Table of Contents

Lectures

Three Topics

- Consequences of electron-electron interactions.
- Magnetism
- Superconductivity

Schrieffer - Theory of Superconductivity
Office Hour: Tues. 2pm.
10 minute quiz the end of Thursday lecture.

Grade Breakdown

1. Quizzes - 30%
2. Midterm - 30%
3. Final Exam - 40%

1 Interactions Between Electrons

1.1 Models

$$H = \sum_i \left(-\frac{\hbar^2}{2m_e} \nabla_i^2 \right) + \sum_i U_{\text{ion}}(\mathbf{r}_i) + \sum_{i \neq j} U_{\text{e-e}}(\mathbf{r}_i - \mathbf{r}_j) \tag{1.1}$$

$$U_{\text{ion}}(\mathbf{r}_i) = -Ze^2 \sum_m |\mathbf{r}_i - \mathbf{R}_m|^{-1} \tag{1.2}$$

$$U_{\text{e-e}}(\mathbf{r}_i - \mathbf{r}_j) = \frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|} \tag{1.3}$$

Now we apply a new notation.

$$n(\mathbf{r}) = \sum_i \delta(\mathbf{r} - \mathbf{r}_i) \tag{1.4}$$

$$U_{\text{ion}} = \int \mathrm{d}\mathbf{r}\, U_{\text{ion}}(\mathbf{r}) n(\mathbf{r}) \tag{1.5}$$

$$U_{\text{e-e}} = \frac{1}{2} \iint \mathrm{d}\mathbf{r}\, \mathrm{d}\mathbf{r}'\, n(\mathbf{r}) n(\mathbf{r}') U_{\text{e-e}}(\mathbf{r} - \mathbf{r}') \tag{1.6}$$

$$U_{\text{e-e}} = \frac{4\pi e^2}{q^2} \quad \text{Fourier Transform (Specific to 3D)} \tag{1.7}$$

$$U_{\text{e-e}} = \frac{2\pi e}{|q|} \quad \text{(2D)}; \qquad \sim \ln|q| \quad \text{(1D)} \tag{1.8}$$

(NOTE: The motivated student should show the 3D result.) Diagonal terms vanish due to phase space argument?

$$U_{\text{e-e}} = \frac{1}{2} \iint \mathrm{d}\mathbf{r}\, \mathrm{d}\mathbf{r}' \sum_{q,q'} n(\mathbf{q}) \mathrm{e}^{-\mathrm{i}\mathbf{q}\cdot\mathbf{r}} n(\mathbf{q}') \mathrm{e}^{-\mathrm{i}\mathbf{q}'\cdot\mathbf{r}'} U_{\text{e-e}}(\mathbf{q}'') \mathrm{e}^{-\mathbf{q}''\cdot(\mathbf{r}-\mathbf{r}')} \tag{1.9}$$

$$\delta(\mathbf{q} + \mathbf{q}'') = \int \mathrm{d}\mathbf{r}\, \mathrm{e}^{-\mathrm{i}(\mathbf{q}+\mathbf{q}'')\cdot\mathbf{r}} \tag{1.10}$$

$$U_{\text{e-e}} = \sum_q n(\mathbf{q}) n(-\mathbf{q}) U(\mathbf{q}) \tag{1.11}$$

1.2 Second Quantization

- Creation operator: $\widehat{a}^\dagger_{\mathbf{k}\sigma}$ (Metals, heavily doped semiconductors).
- Field operator: $\widehat{\psi}^\dagger_\sigma(\mathbf{r}) = \sum_{\mathbf{k}} \phi^*_{\mathbf{k},\sigma}(\mathbf{r})\widehat{a}^\dagger_{\mathbf{k},\sigma}$ (insulator, metal oxides, lightly doped semiconductors).
- Principle of transcription: matrix elements of operators should be the same.

1.2.1 One Particle Operators

$$\widehat{H}^1 = \sum_{\ell,\ell'} \langle \ell \left| H \right| \ell' \rangle \, \widehat{a}^\dagger_{\ell'} \widehat{a}_\ell \tag{1.12}$$

($\widehat{H}^1$ is a one particle second quantized operator. H is a first quantized operator)

$$\left\langle \ell_1 \left| \widehat{H}^1 \right| \ell_2 \right\rangle = \sum_{\ell,\ell'} \langle \ell \left| H \right| \ell' \rangle \left\langle 0 \left| \widehat{a}_{\ell_1} \widehat{a}^\dagger_{\ell'} \widehat{a}_\ell \widehat{a}^\dagger_{\ell_2} \right| 0 \right\rangle \tag{1.13}$$

$$\sum_{\ell} \widehat{a}_\ell \widehat{a}^\dagger_{\ell_2} |0\rangle = \delta_{\ell,\ell_2} \tag{1.14}$$

$$\left\langle \ell_1 \left| \widehat{H}^1 \right| \ell_2 \right\rangle = \langle \ell_1 \left| H \right| \ell_2 \rangle \tag{1.15}$$

Review

- We are most interested in the interactions between electrons and the ions and the electron-electron interaction.
- It is most physically reasonable to discuss the physics in terms of creation and annihilation operators.
- How do we go about doing this? The goal of Heisenberg is to produce the same observables as the first quantized operators (get the same matrix elements).

1.2.2 Two Particle Operators

$$\widehat{H}^{(2)} = \sum_{\ell\ell'\ell''\ell'''} H^{(2)}_{\ell\ell'\ell''\ell'''} \widehat{a}^\dagger_\ell \widehat{a}^\dagger_{\ell'} \widehat{a}_{\ell''} \widehat{a}_{\ell'''} \tag{1.16}$$

$$H^{(2)}_{\ell\ell'\ell''\ell'''} = \iint \mathrm{d}\mathbf{r}\, \mathrm{d}\mathbf{r}' \phi^*_\ell(\mathbf{r}) \phi^*_{\ell'}(\mathbf{r}') H^{(2)}(\mathbf{r}-\mathbf{r}') \phi_{\ell''}(\mathbf{r}) \phi_{\ell'''}(\mathbf{r}') \tag{1.17}$$

(ℓ refers to a generic quantum number)

1.3 Equivalent formulation using field operators

$$\widehat{\psi}(\mathbf{r}) = \sum_{\mathbf{k}} \phi_{\mathbf{k}}(\mathbf{r}) \widehat{a}_{\mathbf{k}} \tag{1.18}$$

$$\widehat{H}^{(1)} = \int \mathrm{d}\mathbf{r}\ \widehat{\psi}^\dagger(\mathbf{r}) H^{(1)}(\mathbf{r}) \widehat{\psi}(\mathbf{r}) \tag{1.19}$$

(Motivated student can prove this.)

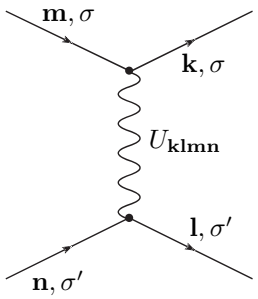
1.3.1 For the electron system

$$\widehat{H} = \sum H_{\mathbf{k},\mathbf{l},\sigma} a^\dagger_{\mathbf{k},\sigma} a_{\mathbf{l},\sigma} + \frac{1}{2} \sum U_{\mathbf{klmn}} a^\dagger_{\mathbf{k},\sigma} a^\dagger_{\mathbf{l}\sigma} a_{\mathbf{m}\sigma} a_{\mathbf{n}\sigma} \tag{1.20}$$

$$H_{\mathbf{kl}} \equiv \int \mathrm{d}\mathbf{r}\ \phi^*_{\mathbf{k}}(\mathbf{r}) \left(-\frac{\hbar^2}{2m} \nabla^2 + U_{\text{ion}}(\mathbf{r}) \right) \phi_{\mathbf{l}}(\mathbf{r}) \tag{1.21}$$

$$U_{\mathbf{klmn}} = \iint \mathrm{d}\mathbf{r}\, \mathrm{d}\mathbf{r}' \phi^*_{\mathbf{k}}(\mathbf{r}) \phi^*_{\mathbf{l}}(\mathbf{r}') U_{\text{e-e}}(\mathbf{r}-\mathbf{r}') \phi_{\mathbf{m}}(\mathbf{r}) \phi_{\mathbf{n}}(\mathbf{r}') \tag{1.22}$$

- Intuition tells us that propagation does not cause spin to flip is reason why spins are the same in kinetic term. Counterexample: spin in magnetic field. In heavier elements, spin-orbit coupling will flip the spin w/o electron-electron interaction.
- Feynman diagram can be used to describe an interaction.



- Density interaction is $a^\dagger a$, not $a^\dagger a^\dagger aa$.
- Normal Ordering: all destruction operators should be moved to the right.
- If we calculate the effective mass of electrons coming from a photon, the effective mass is infinite, so we do Renormalization.
- Imagine that the mass of the electron is infinite as well. When you absorb the infinity from the vacuum fluctuations, the resulting mass is the one you observe.
- Vacuum fluctuations: Viewpoint is that as a photon is travelling there is a particle-antiparticle pair and if we calculate the contributions to the mass, it is infinite. Electron's effective energy and mass are infinity. When combined with vacuum fluctuations then result is what we observe. Putting annihilation operators on the right gets rid of these "ghost" particles.

2 Models for Electrons in Solids

2.1 Jellium Model

- Smear out the positive ions into a homogeneous background charge.
- Eigenstates are plane waves

$$\phi_{\mathbf{k},\sigma}(\mathbf{r}) = \frac{1}{\sqrt{V}} \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}} \eta_\sigma \qquad \eta_\uparrow = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad \eta_\downarrow = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \tag{2.1}$$

$$H^{(1)} \left|\phi_{\mathbf{k},\sigma}\right\rangle = \varepsilon_{\mathbf{k},\sigma} \left|\phi_{\mathbf{k},\sigma}\right\rangle \tag{2.2}$$

$$\left\langle \phi_{\mathbf{l}} \middle| H^{(1)} \middle| \phi_{\mathbf{k}} \right\rangle = \delta_{\mathbf{kl}} \varepsilon_{\mathbf{k}} \tag{2.3}$$

$$\widehat{H} = \sum_{\mathbf{k}\sigma} \varepsilon_{\mathbf{k}} \widehat{c}^\dagger_{\mathbf{k}\sigma} \widehat{c}_{\mathbf{k}\sigma} + \frac{1}{2V} \sum_{\mathbf{q}} U_{\text{e-e}}(\mathbf{q}) \widehat{n}(\mathbf{q}) \widehat{n}(-\mathbf{q}) \tag{2.4}$$

$$= \sum_{\mathbf{k}\sigma} \varepsilon_{\mathbf{k}} \widehat{c}^\dagger_{\mathbf{k}\sigma} \widehat{c}_{\mathbf{k}\sigma} + \frac{1}{2V} \sum_{\substack{\mathbf{q},\mathbf{k},\mathbf{k}' \\ \sigma,\sigma'}} U_{\text{e-e}}(\mathbf{q}) \widehat{c}^\dagger_{\mathbf{k}-\mathbf{q},\sigma} \widehat{c}^\dagger_{\mathbf{k}'+\mathbf{q},\sigma'} \widehat{c}_{\mathbf{k}',\sigma} \widehat{c}_{\mathbf{k},\sigma} \tag{2.5}$$

Second term is Fourier transform of the interaction Hamiltonian (interaction between density waves). $n(\mathbf{q})$ is a density fluctuation of the gas with wavenumber $\mathbf{q}$. (Claim High Tc superconductors have charge density waves.) KNOW THIS HAMILTONIAN. Claim that four out of fifteen will need to know this for our orals!

$$\widehat{n}(\mathbf{q}) = \sum_{\mathbf{k}} \widehat{c}^\dagger_{\mathbf{k}+\mathbf{q}} c_{\mathbf{k}} \qquad\qquad \widehat{n}(\mathbf{r}) = \widehat{\psi}^\dagger(\mathbf{r}) \widehat{\psi}(\mathbf{r}) \tag{2.6}$$

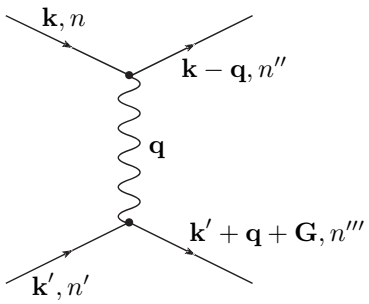
(Motivated student can take field formulation to get second quantized formulation of the above equations). First equation: we annihilate and create an electron with momentum difference $\mathbf{q}$.

