The story so far:

- Electronic properties of solids are dictated by band structure.
- Top-down, bands can be viewed as a consequence of the potential of the ion cores, determined by their spatial arrangement, with boundary conditions leading to discretization of allowed “momenta”.
- Bottom-up, bands are a consequence of the constituent atoms and their chemical bonding.
- Deviations from an infinite, perfect crystal lattice can have profound effects on band structure - surface states, charge transfer at interfaces.
Today:

• Screening - another length scale
  
  How far away from a charged site are the effects of that charge felt?

  How justified are we in ignoring electron-electron interactions?
How do electrons respond to a fixed, charged impurity?

Impurities affect local potential energy of electrons. Far from impurities, electrons are unaffected. Over what length scale do the effects extend?

Remember basic E&M:

\[ \nabla \cdot \varepsilon_0 \mathbf{E} = \rho \]

where \( \rho \) is the total charge density, background + induced.

\[ \nabla \cdot \varepsilon_0 \varepsilon \mathbf{E} = \rho_{\text{ext}} \]

\[ \mathbf{E} = -\nabla \phi \]

where \( \phi \) is the total electric potential.

\[ \nabla^2 \phi = -\frac{1}{\varepsilon_0} \rho, \]
Response of system

Work with Fourier components to handle arbitrary impurity potentials.

Total potential = impurity potential + contribution from electronic response

\[ \varphi(K) = \varphi_{ext}(K) + \delta\varphi(K), \]
\[ \rho(K) = -en + \delta\rho(K) \]

Total charge density = original + contribution from electronic response

Poisson’s equation becomes

\[ K^2 \varphi = \frac{1}{\varepsilon_0} \rho(K), \]

and the dielectric function:

\[ \varepsilon(K) = \frac{\rho_{ext}(K)}{\rho(K)} = 1 - \frac{\delta\rho(K)}{\rho(K)}, \]
Relating charge density back to potential

Work out the case for a metal (degenerate Fermi gas):

How does the charge density vary with local changes in the potential? Recall

Recall density of states:

\[ \nu_{3d}(E) \equiv \left( \frac{\partial n_{3d}}{\partial E} \right) \rightarrow (\delta n_{3d}) = \nu_{3d}(E)(\delta E) \]

Local effective energy change = \( e\phi \), \( \delta\rho = -e(\delta n) \)
Thomas-Fermi screening length

Plugging into the expression for the dielectric function,

$$\varepsilon(K) = 1 + K^{-2}r_{TF}^{-2}$$

where

$$r_{TF} \equiv \left( \frac{e^2}{\varepsilon_0 \nu_{3d}(E_F)} \right)^{-1/2}$$

• The Thomas-Fermi length characterizes screening by electron gas.

• Bigger density of states at the Fermi level, shorter screening length!
Plug in some numbers….

\[ r_{TF} \equiv \left( \frac{e^2}{\varepsilon_0 \nu(E_F)} \right)^{-1/2} \]

In 3d, for a free Fermi gas with \( n_{3d} \sim 10^{23} \text{ cm}^{-3} \),
plug in and find \( r_{TF} \sim 0.1 \text{ nm} \).!

- In a “good metal”, charged impurities are screened by the electrons over very short length scales!
- That is, \( n \) is so high that only a very slight shift in the positions of electrons right near the impurity are enough to shield the rest of the electrons.
Point impurity

\[ \varepsilon(K) = \frac{\varphi_{ext}(K)}{\varphi(K)}, \quad \varepsilon(K) = 1 + K^{-2}r_{TF}^{-2} \]

For point impurity with charge \( q \),

\[ \varphi_{ext}(K) = \frac{q}{4\pi\varepsilon_0} \frac{1}{K^2} \]

\[ \rightarrow \varphi(K) = \frac{q}{4\pi\varepsilon_0} \frac{1}{K^2 + r_{TF}^{-2}}, \]

Transforming back,

\[ \varphi(r) = \frac{q}{4\pi\varepsilon_0} \frac{1}{r} \exp(-r / r_{TF}), \]

Point impurity is exponentially screened!
A complication: Friedel oscillations

Our point-impurity analysis that gave exponential screening isn’t quite right.

Electrons can’t respond to spatial potential variations at arbitrarily high $K$ values (with arbitrarily short length scales).

