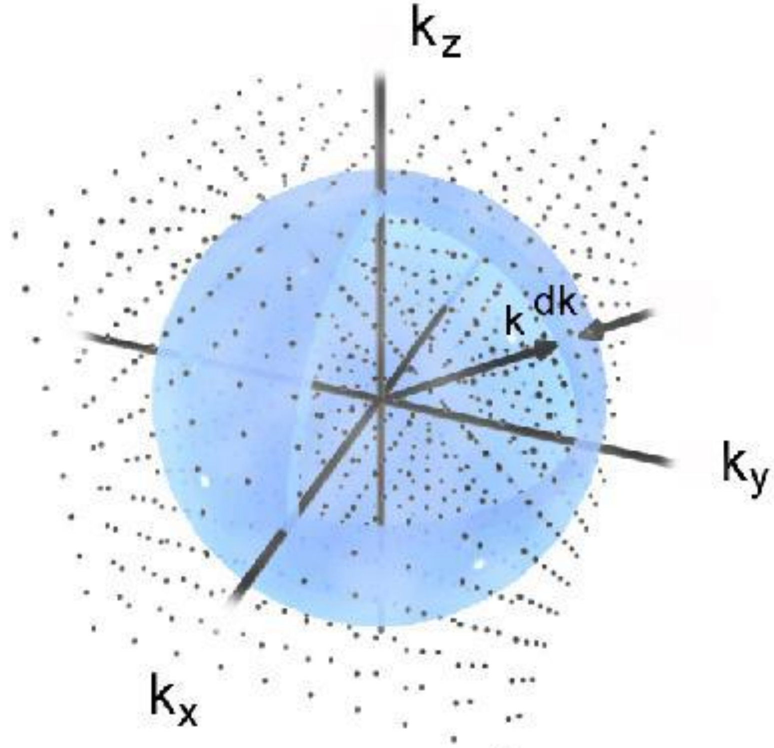


The k space volume taken up by each allowed state is

$\pi^3 / L_x L_y L_z \quad = \pi^3/V$

The number of states available for a given magnitude of wavevector $|k|$ is found by constructing a spherical shell of radius $|k|$ and thickness *dk.*

Allowed states can be plotted as grid of points in k-space



The volume of this spherical shell in k space is $4\pi k^2 dk$

The state density in k space (No. of states per volume in k space)

$= V/\pi^3$

The number of k states within the spherical shell = the k space volume times the k space state density

$$g(k)dk = 4\pi k^2\left[\frac{V}{\pi^3}\right]dk$$

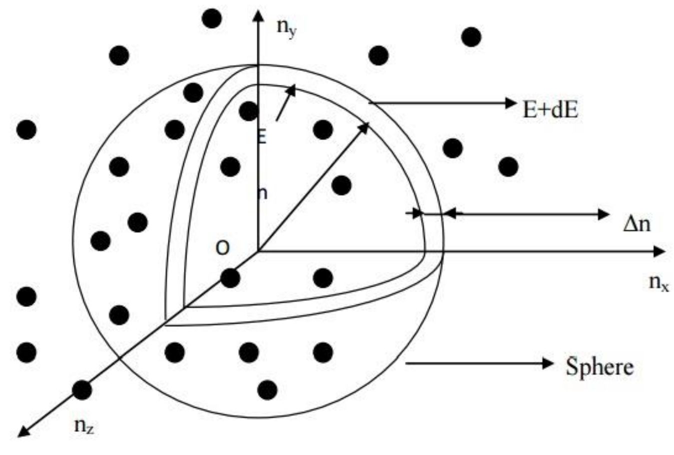
As each k state can hold 2 electrons (of opposite spins), so the number of electron states is:

$$g(k)dk = 8\pi k^2\left[\frac{V}{\pi^3}\right]dk$$

We should count only the positive values of n_x n_y and n_z

Hence the allowed states will be in the positive octant of the spherical shell and thus will be 1/8 of the previous expression

$$g(k)dk = \pi k^2 \left[\frac{V}{\pi^3}\right] dk = \left[\frac{Vk^2}{\pi^2}\right] dk$$



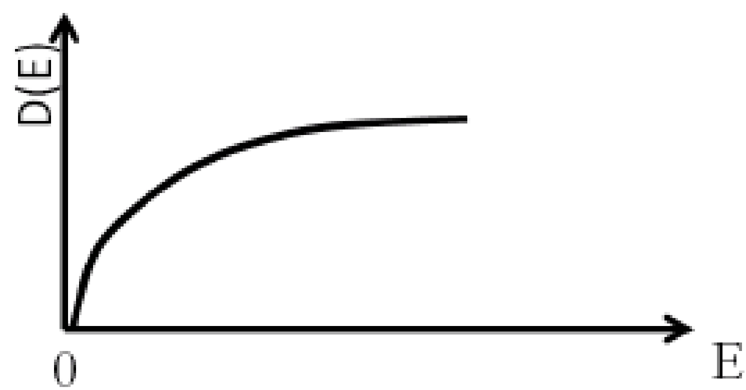
Using dispersion relation for electron energy $E = \frac{\hbar^2 k^2}{2m^*}$

we get $2kdk = \frac{2m^* dE}{\hbar^2}$

now substitute *dk* and *k* in terms of *E in* the expressions for *g(k) dk* to obtain *g(E) dE.*

Next divide *g(E) dE* by *V* to get number of electron states per unit volume over an energy range *dE* and we get density of states function

$$\mathbf{D(E)} = \frac{\mathbf{1}}{\mathbf{2\pi^2}}\left(\frac{\mathbf{2m^*}}{\hbar^{\mathbf{2}}}\right)^{\frac{3}{2}}\mathbf{E^{\frac{1}{2}}}$$