2.2 Blöch Functions

- Restore ionic structure.
- We introduce bands (denoted by index n) to the system.

$$\widehat{\psi}_{n,\mathbf{k},\sigma}(\mathbf{r}) \tag{2.7}$$

- Momentum is conserved up to a reciprocal lattice vector $\mathbf{G}$ (crystal momentum is conserved).



Two more summation indices:

1. band index n
2. reciprocal lattice vector $\mathbf{G}$

$$\mathbf{G}=0 \qquad \text{direct} \qquad\qquad \mathbf{G}\neq 0 \qquad \text{Umklapp} \tag{2.8}$$

2.3 Hubbard Model

- Anderson claimed it holds key for High Tc Superconductivity (they are metal oxides)
- Uses field operators.
- Suitable for localized orbitals: insulators, metal oxides (High Tc S.C.), lightly doped semiconductors
- Use Wannier states as our basis instead of Blöch functions.
- Most studied Hamiltonian of the last 20 years.

$$H^{(1)}=\int \mathrm{d}\mathbf{r}\ \phi_i^*(\mathbf{r}-\mathbf{R}_i)\left(-\frac{\hbar^2}{2m}\nabla^2+U_{\text{ion}}(\mathbf{r})\right)\phi_j(\mathbf{r}-\mathbf{R}_j) \tag{2.9}$$

Biggest is when $i=j$, the diagonal term.

$$H^{(1)}=\varepsilon\sum_i c_i^\dagger c_i \tag{2.10}$$

Assume energy is the same on every site since the atoms are identical.
Next biggest: $i=j+\delta$, nearest neighbor.

$$H^{(1)}=t\sum_{\langle i,j\rangle} c_i^\dagger c_j \tag{2.11}$$

Physical meaning is that this term is the hopping term.

2.3.1 Two Particle Hamiltonian

The biggest term is the diagonal term.

$$H^{(2)}=U\sum \widehat{n}_{i,\sigma}\widehat{n}_{i,-\sigma} \tag{2.12}$$

$$\widehat{H}=t\sum_{\langle i,j\rangle,\sigma}\widehat{c}_{i,\sigma}^\dagger\widehat{c}_{j,\sigma}+U\sum_{i,\sigma}\widehat{n}_{i,\sigma}\widehat{n}_{i,-\sigma} \tag{2.13}$$

Can also consider

- Next nearest neighbor hopping t'
- Neighbor repulsions V.

Last Time

- Derived Hubbard Model, simplest model capturing interactions between electrons.

Additional terms

$$V \sum_{ij} n_i n_j \qquad \begin{array}{c}\text{First(second) neighbor Coulomb interaction}\\ \text{(long-range portion of Coulomb dropped because of screening)}\end{array} \tag{2.14}$$

$$t' \sum_{\substack{ij\\ \text{n.n.n.}}} c^\dagger_{i\sigma} c_{j\sigma} \qquad \text{Next nearest neighbor hopping} \tag{2.15}$$

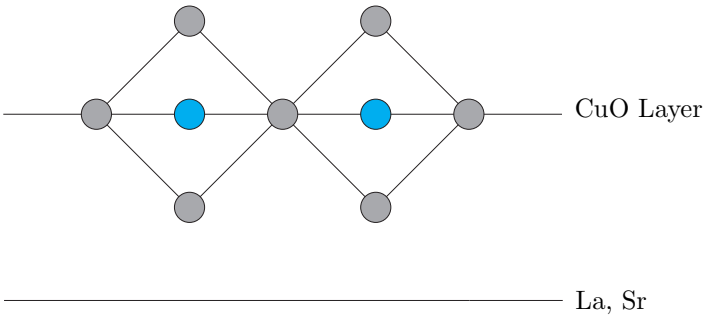
2.3.2 High-Temperature Superconductors

Typical values for a high-T_c superconductor

$$t \sim 0.5 \text{ eV} \qquad U \sim 5 \text{ eV} \tag{2.16}$$

$$t' \sim 0.1 \text{ eV} \qquad V \sim 1 - 2 \text{ eV} \tag{2.17}$$

What happens when we add disorder? (Example: $La_{2-x}Sr_xCuO_4$)



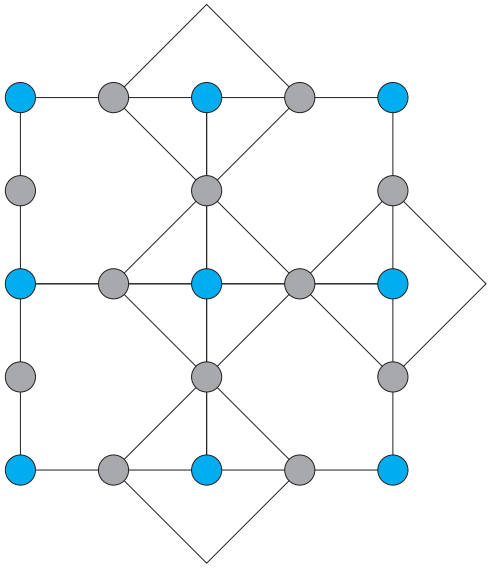


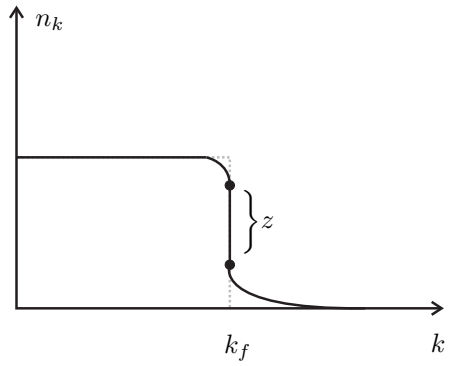
Figure 1: Blue: Cu, Grey: O

Zhang-Rice claim that we view the chemically correct (more complicated) structure as a series of a single type of site.

2.4 Perturbation Theory in U

$$|\phi\rangle = |\mathrm{FS}\rangle + \frac{U}{V} + \sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} \frac{1}{\varepsilon_{\mathbf{k}} + \varepsilon_{\mathbf{k}'} - \varepsilon_{\mathbf{k}+\mathbf{q}} + \varepsilon_{\mathbf{k}'-\mathbf{q}}} c^\dagger_{\mathbf{k}+\mathbf{q}} c^\dagger_{\mathbf{k}'-\mathbf{q}} c_{\mathbf{k}'} c_{\mathbf{k}} |\mathrm{FS}\rangle \tag{2.18}$$

$\langle\phi|n_{\mathbf{k}}|\phi\rangle =$



$$z = 1 - \tfrac{1}{4}\ln 2\,[U\cdot\rho(\varepsilon_F)]^2 \qquad \text{“Fermi step”} \tag{2.19}$$

1. Fermi distribution $n_{\mathbf{k}}$ gets rounded
2. Fermi step is diminished ($z < 1$), but non-vanishing (for small U).
3. Finite T the step still exists?
4. Step in Fermi function translates to the strengths of the pole of the Greens function which in turn represents the strength or amplitude of the quasi-particle interaction.

2.4.1 Limits of Perturbation Theory

1. $U\cdot\rho(\varepsilon_F) \sim 1$
   - Fermi step goes to zero.
2. 1D (previous results given for 3D)

$$\langle n_k\rangle \sim 2\,[U\cdot\rho(\varepsilon_F)]\ln|k - k_F| \tag{2.20}$$

   - Zero radius of convergence

Non-perturbative analysis is required.

2.4.2 Luttinger Theorem

Within radius of convergence of perturbation theory, volume of Fermi surface is unchanged.

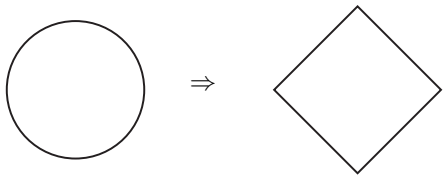


Figure 2: An example of a deformation of a Fermi surface where the volume is unchanged

- Gives rise to zero sound (Oscillation of the Fermi surface).

2.5 Hartree Approximation

Represent the interactions as if the electrons propagate in the average field of the other electrons.

$$\begin{aligned}\widehat{H} = \sum_{\sigma} \int \mathrm{d}\mathbf{r}\ \widehat{\psi}^{\dagger}_{\sigma}(\mathbf{r}) \left[-\frac{\hbar^2}{2m}\nabla^2 + U_{\text{ion}} \right] \widehat{\psi}_{\sigma}(\mathbf{r}) \\ + \sum_{\sigma\sigma'} \int \mathrm{d}\mathbf{r}\,\mathrm{d}\mathbf{r}'\ \widehat{\psi}^{\dagger}_{\sigma}(\mathbf{r}) \left\langle \widehat{\psi}^{\dagger}_{\sigma'}(\mathbf{r}')\widehat{\psi}_{\sigma'}(\mathbf{r}') \right\rangle \widehat{\psi}_{\sigma}(\mathbf{r}) U_{\text{e-e}}(\mathbf{r}-\mathbf{r}')\end{aligned} \tag{2.21}$$

We replaced $\psi^{\dagger}(\mathbf{r}')\psi(\mathbf{r}')$ with its average (or mean-field). This makes the Hamiltonian quadratic (which can be diagonalized). Is our solution self-consistent?

2.5.1 Steps

1. Assume a form for expectation value $\langle\psi^{\dagger}\psi\rangle$.
2. Diagonalize $\widehat{H}$.
3. Determine modified ψ.
4. Recalculate $\langle\psi^{\dagger}\psi\rangle$
5. Repeat from step 2.

This will make the theory self-consistent. Theories that are self-consistent or are mean-field are non-perturbative.

2.6 Fock (exchange) Approximation

- Fock: $\left\langle \widehat{\psi}^{\dagger}_{\sigma}(\mathbf{r})\widehat{\psi}_{\sigma'}(\mathbf{r}') \right\rangle$
- $\widehat{H}$ is quadratic (good), but non-local (bad)

$$\sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} U(\mathbf{q}) \widehat{c}^{\dagger}_{\mathbf{k}+\mathbf{q},\sigma} \widehat{c}^{\dagger}_{\mathbf{k}'-\mathbf{q},\sigma'} \widehat{c}_{\mathbf{k}',\sigma'} \widehat{c}_{\mathbf{k},\sigma} \tag{2.22}$$

$$\left\langle \widehat{c}^{\dagger}_{\mathbf{k}+\mathbf{q},\sigma} \widehat{c}_{\mathbf{k}',\sigma'} \right\rangle = \delta_{\mathbf{k}+\mathbf{q},\mathbf{k}'} \delta_{\sigma,\sigma'} \left\langle \widehat{c}^{\dagger}_{\mathbf{k}',\sigma'} \widehat{c}_{\mathbf{k}',\sigma'} \right\rangle \tag{2.23}$$

Remaining term

$$\widehat{c}^{\dagger}_{\mathbf{k}'-\mathbf{q},\sigma'} \widehat{c}_{\mathbf{k},\sigma} = \widehat{c}^{\dagger}_{\mathbf{k},\sigma} \widehat{c}_{\mathbf{k},\sigma} \tag{2.24}$$

$$\widehat{H} = \sum_{\mathbf{k},\sigma} \left\{ \varepsilon_{\mathbf{k},\sigma} - \sum_{\mathbf{k}'} U(\mathbf{k}-\mathbf{k}') \left\langle \widehat{c}^{\dagger}_{\mathbf{k}',\sigma} \widehat{c}_{\mathbf{k}',\sigma} \right\rangle \right\} \widehat{c}^{\dagger}_{\mathbf{k},\sigma} \widehat{c}_{\mathbf{k},\sigma} \tag{2.25}$$

2.6.1 Hartree Term

$$U(\mathbf{q}=0) \sum_{\mathbf{k}} \left\langle \widehat{c}^{\dagger}_{\mathbf{k}'} \widehat{c}_{\mathbf{k}'} \right\rangle = U(\mathbf{q}=0) N_e \tag{2.26}$$

Shifts energy of every electron by the same amount.