Shortest wavevector available to electrons is $k_F$, the Fermi wavevector.

Must terminate Fourier series there.

Result is “ringing” - screening charge density oscillates with wavevector $\sim k_F/2$. 
Friedel oscillations

Friedel oscillations of electron density near a charged impurity on an InAs surface.

Accumulating electrons at the surface (increasing + voltage on STM) causes shortening of wavelength of oscillations, as expected.

Screening in lower dimensionality

Consider a 2d system of charges confined in the $z$ direction over a scale $d$.

Dimensional analysis lets us estimate an equivalent screening length for this case:

$$r_{TF} \approx \left( \frac{e^2}{\varepsilon_0 d n_{2d} (E_F)} \right)^{-1/2}$$

Plug in numbers for a 2d electron gas in GaAs:

$m* = 0.067 \, m_0$; $n_{2d} = 5 \times 10^{11} \, \text{cm}^{-2}$; $d = 1 \, \text{nm}$.

Result: $\sim 0.5 \, \text{nm}$ - worse than 3d case.

Actual situation is even worse than that.

*Screening is worse as dimensionality is reduced!*
Consequence of poor screening: noise

- Consider a localized trap near a geometrically constrained conductor.
- Charge state of that trap affects carriers within $r_{TF}$ of the trap position.
- Charging / discharging of trap can be seen as changes in the conductance.

Ralls et al., PRL 52, 228 (1984)
Depletion widths at interfaces?

- Also need to solve Poisson equation for this case, self-consistently.
- Planar interfaces means only doing 1d problem.
- Most common case we care about is interface between two doped semiconductors - not really degenerate at room temp, usually.

Recall the $p$-$n$ junction:

![Diagram of $p$-$n$ junction with depletion region highlighted]
Also remember: for undoped semiconductors,

\[
n = \left[2 \left(\frac{2\pi m^*_{e} k_{B} T}{\hbar^2}\right)^{3/2} M_{C}\right] \cdot \exp\left(-\frac{E_{C} - E_{F}}{k_{B} T}\right)
\]

\[N_{c}(T), \text{ effective density of states in conduction band}\]

\[
p = \left[2 \left(\frac{2\pi m^*_{h} k_{B} T}{\hbar^2}\right)^{3/2}\right] \cdot \exp\left(-\frac{E_{F} - E_{V}}{k_{B} T}\right)
\]

\[N_{v}(T), \text{ effective density of states in valence band}\]
p-n junction in equilibrium

\[
n(x) = N_c(T) \exp \left[-\frac{[E_c - e\varphi(x) - \mu]}{k_BT}\right]
\]

\[
p(x) = N_v(T) \exp \left[-\frac{[\mu + e\varphi(x) - E_v]}{k_BT}\right]
\]

Spatially uniform \( \mu \), locally varying potential \( \varphi \).

Far from junction (\( x=0 \)), assume all donors/acceptors ionized.

Result:

\[
e \Delta \varphi = e\varphi(\infty) - e\varphi(-\infty) = E_c - E_v + k_BT \ln \left(\frac{N_d N_a}{N_c N_v}\right)
\]

A built-in potential difference across the junction.
Local carrier density varies.

Donated electrons from $n$ side transfer to $p$ side and are accepted, eliminating holes.

Local carrier density on both sides of interface is reduced, and donor / acceptor ions aren’t well-screened.

carrier concentration:

$N_a$  \hspace{2cm} $N_d$

local charge density:

$-d_p$  \hspace{2cm} $d_n$

ionized donors

ionized acceptors
How big is depletion region?

\[ d_{n,p} = \left[ \frac{(N_a / N_d)^{\pm 1} \varepsilon \Delta \phi}{(N_d + N_a) 2\pi e} \right]^{1/2} \]

Can plug in numbers for effective densities of states to find built-in potential \( \Delta \phi \).

Typical \( d \) can be as large as \( \sim 1 \) micron in lightly doped systems (!).

Nanodevices can easily be smaller than depletion widths for low carrier densities…. Clearly can complicate device design.
Basic screening ideas

- Mobile charges (carriers) redistribute themselves in response to a given charged object, consistent with Poisson equation - minimizes electrostatic potential energy.
- When carrier densities (and dimensionality) are high, only a small rearrangement is required to fully screen charges.
- This implies that the gas of electrons must have screening correlations within *itself*.
- Each electron must have a “correlation hole”.