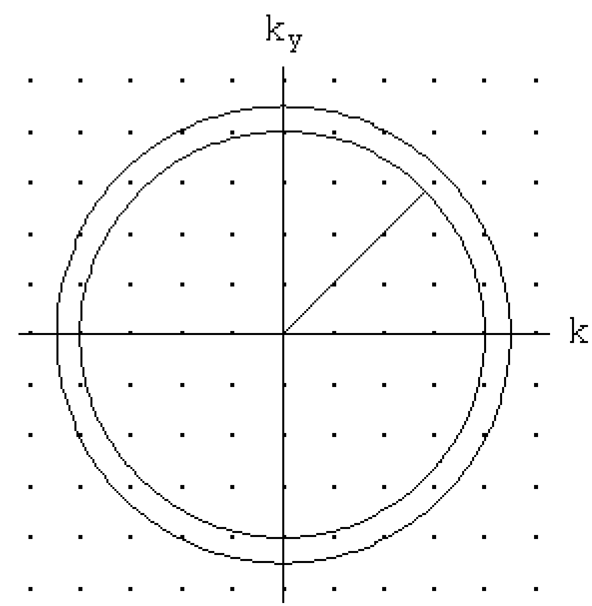
Confining the electron in the *x-y* plane, the wavevector z-component k_z=0

The allowed states in k space becomes a 2 dimensional lattice of k_x and k_y values, spaced $\frac{\pi}{L_{x,y}}$

The state density in k space (No. of states per volume in k space)

$= A/\pi^2$

The number of states available at a given $|k|$ is found using an annular region of radius $|k|$ and thickness dk



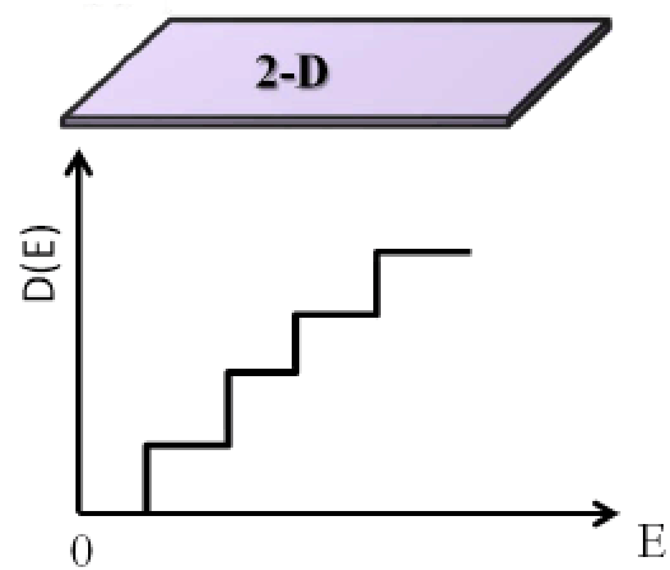
As should count only the positive values of n_x and n_y
the allowed states will be in the positive quadrant of the circle.

Thus a factor of ¼ is multiplied to calculate number of states in the annular ring

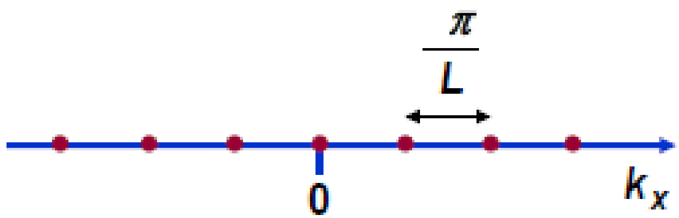
$$g(k)dk = \left[\frac{A}{\pi^2}\right] 2\pi k dk \times 2 \text{ spin states } \div 4 \text{ equivalent states} = k\left[\frac{A}{\pi}\right] dk$$

The density of states for 2D material is:

$$D(E) = \frac{m^*}{\pi \hbar^2}$$

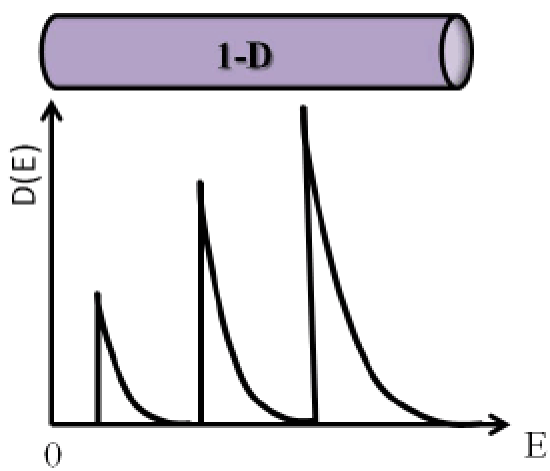


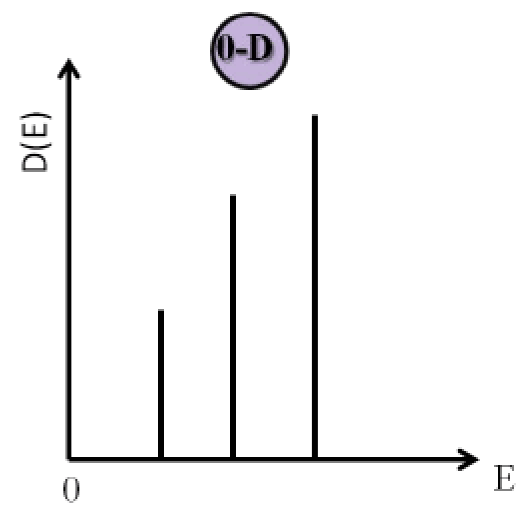
This expression is independent of energy E