- Turns out this number is canceled out by ionic contribution (Only true for simplest interaction problems).

Last Time

- Effects of the interaction
- Perturbation Theory
  - For Strong interaction, Perturbation Theory is not valid.
  - 1D: Breaks down for small interaction
- Approximate quartic interaction term of the Hamiltonian as a quadratic term times the expectation value of the remaining quadratic terms (Hartree Approximation and Fock Approximation).
- Self-Consistent theories are good ways to go beyond perturbative approaches.

2.6.2 Hartree Term Cont.

$$\widehat{H} = \sum_{\mathbf{k},\sigma} \left[\varepsilon_{\mathbf{k},\sigma} - \sum_{\mathbf{k}',\sigma'} U(\mathbf{k}-\mathbf{k}') \left\langle \widehat{c}^\dagger_{\mathbf{k}',\sigma'} \widehat{c}_{\mathbf{k}',\sigma'} \right\rangle \right] \widehat{c}^\dagger_{\mathbf{k},\sigma} \widehat{c}_{\mathbf{k},\sigma} \tag{2.27}$$

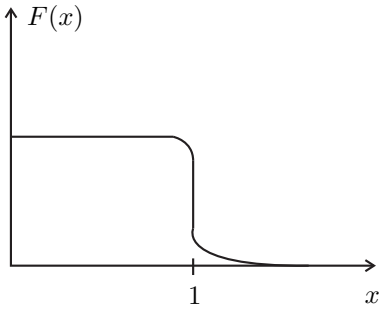
$$\Delta\varepsilon^{\mathrm{F}}_{\mathbf{k},\sigma} = \sum_{\mathbf{k}',\sigma'} U(\mathbf{k}-\mathbf{k}') \left\langle \widehat{c}^\dagger_{\mathbf{k}',\sigma'} \widehat{c}_{\mathbf{k}',\sigma'} \right\rangle \tag{2.28}$$

Calculation of Fock energy shift for spherical FS.

$$\Delta\varepsilon^{\mathrm{F}}_{\mathbf{k},\sigma} = \int_0^{|\mathbf{k}'|<k_F} \mathrm{d}^3\mathbf{k} \, \frac{4\pi e^2}{\left|\mathbf{k}-\mathbf{k}'\right|^2} = \frac{2k_F e^2}{\pi} F\left(\frac{k}{k_F}\right) \tag{2.29}$$

$$F(x) = \frac{1}{2} + \frac{1-x^2}{4x} \ln \frac{|1+x|}{|1-x|} \tag{2.30}$$

The motivated student will show the above.



$$\varepsilon^{\mathrm{F}}_{\mathbf{k}} = \frac{\hbar^2 k^2}{2m} - \frac{2k_F e^2}{\pi} F\left(\frac{k}{k_F}\right) \tag{2.31}$$

Can find the effective mass by taking the derivative of the Fock energy with respect to k and evaluate at the FS since all physical processes take place at the FS.

$$\frac{1}{k_F} \frac{\partial \varepsilon^{\mathrm{F}}}{\partial k}\bigg|_{k_F} \sim \frac{1}{m_{\mathrm{eff}}} = \frac{1}{m} \left(1 + \frac{c}{2} \ln \frac{2}{\left|1 - \frac{k}{k_F}\right|} \right) \tag{2.32}$$

Effective mass diverges logarithmically! $m_{\mathrm{eff}} \to 0$

- Okay to use Fock approximation away from Fermi surface
- Effective mass diverges logarithmically near the Fermi surface $\Rightarrow$ Failure of Fock approximation

Correlations Beyond Hartree-Fock

Density-Density Correlator (Correlation Function)

$$S_{\sigma,\sigma'}(\mathbf{r},\mathbf{r}') = \frac{V}{N_e}\langle \widehat{n}_\sigma(\mathbf{r})\widehat{n}_{\sigma'}(\mathbf{r}')\rangle \tag{2.33}$$

Reminder:

$$\widehat{n}_\sigma(\mathbf{r},t) = \widehat{\psi}^\dagger_\sigma(\mathbf{r},t)\widehat{\psi}_\sigma(\mathbf{r},t) \tag{2.34}$$

$$\widehat{n}_\sigma(\mathbf{q}) = \sum_{\mathbf{k}} \widehat{c}^\dagger_{\mathbf{k},\sigma}\widehat{c}_{\mathbf{k}+\mathbf{q},\sigma} \tag{2.35}$$

We wish to work in Fourier space.

$$S_\sigma(\mathbf{q}) = \frac{1}{N_e}\langle \widehat{n}_\sigma(\mathbf{q})\widehat{n}_\sigma(-\mathbf{q})\rangle \tag{2.36}$$

$$= \frac{1}{N_e}\sum_{\mathbf{k},\mathbf{k}'}\left\langle \widehat{c}^\dagger_{\mathbf{k}',\sigma'}\widehat{c}_{\mathbf{k}'+\mathbf{q},\sigma'}\widehat{c}^\dagger_{\mathbf{k},\sigma}\widehat{c}_{\mathbf{k}-\mathbf{q},\sigma}\right\rangle \tag{2.37}$$

$$= \frac{1}{N_e}\sum_{\mathbf{k},\mathbf{k}'}\left\langle \widehat{c}^\dagger_{\mathbf{k}',\sigma'}\widehat{c}_{\mathbf{k}'+\mathbf{q},\sigma'}\widehat{c}^\dagger_{\mathbf{k}+\mathbf{q},\sigma}\widehat{c}_{\mathbf{k},\sigma}\right\rangle \tag{2.38}$$

Consider case when $\mathbf{q} \neq 0$. Only non-vanishing contribution comes from when $\mathbf{k} = \mathbf{k}'$.

$$S(\mathbf{q}) = (-1)^2\left\langle c_{\mathbf{k}+\mathbf{q},\sigma}c^\dagger_{\mathbf{k}+\mathbf{q},\sigma}\right\rangle\left\langle c^\dagger_{\mathbf{k},\sigma}c_{\mathbf{k},\sigma}\right\rangle \tag{2.39}$$

$$\left\langle \widehat{c}^\dagger_{\mathbf{k}}\widehat{c}_{\mathbf{k}}\right\rangle = f(\varepsilon_{\mathbf{k}}) \tag{2.40}$$

$$\left\langle \widehat{c}_{\mathbf{k}+\mathbf{q}}\widehat{c}^\dagger_{\mathbf{k}+\mathbf{q}}\right\rangle = 1 - f(\varepsilon_{\mathbf{k}+\mathbf{q}}) \tag{2.41}$$

$$S(\mathbf{q}) = \frac{2}{N_e}\sum_{\mathbf{k}} f(\varepsilon_{\mathbf{k}})\cdot[1 - f(\varepsilon_{\mathbf{k}+\mathbf{q}})] \tag{2.42}$$

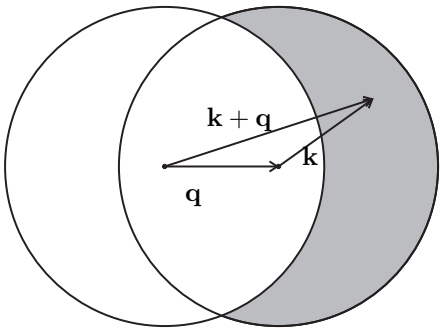


Figure 3: Non-zero contribution is denoted by the shaded area

$\mathbf{k}+\mathbf{q}$ must be outside the FS and $\mathbf{k}$ must be inside the FS.

- $q \to 0$: $S(\mathbf{q}) \to 0$.
- $q > 2k_F$: No more overlap, so we have $S(\mathbf{q}) = 1$
- $0q < 2k_F$: $S(\mathbf{q}) = \frac{3}{5}\frac{|\mathbf{q}|}{k_F} - \frac{1}{16}\left(\frac{|\mathbf{q}|}{k_F}\right)^2$

$$S(\mathbf{r}) = g(\mathbf{r}) = \begin{cases} g^{\mathrm{HF}}_{\uparrow\downarrow}(\mathbf{r}) = 1 \\ g^{\mathrm{HF}}_{\uparrow\uparrow}(\mathbf{r}) = 1 - 9\left[\dfrac{\sin k_F\, r - k_F\, r \cos k_F\, r}{(k_F\, r)^3}\right]^2 \end{cases} \tag{2.43}$$

Within H-F(Hartree-Fock) approximation, the plane wave basis remains appropriate. Only the parameters ($\varepsilon^{\mathrm{F}}_{\mathbf{k}}$, m_{eff}) change. (For the H-F approximation within the Jellium model, the radius of the Fermi sphere remains constant due to Luttinger Theorem.)

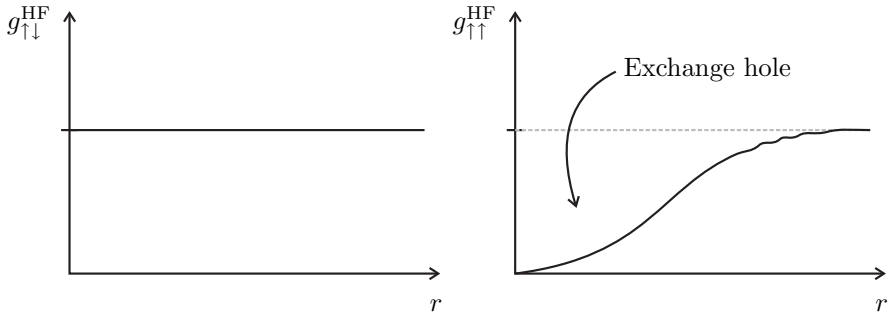


Figure 4: Correlation function in the Hartree-Fock approximation

From the above, we see that correlations for unlike electrons are ignored in the HF approximation (i.e. there no energy cost to put two electrons on the same site). Also, the correlations for like electrons show that two electrons of the same spin cannot be near each other (Pauli). The oscillations in $g^{\mathrm{HF}}_{\uparrow\uparrow}$ were noticed by Friedel. (RKKY)

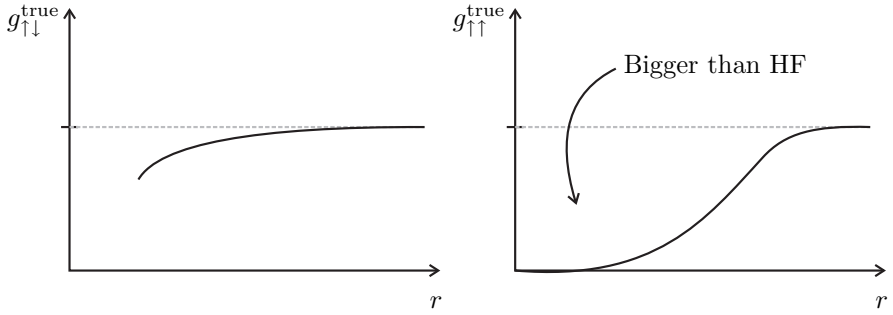


Figure 5: "True" Correlation function

For $g^{\mathrm{true}}_{\uparrow\downarrow}$, the results for small r are not agreed upon. With regard to $g^{\mathrm{true}}_{\uparrow\uparrow}$, the size of the exchange hole is due to two things:

- Pauli principle
- Coulomb repulsion

Spin glasses are due to the fact that the interactions between spins are long range (greater than exponential).

