Lecture 16
Interactions

Marx: Quantitative differences become qualitative ones.

Fitzgerald: The rich are different from us.
Hemingway: Yes, they have more money.

Quotes in P.W. Anderson, "More is different"

Why Electron-Electron Interaction?

- Everything that relates to magnetism (FM, AFM) originates from electron-electron interaction.
- Electron-Electron is dominant in TM and RE elements
- Without E-E, hydrogen molecules or hydrogen solid cannot be understood properly

Landau Fermi Liquid Paradigm

- Replace "electron" by "quasi-electron"
- Quasi-electron is a manybody eigenstate defined by this property (see Anderson CIS)

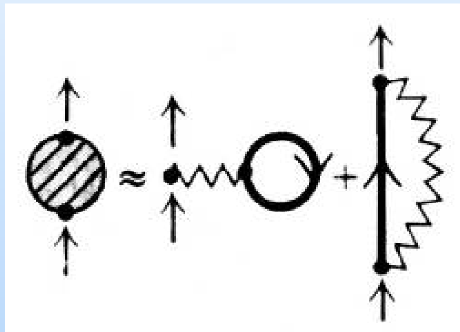
  $$\langle GS | q_{\vec{k}} c^{\dagger}_{\vec{k}} | GS \rangle = \sqrt{Z}$$

  q: quasi-electron,   c: electron
- Phenomenology that is the bedrock principle of many solids (from Si to heavy fermions)
- Not proven generally; Breaks down in 1d (repalced by Luttinger liquid!)
- Lifetime $$\frac{1}{\tau} = a(\varepsilon - \varepsilon_F)^2 + bT^2$$ (Luttinger, PR 121, 942 ('61))

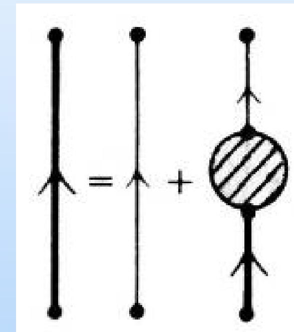
Hartree and Hartree-Fock Approx.

- Approximation to full Green's function (propagator)

Self Energy Σ



Dyson Equation



Direct term

Fetter and Walecka, Quantum Theory of Many-Particle Systems

Exchange term pure QM effect

- Hartree-Fock equation

$$\Psi(\mathbf{r}_1 s_1, \mathbf{r}_2 s_2, \ldots, \mathbf{r}_N s_N) = \begin{vmatrix} \psi_1(\mathbf{r}_1 s_1)\psi_1(\mathbf{r}_2 s_2) & \ldots & \psi_1(\mathbf{r}_N s_N) \\ \psi_2(\mathbf{r}_1 s_1)\psi_2(\mathbf{r}_2 s_2) & \ldots & \psi_2(\mathbf{r}_N s_N) \\ \vdots & & \vdots \\ \psi_N(\mathbf{r}_1 s_1)\psi_N(\mathbf{r}_2 s_2) & \ldots & \psi_N(\mathbf{r}_N s_N) \end{vmatrix}. \quad (17.13)$$

Direct term (Hartree)

$$-\frac{\hbar^2}{2m}\nabla^2\psi_i(\mathbf{r}) + U^{\text{ion}}(\mathbf{r})\psi_i(\mathbf{r}) + U^{\text{el}}(\mathbf{r})\psi_i(\mathbf{r})$$

Exchange term

$$-\sum_j \int d\mathbf{r}' \frac{e^2}{|\mathbf{r}-\mathbf{r}'|}\psi_j{}^*(\mathbf{r}')\psi_i(\mathbf{r}')\psi_j(\mathbf{r})\delta_{s_i s_j} = \varepsilon_i\psi_i(\mathbf{r}), \quad (17.15)$$

Screening

$$\phi_{ext}(\vec{q}) = \epsilon(\vec{q})\phi(\vec{q})$$

$$\rho_{ind}(\vec{q}) = \chi(\vec{q})\phi(\vec{q})$$

$$\epsilon(\vec{q}) = 1 - \frac{4\pi}{q^2}\chi(\vec{q})$$

- Lindhard Susceptibility (Hartree approx, any q)

$$\chi_L(\vec{q}) = \frac{e^2}{V}\sum_{\vec{k},s}\frac{f_{\vec{k}+\frac{1}{2}\vec{q}} - f_{\vec{k}-\frac{1}{2}\vec{q}}}{\varepsilon(\vec{k}+\frac{1}{2}\vec{q}) - \varepsilon(\vec{k}-\frac{1}{2}\vec{q})} = \frac{e^2}{V}\sum_{\vec{k},s}\frac{f_{\vec{k}+\vec{q}} - f_{\vec{k}}}{\varepsilon(\vec{k}+\vec{q}) - \varepsilon(\vec{k})}$$