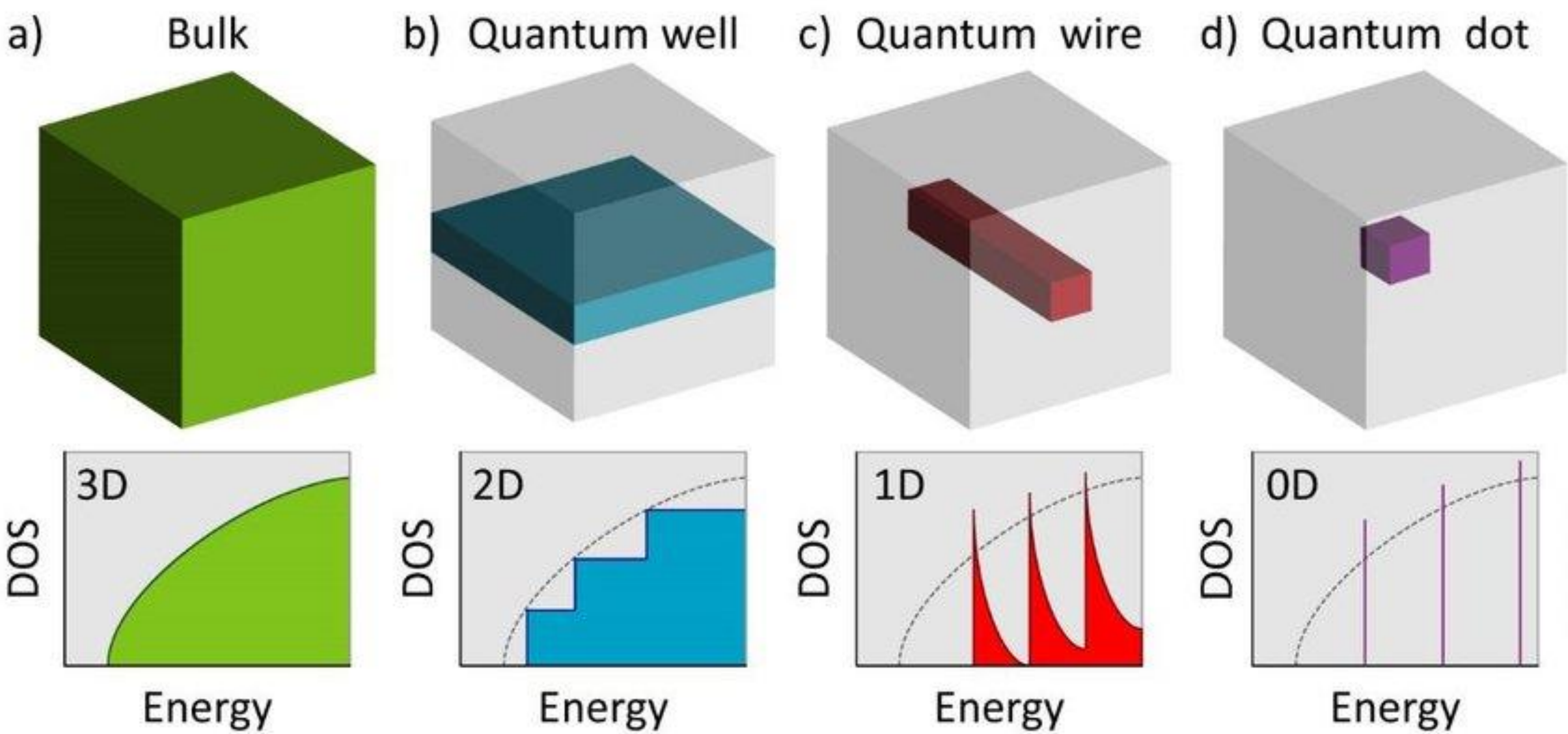


The density of states for 1D material is: $$D(E) = \frac{\sqrt{2m^*}}{\pi\hbar} E^{-\frac{1}{2}}$$

The density of states for 0D material is: $$D(E) = 2\delta(\mathrm{E})$$







a) Bulk
b) Quantum well
c) Quantum wire
d) Quantum dot
3D
2D
1D
0D
DOS
DOS
DOS
DOS
Energy
Energy
Energy
Energy

Electron Transport Physics in Nanoscale Systems

Hydrodynamic and ballistic transport

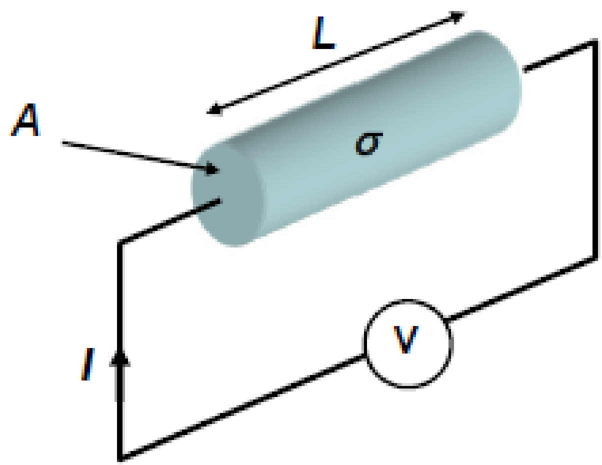
Quantized conductance

Coulomb blockage of tunneling

Coherent carrier transport

Charge density wave and spin density wave transport

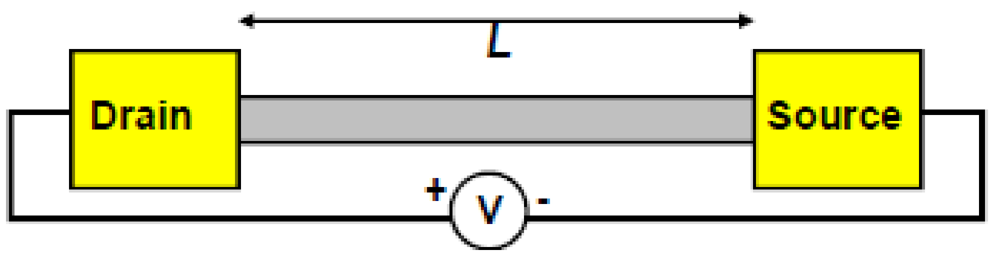
Traditional View of Conductors:

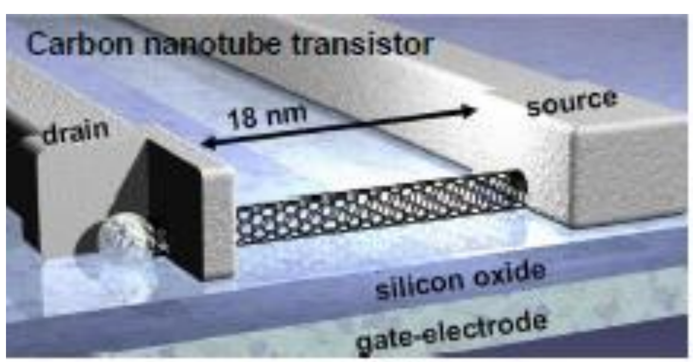


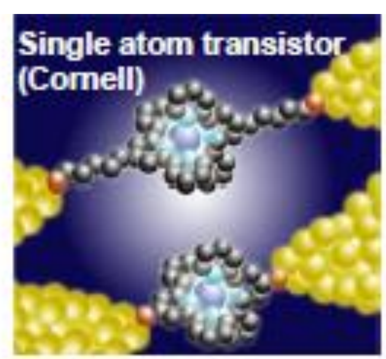
$$J = \sigma E$$

$$I = AJ = A\sigma E = \frac{\sigma A}{L} V = GV = \frac{V}{R}$$

$$\Rightarrow G = \frac{\sigma A}{L} = \frac{1}{R}$$







Important length scales

Elastic mean free path (l_e): average distance the electrons travel without being elastically scattered