2.7 Dynamical Correlations

$$S(\mathbf{q}, t) = \frac{1}{N_e} \sum_{\mathbf{k}\mathbf{k}'\sigma\sigma'} \left\langle \widehat{c}^{\dagger}_{\mathbf{k}',\sigma'}(t)\widehat{c}_{\mathbf{k}'+\mathbf{q},\sigma'}(t)\widehat{c}^{\dagger}_{\mathbf{k}+\mathbf{q},\sigma}(0)\widehat{c}_{\mathbf{k},\sigma}(0) \right\rangle \tag{2.44}$$

$$\widehat{c}^{\dagger}_{\mathbf{k}}(t) = \widehat{c}^{\dagger}_{\mathbf{k}} \mathrm{e}^{\mathrm{i}\varepsilon_{\mathbf{k}} t/\hbar} \tag{2.45}$$

Last Time

- Finished discussion of effects of Fock term
- Discussed effects of correlations
- Described density-density correlation function (static).
  - Hartree-Fock: opposite spin electrons do not see each other
  - HF: like-spins cannot be close to each other (Pauli exclusion principle)

Dynamical Correlations Cont.

$$\hat{c}^\dagger_{\mathbf{k}}(t) = \hat{c}^\dagger_{\mathbf{k}} e^{i\varepsilon_{\mathbf{k}} t/\hbar} \tag{2.46}$$

$$S(\mathbf{q}, t) = \frac{1}{N_e} \sum_{\mathbf{k}} f(\varepsilon_{\mathbf{k}})[1 - f(\varepsilon_{\mathbf{k}-\mathbf{q}})] e^{i(\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}+\mathbf{q}})t/\hbar} \tag{2.47}$$

Only difference between static and dynamical correlations is a complex phase factor. Taking the Fourier transform yields

$$\int_{-\infty}^{\infty} e^{i\omega t} = 2\pi\delta(\omega) \tag{2.48}$$

$$S(\mathbf{q}, \omega) = \frac{2\pi\hbar}{N_e} \sum_{\mathbf{k}} f(\varepsilon_{\mathbf{k}})[1 - f(\varepsilon_{\mathbf{k}+\mathbf{q}})] \cdot \delta\left(\hbar\omega - (\varepsilon_{\mathbf{k}+\mathbf{q}} - \varepsilon_{\mathbf{k}})\right) \tag{2.49}$$

$S \neq 0$ only if $\omega = \varepsilon_{\mathbf{k}+\mathbf{q}} - \varepsilon_{\mathbf{k}}$, "Fermi's Golden Rule".

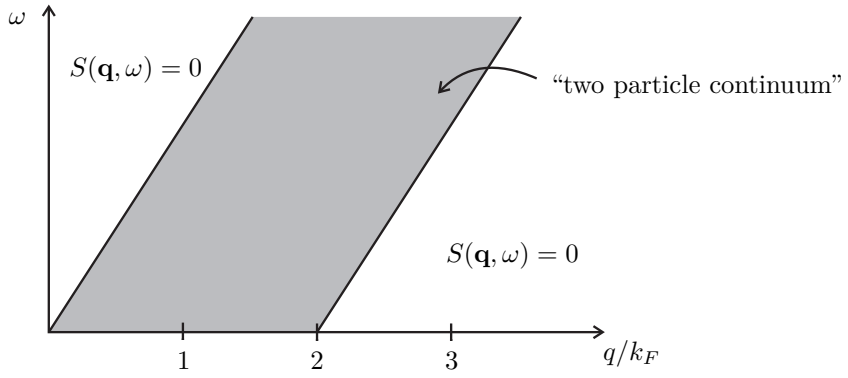


Figure 6: In the shaded region, $S(\mathbf{q}, \omega) \neq 0$.

2.8 Response of Electrons to External Perturbation

Insert extra charges into your system, i.e. place $\rho_{\text{ext}}(\mathbf{r}, t)$, and calculate response.

$$\rho(\mathbf{r}, t) = \rho_{\text{ext}}(\mathbf{r}, t) + \rho_{\text{ind}}(\mathbf{r}, t) \tag{2.50}$$

$$\varphi(\mathbf{r}, t) = \frac{1}{\epsilon_r} \varphi_{\text{ext}}(\mathbf{r}, t) \tag{2.51}$$

$$\nabla^2\varphi = -4\pi\rho \qquad q^2\varphi(q) = 4\pi\rho(q) \tag{2.52}$$

$$\nabla^2\varphi_{\text{ext}} = -4\pi\rho_{\text{ext}} \qquad q^2\varphi_{\text{ext}}(q) = 4\pi\rho_{\text{ext}}(q) \tag{2.53}$$

$$\tag{2.54}$$

$$\rho(\mathbf{q}) = \frac{1}{\epsilon_r}\rho_{\text{ext}}(\mathbf{q}) \tag{2.55}$$

$$\frac{1}{\epsilon_r} = \frac{\rho_{\text{ext}} + \rho_{\text{ind}}}{\rho_{\text{ext}}} = 1 + \frac{\rho_{\text{ind}}}{\rho_{\text{ext}}} \tag{2.56}$$

$$= 1 + \frac{4\pi}{q^2}\frac{\rho_{\text{ind}}}{\varphi_{\text{ext}}} \tag{2.57}$$

$$\rho_{\text{ind}} = -en_{\text{ind}} \tag{2.58}$$

$$U = -e\varphi \tag{2.59}$$

$$\frac{\rho_{\text{ind}}}{\varphi_{\text{ext}}} = e^2\frac{n_{\text{ind}}}{U} \tag{2.60}$$

$$\frac{1}{\epsilon_r} = 1 + \frac{4\pi e^2}{q^2}\frac{n_{\text{ind}}}{U} \tag{2.61}$$

$\frac{4\pi e^2}{q^2}$ is the Fourier transform of the Coulomb interaction.

$$n(\mathbf{r},t) = \left\langle \psi \middle| \mathrm{e}^{\mathrm{i}(\widehat{H}+\widehat{H}_{\text{ext}})t}\widehat{n}(\mathbf{r})\mathrm{e}^{-\mathrm{i}(\widehat{H}+\widehat{H}_{\text{ext}})t} \middle| \psi \right\rangle \tag{2.62}$$

If $\widehat{H}_{\text{ext}} = \widehat{H}_{\text{ext}}(t)$, then

$$n(\mathbf{r},t) = \left\langle \psi \middle| \exp\left[\mathrm{i}\int_{-\infty}^{t} \widehat{H}_{\text{ext}}(t')\,\mathrm{d}t'\right] \mathrm{e}^{\mathrm{i}\widehat{H}t}\widehat{n}(\mathbf{r})\mathrm{e}^{-\mathrm{i}\widehat{H}t} \exp\left[-\mathrm{i}\int_{-\infty}^{t} \widehat{H}_{\text{ext}}(t')\,\mathrm{d}t'\right] \middle| \psi \right\rangle \tag{2.63}$$

The above formula is the "interaction representation".

2.8.1 Linear Response

Expand the exponential to first order

$$\widehat{n}(\mathbf{r},t) = \mathrm{e}^{\mathrm{i}\widehat{H}t}\widehat{n}(\mathbf{r})\mathrm{e}^{-\mathrm{i}\widehat{H}t} \tag{2.64}$$

$$n(\mathbf{r},t) = \left\langle \psi \middle| \left[1 + \mathrm{i}\int_{-\infty}^{t} \widehat{H}_{\text{ext}}(t')\,\mathrm{d}t'\right] \widehat{n}(\mathbf{r},t) \left[1 - \mathrm{i}\int_{-\infty}^{t} \widehat{H}_{\text{ext}}(t')\,\mathrm{d}t'\right] \middle| \psi \right\rangle \tag{2.65}$$

$$= n_0 + n_{\text{ind}} \tag{2.66}$$

$$n_{\text{ind}}(\mathbf{r},t) = \mathrm{i}\int_{-\infty}^{t} \mathrm{d}t' \ \left\langle \psi \middle| \left[\widehat{H}_{\text{ext}}(t'), \widehat{n}(\mathbf{r},t)\right] \middle| \psi \right\rangle \tag{2.67}$$

$$\widehat{H}_{\text{ext}}(t') = \int \mathrm{d}\mathbf{r}'\ U_{\text{ext}}(\mathbf{r}',t')\widehat{n}(\mathbf{r}',t') \tag{2.68}$$

$$n_{\text{ind}}(\mathbf{r},t) = \mathrm{i}\int_{-\infty}^{t} \mathrm{d}t' \int \mathrm{d}\mathbf{r}\ \langle\psi|\left[\widehat{n}(\mathbf{r}',t'), \widehat{n}(\mathbf{r},t)\right]|\psi\rangle\, U(\mathbf{r}',t') \tag{2.69}$$

$$\Pi(\mathbf{r}-\mathbf{r}', t-t') = \langle\psi|\left[\widehat{n}(\mathbf{r}',t'), \widehat{n}(\mathbf{r},t)\right]|\psi\rangle \tag{2.70}$$

Next, since we note that we have a convolution, we immediately go to Fourier space since the convolution is a product.

$$n_{\text{ind}}(\mathbf{q},\omega) = \Pi(\mathbf{q},\omega)\cdot U_{\text{ext}}(\mathbf{q},\omega) \tag{2.71}$$

$$\frac{n_{\text{ind}}}{U} = \Pi(\mathbf{q},\omega) \tag{2.72}$$

$$\frac{1}{\epsilon_r} = 1 + \frac{4\pi e^2}{q^2}\cdot\Pi(\mathbf{q},\omega) \tag{2.73}$$

Kubo-Greenwood discovered that the commutator-type correlation function gives the linear response to external perturbations.

Π is a retarded correlator. There are no restrictions in space, but $t' < t$ in time. Let us consider the Fourier Transform.

$$\Pi(\mathbf{q},\omega) = \mathrm{i}\int_{-\infty}^{t} \langle\psi\big|[\widehat{n}(\mathbf{q},t'),\widehat{n}(-\mathbf{q},t)]\big|\psi\rangle\,\mathrm{d}t' \tag{2.74}$$

$$= \mathrm{i}\int_{-\infty}^{0} \mathrm{d}t\ \mathrm{e}^{\mathrm{i}\omega t}\,\langle\psi\big|[\widehat{n}(\mathbf{q},t'),\widehat{n}(-\mathbf{q},0)]\big|\psi\rangle\,\mathrm{d}t' \tag{2.75}$$

"$-\infty$": Adiabatic switching.

$$\lim_{\delta\to 0} U_{\mathrm{ext}}\mathrm{e}^{\delta t}\Big|_{t\in[-\infty,0]} \tag{2.76}$$

$$\mathrm{Re}\int \mathrm{e}^{\mathrm{i}(\omega-\Delta\varepsilon)t}U(t) \to \frac{1}{\omega-\Delta\varepsilon+\mathrm{i}\delta} \tag{2.77}$$

Turning on the interaction slowly pushes the pole off the real axis.

Last Time

- Studying collective behavior of interaction electrons
- Determined generic formula of the linear response of the system.
- Correlation functions of the system will capture the response of the system more appropriately.
- Commutator correlation function
- Derived for specific case but is generally true.

