Mobility

2003

High-performance thin-film transistors using semiconductor nanowires and nanoribbons

Xiangfeng Duan[1,2], Chunming Niu[1,2], Vijendra Sahi[1,2], Jian Chen[2],
J. Wallace Parce[2], Stephen Empedocles[2] & Jay L. Goldman[1,2]

[1]Nanosys, Inc., Advanced Research Center, 200 Boston Ave, Medford,
Massachusetts 02155, USA
[2]Nanosys, Inc., 2625 Hanover Street, Palo Alto, California 94304, USA

Thin-film transistors (TFTs) are the fundamental building blocks for the rapidly growing field of macroelectronics[1,2]. The use of plastic substrates is also increasing in importance owing to their light weight, flexibility, shock resistance and low cost[3,4]. Current polycrystalline-Si TFT technology is difficult to implement on plastics because of the high process temperatures required[1,2]. Amorphous-Si and organic semiconductor[5,6] TFTs, which can be

processed at lower temperatures, but are limited by poor carrier mobility. As a result, applications that require even modest computation, control or communication functions on plastics cannot be addressed by existing TFT technology. Alternative semiconductor materials[7,8] that could form TFTs with performance comparable to or better than polycrystalline or single-crystal Si, and which can be processed at low temperatures over large-area plastic substrates, should not only improve the existing technologies, but also enable new applications in flexible, wearable and disposable electronics. Here we report the fabrication of TFTs using oriented Si nanowire thin films or CdS nanoribbons as semiconducting channels. We show that high-performance TFTs can be produced on various substrates, including plastics, using a low-temperature assembly process. Our approach is general to a broad range of materials including high-mobility materials (such as InAs or InP).

2006

Ge/Si nanowire heterostructures as high-performance field-effect transistors

Jie Xiang[1]*, Wei Lu[1]*, Yongjie Hu[1], Yue Wu[1], Hao Yan[1] & Charles M. Lieber[1,2]

Semiconducting carbon nanotubes[1,2] and nanowires[3] are potential alternatives to planar metal-oxide-semiconductor field-effect transistors (MOSFETs)[4] owing, for example, to their unique electronic structure and reduced carrier scattering caused by one-dimensional quantum confinement effects[1,5]. Studies have demonstrated long carrier mean free paths at room temperature in both carbon nanotubes[1,6] and Ge/Si core/shell nanowires[7]. In the case of carbon nanotube FETs, devices have been fabricated that work close to the ballistic limit[8]. Applications of high-performance carbon nanotube FETs have been hindered, however, by difficulties in producing uniform semiconducting nanotubes, a factor not limiting nanowires, which have been prepared with reproducible electronic properties in high yield as required for large-scale integrated systems[3,9,10]. Yet whether nanowire field-

effect transistors (NWFETs) can indeed outperform their planar counterparts is still unclear[4]. Here we report studies on Ge/Si core/shell nanowire heterostructures configured as FETs using high-κ dielectrics in a top-gate geometry. The clean one-dimensional hole-gas in the Ge/Si nanowire heterostructures[7] and enhanced gate coupling with high-κ dielectrics give high-performance FETs values of the scaled transconductance ($3.3\,\mathrm{mS}\,\mu\mathrm{m}^{-1}$) and on-current ($2.1\,\mathrm{mA}\,\mu\mathrm{m}^{-1}$) that are three to four times greater than state-of-the-art MOSFETs and are the highest obtained on NWFETs. Furthermore, comparison of the intrinsic switching delay, $\tau = CV/I$, which represents a key metric for device applications[4,11], shows that the performance of Ge/Si NWFETs is comparable to similar length carbon nanotube FETs and substantially exceeds the length-dependent scaling of planar silicon MOSFETs.

2011

Single-layer MoS$_2$ transistors

B. Radisavljevic[1], A. Radenovic[2], J. Brivio[1], V. Giacometti[1] and A. Kis[1]*

Two-dimensional materials are attractive for use in next-generation nanoelectronic devices because, compared to one-dimensional materials, it is relatively easy to fabricate complex structures from them. The most widely studied two-dimensional material is graphene[1,2], both because of its rich physics[3-5] and its high mobility[6]. However, pristine graphene does not have a bandgap, a property that is essential for many applications, including transistors[7]. Engineering a graphene bandgap increases fabrication complexity and either reduces mobilities to the level of strained silicon films[8-13] or requires high voltages[14,15]. Although single layers of MoS$_2$ have a large intrinsic

bandgap of 1.8 eV (ref. 16), previously reported mobilities in the 0.5–3 $cm^2 V^{-1} s^{-1}$ range[17] are too low for practical devices. Here, we use a halfnium oxide gate dielectric to demonstrate a room-temperature single-layer MoS_2 mobility of at least 200 $cm^2 V^{-1} s^{-1}$, similar to that of graphene nanoribbons, and demonstrate transistors with room-temperature current on/off ratios of 1×10^8 and ultralow standby power dissipation. Because monolayer MoS_2 has a direct bandgap[16,18], it can be used to construct interband tunnel FETs[19], which offer lower power consumption than classical transistors. Monolayer MoS_2 could also complement graphene in applications that require thin transparent semiconductors, such as optoelectronics and energy harvesting.

2015

Silicene field-effect transistors operating at room temperature

Li Tao[1], Eugenio Cinquanta[2], Daniele Chiappe[2], Carlo Grazianetti[2], Marco Fanciulli[2], Madan Dubey[3], Alessandro Molle[2]* and Deji Akinwande[1]*

Free-standing silicene, a silicon analogue of graphene, has a buckled honeycomb lattice[1] and, because of its Dirac bandstructure[2,3] combined with its sensitive surface, offers the potential for a widely tunable two-dimensional monolayer, where external fields and interface interactions can be exploited to influence fundamental properties such as bandgap[4] and band character[5] for future nanoelectronic devices[6,7]. The quantum spin Hall effect[3], chiral superconductivity[8], giant magnetoresistance[9] and various exotic field-dependent states[7] have been predicted in monolayer silicene. Despite recent progress regarding the epitaxial synthesis of silicene[8-10] and investigation of its electronic properties[11,13-15], to date there has

been no report of experimental silicene devices because of its air stability issue[16]. Here, we report a silicene field-effect transistor, corroborating theoretical expectations regarding its ambipolar Dirac charge transport[17], with a measured room-temperature mobility of $\sim 100 \ \mathrm{cm^2 \ V^{-1} \ s^{-1}}$ attributed to acoustic phonon-limited transport[18] and grain boundary scattering. These results are enabled by a growth–transfer–fabrication process that we have devised—silicene encapsulated delamination with native electrodes. This approach addresses a major challenge for material preservation of silicene during transfer and device fabrication and is applicable to other air-sensitive two-dimensional materials such as germanene[2-4] and phosphorene[19,20]. Silicene's allotropic affinity with bulk silicon and its low-temperature synthesis compared with graphene or alternative two-dimensional semiconductors suggest a more direct integration with ubiquitous semiconductor technology.

Who is conducting?

# Who is conducting?

Electrons

# Who is conducting?

Electrons

How?