$l_e = v_F \tau_e$. v_F denotes the Fermi velocity of the electrons

Phase coherent length (l_Φ): average distance the electrons travel before their phase is randomized

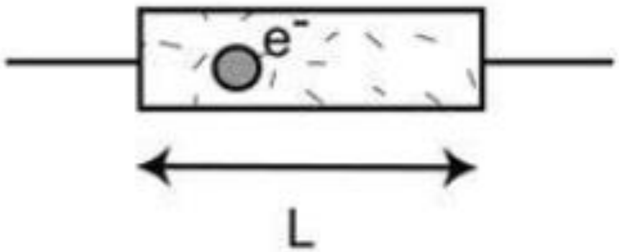
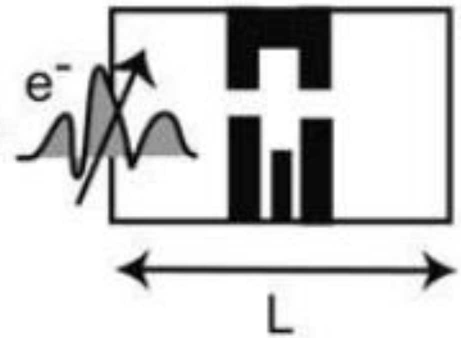
$l_\Phi = v_F \tau_\Phi$. τ_Φ denotes the dephasing time of the electrons

Fermi wavelength (λ_F): de Broglie wavelength of Fermi electrons

in $d = 3$: $\lambda_F = 2^{3/2}(\pi/3n)^{1/3}$

in $d = 2$: $\lambda_F = (2\pi/n)^{1/2}$

in $d = 1$: $\lambda_F = 4/n$

conventional device: 		mesoscopic device: 	
$L \gg l_e$	diffusive	$L \lesssim l_e$	ballistic
$L \gg l_\phi$	incoherent	$L \lesssim l_\phi$	phase coherent
$L \gg \lambda_F$	no size quantization	$L \lesssim \lambda_F$	size quantization
$e^2/C < k_B\Theta$	no single electron charging	$e^2/C \gtrsim k_B\Theta$	single electron charging effects
$L \gg l_s$	no spin effects	$L \lesssim l_s$	spin effects

Conduction at the macroscale

- Large number of states contribute to overall current
- Large number of electrons
- Resistivity, mobility, electric field, bias voltage, macrocopic currents are well-defined
- Quantum effects are averaged out by thermal effects

Conduction at the nanoscale

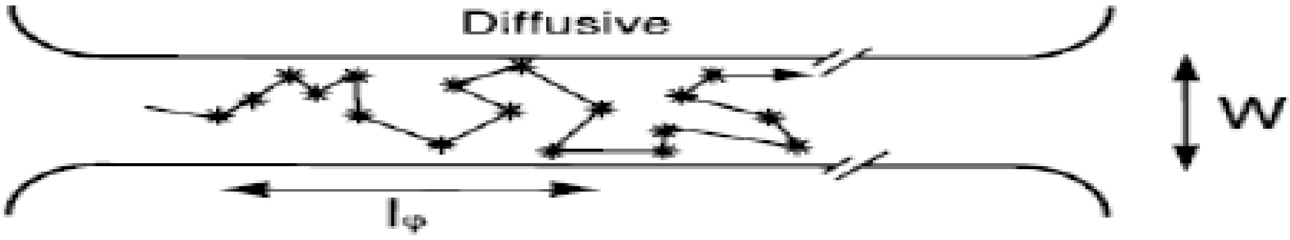
- Small number of states can affect the overall current
- Wavefunction coherence lengths are comparable to characteristic device dimensions
- Single electrons charging effects can be significant
- These can amount to overall macroscopic electronic properties that show deviations from bulk electronic properties

Ballistic, quasi-ballistic and diffusive transport

The transport in low-dimensional electron systems can be classified intothree regimes:
diffusive, **ballistic** and **quasi-ballistic.**

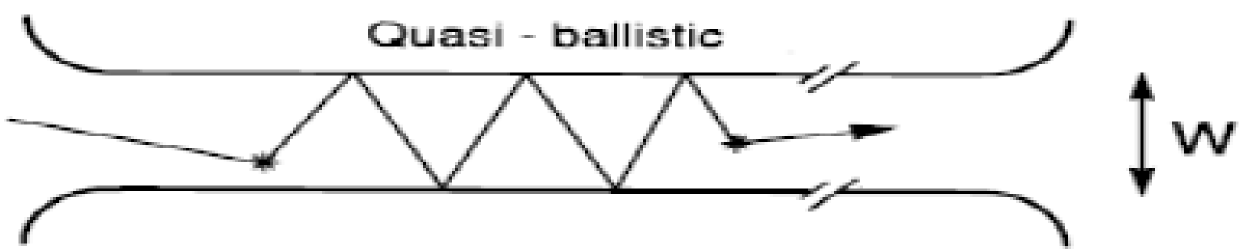
In the **diffusive regime** both the length L and the width W of the conductor are much larger than the electron mean free path, W,L > ℓe

The transport properties are dominated by elastic scattering and can be expressed by classical Drude theory



If the width of the conductor is smaller than the ℓe, but the length larger,
W < ℓe < L, the transport is said to be **quasi-ballistic**.

This is an intermediate regime in which both impurity and boundary scattering become important.