2.9 Models of Dielectric Functions

2.9.1 Thomas-Fermi Approximation

$$\nabla^2 U(\mathbf{r}) = 4\pi e\left[\rho_{\text{ext}}(\mathbf{r}) + \rho_{\text{scr}}(\mathbf{r})\right] = 4\pi e\rho(\mathbf{r}) \tag{2.78}$$

$$\rho(\mathbf{r}) = -en(\mathbf{r}) \qquad n(\mathbf{r}) \equiv \text{Number density} \tag{2.79}$$

(Note: U is potential energy.) Assume that locally the system is a free electron system.

$$n = \frac{k_F^3(\mathbf{r})}{3\pi^2} \qquad \left[2 \cdot \frac{4}{3}\left(\frac{k_F}{2\pi}\right)^3 \pi = n_0\right] \tag{2.80}$$

Introduce a space-dependent Fermi momentum as a result of the test charge. Since the test charge is a spatially varying quantity, it is reasonable that its effect on the Fermi momentum is also spatially variable.

$$E_F = \frac{k_F^2(\mathbf{r})}{2m} + U(\mathbf{r}) \tag{2.81}$$

$$k_F^3(\mathbf{r}) = [2m(E_F - U(\mathbf{R}))]^{3/2} \tag{2.82}$$

$$n(\mathbf{r}) = n_0 \cdot \left(1 - \frac{U(\mathbf{r})}{E_F}\right)^{3/2} \tag{2.83}$$

$$n_0 = \frac{k_{F,0}^3}{3\pi^2} \tag{2.84}$$

$$\nabla^2 U(\mathbf{r} = 4\pi e\left[\rho_{\text{ext}} + en_0 - en_0\left(1 - \frac{U(\mathbf{r})}{E_F}\right)^{3/2}\right] \tag{2.85}$$

$$\rho_{\text{scr}}(\mathbf{r}) = en_0 - en_0\left(1 - \frac{U(\mathbf{r})}{E_F}\right)^{3/2} \tag{2.86}$$

When $U = 0$, we have $\rho_{\text{scr}} = 0$. When $U \neq 0$, we have a non-trivial screening charge. Since we are performing a small perturbation, we can expand the term containing $U(\mathbf{r})$ in the parentheses, yielding

$$\nabla^2 U(\mathbf{r}) = 4\pi e\rho_{\text{ext}} + \frac{6\pi n_0 e^2}{E_F} U(\mathbf{r}) \tag{2.87}$$

Transforming to Fourier space yields

$$-q^2 U(\mathbf{q}) = 4\pi e[\rho_{\text{ext}}(\mathbf{q}) + \rho_{\text{scr}}(\mathbf{q})] \tag{2.88}$$

$$\left(-q^2 - q_{\text{TF}}^2\right) U(\mathbf{q}) = 4\pi e\rho_{\text{ext}}(\mathbf{q}) \qquad q_{\text{TF}}^2 = \frac{6\pi n_0 e^2}{E_F} \tag{2.89}$$

$$U(\mathbf{q}) = -\frac{4\pi e\rho_{\text{ext}}(\mathbf{q})}{q^2 + q_{\text{TF}}^2} \tag{2.90}$$

$$\epsilon_r(\mathbf{q}) = \frac{\rho_{\text{ext}}}{\rho_{\text{ext}} + \rho_{\text{scr}}} = \frac{(q^2 + q_{\text{TF}}^2)U(\mathbf{q})/(-4\pi e)}{q^2 U(\mathbf{q})/(-4\pi e)} = \frac{q^2 + q_{\text{TF}}^2}{q^2} \tag{2.91}$$

Note: Kondo problem is that of magnetic impurities.

2.9.2 Special Case: Point Charge

$$\rho_{\text{ext}}(\mathbf{r}) \equiv Q \cdot \delta(\mathbf{r}) \tag{2.92}$$

$$\rho_{\text{ext}}(\mathbf{q}) = Q \cdot \text{const} \tag{2.93}$$

$$U(\mathbf{r}) = \int \frac{\mathrm{d}^d q}{(2\pi)^d} \mathrm{e}^{\mathrm{i}\mathbf{q}\cdot\mathbf{r}} \frac{-4\pi e \cdot Q}{q^2 + q_{\text{TF}}^2} \tag{2.94}$$

$$= -\frac{4\pi e Q}{(2\pi)^3} \cdot 2\pi \int_0^\infty \mathrm{d}q\, q^2 \int_{-1}^1 \mathrm{d}x \mathrm{e}^{\mathrm{i}qrx} \frac{1}{q^2 + q_{\text{TF}}^2} \tag{2.95}$$

$$= -\frac{eQ}{\pi} \int_0^\infty \mathrm{d}q\, \frac{q^2}{q^2 + q_{\text{TF}}^2} \frac{2\sin qr}{qr} \tag{2.96}$$

$$= -\frac{2eQ}{\pi} \frac{1}{r} \int_0^\infty \mathrm{d}q\, \frac{q}{q^2 + q_{\text{TF}}^2} \sin qr \tag{2.97}$$

$$= -\frac{eQ}{\pi} \frac{1}{r} \int_{-\infty}^\infty \mathrm{d}q\, \frac{q}{q^2 + q_{\text{TF}}^2} \sin qr \tag{2.98}$$

We wish to do a contour integral since we have poles at $\pm \mathrm{i} q_{\text{TF}}$.

$$U(\mathbf{r}) = -\frac{eQ}{r} \mathrm{e}^{-q_{\text{TF}} r} \qquad \frac{1}{q_{\text{TF}}} = \left(\frac{E_F}{6\pi e^2 n} \right)^{1/2} = r_{\text{TF}} \tag{2.99}$$

The motivated student will calculate the induced charge density and calculate the integral of the charge density and find that it equals

$$\text{Total screening charge} \equiv \int \mathrm{d}^d r\, \rho_{\text{scr}}(\mathbf{r}) = -Q \tag{2.100}$$

(Derivation assumed that our electrons were free fermions. Thus, our work is not valid for a dielectric or an insulator.) Next level: Fock approximation $\ln(k - k_F)$ in $\varepsilon(\mathbf{k})$. This non-analyticity DESTROYS exponential decay, gives rise to

$$U(\mathbf{r}) \sim \frac{\cos 2k_F r}{r^3} \qquad \text{Friedel Oscillations} \tag{2.101}$$

2.9.3 Self-Consistent Theory

$$\frac{1}{\epsilon_r} = 1 + \frac{4\pi e^2}{q^2} \frac{n_{\text{ind}}(\mathbf{q}, \omega)}{U_{\text{ext}}(\mathbf{q}, \omega)} \tag{2.102}$$

$$U(\mathbf{q}, \omega) = \frac{1}{\epsilon_r} U_{\text{ext}}(\mathbf{q}, \omega) \tag{2.103}$$

$$\frac{1}{\epsilon_r} = 1 + \frac{4\pi e^2}{q^2} \frac{n_{\text{ind}}(\mathbf{q}, \omega)}{U(\mathbf{q}, \omega)} \frac{1}{\epsilon_r} \tag{2.104}$$

$$\epsilon_r = 1 - \frac{4\pi e^2}{q^2} \frac{n_{\text{ind}}(\mathbf{q}, \omega)}{U(\mathbf{q}, \omega)} \tag{2.105}$$

Both ϵ_r and $1/\epsilon_r$ represent a response to the system. $1/\epsilon_r$ is the response to an external perturbation. ϵ_r is the response to any kind of potential.

Last Time

- System's response will be related to its correlation
- Referred to as retarded since they require times from negative infinity
- Thomas-Fermi approximation: Assume perturbation is not too strong. Can view the electron locally as being a Fermi system with the parameters (Fermi momentum) being spatially dependent. Fermi energy must remain constant since the system is in equilibrium.

$$E_F = \frac{k_F^2(\mathbf{r})}{2m} + U(\mathbf{r})$$

- For case of a single point charge: Get induced screening cloud with exponential decay.
- $1/\epsilon_r$ is the response to external perturbations.
- ϵ_r is the response to all of the perturbations.

Question

Why do we work in second quantization?
It is very natural to work in this formulation. Many of the physical processes result in changes in particle number (absorption of a photon by a solid). It is first quantized functions times bookkeeping. Will later learn that superconducting state will be very hard to write in first quantized form. It is very hard to mix wavefuctions that describe different particle numbers.

Self-Consistency Screening cont.

$$\frac{1}{\epsilon_r} = 1 + U_0 \frac{n_{\text{in}}}{U_{\text{ext}}} \qquad U_0 = \frac{4\pi e^2}{q^2} \tag{2.106}$$

U_0 is the bare Coulomb interaction.

$$\frac{1}{\epsilon_r} = 1 + U_0 \Pi(\mathbf{q}, \omega) \tag{2.107}$$

$$\epsilon_r = 1 - U_0 \frac{n_{\text{ind}}}{U} = 1 - U_0 \widetilde{\Pi}(\mathbf{q}, \omega) \tag{2.108}$$

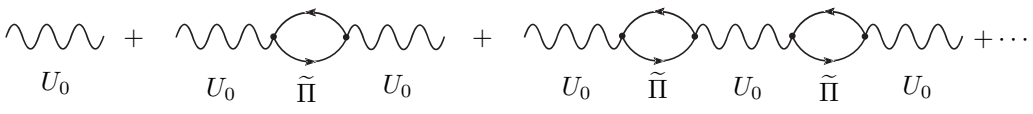
$$1 + U_0 \Pi = \frac{1}{1 - U_0 \widetilde{\Pi}} \tag{2.109}$$

$$\Pi = \frac{\widetilde{\Pi}}{1 - U_0 \widetilde{\Pi}} \tag{2.110}$$

$$\frac{1}{\epsilon_r} = 1 + U_0 \Pi = 1 + U_{\text{eff}} \widetilde{\Pi} \tag{2.111}$$

$$U_{\text{eff}} = \frac{U_0}{1 - U_0 \widetilde{\Pi}} = U_0 + U_0 \widetilde{\Pi} U_0 + \cdots \tag{2.112}$$

Looks like a geometric series. Indeed, one can visualize this as



Viewing as an effective interaction and viewing as an effective correlation are physically equivalent.

Effective Interaction as a geometric series:

- Originally called the Random Phase Approximation(RPA)
- David Bohm and David Pines
- First attempt to take a series and sum it up to infinite order in the interaction.
- Contains high order (∞) powers of U_0.
- Non-perturbative result.
- Need $U_0\widetilde{\Pi}$
- It is a subset. Need to convince audience that this is the most important subset of perturbative corrections. It is conceivable that another subset will be more important. For example, in superconductivity we have a solution which is similar to RPA but yields a different set of diagrams.