Role of Electrons in Solids

- **Electrons are responsible for binding of crystals -- they are the "glue" that hold the nuclei together**

  Types of binding (see next slide)

   Van der Waals - electronic polarizability

   Ionic - electron transfer

   Covalent - electron bonds

- **Electrons are responsible for important properties:**

  Electrical conductivity in metals

  (But why are some solids insulators?)
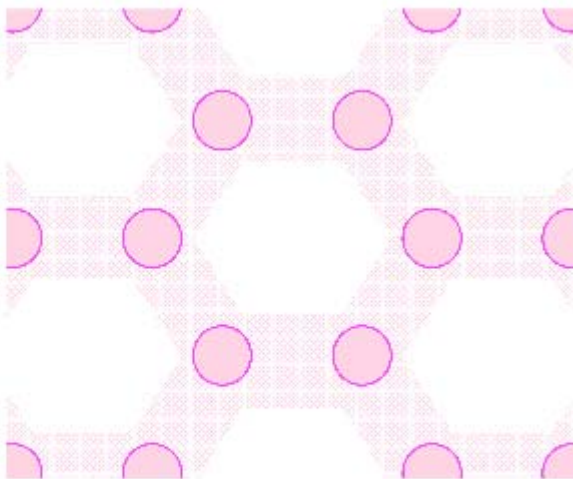
  Magnetism

  Optical properties

   . . . .
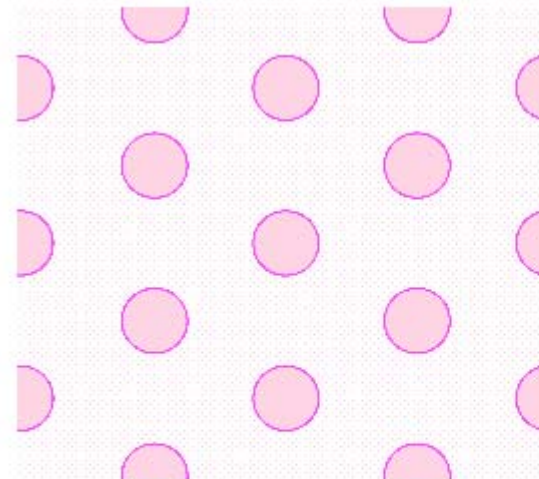
Characteristic types of binding
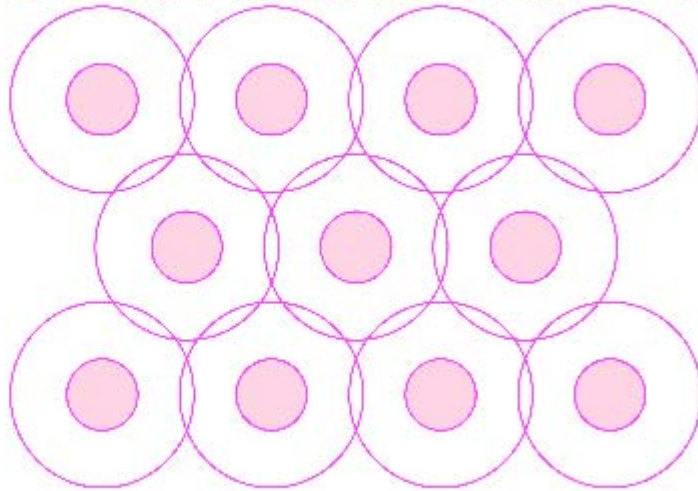
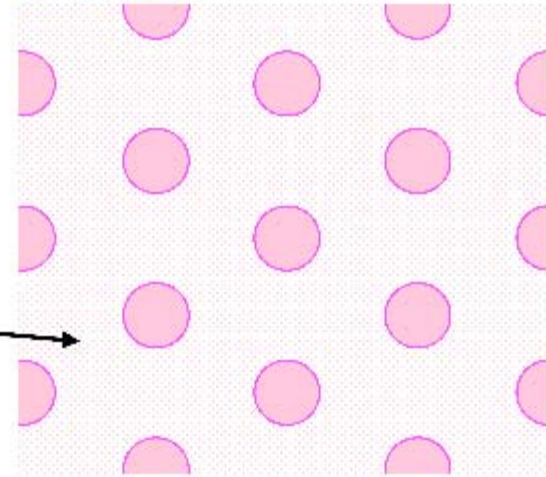**Closed-Shell Binding Van der Waals**
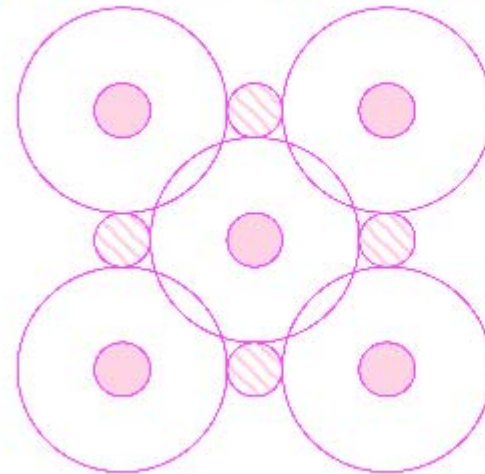
Ionic Binding

Covalent Binding

Metallic Binding

Starting Point for Understanding Electrons in Solids

- **Nature of a metal:** Electrons can become "free of the nuclei" and move between nuclei since we observe electrical conductivity

- **Electron Gas** Simplest possible model for a metal - electrons are completely "free of the nuclei" - nuclei are replaced by a smooth background -- **"Electrons in a box"**
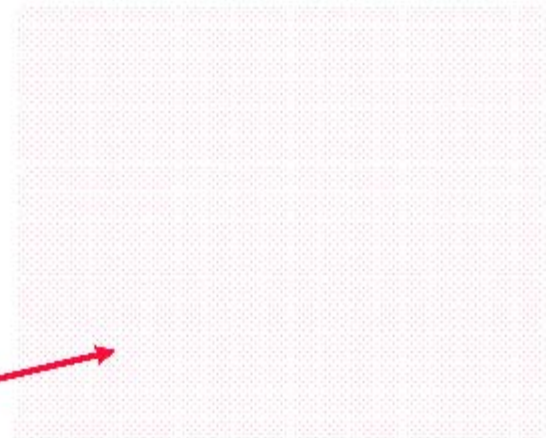
Electron Gas - History

- **Electron Gas** model predates quantum mechanics

- **Electrons Discovered in 1897**

- **Drude-Lorentz Model (1905)- Electrons - classical particles free to move in a box**

- **Model: All electrons contribute to conductivity. Works! Still used!**

- **But same model predicted that all electrons contribute to heat capacity. Disaster. Heat capacity is MUCH less than predicted.**
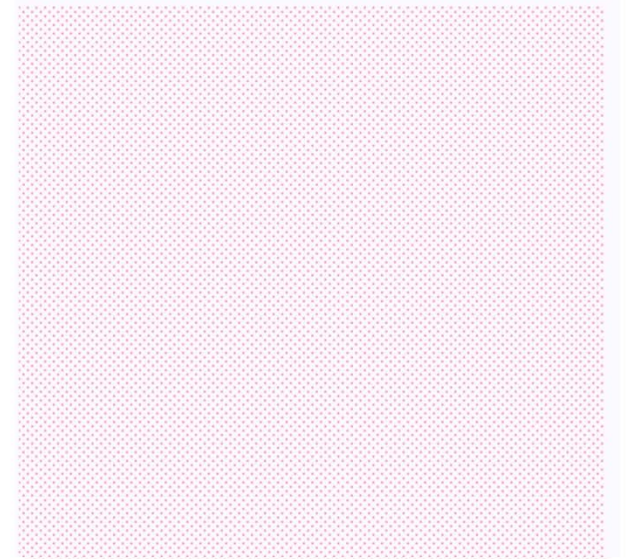
The free electron theory of metals
The Drude theory of metals

