

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:

$$\nabla \cdot \epsilon_0 \mathbf{E} = \rho$$

where ρ is the total charge density, background + induced.

$$\nabla \cdot \epsilon_0 \epsilon \mathbf{E} = \rho_{ext}$$

$$\mathbf{E} = -\nabla \phi$$

where ϕ is the total electric potential.

$$\nabla^2 \phi = -\frac{1}{\epsilon_0} \rho,$$

Response of system

Work with Fourier components to handle arbitrary impurity potentials.

Total potential = impurity potential + contribution from electronic response

$$\varphi(\mathbf{K}) = \varphi_{ext}(\mathbf{K}) + \delta\varphi(\mathbf{K}),$$

$$\rho(\mathbf{K}) = -en + \delta\rho(\mathbf{K})$$

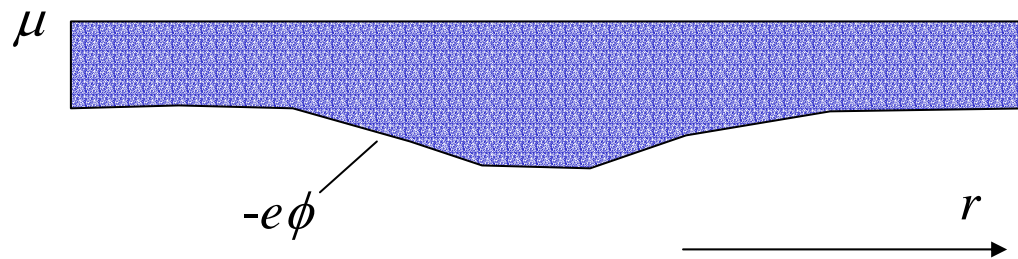
Total charge density = original + contribution from electronic response

Poisson's equation becomes
$$K^2\varphi = \frac{1}{\epsilon_0}\rho(\mathbf{K}),$$

and the dielectric function:
$$\epsilon(\mathbf{K}) = \frac{\rho_{ext}(\mathbf{K})}{\rho(\mathbf{K})} = 1 - \frac{\delta\rho(\mathbf{K})}{\rho(\mathbf{K})},$$

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:

$$v_{3d}(E) \equiv \left(\frac{\partial n_{3d}}{\partial E} \right) \longrightarrow (\delta n_{3d}) = v_{3d}(E)(\delta E)$$

Local effective energy change = $e\phi$, $\delta\rho = -e(\delta n)$

Thomas-Fermi screening length

Plugging into the expression for the dielectric function,

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

where

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

- The Thomas-Fermi length characterizes screening by electron gas.
- Bigger density of states at the Fermi level, shorter screening length!

Plug in some numbers....

$$r_{TF} \equiv \left(\frac{e^2}{\epsilon_0} \nu(E_F) \right)^{-1/2}$$

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

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

For point impurity with charge q ,

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

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

Transforming back,

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

Point impurity is exponentially screened!