Now, let us find the correlation function $\widetilde{\Pi}$.

$$\widetilde{\Pi} = \mathrm{i}\int_{-\infty}^{0} \mathrm{d}t\ \mathrm{e}^{\mathrm{i}\omega t}\,\langle[\widehat{n}(\mathbf{q},t),\widehat{n}(-\mathbf{q},0)]\rangle \tag{2.113}$$

Assume free electron gas

$$\widetilde{\Pi} = \mathrm{i}\int_{-\infty}^{0} \mathrm{d}t\ \mathrm{e}^{\mathrm{i}\omega t}\frac{1}{V}\sum_{\mathbf{k},\sigma}\left\{f(\varepsilon_{\mathbf{k}})[1-f(\varepsilon_{\mathbf{k}+\mathbf{q}})]\mathrm{e}^{\mathrm{i}(\varepsilon_{\mathbf{k}}-\varepsilon_{\mathbf{k}+\mathbf{q}})t} - f(\varepsilon_{\mathbf{k}+\mathbf{q}})[1-f(\varepsilon_{\mathbf{k}})]\mathrm{e}^{\mathrm{i}(\varepsilon_{\mathbf{k}}-\varepsilon_{\mathbf{k}+\mathbf{q}})t}\right\} \tag{2.114}$$

$$= \mathrm{i}\int_{-\infty}^{0} \mathrm{d}t\frac{1}{V}\sum_{\mathbf{k},\sigma}\mathrm{e}^{\mathrm{i}(\omega-(\varepsilon_{\mathbf{k}+\mathbf{q}}-\varepsilon_{\mathbf{k}}))t}[f(\varepsilon_{\mathbf{k}})-f(\varepsilon_{\mathbf{k}+\mathbf{q}})] \tag{2.115}$$

$$= \frac{1}{V}\sum_{\mathbf{k},\sigma}\frac{f(\varepsilon_{\mathbf{k}})-f(\varepsilon_{\mathbf{k}+\mathbf{q}})}{\omega-(\varepsilon_{\mathbf{k}+\mathbf{q}}-\varepsilon_{\mathbf{k}})+\mathrm{i}\delta} \tag{2.116}$$

Plugging this back into our formula for the dielectric constant yields

$$\boxed{\epsilon_r^{\mathrm{RPA}}(\mathbf{q},\omega) = 1 - \frac{4\pi e^2}{q^2}\cdot\frac{2}{V}\sum_{\mathbf{k}}\frac{f(\varepsilon_{\mathbf{k}})-f(\varepsilon_{\mathbf{k}+\mathbf{q}})}{\omega-(\varepsilon_{\mathbf{k}+\mathbf{q}}-\varepsilon_{\mathbf{k}})+\mathrm{i}\delta}} \tag{2.117}$$

Memorize the above formula!

$$\epsilon_r = \epsilon_r' + \mathrm{i}\epsilon_r'' \tag{2.118}$$

$$\epsilon_r' = 1 - \frac{4\pi e^2}{q^2}\frac{2}{V}\mathcal{P}\sum_{\mathbf{k}}\frac{f(\varepsilon_{\mathbf{k}})-f(\varepsilon_{\mathbf{k}+\mathbf{q}})}{\omega-(\varepsilon_{\mathbf{k}+\mathbf{q}}-\varepsilon_{\mathbf{k}})+\mathrm{i}\delta} \tag{2.119}$$

$$\epsilon_r'' = \frac{4\pi^2 e^2}{q^2}\cdot\frac{2}{V}\sum_{\mathbf{k}}[f(\varepsilon_{\mathbf{k}})-f(\varepsilon_{\mathbf{k}+\mathbf{q}})]\delta(\omega-(\varepsilon_{\mathbf{k}+\mathbf{q}}-\varepsilon_{\mathbf{k}})) \tag{2.120}$$

Principle Part($\mathcal{P}$): (Look this up in Boas and Arfken to refresh)

$$f(x) = \frac{1}{x} = P(\tfrac{1}{x}) + \mathrm{i}\pi\delta(x) \tag{2.121}$$

$$\int_{-\infty}^{\infty}\mathrm{d}x\ \frac{1}{x}g(x) = \int_{-\infty}^{-\epsilon} + \int_{\epsilon}^{\infty}\mathrm{d}x\ \frac{1}{x}g(x) + \mathrm{i}\pi g(0) \tag{2.122}$$

Last Time

- Linear response
- Studying model dielectric functions
- Thomas-Fermi approach
- Difference between $1/\epsilon$ and ϵ. $1/\epsilon$ is response to external perturbation. ϵ is response to total potential.
- Determined ϵ for a point charge.

$$\epsilon_r' = 1 - \frac{4\pi e^2}{q^2}\frac{2}{V}\mathcal{P}\sum_{\mathbf{k}}\frac{f(\varepsilon_{\mathbf{k}}) - f(\varepsilon_{\mathbf{k+q}})}{\omega - (\varepsilon_{\mathbf{k+q}} - \varepsilon_{\mathbf{k}}) + \mathrm{i}\delta} \tag{2.123}$$

2.9.4 Limiting Cases

The order of the limits is important. Many of these response functions are not analytic, thus the order is important and physical circumstances can aid in determining the proper order. Example: a photon is wiggling electrons at very high frequency but low momentum. In contrast, the phonons are wiggling at low frequency but high momentum.

1. $\omega \to 0$, $\mathbf{q} \to 0$

   As $\mathbf{q} \to 0$, we Taylor expand $f(\varepsilon_{\mathbf{k}}) - f(\varepsilon_{\mathbf{k+q}})$

$$\epsilon_r' = 1 - \frac{4\pi e^2}{q^2}\frac{2}{V}\sum_{\mathbf{k}}\frac{-\frac{\partial f}{\partial \varepsilon}(\varepsilon_{\mathbf{k+q}} - \varepsilon_{\mathbf{k}})}{-(\varepsilon_{\mathbf{k+q}} - \varepsilon_{\mathbf{k}})} \tag{2.124}$$

$$= 1 - \frac{8\pi e^2}{q^2}\int \frac{\mathrm{d}^3k}{(2\pi)^3}\frac{\partial f}{\partial \varepsilon} \tag{2.125}$$

   Convert to energy integral.

$$\varepsilon = \frac{k^2}{2m} \to k = \sqrt{2m\varepsilon} \tag{2.126}$$

$$\mathrm{d}k = \sqrt{2m}\,\frac{1}{2\sqrt{\varepsilon}}\,\mathrm{d}\varepsilon \tag{2.127}$$

$$\frac{\partial f}{\partial \varepsilon} = -\delta(\varepsilon - \varepsilon_F) \tag{2.128}$$

$$\epsilon_r' = 1 + \frac{8\pi e^2}{q^2}\frac{4\pi}{8\pi^3}\int_0^\infty \mathrm{d}\varepsilon\,\sqrt{2m}\,\frac{1}{2}\,\frac{1}{\sqrt{\varepsilon}}\,2m\varepsilon\cdot\delta(\varepsilon - \varepsilon_F) \tag{2.129}$$

$$= 1 + \frac{e^2}{q^2}\cdot\frac{4}{\pi}\cdot\sqrt{2}\cdot m^{3/2}\int_0^\infty \mathrm{d}\varepsilon\,\sqrt{\varepsilon}\cdot\delta(\varepsilon - \varepsilon_F) \tag{2.130}$$

$$= 1 + \frac{e^2}{q^2}\cdot\frac{4\sqrt{2}}{\pi}m^{3/2}\cdot\sqrt{\varepsilon_F} = 1 + \frac{4me^2k_F}{\pi q^2} \tag{2.131}$$

$$\epsilon^{\mathrm{TF}} = 1 + \frac{q_{\mathrm{TF}}^2}{q^2} \qquad q_{\mathrm{TF}}^2 = \frac{6\pi e^2 n_0}{\varepsilon_F} = \frac{6\pi e^2\frac{k_F^3}{3\pi^2}}{\frac{k_F^2}{2m}} = \frac{4me^2k_F}{\pi} \tag{2.132}$$

2. $\mathbf{q} \to 0$, $\omega \to 0$

$$\epsilon_r' = 1 - \frac{4\pi e^2}{q^2}\cdot\frac{2}{V}\sum_{\mathbf{k}} f(\varepsilon_{\mathbf{k}})\cdot\left[\frac{1}{\omega - (\varepsilon_{\mathbf{k+q}} - \varepsilon_{\mathbf{k}})} - \frac{1}{\omega - (\varepsilon_{\mathbf{k+q}} + \varepsilon_{\mathbf{k}})}\right] \tag{2.133}$$

Shifted $\mathbf{k} \to \mathbf{k} - \mathbf{q}$ in second term.

$$\epsilon_r' = 1 - \frac{4\pi e^2}{q^2} \cdot \frac{2}{V} \sum_{\mathbf{k}} f(\varepsilon_{\mathbf{k}}) \cdot \frac{2(\varepsilon_{\mathbf{k}+\mathbf{q}} - \varepsilon_{\mathbf{k}})}{\omega^2 - (\varepsilon_{\mathbf{k}+\mathbf{q}} - \varepsilon_{\mathbf{k}})^2} \tag{2.134}$$

$$= 1 - \frac{4\pi e^2}{q^2} \cdot \frac{2}{V} \sum_{\mathbf{k}} f(\varepsilon_{\mathbf{k}}) \cdot \frac{2\left[2\frac{\mathbf{k}\cdot\mathbf{q}}{2m} + \frac{q^2}{2m}\right]}{\omega^2} \tag{2.135}$$

In the denominator, we let $q \to 0$, resulting in no k or q dependence. Next, in the numerator $\mathbf{k}\cdot\mathbf{q} = kq\cos\theta$ and $\int \mathrm{d}\mathbf{k}\, \mathbf{k}\cdot\mathbf{q} = 0$.

$$\epsilon_r' = 1 - \frac{4\pi e^2}{q^2} \cdot \frac{q^2}{m\omega^2} \cdot \frac{2}{V} \sum_{\mathbf{k}} f(\varepsilon_{\mathbf{k}}) \tag{2.136}$$

Thus, we have

$$\boxed{\epsilon_r' = 1 - \frac{\omega_{\mathrm{pl}}^2}{\omega^2}} \qquad \omega_{\mathrm{pl}}^2 = \frac{4\pi e^2 n}{m} \tag{2.137}$$

where ω_{pl} is the plasma frequency! Next, recall

$$\frac{1}{\epsilon_r} = 1 + \frac{4\pi e^2}{q^2} \frac{n_{\mathrm{ind}}}{U_{\mathrm{ext}}} \tag{2.138}$$

If ω of U_{ext} is ω_{pl}, the system will produce a huge response (plasma oscillations). This is a homogeneous excitation with the overall center of charge for the positive charges and negative charges oscillate out of phase.

3. $\omega \to 0$, q finite

$$\epsilon_r' = 1 + \frac{q_{\mathrm{TF}}^2}{q^2}\left[\frac{1}{2} + \frac{1}{4x}(1-x^2)\ln\frac{|x+1|}{|x-1|}\right] \qquad x \equiv \frac{q}{2k_F} \tag{2.139}$$

As $q \to 0$ ($x \to 0$) the above reduces to Thomas-Fermi results. First calculated by Lindhard. Note: Non-analytic at $x \sim 1$. If we FT back to real space, we find the screening cloud n_{ind} to be

$$n_{\mathrm{ind}}(\mathbf{r}) = Q \cdot \frac{\cos 2k_F r}{r^3} \tag{2.140}$$

This differs from Thomas-Fermi as the screening cloud oscillates in density. Because of the non-analyticity, the large q behavior influences the large r behavior. A consequence of the Fermi surface is that response functions are oscillatory with a power law envelope. Decays exponentially?

4. Low dimensions

$$\epsilon_r(\omega = 0, \mathbf{q}) = 1 + \frac{q_{\mathrm{TF}}^2}{q^2} F\left(\frac{q}{2k_F}\right) \tag{2.141}$$

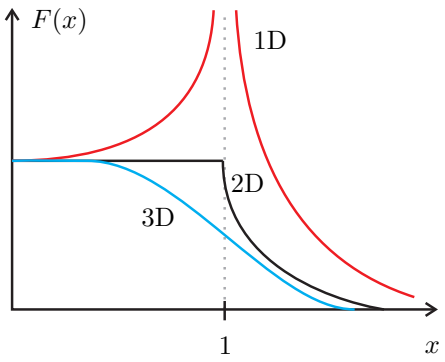


Figure 7: Fermi function in 1(red), 2(black) and 3(blue) dimensions

$1/\epsilon$ diverging is a good way of capturing excitations of the system. ϵ diverging is a good way of finding instabilities of the system. The natural excitations of the system will be bosons (electron-hole pairs). The instability manifests itself by the nature of the excitations from electronic to bosonic. Example: Superconductivity.

5. "Nesting" Everything we have done previously assumed that the Fermi surface is spherical, i.e. that everything is isotropic or that there is no dependence on the angle. What happens if the Fermi surface is anisotropic?

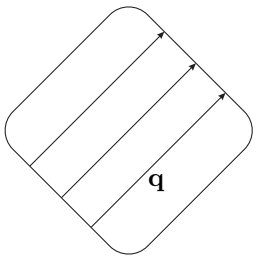


Figure 8: Example of nesting for a rectangular Fermi surface

The phase space for a given q where the energy difference is small (~ 0) is much larger when we move away from a spherical Fermi surface.

$$\epsilon_r \sim \sum \frac{1}{\varepsilon_{\mathbf{k}+\mathbf{q}} - \varepsilon_{\mathbf{k}}} \qquad \text{large} \tag{2.142}$$

ϵ_r can diverge.