Paul Drude (1900): theory of electrical and thermal conduction in a metal
application of the kinetic theory of gases to a metal,
which is considered as a gas of electrons

mobile negatively charged electrons are confined in a
metal by attraction to immobile positively charged ions

isolated atom in a metal
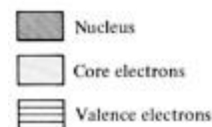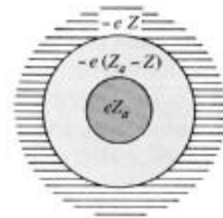
nucleus charge eZ_a
Z <u>valence electrons</u> are weakly bound to the nucleus (participate in chemical reactions)
$Z_a - Z$ <u>core electrons</u> are tightly bound to the nucleus (play much less of a role in chemical reactions)
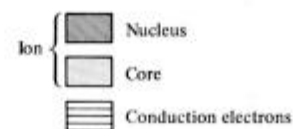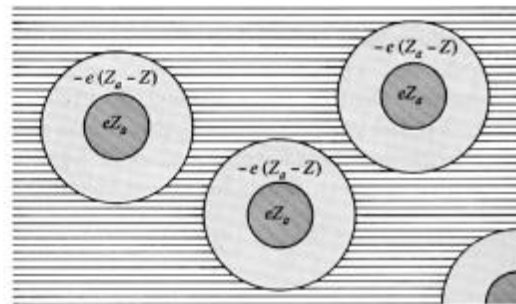
in a metal – the <u>core electrons</u> remain bound to the nucleus to form the metallic ion
the <u>valence electrons</u> wander far away from their parent atoms
called <u>conduction electrons</u> or <u>electrons</u>

density of conduction electrons in metals $\sim 10^{22} - 10^{23}$ cm^{-3}

r_s – measure of electronic density
r_s is radius of a sphere whose volume is equal to the volume per electron

$$\frac{4\pi r_s^3}{3} = \frac{V}{N} = \frac{1}{n} \qquad r_s = \left(\frac{3}{4\pi n}\right)^{1/3} \sim \frac{1}{n^{1/3}}$$

mean inter-electron spacing

in metals $r_s \sim 1 - 3$ Å $(1$ Å$ = 10^{-8}$ cm$)$ $\qquad r_s/a_0 \sim 2 - 6$

$$a_0 = \frac{\hbar^2}{me^2} = 0.529\text{Å} - \text{Bohr radius}$$

● electron densities are thousands times greater than those of a gas at normal conditions
● there are strong electron-electron and electron-ion electromagnetic interactions
↓

in spite of this the Drude theory treats the electron gas
by the methods of the kinetic theory of a neutral dilute gas

The basic assumptions of the Drude model

1. between collisions the interaction of a given electron
with the other electrons is neglected ⟵————————— independent electron approximation
and with the ions is neglected ⟵————————— free electron approximation

2. collisions are instantaneous events
Drude considered electron scattering off
the impenetrable ion cores
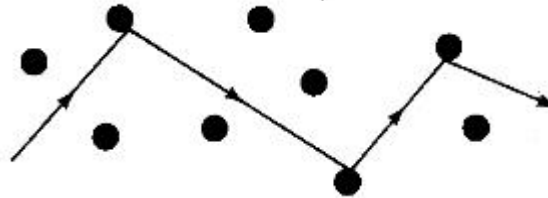
the specific mechanism of the electron scattering is not considered below

3. an electron experiences a collision with a probability per unit time $1/\tau$
dt/τ – probability to undergo a collision within small time dt
randomly picked electron travels for a time τ before the next collision
τ is known as the <u>relaxation time</u>, the <u>collision time</u>, or the <u>mean free time</u>
τ is independent of an electron position and velocity

4. after each collision an electron emerges with a velocity that is randomly directed and
with a speed appropriate to the local temperature

DC electrical conductivity of a metal

$V = RI$ Ohm's low

the Drude model provides an estimate for the resistance

introduce characteristics of the metal which are independent on the shape of the wire

$$\mathbf{E} = \rho\mathbf{j} \qquad\qquad \mathbf{j} = \sigma\mathbf{E}$$

$j=I/A$ – the current density
ρ – the resistivity
$R = \rho L/A$ – the resistance
$\sigma = 1/\rho$ – the conductivity
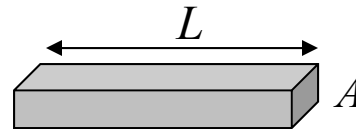
$$\mathbf{j} = -en\mathbf{v}$$

$\mathbf{v}$ is the average electron velocity

$$\mathbf{v} = -\frac{e\mathbf{E}}{m}\tau \qquad\qquad \mathbf{j} = \left(\frac{ne^2\tau}{m}\right)\mathbf{E}$$

$$\mathbf{j} = \sigma\mathbf{E} \qquad \sigma = \frac{ne^2\tau}{m}$$

$$\tau = \frac{m}{\rho n e^2}$$

at room temperatures
resistivities of metals are typically of the order of microohm centimeters (μohm-cm)
and τ is typically $10^{-14} - 10^{-15}$ s

mean free path $l = v_0 \tau$
v_0 – the average electron speed
l measures the average distance an electron travels between collisions
estimate for v_0 at Drude's time $1/2 \, m v_0^2 = 3/2 \, k_B T \rightarrow v_0 \sim 10^7$ cm/s $\rightarrow l \sim 1 - 10$ Å
consistent with Drude's view that collisions are due to electron bumping into ions

at low temperatures very long mean free path can be achieved
$l > 1$ cm $\sim 10^8$ interatomic spacings!
the electrons do not simply bump off the ions!

the Drude model can be applied where
a precise understanding of the scattering mechanism is not required

particular cases: electric conductivity in spatially uniform static magnetic field
and in spatially uniform time-dependent electric field

Very disordered metals and semiconductors

Motion under the influence of the force $\mathbf{f}(t)$ due to spatially uniform electric and/or magnetic fields

Equation of motion
for the momentum per electron

$$\frac{d\mathbf{p}(t)}{dt} = -\frac{\mathbf{p}(t)}{\tau} + \mathbf{f}(t)$$

average momentum → average velocity →

$$\mathbf{p}(t) = m\mathbf{v}(t)$$

Electron collisions introduce a frictional damping term for the momentum per electron

Free electron model:
Works best for alkali metals (Group I: Li, Na, K, Cs, Rb)

Successes of classical model:
Ohm's law.
σ / κ

Failures of classical model:
Heat capacity.
Magnetic susceptibility.
Mean free path.

Drude model ~ Quantum model

Quantum Mechanics

- **1911: Bohr Model for H**

- **1923: Wave Nature of Particles Proposed**
  Prince Louis de Broglie

- **1924-26: Development of Quantum Mechanics - Schrodinger equation**

- **1924: Bose-Einstein Statistics for Identical Particles (phonons, ...)**

- **1925-26: Pauli Exclusion Principle, Fermi-Dirac Statistics (electrons, ...)**

- **1925: Spin of the Electron (spin = 1/2)**
  G. E. Uhlenbeck and S. Goudsmit

Schrodinger

SUMMARY OF PHOTON PROPERTIES

Relation between particle and wave properties of light

Energy and frequency $E = h\nu$

Relativistic formula relating energy and momentum $\Rightarrow$ $E^2 = p^2 c^2 + m^2 c^4$

For light $E = pc$ and $c = \lambda\nu$

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

Also commonly write these as

$E = \hbar\omega$ $\quad p = \hbar k \quad$ $\omega = 2\pi\nu$ $\quad$ wavevector $k = \dfrac{2\pi}{\lambda}$ $\quad \hbar = \dfrac{h}{2\pi}$

angular frequency $\qquad\qquad$ hbar

MATTER WAVES

We have seen that light comes in discrete units (photons) with particle properties (energy and momentum) that are related to the wave-like properties of frequency and wavelength.