A complication: Friedel oscillations

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

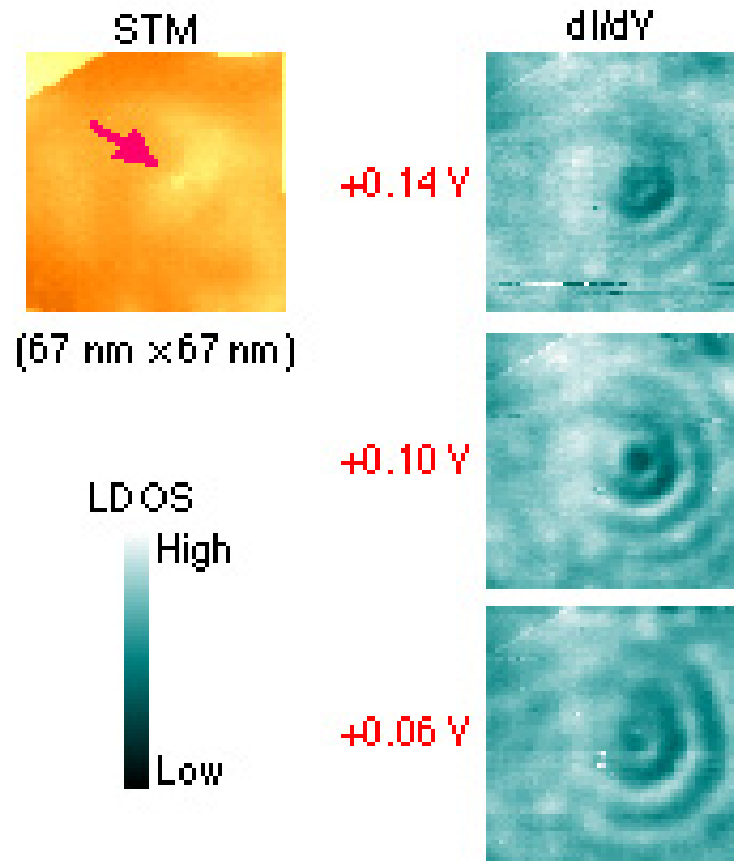
Electrons can't respond to spatial potential variations at arbitrarily high K values (with arbitrarily short length scales).

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.

Kanisawa *et al.*, *Phys. Rev. Lett.* **86**, 3384 (2001).

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:

$$r_{TF} \approx \left(\frac{e^2}{\epsilon_0 d} \nu_{2d}(E_F) \right)^{-1/2}$$

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

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

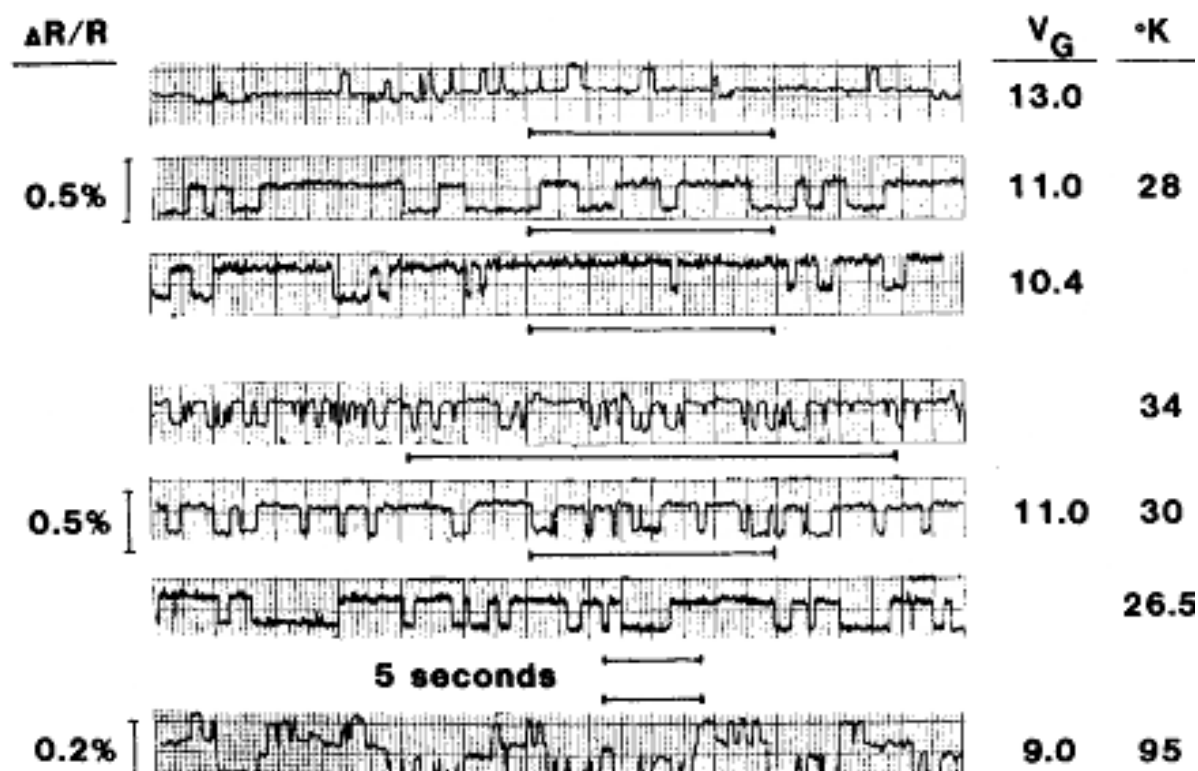
Result: ~ 0.5 nm - worse than 3d case.