- Reduces to Thomas-Fermi for small q

$$\chi_{TF}(\vec{q}) \approx -\frac{e^2}{V}\sum_{\vec{k},s}\frac{\partial f_{\vec{k}}}{\partial \mu} = -e^2\frac{\partial n_0}{\partial \mu}$$

Thomas-Fermi Screening

- Very effective screening at long λ

$$\phi_{ext}(\vec{q}) = \epsilon(\vec{q})\phi(\vec{q})$$

$$\rho_{ind}(\vec{q}) = \chi(\vec{q})\phi(\vec{q})$$

$$\epsilon(\vec{q}) = 1 - \frac{4\pi}{q^2}\chi(\vec{q})$$

$$\chi(\vec{q}) \approx -\frac{e^2}{V}\sum_{\vec{k},s}\frac{\partial f_{\vec{k}}}{\partial \mu} = -e^2\frac{\partial n_0}{\partial \mu}$$

$$k_0^2 = 4\pi e^2 \frac{\partial n_0}{\partial \mu}$$

$$\epsilon(\vec{q}) = 1 + \frac{k_0^2}{q^2}$$

$$\phi(\vec{r}) = \frac{Q_{ext}}{r}e^{-k_0 r}$$

$$\frac{\partial n_0}{\partial \mu} \approx g(\varepsilon_F) = \frac{m k_F}{\hbar^2 \pi^2}$$

- Screened Coulomb
- Very short screening length

$$k_0 = \frac{2.95}{(r_s/a_0)^{1/2}}\text{Å}^{-1}$$

$$k_0 \sim k_F \sim O(1)\text{Å}^{-1}$$

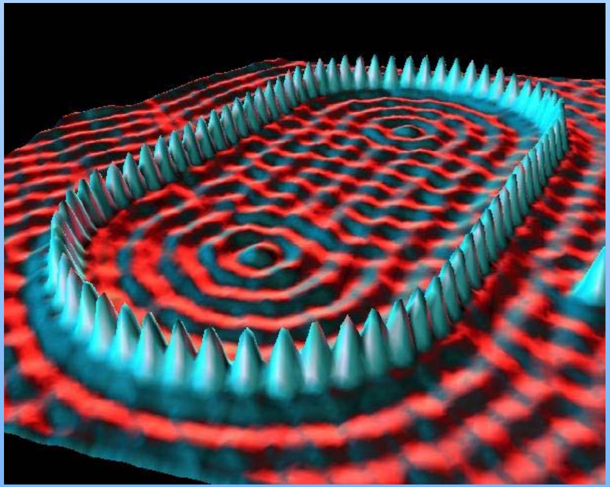
Lindhard-Specific Screening

- At short λ (~ $1/k_F$)

  χ (q) generally has singularity at $q=2k_F$

$$\phi(\vec{r}) \sim \frac{1}{r^3} \cos 2k_F r$$

- Friedel (or Ruderman-Kittel) Oscillations



http://www.aip.org/png/images/stm2.jpg

Don Eigler, IBM

Lindhard Over-Screening

$\rho_{ind}(\vec{q}) = \chi(\vec{q})\phi(\vec{q})$

- FS Nesting (below) or van-Hove singularity can lead to divergence of χ at $q=2k_F$ (CDW), T=0

$$\chi_L(\vec{q}) = \frac{e^2}{V}\sum_{\vec{k},s}\frac{f_{\vec{k}+\vec{q}} - f_{\vec{k}}}{\varepsilon(\vec{k}+\vec{q}) - \varepsilon(\vec{k})}$$

χ grows as T decreases.
CDW happens if χ is large enough.