In 1923 Prince Louis de Broglie postulated that ordinary matter can have wave-like properties, with the wavelength λ related to momentum p in the same way as for light

de Broglie relation

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

Planck's constant

$$h = 6.63 \times 10^{-34}\, \text{Js}$$

de Broglie wavelength

Wavelength depends on momentum, not on the physical size of the particle

$$E = h\nu \qquad p = \frac{h}{\lambda}$$

Estimate some de Broglie wavelengths

• Wavelength of electron with 50eV kinetic energy

$$K = \frac{p^2}{2m_e} = \frac{h^2}{2m_e\lambda^2} \Rightarrow \lambda = \frac{h}{\sqrt{2m_e K}} = 1.7 \times 10^{-10}\,\text{m}$$

• Wavelength of Nitrogen molecule at room temp.

$$K = \frac{3kT}{2}, \quad \text{Mass} = 28\text{m}_u$$

$$\lambda = \frac{h}{\sqrt{3MkT}} = 2.8 \times 10^{-11}\,\text{m}$$

• Wavelength of Rubidium(87) atom at 50nK

$$\lambda = \frac{h}{\sqrt{3MkT}} = 1.2 \times 10^{-6}\,\text{m}$$

The Sommerfeld theory of metals

the Drude model: electronic velocity distribution is given by the classical <u>Maxwell-Boltzmann distribution</u>

$$f_{MB}(\mathbf{v}) = n \left(\frac{m}{2\pi k_B T} \right)^{3/2} \exp\left(-\frac{mv^2}{2k_B T} \right)$$

the Sommerfeld model: electronic velocity distribution is given by the quantum <u>Fermi-Dirac distribution</u>

$$f_{FD}(\mathbf{v}) = \frac{(m/\hbar)^3}{4\pi^3} \frac{1}{\exp\left(\dfrac{\frac{1}{2}mv^2 - k_B T_0}{k_B T} \right) + 1}$$

<u>Pauli exclusion principle:</u> at most one electron can occupy any single electron level

$$n = \int d\mathbf{v} f(\mathbf{v})$$ normalization condition $\longrightarrow T_0$

Energy Levels in One Dimension

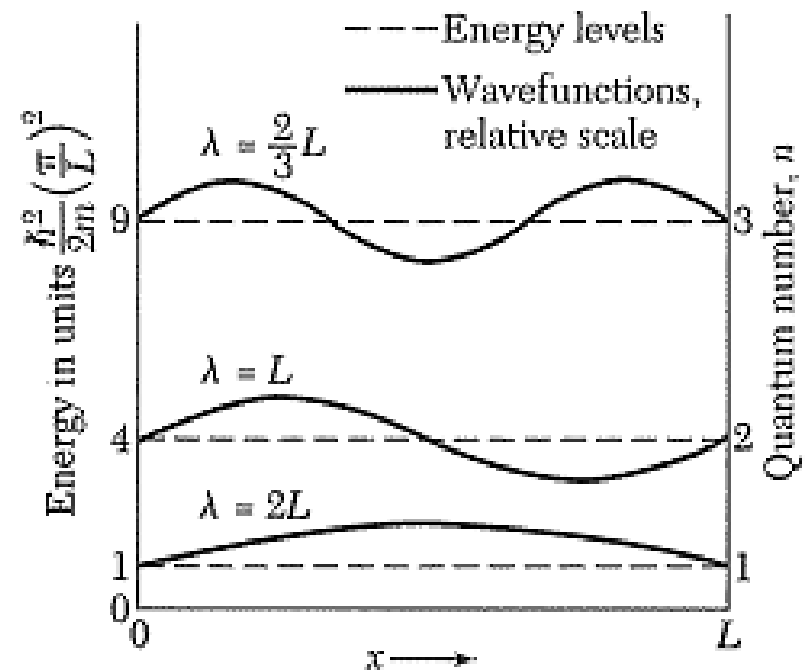$$H\psi_n = -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = \varepsilon_n\psi_n$$

Orbital: solution of a 1-e Schrodinger equation

Boundary conditions: $\psi_n(0) = \psi_n(L) = 0$ Particle in a box

$$\psi_n = A\sin\left(\frac{n\pi}{L}x\right) = A\sin\left(\frac{2\pi}{\lambda_n}x\right)$$

$$n = 1, 2, \cdots \qquad \lambda_n = \frac{2}{n}L$$

$$\varepsilon_n = \frac{\hbar^2}{2m}\left(\frac{n\pi}{L}\right)^2$$

Pauli-exclusion principle: No two electrons can occupy the same quantum state.

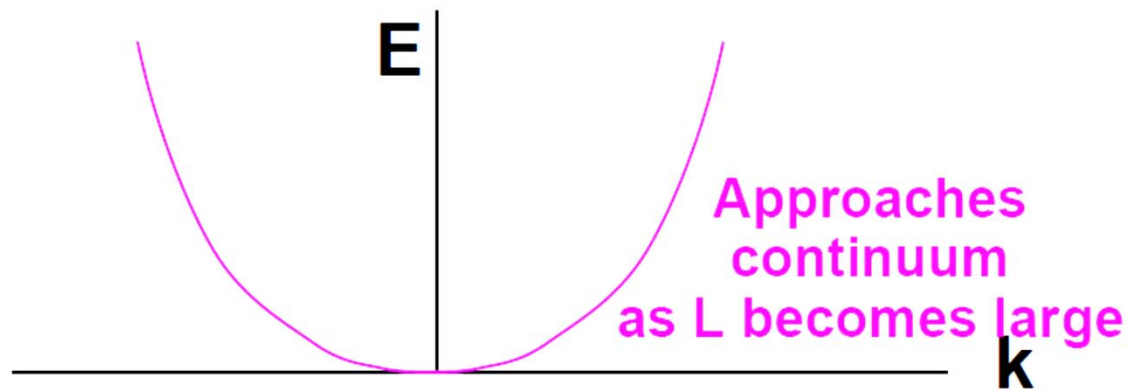Quantum numbers for free electrons: (n, m_s) $m_s = \uparrow, \downarrow$

Degeneracy: number of orbitals having the same energy.

Fermi energy ε_F = energy of topmost filled orbital when system is in ground state.

N free electrons: $\varepsilon_F = \dfrac{\hbar^2}{2m}\left(\dfrac{n_F \pi}{L}\right)^2$ $n_F = \dfrac{N}{2}$

E

Approaches continuum as L becomes large

k

consider noninteracting electrons

electron wave function
associated with a level of energy E
satisfies the <u>Schrodinger equation</u>

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)\psi(r)=E\psi(r)$$

periodic
boundary
conditions

$$\psi(x,y,z+L)=\psi(x,y,z)$$
$$\psi(x,y+L,z)=\psi(x,y,z)$$
$$\psi(x+L,y,z)=\psi(x,y,z)$$

3D:

L

a solution neglecting
the boundary conditions

$$\psi_{\mathbf{k}}(\mathbf{r})=\frac{1}{\sqrt{V}}e^{i\mathbf{k}\cdot\mathbf{r}}$$

1D: ———————

normalization constant: probability
of finding the electron somewhere
in the whole volume V is unity

$$1=\int d\mathbf{r}\,|\psi(\mathbf{r})|^2$$

energy

$$E(\mathbf{k})=\frac{\hbar^2 k^2}{2m}$$

momentum

$$\mathbf{p}=\hbar\mathbf{k}$$
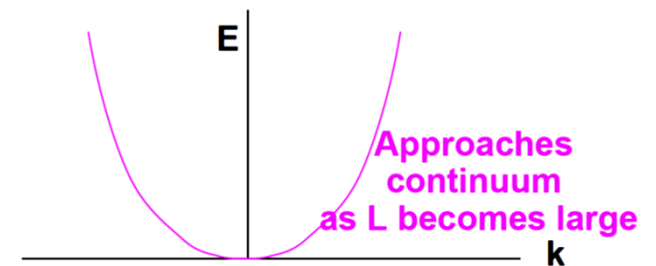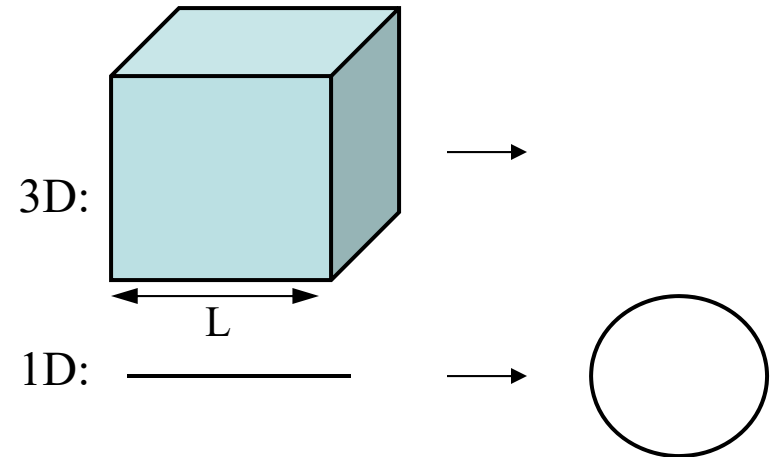
velocity