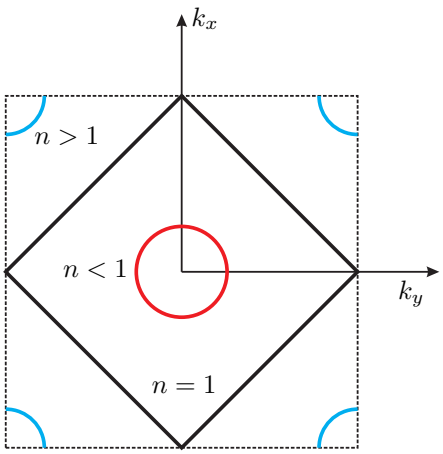


Figure 9: Fermi surface for the 2D Hubbard model at less than (red), equal to (black), and greater than (blue) half-filling

Nesting in 2D Hubbard model represents instability of anti-ferromagnetism. Reference for Nesting by Ruralds-Virosztek "Nested Fermi-Liquid Theory".

Last Time / Announcement

- No class next Tuesday. Replacement class 5/16 from 12:30-2:00pm.
- Looked at general formula given by RPA theory.
- Studied small q behavior and found Thomas-Fermi result
- Studied small ω behavior and recovered behavior of plasmas.

2.9.5 Effect of finite relaxation time

Previously assumed in RPA that wave functions were plane waves. What happens if there is disorder? The plane waves will cease to be eigenstates. Let us add an exponential decay to the plane waves.

$$\hat{c}^p_{\mathbf{k}}(t) = \hat{c}^p_{\mathbf{k}} \mathrm{e}^{-\mathrm{i}\varepsilon_{\mathbf{k}} t} \Rightarrow \hat{c}^p_{\mathbf{k}} \mathrm{e}^{-\mathrm{i}\varepsilon_{\mathbf{k}} t} \cdot \mathrm{e}^{-t/2\tau} = \hat{c}^p_{\mathbf{k}} \mathrm{e}^{-\mathrm{i}\left(\varepsilon_{\mathbf{k}} - \frac{\mathrm{i}}{2\tau}\right)t} \tag{2.143}$$

Shift frequency to complex plane. For holes, we find

$$\hat{c}^p_{\mathbf{k}}(t) = \cdots = \hat{c}^p_{\mathbf{k}} \mathrm{e}^{-\mathrm{i}\left(\varepsilon_{\mathbf{k}} + \frac{\mathrm{i}}{2\tau}\right)t} \tag{2.144}$$

Holes can be viewed as particles moving backwards in time. Applying to RPA formula

$$\epsilon_r = 1 - \frac{4\pi e^2}{q^2} \frac{2}{V} \sum_{\mathbf{k}} \frac{f(\varepsilon_{\mathbf{k}}) - f(\varepsilon_{\mathbf{k}+\mathbf{q}})}{\omega - (\varepsilon_{\mathbf{k}+\mathbf{q}} - \varepsilon_{\mathbf{k}}) + \frac{\mathrm{i}}{\tau}} \tag{2.145}$$

$\varepsilon_{\mathbf{k}+\mathbf{q}}$ is the energy of an electron, and $\varepsilon_{\mathbf{k}}$ is the energy of the corresponding hole. RPA is describing the creation of a particle-hole pair. i/τ is referred to as the "self-energy" Σ of the Green's function.

2.9.6 Connection in RPA

Maxwell's equation

$$\mathbf{E} = -\nabla\varphi \tag{2.146}$$
$$\mathbf{E} = -\mathrm{i}\mathbf{q}\varphi \tag{2.147}$$
$$e\mathbf{E} = \mathrm{i}\mathbf{q}(-e\varphi) = \mathrm{i}qU \tag{2.148}$$
$$-\mathrm{i}e\mathbf{q}\cdot\mathbf{E} = q^2 U \tag{2.149}$$

The dielectric constant becomes

$$\epsilon_r = 1 - \frac{4\pi e^2}{q^2}\frac{n_{\mathrm{ind}}}{U} = 1 + \mathrm{i}\frac{1}{\epsilon_0}\frac{\rho_{\mathrm{ind}}}{\mathbf{q}\cdot\mathbf{E}} \qquad (\rho = -en) \qquad \frac{1}{4\pi\epsilon_0} \text{ extra factor} \tag{2.150}$$

Conductivity is related to currents. Continuity equation relates density to current.

$$\nabla\cdot\mathbf{j}(\mathbf{r},t) + \frac{\partial\rho(\mathbf{r},t)}{\partial t} = 0 \tag{2.151}$$
$$\mathrm{i}\mathbf{q}\cdot\mathbf{j}(\mathbf{q},\omega) - \mathrm{i}\omega\rho(\mathbf{q},\omega) = 0 \tag{2.152}$$

Solving for the density

$$\rho = \frac{\mathbf{q}\cdot\mathbf{j}}{\omega} \tag{2.153}$$

Recall Ohm's Law

$$\mathbf{j}(\mathbf{q},\omega) = \sigma(\mathbf{q},\omega)\mathbf{E}(\mathbf{q},\omega) \tag{2.154}$$

Inserting into our equation for ϵ_r yields

$$\boxed{\epsilon_r(\mathbf{q},\omega) = 1 + \mathrm{i}\frac{1}{\epsilon_0}\frac{\sigma(\mathbf{q},\omega)}{\omega}} \qquad \epsilon(\mathbf{q},\omega) = \epsilon_0 + \mathrm{i}\frac{\sigma(\mathbf{q},\omega)}{\omega} \tag{2.155}$$

Now recall that

$$\epsilon_r(\mathbf{q},\omega) = 1 - \frac{4\pi e^2}{q^2}\widetilde{\Pi}(\mathbf{q},\omega) = 1 - \frac{1}{\epsilon_0}\frac{e^2}{q^2}\widetilde{\Pi}(\mathbf{q},\omega) \tag{2.156}$$

$$\sigma(\mathbf{q},\omega) = \frac{\mathrm{i}\omega e^2}{q^2}\widetilde{\Pi}(\mathbf{q},\omega) \tag{2.157}$$

In the finite ω, $\mathbf{q} \to 0$ limit we have calculated $\widetilde{\Pi}$ for the plasmons

$$\widetilde{\Pi}(\mathbf{q},\omega) = \frac{n_e q^2}{m\omega} \tag{2.158}$$

$$\sigma(\omega) = \lim_{\mathbf{q}\to 0}\sigma(\mathbf{q},\omega) = \frac{\mathrm{i}n_e e^2}{m\omega} \tag{2.159}$$

This is the conductivity for a free electron. If the electron lifetime is finite, then $\omega \to \omega + \frac{\mathrm{i}}{\tau}$

$$\sigma(\omega) = \frac{n_e e^2}{m}\frac{1}{\omega + \frac{\mathrm{i}}{\tau}} \tag{2.160}$$

In the limit where $\omega \to 0$, we find

$$\boxed{\sigma(\omega = 0) = \frac{n_e e^2 \tau}{m}} \qquad \text{Recovered Drüde form} \tag{2.161}$$

For general q, ω

$$\rho = \frac{1}{\omega}\mathbf{q}\cdot j \qquad\qquad n = \frac{1}{\omega}\mathbf{q}\cdot\mathbf{j}_n \tag{2.162}$$

The conductivity becomes

$$\sigma = \frac{\mathrm{i}\omega e^2}{q^2}\left(-\frac{\mathrm{i}}{V}\right)\int_0^\infty \mathrm{d}t\ \mathrm{e}^{\mathrm{i}\omega t}\left\langle[n(\mathbf{q},t), n(-\mathbf{q},0)]\right\rangle \tag{2.163}$$

$$= \frac{e^2}{\omega}\frac{1}{V}\int_0^\infty \mathrm{d}t\ \mathrm{e}^{\mathrm{i}\omega t}\left\langle[\mathbf{j}(\mathbf{q},t), \mathbf{j}(-\mathbf{q},0)]\right\rangle \qquad \text{Kubo-Greenwood} \tag{2.164}$$

Full formula is

$$\sigma = \frac{e^2}{\omega}\frac{1}{V}\int_0^\infty \mathrm{d}t; \mathrm{e}^{\mathrm{i}\omega t}\left\langle[\mathbf{j}(\mathbf{q},t), \mathbf{j}(-\mathbf{q},0)]\right\rangle + \frac{\mathrm{i}ne^2}{m\omega^2} \tag{2.165}$$

Where does the second term come from?

$$\widehat{H} = \frac{\widehat{p}^2}{2m} \to \frac{(\widehat{\mathbf{p}} - \frac{e}{c}\widehat{\mathbf{A}})^2}{2m} = \frac{\widehat{p}^2}{2m} + \frac{e}{2mc}\left[\widehat{\mathbf{p}}\cdot\widehat{\mathbf{A}} + \widehat{\mathbf{A}}\cdot\widehat{\mathbf{p}}\right] \tag{2.166}$$

$$\mathbf{v} = \mathrm{i}[\widehat{H}, \widehat{r}] = \frac{\widehat{\mathbf{p}}}{m} + \frac{e}{mc}\widehat{\mathbf{A}} \tag{2.167}$$

Last Time

- Studied effect of finite relaxation time
- Determined relationship between ϵ and σ in general.

$$\epsilon(\mathbf{q},\omega) = \epsilon_0 + \mathrm{i}\frac{\sigma(\mathbf{q},\omega)}{\omega}$$

- What happens when we add this effect to RPA.
- In the $\mathbf{q} \to 0$, $\omega \to 0$ limit, we get the Drüde form for the conductivity.
- Related conductivity to current-current correlation function (Kubo-Greenwood).

2.10 Response to Magnetic Perturbation

In a magnetic field

$$\varepsilon(H) = \varepsilon(H=0) - \frac{1}{2}g\mu_B\boldsymbol{\sigma}\cdot\mathbf{H} \tag{2.168}$$

$\boldsymbol{\sigma}$ is the spin of the electron. μ_B is the Bohr magneton. g is the gyro-magnetic ratio. Response of the system (susceptibility) is

$$\chi \equiv \frac{M}{H_{\text{ext}}} = \frac{\mathrm{i}}{\hbar}\mu_0\int_0^\infty \mathrm{d}t\ \mathrm{e}^{\mathrm{i}\omega t}\left\langle[m(\mathbf{q},t), m(-\mathbf{q},0)]\right\rangle \tag{2.169}$$

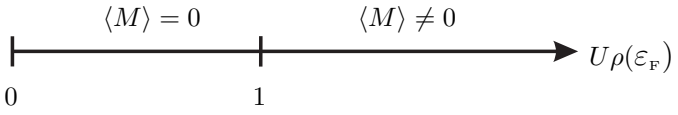
Correlation function of the quantity the external field couples to.

$$\chi(0,0) = \chi_0 = \frac{1}{2}g^2\mu_B^2\rho(\varepsilon_F) \qquad \text{Pauli magnetic susceptibility} \tag{2.170}$$

$\rho(\varepsilon_F)$ is the DOS at the Fermi Surface, $\dfrac{mk_F}{2\pi^2}$ (3D). The susceptibility in the RPA approximation is

$$\boxed{\chi^{\text{RPA}} = \frac{\chi_0}{1 - U\cdot\rho(\varepsilon_F)}} \tag{2.171}$$

A magnetic response is enhanced because of an electric interaction. Stoner instability is when $\chi \to \infty$ as U increases. Stoner criterion indicates the onset of a ferromagnetic instability. $\langle M\rangle \neq 0$



Hartree approximation: Allow different densities for up and down electrons.

$$\left\langle\psi_\uparrow^\dagger\psi_\uparrow\right\rangle \neq \left\langle\psi_\downarrow^\dagger\psi_\downarrow\right\rangle \tag{2.172}$$