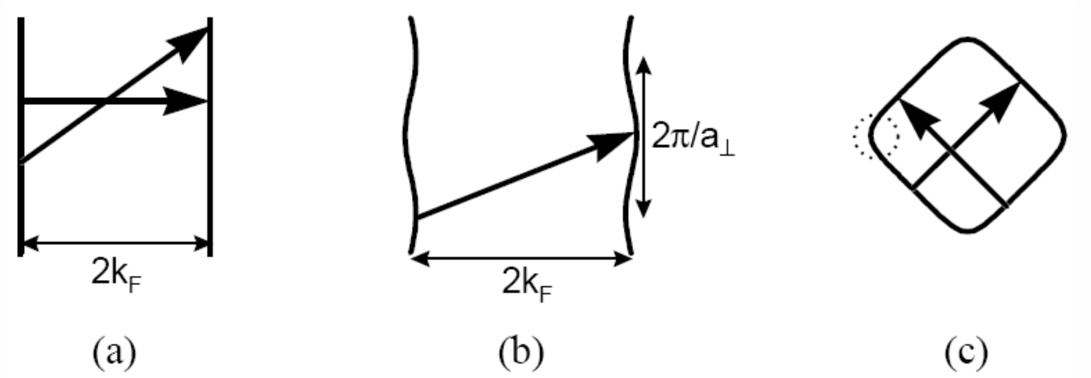
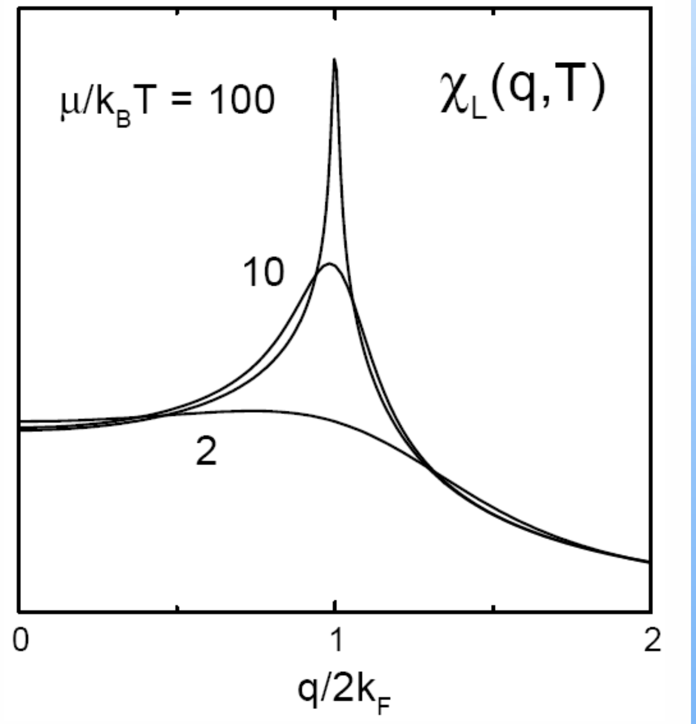


Figure 2.4: Examples of nesting FS's. For illustration a two spatial dimensional world is considered. (a) A 1 dimensional FS which is nested by an infinite number of vectors $(2k_F, x)$ for any value of x. (b) A small amount of modulation picks out the unique nesting vector $(2k_F, \frac{\pi}{a_\perp})$, where $a_\perp$ is the unit cell distance along the easy conducting direction. (c) A fully 2-dimensional FS with alternative partial nesting vectors. The states at corners are never nested in any case.



Mean Field and Beyond...

$$H = -J \sum_{\langle i,j\rangle = nn} \vec{S_i} \cdot \vec{S_j}$$

n.n. = nearest neighbor

$$\vec{S_i} = \underbrace{\langle \vec{S_i} \rangle}_{\text{Thermo-dynamic average}} + \delta \vec{S_i} \qquad \delta \vec{S_i} = \vec{S_i} - \langle \vec{S_i} \rangle$$

$$H = -J \sum_{\langle i,j\rangle = nn} \vec{S_i} \cdot \vec{S_j} \approx -J \sum_i \vec{S_i} \cdot \sum_{j=nn} \langle \vec{S_j} \rangle$$

$\langle \vec{S_i} \rangle$ = uniform for FM, alternating for AFM

z = coordination # = # of n.n.