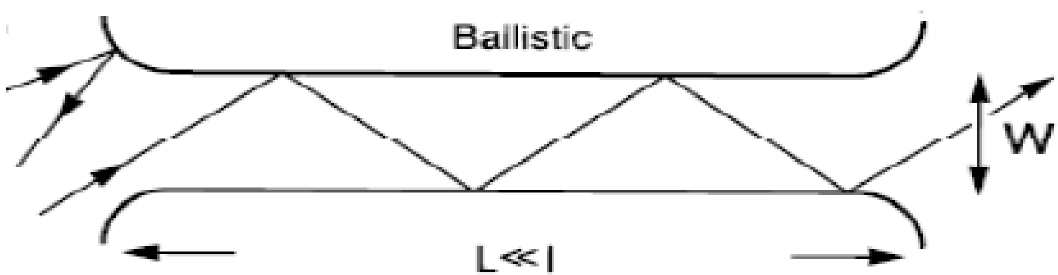


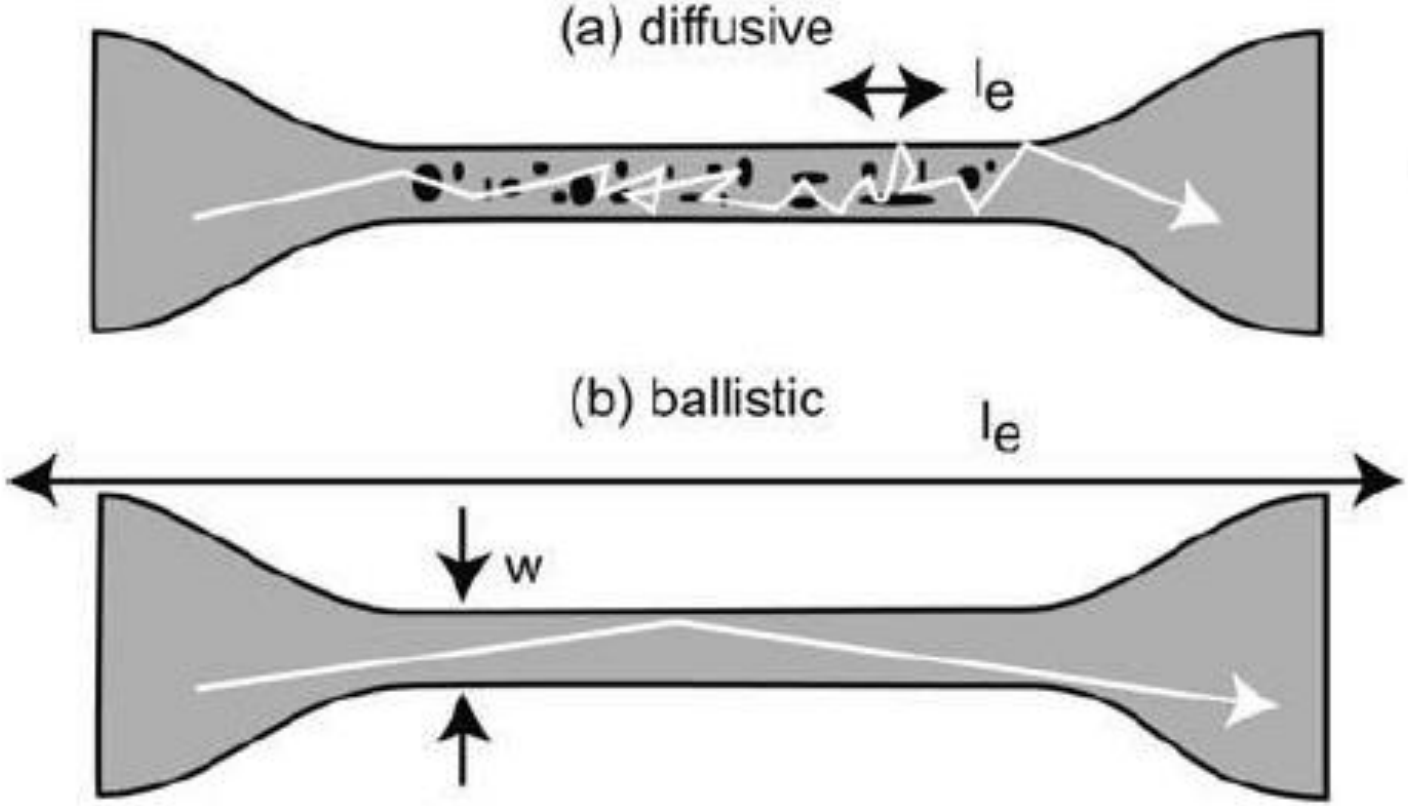
Ballistic transport occurs when the mean free path is larger than both the width and length of the conductor, $\ell e > W,L$.

In this case electrons do not scatter from impurities but only from the boundaries of the conductor.

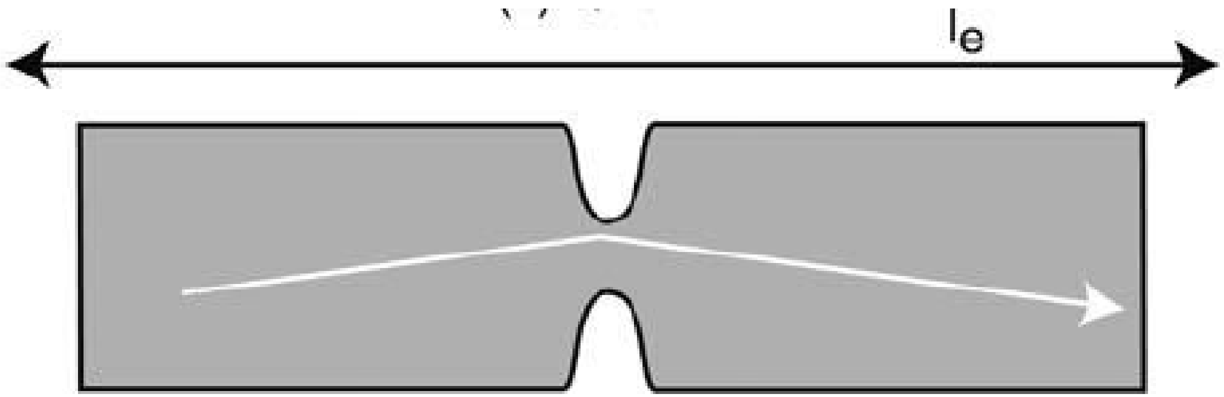
Backscattering at the entrance of the constriction results in a non-zero resistance in the ballistic regime.