$$\mathbf{v}=\frac{\hbar\mathbf{k}}{m}$$

$$E=\frac{p^2}{2m}=\frac{1}{2}mv^2$$

wave vector

$$\mathbf{k}$$

de Broglie
wavelength

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

E

**Approaches
continuum
as L becomes large**

k

$$\psi(x, y, z + L) = \psi(x, y, z)$$

$$\psi_{\mathbf{k}}(\mathbf{r}) = \frac{1}{\sqrt{V}} e^{i\mathbf{k}\cdot\mathbf{r}} \qquad \psi(x, y + L, z) = \psi(x, y, z)$$

$$\psi(x + L, y, z) = \psi(x, y, z)$$

apply the boundary conditions $\quad e^{ik_x L} = e^{ik_y L} = e^{ik_z L} = 1$

components of $\mathbf{k}$ must be $\qquad k_x = \dfrac{2\pi}{L} n_x, \; k_y = \dfrac{2\pi}{L} n_y, \; k_z = \dfrac{2\pi}{L} n_z$

n_x, n_y, n_z integers

the area per point $\qquad \left(\dfrac{2\pi}{L}\right)^2$

the volume per point $\qquad \left(\dfrac{2\pi}{L}\right)^3 = \dfrac{(2\pi)^3}{V}$

k-space

a region of k-space of volume Ω contains $\qquad \dfrac{\Omega}{(2\pi/L)^3} = \dfrac{\Omega V}{(2\pi)^3} \qquad$ states i.e. allowed values of k

the number of states per unit volume of k-space, k-space density of states $\qquad \dfrac{V}{(2\pi)^3}$
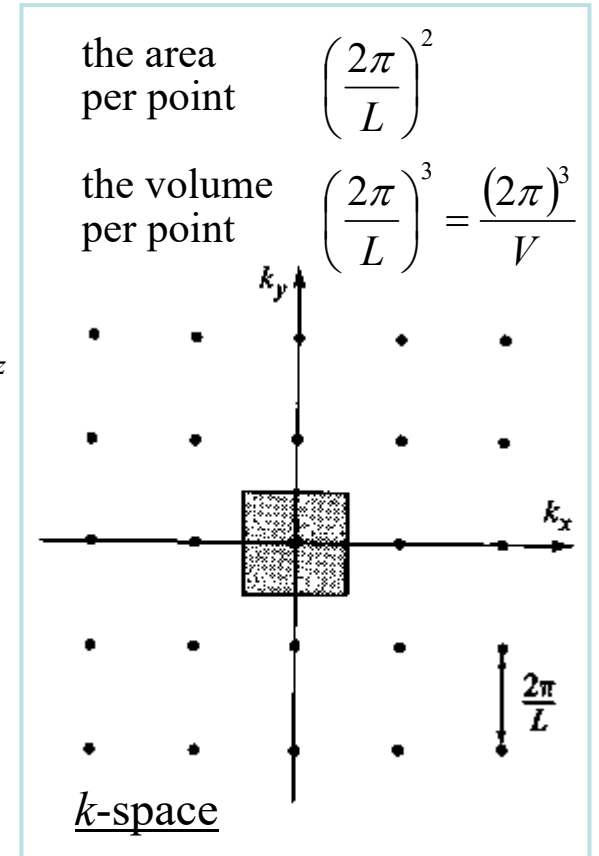
consider T=0

the Pauli exclusion principle postulates that only one electron can occupy a single state
therefore, as electrons are added to a system, they will fill the states in a system
like water fills a bucket – first the lower energy states and then the higher energy states

the <u>ground state</u> of the N-electron system is formed by occupying all single-particle levels with $k < k_F$

state of the lowest energy   volume   density of states

the number of allowed values of
k within the sphere of radius k_F

$$\left(\frac{4\pi k_F^{\ 3}}{3}\right)\frac{V}{(2\pi)^3} = \frac{k_F^{\ 3}}{6\pi^2}V$$

to accommodate N electrons
2 electrons per k-level due to spin

$$N = 2\frac{k_F^{\ 3}}{6\pi^2}V$$

$$n = \frac{k_F^{\ 3}}{3\pi^2}$$

<u>Fermi sphere</u>

<u>Fermi surface</u>
at energy E_F
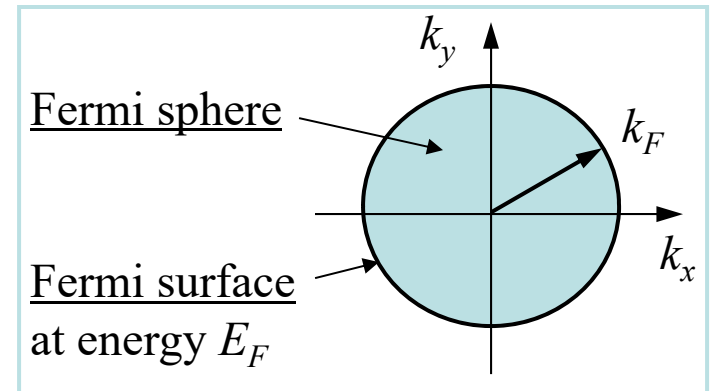
Fermi wave vector	k_F	~10^8 cm^{-1}
Fermi energy	$E_F = \hbar^2 k_F^{\ 2}/2m$	~1-10 eV
Fermi temperature	$T_F = E_F/k_B$	~10^4-10^5 K
Fermi momentum	$p_F = \hbar k_F$	
Fermi velocity	$v_F = \hbar k_F/m$	~10^8 cm/s

compare to the classical thermal velocity

$$v_{thermal} = (3k_B T/m)^{1/2} \sim 10^7 \text{ cm/s at T=300K}$$

$$0 \qquad \text{at T=0}$$

$$k_F = (3\pi^2 n)^{1/3}$$

$$E_F = \frac{\hbar^2}{2m}(3\pi^2 n)^{2/3}$$

$$v_F = \frac{\hbar}{m}(3\pi^2 n)^{1/3}$$

Table 1 Calculated free electron Fermi surface parameters for metals at room temperature

(Except for Na, K, Rb, Cs at 5 K and Li at 78 K)

Valency	Metal	Electron concentration, in cm^{-3}	Radius[a] parameter r_n	Fermi wavevector, in cm^{-1}	Fermi velocity, in $cm\ s^{-1}$	Fermi energy, in eV	Fermi temperature $T_F = \epsilon_F/k_B$, in deg K
1	Li	4.70×10^{22}	3.25	1.11×10^8	1.29×10^8	4.72	5.48×10^4
	Na	2.65	3.93	0.92	1.07	3.23	3.75
	K	1.40	4.86	0.75	0.86	2.12	2.46
	Rb	1.15	5.20	0.70	0.81	1.85	2.15
	Cs	0.91	5.63	0.64	0.75	1.58	1.83
	Cu	8.45	2.67	1.36	1.57	7.00	8.12
	Ag	5.85	3.02	1.20	1.39	5.48	6.36
	Au	5.90	3.01	1.20	1.39	5.51	6.39
2	Be	24.2	1.88	1.93	2.23	14.14	16.41
	Mg	8.60	2.65	1.37	1.58	7.13	8.27
	Ca	4.60	3.27	1.11	1.28	4.68	5.43
	Sr	3.56	3.56	1.02	1.18	3.95	4.58
	Ba	3.20	3.69	0.98	1.13	3.65	4.24
	Zn	13.10	2.31	1.57	1.82	9.39	10.90
	Cd	9.28	2.59	1.40	1.62	7.46	8.66
3	Al	18.06	2.07	1.75	2.02	11.63	13.49
	Ga	15.30	2.19	1.65	1.91	10.35	12.01
	In	11.49	2.41	1.50	1.74	8.60	9.98
4	Pb	13.20	2.30	1.57	1.82	9.37	10.87
	Sn(w)	14.48	2.23	1.62	1.88	10.03	11.64