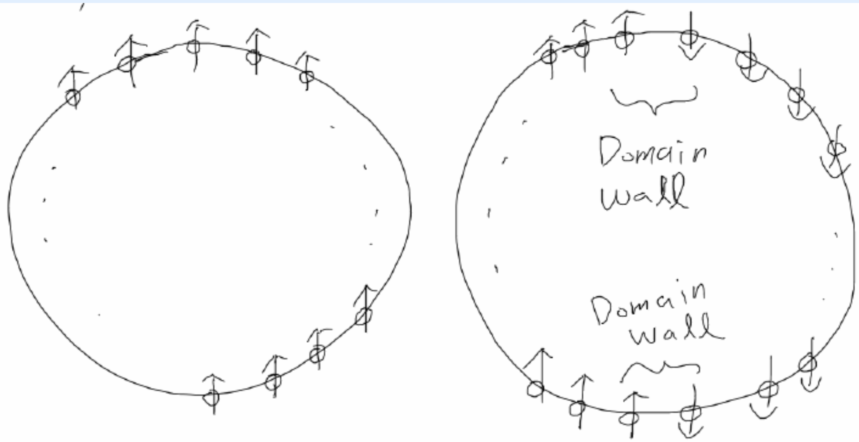
$$H = -\sum_i \vec{S_i} \cdot \left(J z \langle \vec{S} \rangle \right)$$

↖ FM

$$\vec{B_i} \propto J z \vec{M}$$

MF theory works better as the spatial dimension increases.

Why Mean-Field Theory Completely Breaks Down in One Dimension



$E = E_0$ $\quad$ $S = 0$

$E = E_0 + J$ $\quad$ $S \propto \log N$

$F_0 = E - TS = E_0$

$F_1 = E - TS = E_0 + J - T k_B \log N$

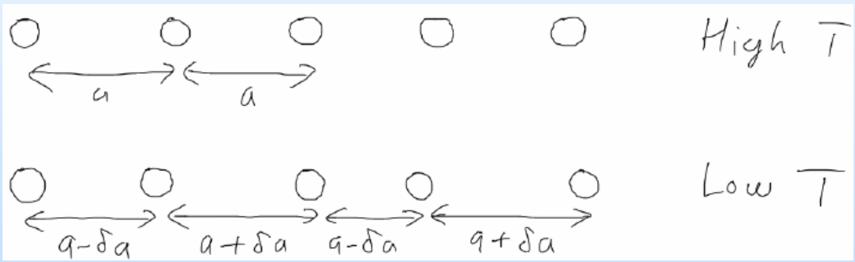
$F_1 < F_0$ for any finite T

Can continue with more domains

Long range order breaks into many many short range orders which fluctuate in time, space (unless pinned by impurities)

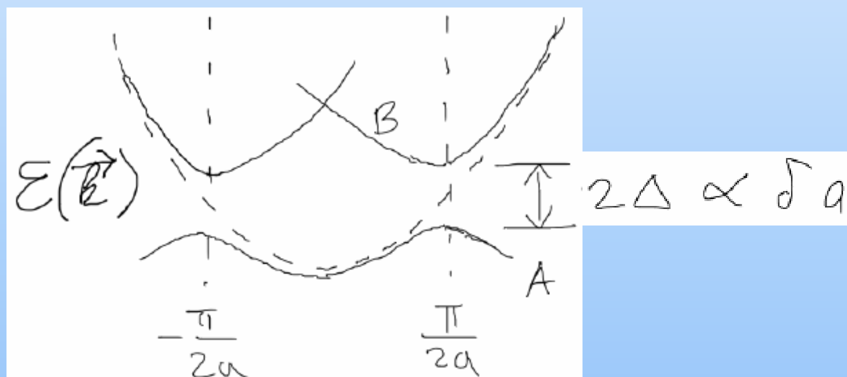
- Mermin-Wagner Theorem : No long range order (i.e. no phase transition) in 1D or 2D with short range interactions

Peierls Instability (Charge Density Wave)



mono-valent

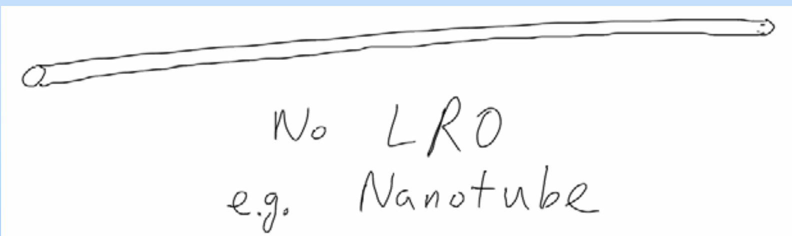
High T : metal
Low T : insulator



- Analogous Physics in Spin Density Wave (Cr), and Spin Peierls ($CuGeO_3$) Transitions

Wait … What Really Happens in Peierls Systems

- This was a mean-field picture! And, we did not condier Mermin-Wagner theorem.