The limiting contact resistance depends on the geometry of the sample, and not its length; therefore the **transport properties cannot be expressed in terms of local quantities**, such as conductivity, as is the case in diffusive transport.



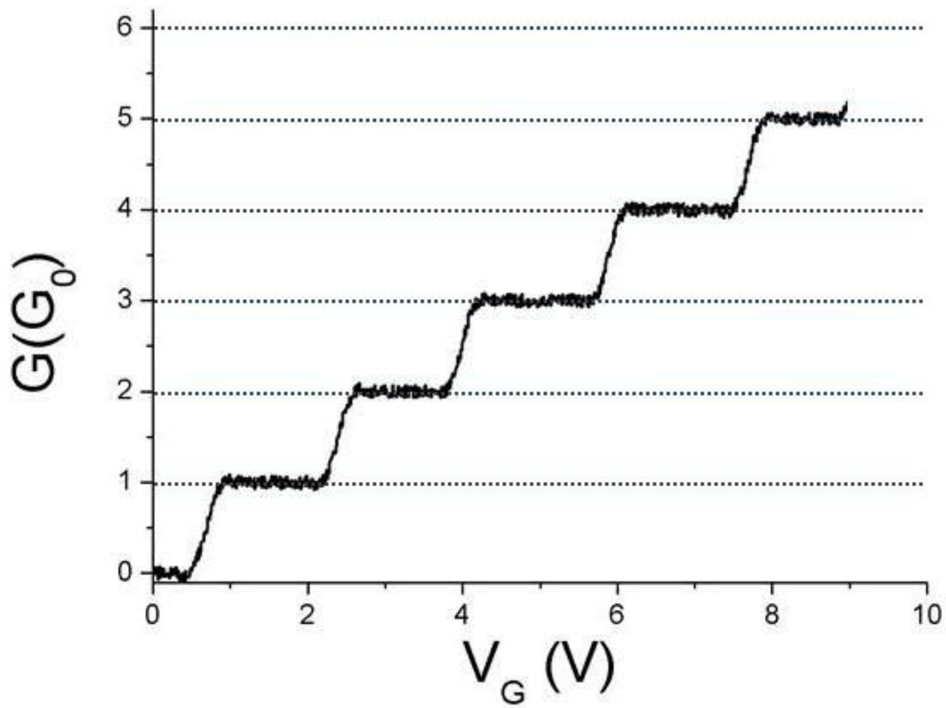

(a) diffusive
l_e
(b) ballistic
l_e
w

If a width of constriction is small enough it forms a one dimensional conductor, known as **a quantum point contact**



Quantisation and the Landauer formalism

Measurements of the conductance G =dI/dV reveal that it does not fall in a smooth fashion, but instead exhibits plateaus and rises

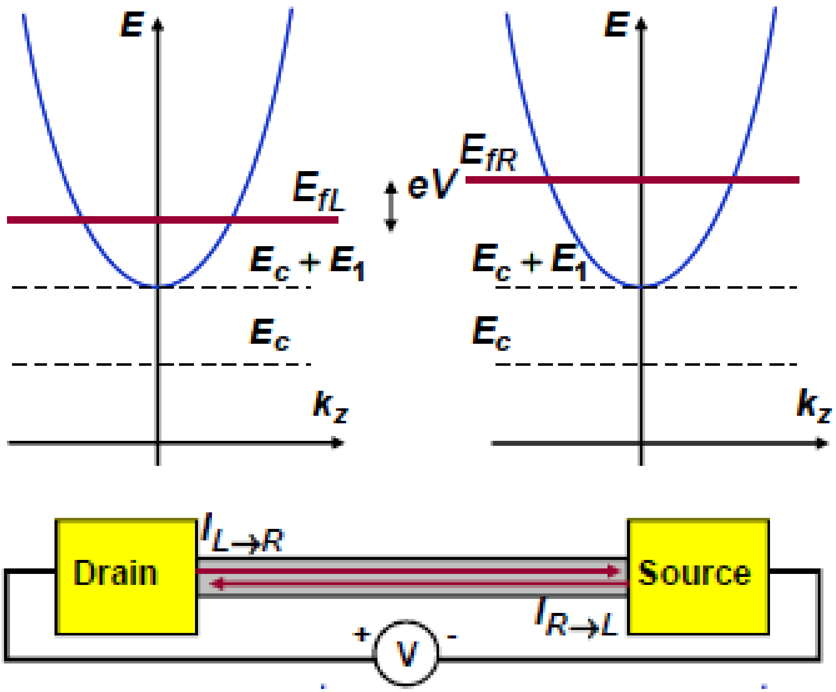


On the plateaus the conductance is quantised at integer multiples $\frac{2e^2}{h}$

The voltage source will raise the chemical potential (or the Fermi level) on one side of the conductor with respect to the other by an amount eV

Electrons do not scatter in the quantum wire. Therefore:

- All electrons that enter the wire from the left contact make it to the right contact
- All electrons that enter the wire from the right contact make it to the left contact



Total Current:

The net current is the sum of the currents due to the right-moving and left-moving electrons:

$$I = I_{L\to R} + I_{R\to L}$$

$$I = \frac{e}{\pi \hbar}(eV) \qquad I = GV$$

$$= \frac{e^2}{\pi \hbar} V \qquad \Rightarrow \; G = \frac{e^2}{\pi \hbar} = 7.72\times 10^{-5}\ \text{S}$$

The quantum of resistance is therefore: $R_Q = \frac{1}{G_Q} = \frac{\pi \hbar}{e^2} = 12.95\ \text{k}\Omega$