[a]The dimensionless radius parameter is defined as $r_n = r_0/a_H$, where a_H is the first Bohr radius and r_0 is the radius of a sphere that contains one electron.

density of states

total number of states with wave vector $< k$

$$N = \frac{V}{3\pi^2} k^3$$

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

total number of states with energy $< E$

$$N = \frac{V}{3\pi^2} \left(\frac{2mE}{\hbar^2} \right)^{3/2}$$

the <u>density of states</u> – number of states per unit energy

$$D(E) = \frac{dN}{dE} = \frac{V}{2\pi^2} \left(\frac{2m}{\hbar^2} \right)^{3/2} \sqrt{E}$$

the <u>density of states per unit volume</u> or the <u>density of states</u>

$$D(E) = \frac{dn}{dE} = \frac{1}{2\pi^2} \left(\frac{2m}{\hbar^2} \right)^{3/2} \sqrt{E}$$

<u>k-space density of states</u> – the number of states per unit volume of k-space

$$\frac{V}{(2\pi)^3}$$

Ground state energy of N electrons

add up the energies of all electron states inside the Fermi sphere

$$E = 2 \sum_{k<k_F} \frac{\hbar^2}{2m} k^2$$

volume of k-space per state

$$\Delta \mathbf{k} = 8\pi^3 / V$$

$\forall$ smooth $F(\mathbf{k})$

$$\sum_{\mathbf{k}} F(\mathbf{k}) = \frac{V}{8\pi^3} \sum_{\mathbf{k}} F(\mathbf{k}) \Delta \mathbf{k} \xrightarrow{\Delta \mathbf{k} \to 0 \, i.e. \, V \to \infty} \frac{V}{8\pi^3} \int F(\mathbf{k}) d\mathbf{k}$$

the energy density

$$\frac{E}{V} = \frac{1}{4\pi^3} \int_{k<k_F} d\mathbf{k} \frac{\hbar^2 k^2}{2m} = \frac{1}{\pi^2} \frac{\hbar^2 k_F^5}{10m}$$

$$F(\mathbf{k}) = \frac{\hbar^2 k^2}{2m}$$

$$d\mathbf{k} = 4\pi k^2 dk$$

3D➔1D

the energy per electron in the ground state

$$\frac{E}{N} = \frac{3}{10} \frac{\hbar^2 k_F^2}{m} = \frac{3}{5} E_F$$

$$N = \frac{k_F^3}{3\pi^2} V$$

remarks on statistics I

in quantum mechanics particles are indistinguishable

systems where particles are exchanged are identical

exchange of identical particles can lead to changing of the system wavefunction by a phase factor only

$$\psi(\xi_1,\xi_2) = e^{i\alpha}\psi(\xi_2,\xi_1)$$

system of N=2 particles ξ_1, ξ_2 - coordinates and spins for each of the particles

repeated particle exchange $\rightarrow e^{2i\alpha} = 1 \longrightarrow \psi(\xi_1,\xi_2) = \pm\psi(\xi_2,\xi_1)$

antisymmetric wavefunction with respect to the exchange of particles

$$\psi(\xi_1,\xi_2) = \frac{1}{\sqrt{2}}\left[\psi_{p_1}(\xi_1)\psi_{p_2}(\xi_2) - \psi_{p_1}(\xi_2)\psi_{p_2}(\xi_1)\right]$$

symmetric wavefunction with respect to the exchange of particles

$$\psi(\xi_1,\xi_2) = \frac{1}{\sqrt{2}}\left[\psi_{p_1}(\xi_1)\psi_{p_2}(\xi_2) + \psi_{p_1}(\xi_2)\psi_{p_2}(\xi_1)\right]$$

p_1, p_2 – single particle states

fermions are particles which have half-integer spin the wavefunction which describes a collection of fermions must be antisymmetric with respect to the exchange of identical particles

fermions: electron, proton, neutron

if $p_1 = p_2$ $\psi = 0$
$\rightarrow$ at most one fermion can occupy any single particle state – Pauli principle

obey Fermi-Dirac statistics

bosons are particles which have integer spin the wavefunction which describes a collection of bosons must be symmetric with respect to the exchange of identical particles

bosons: photon, Cooper pair, H atom, exciton

unlimited number of bosons can occupy a single particle state

obey Bose-Einstein statistics

Observed fact: only symmetrical and antisymmetrical wave functions are `found' in nature. Both types satisfy required probability density equality, but only antisymmetrical ones entail the Exclusion principle (if $x1 = x2$ then $\psi = 0$, i.e. there is no corresponding quantum state.)

distribution function $f(E) \rightarrow$ probability that a state at energy E will be occupied at thermal equilibrium

fermions
particles with
half-integer spins

Fermi-Dirac
distribution
function

$$f_{FD}(E) = \frac{1}{\exp\left(\dfrac{E - \mu}{k_B T}\right) + 1}$$

degenerate
Fermi gas
$f_{FD}(\mathbf{k}) < 1$

bosons
particles with
integer spins

Bose-Einstein
distribution
function

$$f_{BE}(E) = \frac{1}{\exp\left(\dfrac{E - \mu}{k_B T}\right) - 1}$$

degenerate
Bose gas
$f_{BE}(\mathbf{k})$ can be any

both fermions and
bosons at high T
when $E - \mu \gg k_B T$

Maxwell-Boltzmann
distribution
function

$$f_{MB}(E) = \exp\left(\frac{\mu - E}{k_B T}\right)$$

classical
gas
$f_{MB}(\mathbf{k}) \ll 1$

$$n = \int dE n(E) = \int dE D(E) f(E)$$

$\mu = \mu(n, T) -$ <u>chemical potential</u>

remarks on statistics II

BE and FD distributions differ from the classical MB distribution
because the particles they describe are <u>indistinguishable.</u>
Particles are considered to be indistinguishable if their <u>wave packets</u>
overlap significantly.
Two particles can be considered to be <u>distinguishable</u>
if their separation is large compared to their de Broglie wavelength.

thermal de Broglie wavelength

$$\lambda_{dB} = \left(\frac{2\pi\hbar^2}{mk_B T}\right)^{1/2} \sim \frac{h}{p}$$

particles become indistinguishable when

$$\lambda_{dB} \sim d = n^{-1/3}$$

i.e. at temperatures below

$$T_{dB} = \frac{2\pi\hbar^2}{mk_B} n^{2/3}$$

at $T < T_{dB}$ f_{BE} and f_{FD} are strongly different from f_{MB}
at $T \gg T_{dB}$ $f_{BE} \approx f_{FD} \approx f_{MB}$
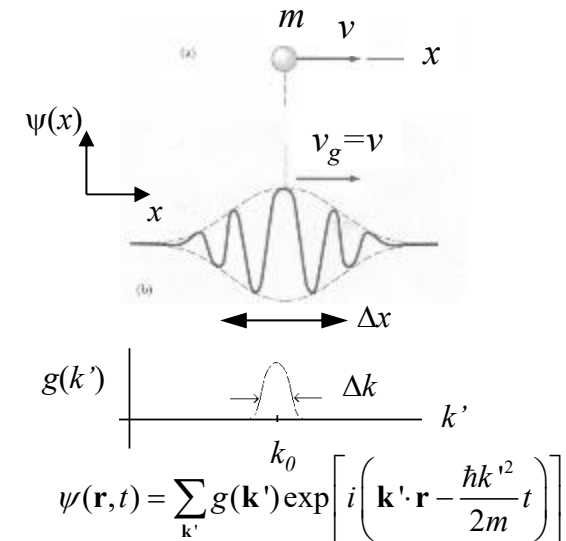
electron gas in metals:
$n = 10^{22}$ cm^{-3}, $m = m_e \rightarrow T_{dB} \sim 3\times 10^4$ K

gas of Rb atoms:
$n = 10^{15}$ cm^{-3}, $m_{atom} = 10^5 m_e \rightarrow T_{dB} \sim 5\times 10^{-6}$ K

excitons in GaAs QW
$n = 10^{10}$ cm^{-2}, $m_{exciton} = 0.2\, m_e \rightarrow T_{dB} \sim 1$ K

$$\psi(\mathbf{r},t) = \sum_{\mathbf{k'}} g(\mathbf{k'})\exp\left[i\left(\mathbf{k'}\cdot\mathbf{r} - \frac{\hbar k'^2}{2m}t\right)\right]$$