Neutron Diffraction, X-ray Diffraction, Photoemission Spectroscopy, Pauli Susceptibility, Resistivity etc. can examine these strange behaviors on quasi-1D materials

$T \approx T_{MF}$

$T \gg T_{MF}$	Nothing
$T \approx T_{MF}$	Fluctuating SRO show up (confined to chains)
$T \approx T_{3D}$ ($T_{3D} \ll T_{MF}$)	Real LRO phase transition

Other Novel (Low-Dim) Physics

- Spin-and-charge separation
- Luttinger liquid state of electrons
- Nanotubes, graphene, graphite
- Massless Dirac particles in graphene
- Quantized conductance
- Metal-Insulator transition
- Quantum dots – Coulomb blockade, Kondo resonance, …
- Quantum Hall Effect
- Magnetic multi-layers
- …

I was like a boy playing on the sea-shore, and diverting myself now and then finding a smoother pebble or a prettier shell than ordinary, whilst the great ocean of truth lay all undiscovered before me.

Stoner Ferromagnetism

- Just like Pauli Para-magnetism theory, but with internal field

$$\varepsilon_{\vec{k}\uparrow} = \varepsilon_{\vec{k}} + U n_{\downarrow}$$

$$\varepsilon_{\vec{k}\downarrow} = \varepsilon_{\vec{k}} + U n_{\uparrow}$$

Exchange energy $U > 0$

$$M = \mu_B (n_{\uparrow} - n_{\downarrow})$$

$$\varepsilon_{k\uparrow} = \varepsilon_{\vec{k}} + U \cdot \frac{n}{2} - U \frac{M}{2\mu_B}$$

$$\varepsilon_{k\downarrow} = \varepsilon_{\vec{k}} + U \cdot \frac{n}{2} + U \cdot \frac{M}{2\mu_B}$$

$$n = n_{\uparrow} + n_{\downarrow}$$

$n, n_{\uparrow}, n_{\downarrow}$: # densities

- Self consistency requires that

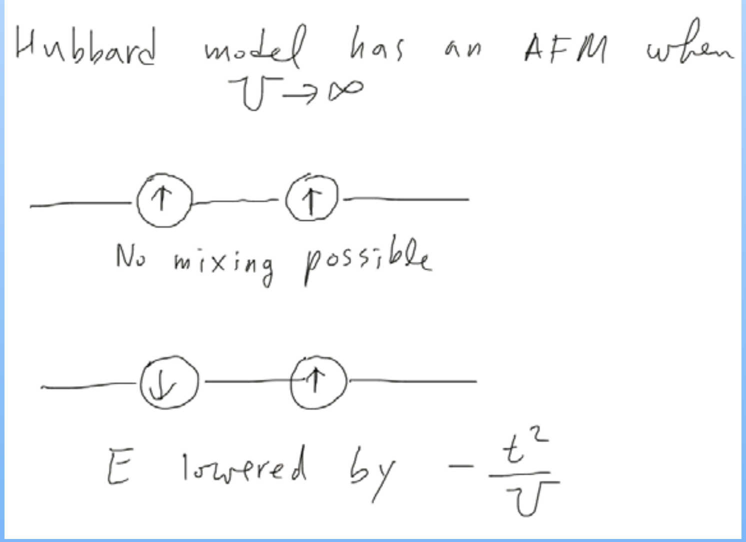
$$\frac{g(\varepsilon_F)}{N} \cdot U = 1$$

(Stoner criterion)

Hubbard Model and (A)FM

$$H = -t \sum_{<i,j>,\sigma} c_{i,\sigma}^{\dagger} c_{j,\sigma} + U \sum_{i=1}^{N} n_{i\uparrow} n_{i\downarrow}$$