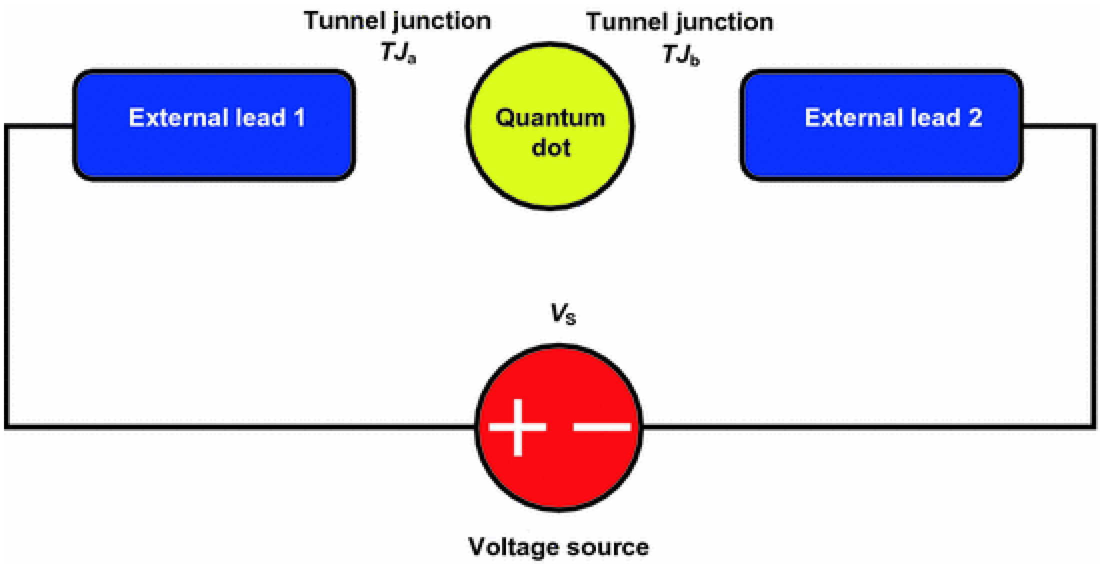
The Quantum of Conductance:

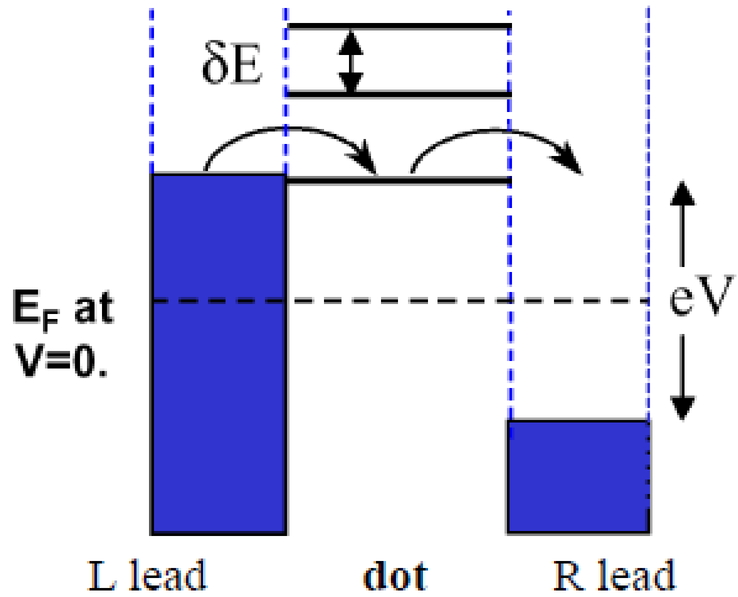
- The quantum of conductance is the smallest possible non-zero conductance of a completely ballistic conductor. Equivalently, the quantum of resistance is the highest possible resistance of a completely ballistic conductor.

- All completely ballistic conductors (whether in 1D, 2D, or 3D) will have conductance that is in multiples of the quantum conductance value (one can think of ballistic conductance in 2D and 3D as a number of 1D conductors in parallel)