Actual situation is even worse than that.

Screening is worse as dimensionality is reduced!

Consequence of poor screening: noise

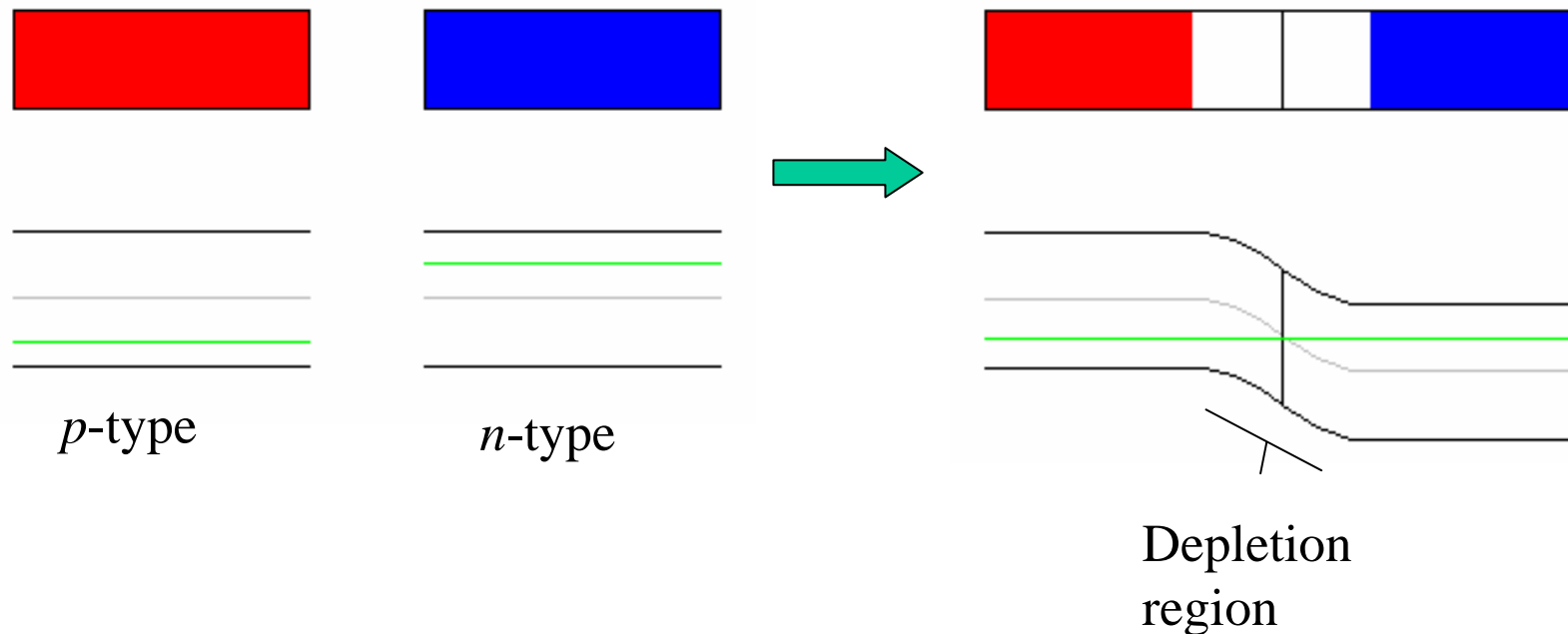
- Consider a localized trap near a geometrically constrained conductor.
- Charge state of that trap affects carriers within r_{TF} of the trap position.
- Charging / discharging of trap can be seen as changes in the conductance.