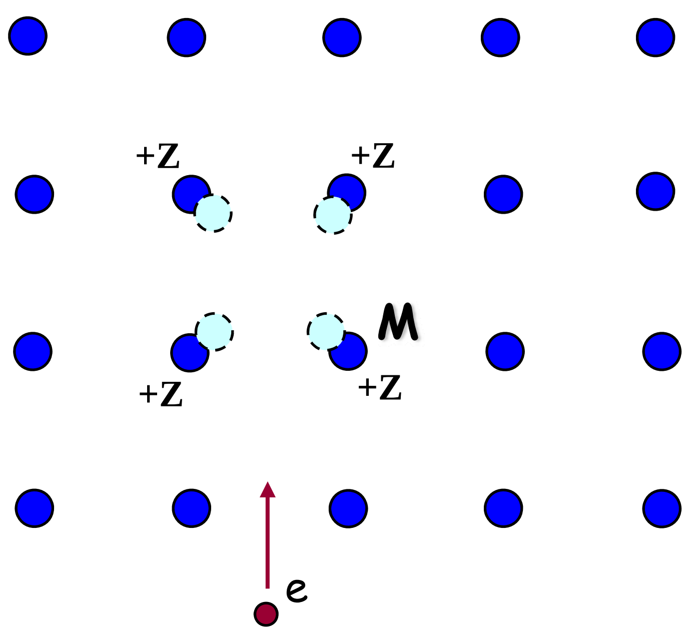
- Hubbard Model provides a basis for the Stoner FM (small U)
- Hubbard Model also provides a basis for an AFM in the opposite limit of large U



AFM MH Insulator

Electron-Phonon Interaction: BCS theory

PHONON MEDIATED PAIRING



Pairs of electrons: **Cooper pairs**

Superconducting gap: Δ

El-ph coupling constant: λ

$$T_c \sim \omega_{ph} \exp(-1/\lambda) \sim M^{-1/2}$$

e-ph wins e-e at low freq. (**Slow Wins!**)

Emergence of Debye Phonon in Metal

Ion-Ion interaction without screening: Phonon Mode is NOT Debye-like!

$$\Omega_p{}^2 = \frac{4\pi n_i (Ze)^2}{M} = \left(\frac{Zm}{M}\right)\omega_p{}^2$$

$$\omega_p{}^2 = \frac{4\pi n_e e^2}{m}$$

Ion-Ion interaction with screening: Phonon Mode is LIKE Debye, as observed.

$$\omega(\mathbf{k})^2 = \frac{\Omega_p{}^2}{\epsilon(\mathbf{k})}$$

$$\epsilon(\mathbf{k}) = 1 + \frac{k_0{}^2}{k^2}$$

$$\omega(\mathbf{k}) \approx ck, \quad c^2 = \frac{\Omega_p{}^2}{k_0{}^2} = \frac{Zm}{M}\frac{\omega_p{}^2}{k_0{}^2}$$

Screening by both electrons and phonons

$$\epsilon\phi^{\text{total}} = \phi^{\text{ext}}.$$

$$\epsilon^{\text{el}}\phi^{\text{total}} = \phi^{\text{ext}} + \phi^{\text{ion}}$$

$$\epsilon^{\text{ion}}_{\text{bare}}\phi^{\text{total}} = \phi^{\text{ext}} + \phi^{\text{el}}$$

$$\epsilon = \epsilon^{\text{el}} + \epsilon^{\text{ion}}_{\text{bare}} - 1.$$

Or, think in terms of "dressed ions"

$$\phi^{\text{total}} = \frac{1}{\epsilon^{\text{ion}}_{\text{dressed}}}\frac{1}{\epsilon^{\text{el}}}\phi^{\text{ext}}$$

$$\frac{1}{\epsilon} = \frac{1}{\epsilon^{\text{ion}}_{\text{dressed}}}\frac{1}{\epsilon^{\text{el}}}$$

$$\epsilon^{\text{ion}}_{\text{dressed}} = 1 + \frac{1}{\epsilon^{\text{el}}}(\epsilon^{\text{ion}}_{\text{bare}} - 1).$$

$$\epsilon^{\text{ion}}_{\text{bare}} = 1 - \frac{\Omega_p{}^2}{\omega^2}$$ Just like Plasmon

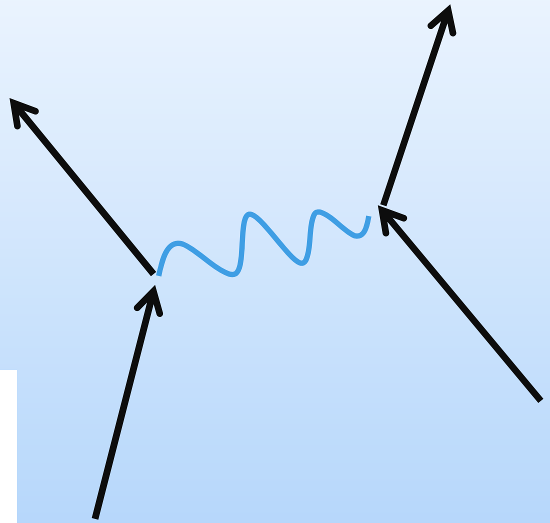
$$\epsilon = 1 + \frac{k_0{}^2}{q^2} - \frac{\Omega_p{}^2}{\omega^2},$$