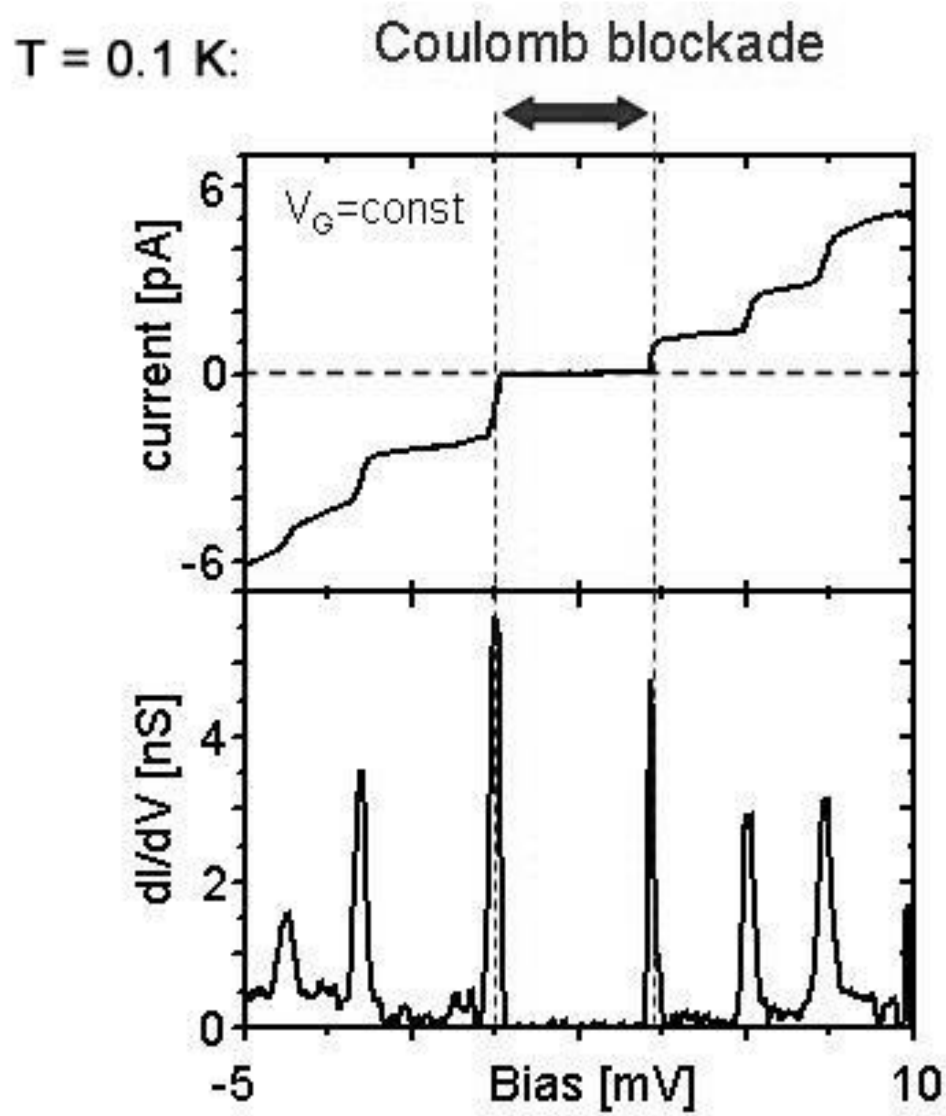
Coulomb Blockade: Non-linear Transport

The single-electron transistor consists of a metallic island, placed between two tunneling junctions connected to a drain and a source and has a gate electrode as in a normal field-effect transistor.
The tunneling junctions are simply a thin (<10 nm) oxide layer between the island and the electrodes.





δE
E_F at
V=0.
eV
L lead
dot
R lead



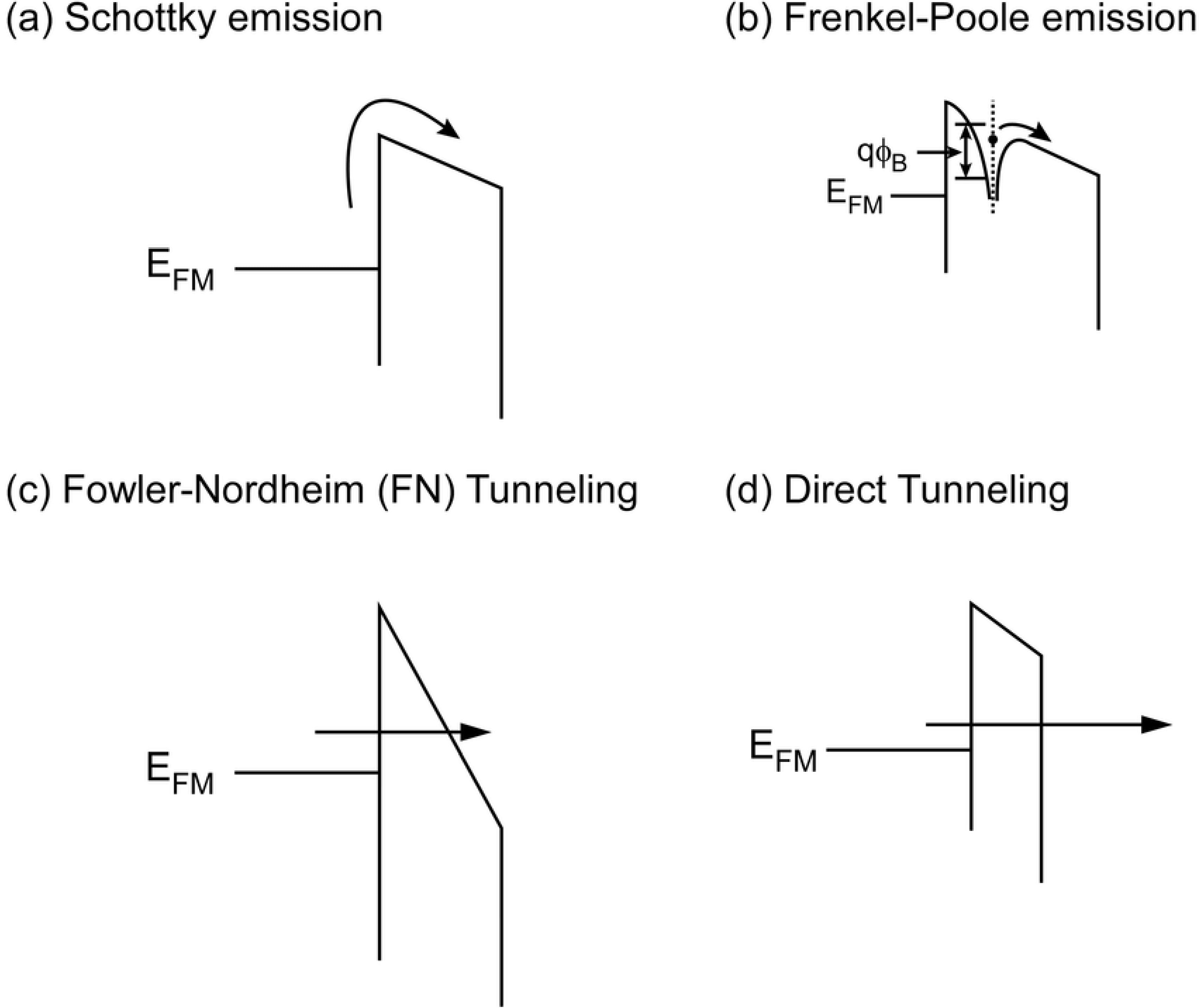
T = 0.1 K:
Coulomb blockade
V_G=const
current [pA]
6
0
-6
dI/dV [nS]
4
2
0
-5
Bias [mV]
10

The conductance through a small grain weakly coupled to metallic leads shows periodic dependence on the voltage applied to a gate electrode.

This phenomenon is observed in both metallic and semiconductor devices, and is commonly referred to as the Coulomb blockade.

This behavior of conductance is caused by electrostatic energy arising due to a change in the charge of the grain(quantum dot) by an electron tunneling through it.

The Coulomb blockade is typically observed in structures with a well defined quantum dot, which is separated from the leads by tunneling barriers


(a) Schottky emission
E_{FM}
(b) Frenkel-Poole emission
$q\phi_B$
E_{FM}
(c) Fowler-Nordheim (FN) Tunneling
E_{FM}
(d) Direct Tunneling
E_{FM}