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:



Also remember: for undoped semiconductors,

$$n = \underbrace{\left[2 \left(\frac{2\pi m_{*e} k_B T}{\hbar^2} \right)^{3/2} M_C \right]}_{N_c(T)} \cdot \exp\left(-\frac{E_C - E_F}{k_B T} \right)$$

$N_c(T)$, effective density of states in conduction band

$$p = \underbrace{\left[2 \left(\frac{2\pi m_{*h} k_B T}{\hbar^2} \right)^{3/2} \right]}_{N_v(T)} \cdot \exp\left(-\frac{E_F - E_V}{k_B T} \right)$$

$N_v(T)$, effective density of states in valence band

p-n junction in equilibrium

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

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

Spatially uniform μ , locally varying potential ϕ .

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

Result:

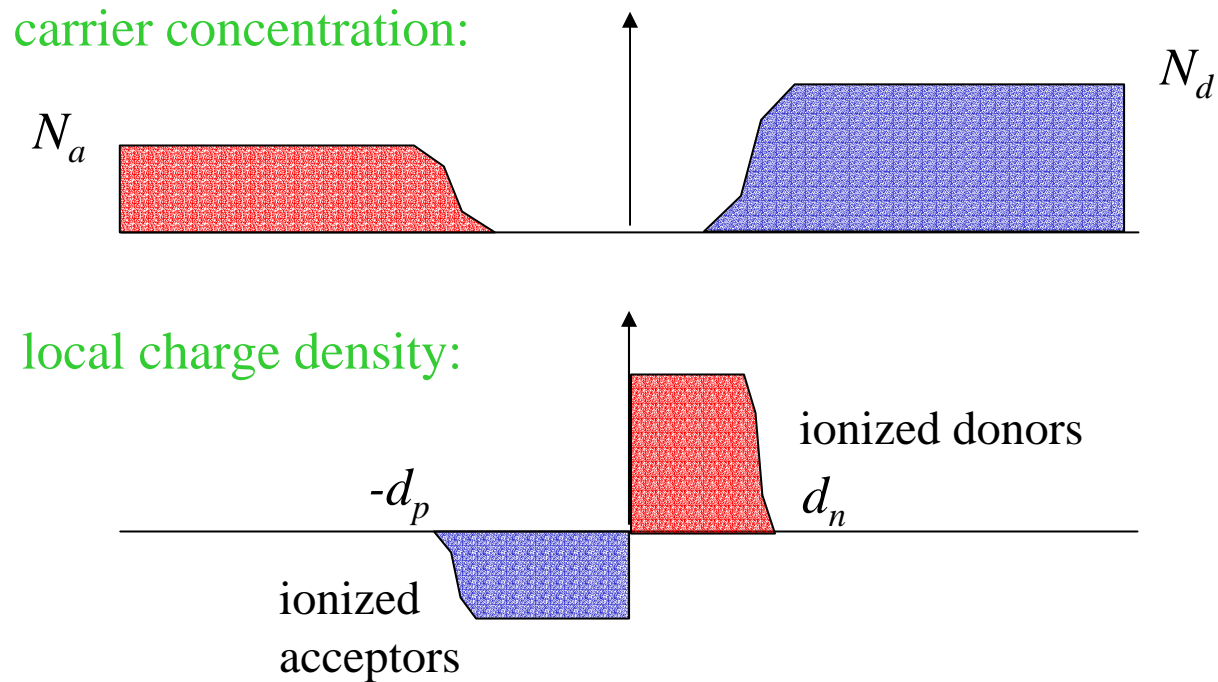
$$e\Delta\phi = e\phi(\infty) - e\phi(-\infty) = E_c - E_v + k_B T \ln\left(\frac{N_d N_a}{N_c N_v}\right)$$

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.



How big is depletion region?

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

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

Typical d can be as large as ~ 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:

average electron-electron potential energy

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 ~ 2 ; Cs ~ 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