A particle is represented by a
<u>wave group or wave packets</u>
of limited spatial extent,
which is a superposition of many matter
waves with a spread of wavelengths
centered on $\lambda_0 = h/p$

The wave group moves
with a speed v_g – <u>the group speed,</u>
which is identical to the classical
particle speed

Heisenberg uncertainty principle, 1927:
If a measurement of position is made with
precision Δx and a simultaneous
measurement of momentum in the x
direction is made with precision Δp_x,
then
$$\Delta p_x \Delta x \geq \hbar/2$$

Density of conduction electrons in metals $\sim 10^{22} - 10^{23}$ cm^{-3}

r_s – measure of electronic density
r_s is radius of a sphere whose volume is equal to the volume per electron

$$\frac{4\pi r_s^3}{3} = \frac{V}{N} = \frac{1}{n} \qquad r_s = \left(\frac{3}{4\pi n}\right)^{1/3} \sim \frac{1}{n^{1/3}}$$

mean inter-electron spacing

in metals $r_s \sim 1 - 3$ Å (1 Å = 10^{-8} cm) $\qquad r_s/a_0 \sim 2 - 6$

$$a_0 = \frac{\hbar^2}{me^2} = 0.529\text{Å} - \text{Bohr radius}$$

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Estimate some de Broglie wavelengths

• Wavelength of electron with 50eV kinetic energy

$$K = \frac{p^2}{2m_e} = \frac{h^2}{2m_e\lambda^2} \Rightarrow \lambda = \frac{h}{\sqrt{2m_e K}} = 1.7 \times 10^{-10}\,\text{m}$$

Electron occupation

density of states $\qquad D(E) = \dfrac{dn}{dE} = \dfrac{1}{2\pi^2}\left(\dfrac{2m}{\hbar^2}\right)^{3/2}\sqrt{E}$

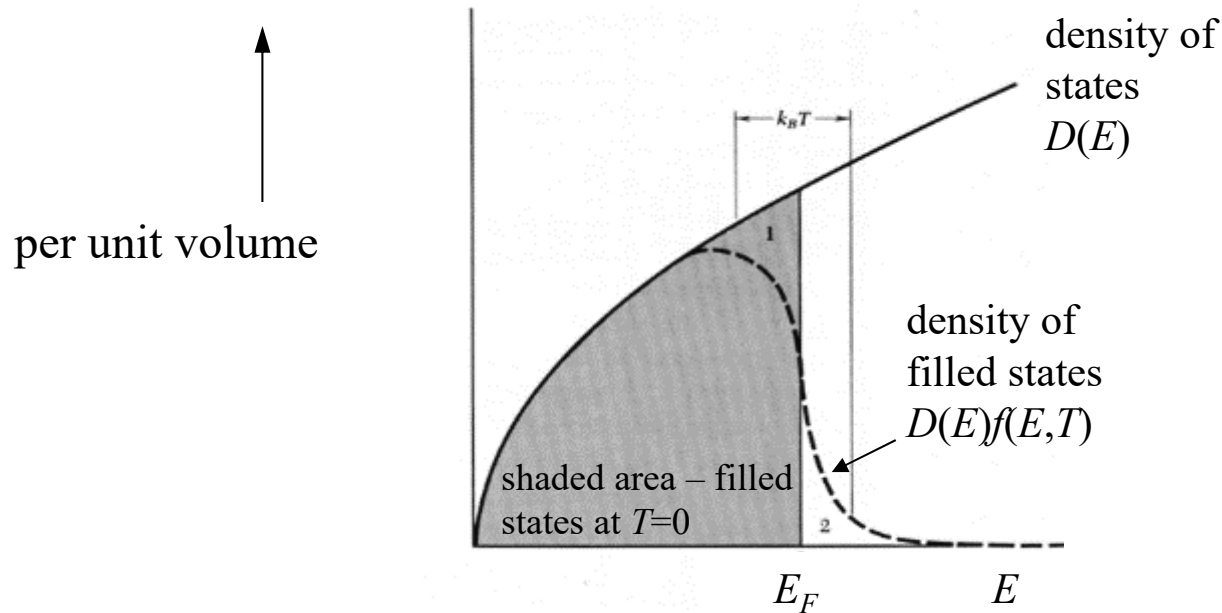$\uparrow$ 3D

distribution function $\quad f(E) = \dfrac{1}{\exp\left(\dfrac{E-\mu}{k_B T}\right)+1}$ $\qquad \lim\limits_{T\to 0} f(E) = 1, \quad E < \mu$

$\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad = 0 \quad E > \mu$

$$n = \int dE\, D(E) f(E) \rightarrow \mu \qquad\qquad \lim\limits_{T\to 0}\mu = E_F$$

$$D(E)dE = \frac{1}{V} \times [\text{the number of states in the energy range from } E \text{ to } E + dE]$$

$$D(E)f(E)dE = \frac{1}{V} \times [\text{the number of \underline{filled} states in the energy range from } E \text{ to } E + dE]$$

per unit volume

density of states $D(E)$

density of filled states $D(E)f(E,T)$

shaded area – filled states at T=0

E_F $\qquad E$

Effect of Temperature on the Fermi-Dirac Distribution

Fermi-Dirac distribution : $\quad f(\varepsilon) = \dfrac{1}{e^{\beta(\varepsilon-\mu)}+1}$ $\qquad \beta = \dfrac{1}{k_B T}$

Chemical potential $\mu = \mu(T)$ is determined by $\quad N = \int d\varepsilon \, g(\varepsilon) f(\varepsilon)$ $\qquad g =$ density of states
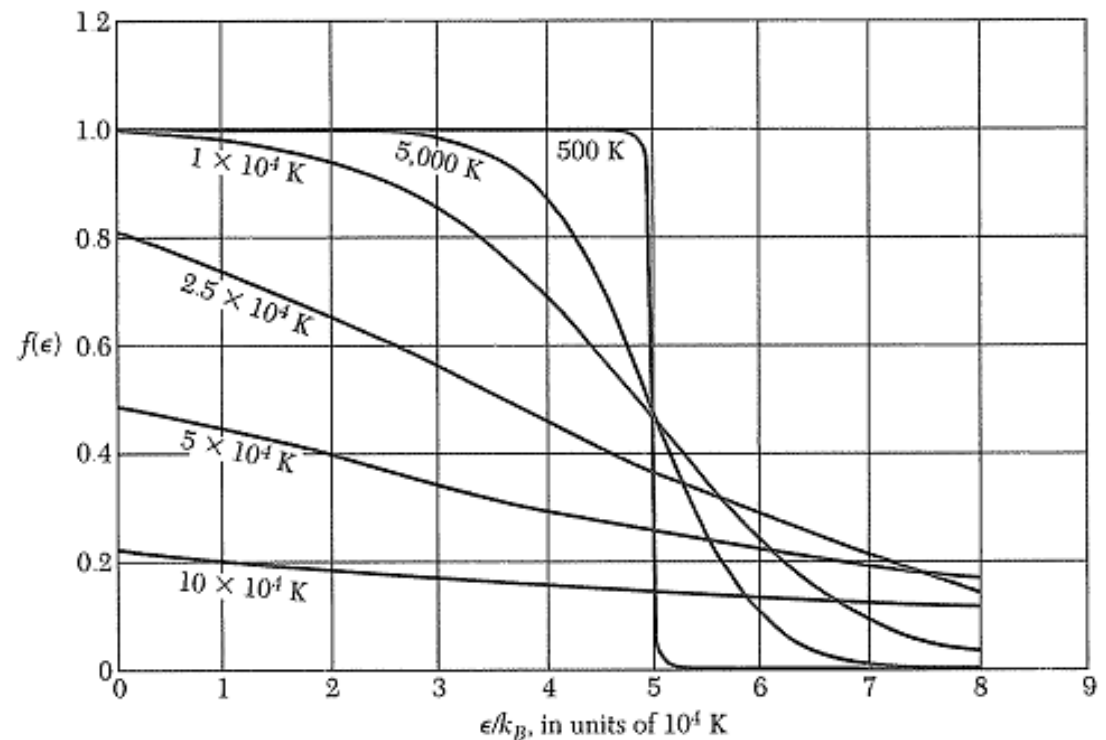
At $T = 0$: $\quad f(\varepsilon) = \begin{cases} 1 \\ 0 \end{cases}$ for $\quad \begin{matrix} \varepsilon < \mu \\ \varepsilon > \mu \end{matrix}$