Not Surprisingly …

$$\epsilon^{\text{ion}}_{\text{dressed}} = 1 - \frac{\Omega_p{}^2/\epsilon^{\text{el}}}{\omega^2} = 1 - \frac{\omega(\mathbf{q})^2}{\omega^2},$$

Effective Electron-Electron Interaction

$$\frac{1}{\epsilon} = \left(\frac{1}{1 + k_0{}^2/q^2}\right)\left(\frac{\omega^2}{\omega^2 - \omega(\mathbf{q})^2}\right)$$



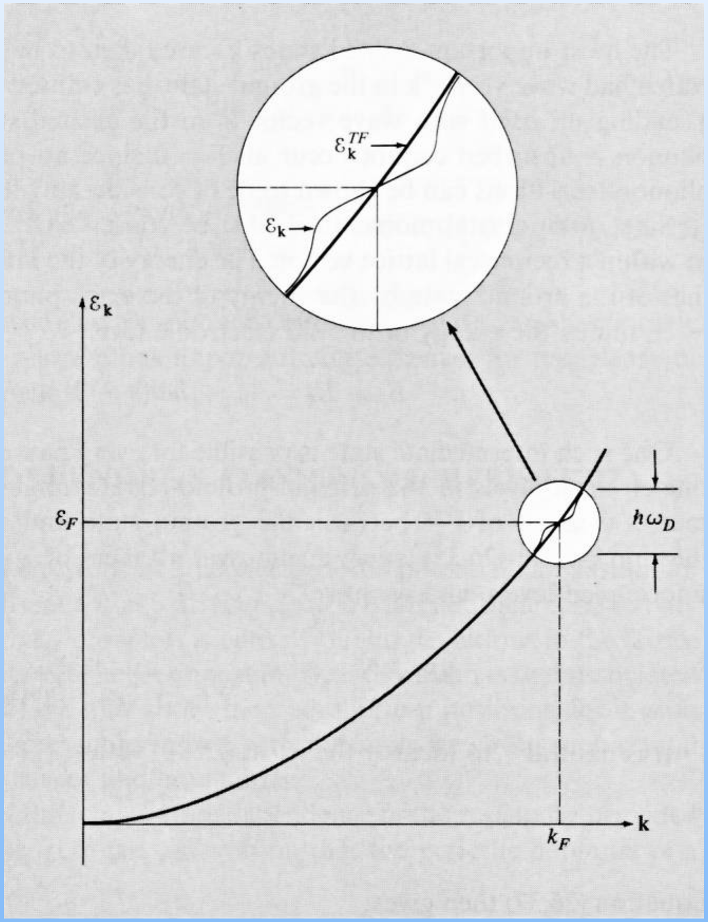
$$\frac{4\pi e^2}{k^2} \to \frac{4\pi e^2}{k^2\epsilon} = \frac{4\pi e^2}{k^2 + k_0{}^2}\left(1 + \frac{\omega(\mathbf{k})^2}{\omega^2 - \omega(\mathbf{k})^2}\right).$$

$$v^{\mathrm{eff}}_{\mathbf{k},\mathbf{k}'} = \frac{4\pi e^2}{q^2 + k_0{}^2}\left[1 + \frac{\omega(\mathbf{q})^2}{\omega^2 - \omega(\mathbf{q})^2}\right]; \qquad \mathbf{q} = \mathbf{k} - \mathbf{k}', \quad \omega = \frac{\mathcal{E}_{\mathbf{k}} - \mathcal{E}_{\mathbf{k}'}}{\hbar}.$$

- Attractive Interaction due to Retardation!