How important are these electron-electron interaction effects?
Quantifying electron-electron interactions

Natural parameter to use:

$$\frac{\text{average electron-electron potential energy}}{\text{average electron kinetic energy}}$$

How does this ratio depend on density and dimensionality?

Typical interelectron potential energy $\sim 1/r \sim (n_d)^{1/d}$

Typical kinetic energy $\sim E_F$.

Remember, $E_F \sim n_{3d}^{2/3}$, in 3d

$E_F \sim n_{2d}$, in 2d

$E_F \sim n_{1d}^2$, in 1d
Variation with density

Result: ratio $\sim n_{3d}^{-1/3}$, in 3d  
ratio $\sim n_{2d}^{-1/2}$, in 2d  
ratio $\sim n_{1d}^{-1}$, in 1d

• Electron-electron interactions become proportionately less important as carrier densities are increased.

• In all dimensionalities, at sufficiently low carrier densities interaction effects dominate.

• As density is decreased, systems of lower dimensionality expected to show interaction effects first.
A related useful quantity, \( r_s \)

\[
  r_s^3 = \left( \frac{4\pi}{3} a_0^3 n_{3d} \right)^{-1}
\]

- Measures interparticle separation in Bohr radii.
- Proportional to the ratio from above in 3d.
- Simple interpretation would suggest that interactions may be relevant once \( r_s > \sim 1 \).

In a typical metal? Al \( \sim 2 \); Cs \( \sim 6 \).

- Not obvious that interactions effects are really small.
- At \( r_s \sim 100 \) in 3d, energetically favorable for electrons to form an ordered bcc lattice!
- At \( r_s \sim 37 \) in 2d, electrons predicted to form a triangular lattice.

These last two are called **Wigner crystallization**. Not yet unambiguously observed.
Electron-electron scattering I

Electron-electron scattering processes can shorten the lifetime of a particular state. How much so?

Start with a full Fermi sea at $T=0$, and drop in an extra electron at some energy $E_1 > E_F$.

Let it interact with another electron with energy $E_2$.

We know $E_2 < E_F$, since all other states are empty.

Final states $E_3$ and $E_4$ have to be unoccupied for scattering to occur: $E_3, E_4 > E_F$.

Conservation of energy: $E_1 + E_2 = E_3 + E_4$

As $E_1$ approaches $E_F$, the number of available states that satisfy these conditions drops to zero!

EE scattering time at $T = 0$ for an electron in single-particle state with energy $E_F$ is infinite!
Electron-electron scattering II - finite $T$

At finite $T$, there are now some empty states available near the Fermi level to allow electron-electron scattering.

Pauli principle still leads to reduction of scattering rate from simple estimate by a factor of $(k_B T / E_F)^2$.

Scattering cross-section is also reduced from bare value due to screening. Effective cross section is something like $r_{TF}^2$.

Mean free path from electron-electron scattering:

$$\ell_{ee} \approx \frac{1}{n \sigma} \approx \frac{1}{nr_{TF}^2} \left( \frac{E_F}{k_B T} \right)^2$$

At room $T$, this is something like 1 micron: other scattering processes limit electron motion at room $T$, not electron-electron scattering!
Fermi liquid theory

Interactions *do* take place - there is screening.

Fermi Liquid Theory:
• “Turning on” interactions leads only to simple changes.

• 1-1 correspondence between ground state of interacting and noninteracting systems - Fermi surface still exists.

• 1-1 correspondence between excitations of interacting and noninteracting systems - quasiparticles are still reasonable.

• Basic relationships of noninteracting case still hold: $R \sim T$; $c_V \sim T$; etc.
Luttinger liquids

Under certain extreme conditions, FLT doesn’t hold anymore.

For example, poor screening in 1d means interactions no longer well-accounted for by FLT.

Result:

• Power-law singularity in momentum distribution rather than nice Fermi edge.

• Weird new excitations: spin and charge separation!

System that can exhibit such properties: metallic nanotube.
Next time:

Carbon nanotubes in a nutshell

Chemical approaches to understanding and synthesizing nanoparticles