$\rightarrow \qquad \mu(0) = \varepsilon_F$

For all T: $\qquad f(\mu) = \dfrac{1}{2}$

For $\varepsilon \gg \mu$: $\quad f(\varepsilon) \square \, e^{-\beta(\varepsilon-\mu)}$

(Boltzmann distribution)

3D e-gas

Electrical conductivity and Ohm's law

equation of motion
Newton's law

$$m\frac{d\mathbf{v}}{dt} = \hbar\frac{d\mathbf{k}}{dt} = -e\mathbf{E}$$

$$\frac{d\mathbf{p}(t)}{dt} = -\frac{\mathbf{p}(t)}{\tau} + \mathbf{f}(t) = 0$$

in the absence of collisions the Fermi sphere in k-space is displaced as a whole at a uniform rate by a constant applied electric field

$$\mathbf{k}(t) - \mathbf{k}(0) = -\frac{e\mathbf{E}}{\hbar}t$$

$$\mathbf{p} = \mathbf{f}\tau = -e\mathbf{E}\tau$$

because of collisions the displaced Fermi sphere is maintained in a steady state in an electric field

$$\mathbf{k}_{avg} = -\frac{e\mathbf{E}}{\hbar}\tau$$

Fermi sphere

Ohm's law

$$\mathbf{v}_{avg} = \frac{\hbar\mathbf{k}_{avg}}{m} = -\frac{e\mathbf{E}}{m}\tau$$

$$\mathbf{j} = \left(\frac{ne^2\tau}{m}\right)\mathbf{E}$$

$$\mathbf{j} = -ne\mathbf{v}_{avg}$$

$$\sigma = \frac{ne^2\tau}{m}$$

$$\rho = \frac{1}{\sigma} = \frac{m}{ne^2\tau}$$

the mean free path $l = v_F\tau$
because all collisions involve only electrons near the Fermi surface

$v_F \sim 10^8$ cm/s
for pure Cu:

at T=300 K	$\tau \sim 10^{-14}$ s	$l \sim 10^{-6}$ cm = 100 Å
at T=4 K	$\tau \sim 10^{-9}$ s	$l \sim 0.1$ cm

$k_{avg} \ll k_F$ for $n = 10^{22}$ cm^{-3} and $j = 1$ A/mm^2 $v_{avg} = j/ne \sim 0.1$ cm/s $\ll v_F \sim 10^8$ cm/s

Where is the resistance coming from?

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equation of motion
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k_y, k_x, F, k_{avg}
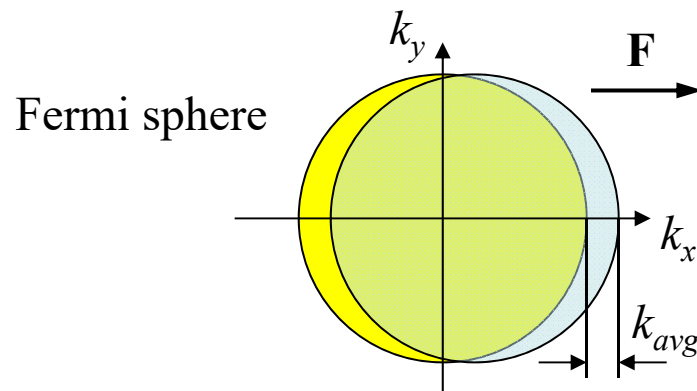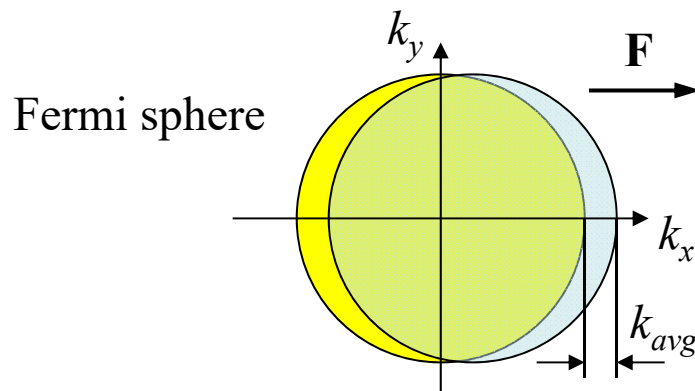
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Ballistic Transport

Ballistic conduction or **Ballistic transport** is the **transport** of electrons in a medium having negligible electrical resistivity caused by scattering. Without scattering, electrons simply obey Newton's second law of motion at non-relativistic speeds.

Carbon nanotubes as long ballistic conductors

C. T. White[*†] **& T. N. Todorov**[*]

* *Department of Materials, University of Oxford, Parks Road, Oxford OX1 3PH, UK*

Early theoretical work on single-walled carbon nanotubes[1–3] predicted that a special achiral subset of these structures known as armchair nanotubes[3] should be metallic. Tans *et al.*[4] have recently confirmed these predictions experimentally and also showed directly that coherent electron transport can be maintained through these nanowires up to distances of at least 140 nm. But single-walled armchair nanotubes are one-dimensional conductors with only two open conduction channels (energy subbands in a laterally confined system that cross the Fermi level)[1–3]. Hence, with increasing length, their conduction electrons ultimately become localized[5] owing to residual disorder in the tube which is inevitably produced by interactions between the tube and its environment. We present here calculations which show, however, that unlike normal metallic wires, conduction electrons in armchair nanotubes experience an effective disorder averaged over the tube's circumference, leading to electron mean free paths that increase with nanotube diameter. This increase should result in exceptional ballistic transport properties and localization lengths of 10 μm or more for tubes with the diameters that are typically produced experimentally[6].

Ballistic carbon nanotube field-effect transistors

Ali Javey[1], Jing Guo[2], Qian Wang[1], Mark Lundstrom[2] & Hongjie Dai[1]

[1]Department of Chemistry, Stanford University, California 94305, USA
[2]School of Electrical and Computer Engineering, Purdue University,
West Lafayette, Indiana 47907, USA

A common feature of the single-walled carbon-nanotube field-effect transistors fabricated to date has been the presence of a Schottky barrier at the nanotube–metal junctions[1-3]. These energy barriers severely limit transistor conductance in the 'ON' state, and reduce the current delivery capability—a key determinant of device performance. Here we show that contacting semiconducting single-walled nanotubes by palladium, a noble metal with high work function and good wetting interactions with nanotubes, greatly reduces or eliminates the barriers for transport through the valence band of nanotubes. *In situ* modification of the electrode work function by hydrogen is carried out to shed light on the nature of the contacts. With Pd contacts, the 'ON' states of semiconducting nanotubes can behave like ohmically contacted ballistic metallic tubes, exhibiting room-temperature conductance near the ballistic transport limit of $4e^2/h$ (refs 4–6), high current-carrying capability ($\sim 25\,\mu A$ per tube), and Fabry–Perot interferences[5] at low temperatures. Under high voltage operation, the current saturation appears to be set by backscattering of the charge carriers by optical phonons. High-performance ballistic nanotube field-effect transistors with zero or slightly negative Schottky barriers are thus realized.