  (for ω on the order of or less than ω_D: Basis for BCS)

Electron Dispersion Change ("Kink")

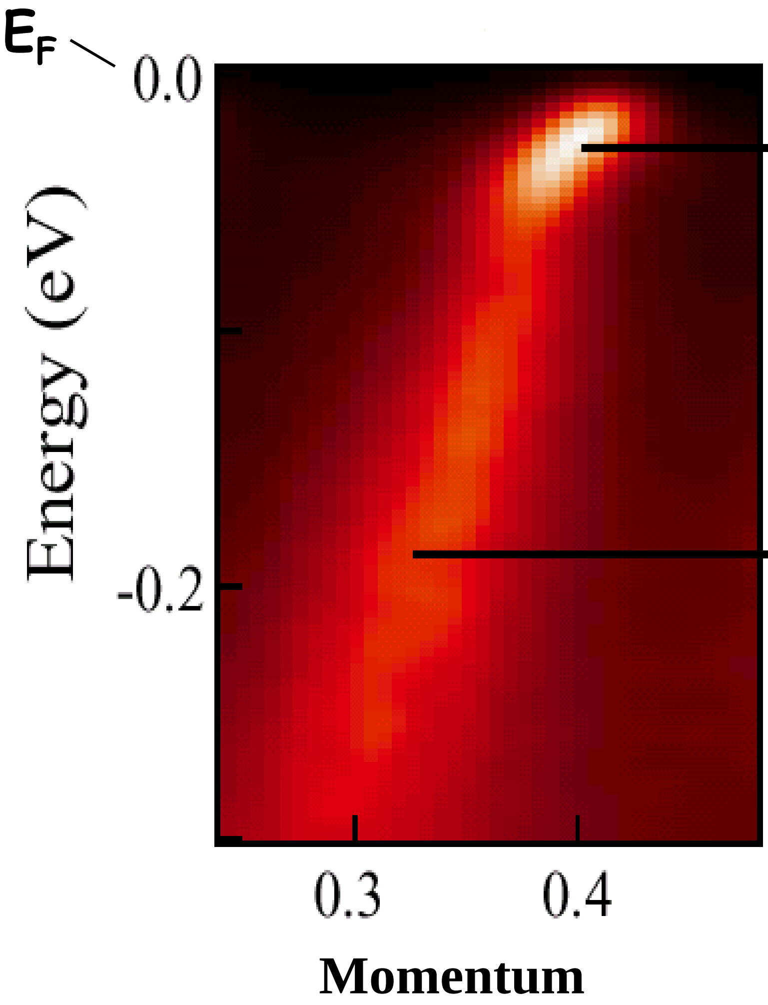


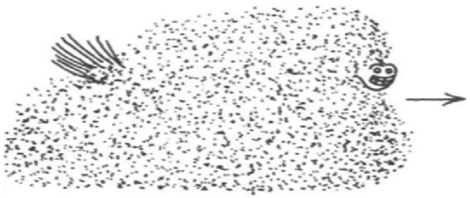
- Observed for simple metals such as Be, Mo, W, etc.
- Highly debated in HTSC

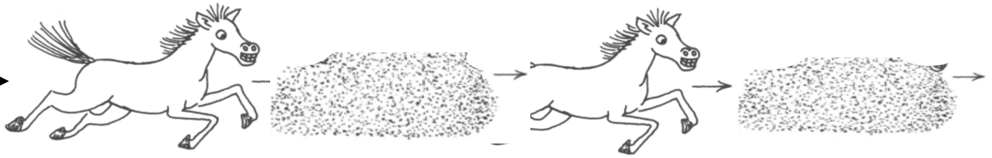
Read: 519-521 of A&M or Schrieffer "Theory of Superconductivity"

Heavy Quasi-Particle at Low Energy …

Change of Velocity due to El-Ph Interaction







Electron-Phonon Interaction

- Can interpret the energy lowering as being due to electron-phonon interaction (pages 522-523)

$$|g_{\mathbf{k},\mathbf{k}'}|^2 = \frac{1}{V} \frac{4\pi e^2}{|\mathbf{k} - \mathbf{k}'|^2 + k_0{}^2} \frac{1}{2} \hbar\omega_{\mathbf{k}-\mathbf{k}'}$$

$$|g_{\mathbf{k},\mathbf{k}'}|^2 \approx \frac{\hbar\omega(\mathbf{k} - \mathbf{k}')\mathcal{E}_F}{3n_e V} = \frac{\hbar\omega(\mathbf{k} - \mathbf{k}')\mathcal{E}_F}{3NZ}, \qquad |\mathbf{k} - \mathbf{k}'| \ll k_0.$$

- Important element in giving Bloch T^5 law of resistivity at low T (read A&M pages 525-526)
- E-Ph important for Peierls transition

  Compeition between Cooper channel and Peierls channel!