Energies of up and down spin electrons will shift differently. Systems that want to be antiferromagnetic have the same Stoner relation but not at $\mathbf{q} = 0$, instead at $\mathbf{q} \neq 0$. $\chi(\mathbf{q}_{\text{AF}}) \to \infty$

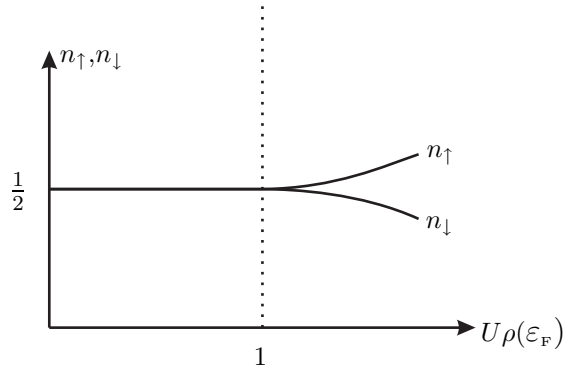


Figure 10: Electron density versus $U\rho(\varepsilon_F)$

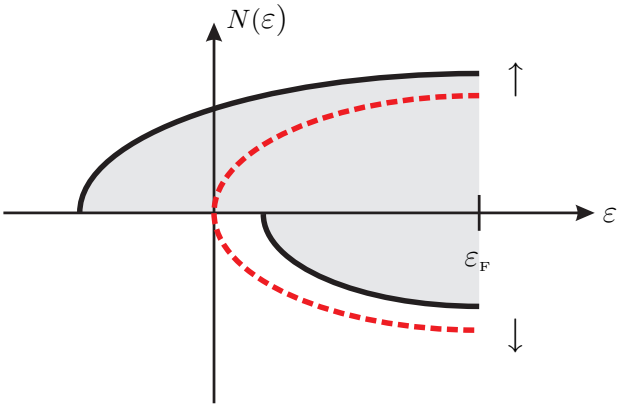


Figure 11: Density of States for up and down spin electrons with (solid black) and without (dashed red) applied magnetic field

3 Scattering Experiments

Previously looked at what happens when you expose a system to a large external perturbation.

3.1 Electron Scattering

Interaction: Coulomb

$$V = \sum_{\mathbf{R},\mathbf{r}^\alpha} e \cdot e^\alpha V(\mathbf{R} - \mathbf{r}^\alpha) = e \int \mathrm{d}^d r \; V(\mathbf{R} - \mathbf{r}) \rho(\mathbf{r}) \tag{3.1}$$

Fermi's Golden Rule

$$P_{\mathrm{i}\to\mathrm{f}} = \frac{2\pi}{\hbar} |V_{\mathrm{f\,i}}|^2 \delta(E_f - E_i - \hbar\omega) \tag{3.2}$$

$$\langle t_f e_f | V | t_i e_i \rangle = V_{\mathrm{f\,i}} \tag{3.3}$$

1. electron matrix element

$$\langle k_F | V(\mathbf{R} - \mathbf{r}) | k_i \rangle = V(\mathbf{k}) \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{r}} \qquad \mathbf{k} = \mathbf{k}_f - \mathbf{k}_i \tag{3.4}$$

2. target/ion matrix element

$$V_{\mathrm{f\,i}} = eV(\mathbf{k}) \int \mathrm{d}^d r \; \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{r}} \langle i | \widehat{\rho}(\mathbf{r}) | f \rangle \tag{3.5}$$

Insert $\mathrm{e}^{\mathrm{i}\widehat{H}t}\mathrm{e}^{-\mathrm{i}\widehat{H}t}$ before and after the density operator, yielding

$$\langle i\,|\,\rho(\mathbf{r})\,|\,f\rangle\cdot\delta(E_f-E_i-\hbar\omega)=\int_{-\infty}^{\infty}\mathrm{d}t\;\mathrm{e}^{\mathrm{i}\omega t}\,\langle i\,|\,\rho(\mathbf{r},t)\,|\,f\rangle \tag{3.6}$$

$$P_{i\to f}=\frac{e^2|V(\mathbf{k})|^2}{\hbar^2}\int\mathrm{d}^dr\int\mathrm{d}^dr'\int_{-\infty}^{\infty}\mathrm{d}t\;\mathrm{e}^{\mathrm{i}\omega t}\mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')}\cdot\langle i\,|\,\rho(\mathbf{r},t)\,|\,f\rangle\,\langle f\,|\,\rho(\mathbf{r},0)\,|\,i\rangle \tag{3.7}$$

Summing over all final states yields

$$\boxed{P^{\mathrm{total}}=\frac{e^2|V(\mathbf{k})|^2}{\hbar^2}\int\mathrm{d}^dr\int\mathrm{d}^dr'\int\mathrm{d}t\;\mathrm{e}^{\mathrm{i}\omega t}\mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')}\cdot\langle i\,|\,\rho(\mathbf{r},t)\rho(\mathbf{r},0)\,|\,i\rangle} \tag{3.8}$$

Response to scattering experiments is similar to linear response. We always measure correlation functions.

Last Time

- Considered response to a magnetic perturbation.

$$\chi^{\mathrm{RPA}} = \frac{\chi_0}{1 - U \cdot \rho(\varepsilon_F)} \tag{3.9}$$

- Started discussing scattering experiments
- Calculated the total probability of going from the initial state to the final state. Learned it was related to a correlation function.
- Correlation function is not retarded and does not have a commutator.
- Fluctuation Dissipation Theorem (FDT): There is a numerical factor $\coth k_B T/\hbar\omega$ relating the retarded commutator correlation function with the simple correlation function.
- If you will study disordered systems (glasses), there is a violation of the Fluctuation Dissipation Theorem.

Electron Scattering Cont.

What you measure is not the transition probability but the scattering cross-section σ.

$$\text{incoming flux} \cdot \mathrm{d}\sigma = \sum_f P_{i\to f} \tag{3.10}$$

$$\text{incoming flux} = \frac{\hbar k_i}{m} \tag{3.11}$$

Final state phase space
$$\frac{1}{(2\pi)^3}\,\mathrm{d}^d k_f = \frac{1}{(2\pi)^3} k_f^2\,\mathrm{d}k_f\,\mathrm{d}\Omega_f = \frac{1}{(2\pi)^3}\frac{m_e}{\hbar^2} k_f\,\mathrm{d}\varepsilon_f\,\mathrm{d}\Omega_f \tag{3.12}$$

$$\frac{\mathrm{d}^2\sigma}{\mathrm{d}\varepsilon_f\,\mathrm{d}\Omega_f} = \frac{k_f}{k_i}\frac{m_e^2}{(2\pi)^3}\frac{e^2}{\hbar^5 k^4} S_{\rho\rho}(\mathbf{k},\omega) \qquad \text{Differential cross section} \tag{3.13}$$

Differential cross section is a geometric factor times the density-density correlation function.

$$S_{\rho\rho}(\mathbf{k},\omega) = \int \mathrm{d}t\,\mathrm{d}t'\,\mathrm{d}r\,\mathrm{d}r'\,\mathrm{e}^{\mathrm{i}\omega(t-t')-\mathrm{i}\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')}\,\langle\rho(\mathbf{r},t)\rho(\mathbf{r}',t')\rangle \tag{3.14}$$

3.2 Neutron Scattering

If you bombard a charged particle with an electron, it will interact strongly with the particle. The electron will not penetrate deep into the sample and are better suited for surface probes. Neutrons do not interact strongly with the particle and will probe deeply into the sample.

3.2.1 Interaction with the nuclei via short range forces

$$V = \sum_\alpha V(\mathbf{R} - \mathbf{r}^\alpha) = a\int \mathrm{d}^d r\;\delta(\mathbf{R}-\mathbf{r})n(\mathbf{r}) \tag{3.15}$$

The δ function describes a contact interaction. $n(r)$ is the density of nucleons.

$$\frac{\mathrm{d}^2\sigma}{\mathrm{d}\varepsilon_f\,\mathrm{d}\Omega_f} = \frac{k_f}{k_i}\frac{m_n^2}{(2\pi)^3}\frac{a^2}{\hbar^5} S_{nn}(\mathbf{k},\omega) \tag{3.16}$$

$e/k^2 \to a$, the scattering length and $\rho(\mathbf{r},t) \to n(\mathbf{r},t)$. The first term in $S_{nn}(\mathbf{k},\omega)$: the Bragg peaks at $\omega = 0$, i.e. elastic scattering.

3.2.2 Interaction with the nucleon spin

The neutron spin interacts with the nucleon spin via a dipole interaction.

$$V = 2\mu \sum_{\alpha} S_i(\mathbf{R}) V_{ij}(\mathbf{R}-\mathbf{r}) M_\gamma(\mathbf{r}) \tag{3.17}$$

$$V_{ij}(\mathbf{r}) = -\frac{1}{4\pi}\nabla_i \nabla_j \frac{1}{r} \to \hat{\mathbf{k}}_i \cdot \hat{\mathbf{k}}_j \tag{3.18}$$

$$\frac{\mathrm{d}^2\sigma}{\mathrm{d}\varepsilon_f \, \mathrm{d}\Omega_f} = \frac{k_f}{k_i} \frac{(\mu_n m_n)^2}{(2\pi)^3 \hbar^5} \hat{\mathbf{k}}_i \cdot \hat{\mathbf{k}}_j S_{M_i M_j}(\mathbf{k}, \omega) \tag{3.19}$$

i and j denote the polarization directions.

3.3 Light Scattering

$$\frac{\mathrm{d}^2\sigma}{\mathrm{d}\varepsilon_f \, \mathrm{d}\Omega_f} = \frac{1}{4} \frac{\sqrt{\epsilon}}{(2\pi)^3} \left(\frac{\omega_f}{c}\right)^4 S_{\epsilon\epsilon}(\mathbf{k}, \omega) \tag{3.20}$$

$S_{\epsilon\epsilon}$ is the correlation function of the fluctuations of the dielectric constant. In an isotropic liquid, $S_{\epsilon\epsilon} \sim S_{nn}$. In a liquid crystal, $S_{\epsilon\epsilon}$ consists of many contributions.

3.4 Magnetic Scattering of Neutrons

1. No thermal motion $T = 0$

$$S(\mathbf{k}, \omega) = A \int_{-\infty}^{\infty} \mathrm{d}t \, \mathrm{e}^{\mathrm{i}\omega t} \sum_{\mathbf{R}, \mathbf{R}'} \left\langle \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{R}(0)} \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{R}'(t)} \right\rangle = \delta(\omega) \sum_{\mathbf{G}} \delta(\mathbf{k} - \mathbf{G}) \tag{3.21}$$

   If your system is at $T = 0$, then when neutrons are scattered their energy and momentum will be conserved up to a reciprocal lattice vector. We will have peaks in the directions of the reciprocal lattice vectors. (NOTE: Fermi's Golden rule only applies when the interaction strength is small. If the interaction is strong, then we can have multiple scattering events.)

2. With thermal motion $T \neq 0$. The ions are moving at finite temperatures. $\mathbf{R}(t) = \mathbf{R}_i + \mathbf{u}_i(t)$. The $\mathbf{u}_i(t)$ form phonons, characterizing ionic displacements from equilibrium position.

$$S(\mathbf{k}, t) = \sum_{\mathbf{R}, \mathbf{R}'} \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot(\mathbf{R}-\mathbf{R}')} \left\langle \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{u}(\mathbf{R},0)} \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{u}(\mathbf{R},t)} \right\rangle \tag{3.22}$$

   Theorem:

$$\left\langle \mathrm{e}^{-\mathrm{i}\widehat{A}} \mathrm{e}^{\mathrm{i}\widehat{B}} \right\rangle = \mathrm{e}^{-\frac{1}{2}\left(\langle(\widehat{A}-\widehat{B})^2\rangle - [\widehat{A},\widehat{B}]\right)} \tag{3.23}$$

   This is true only in systems where the expectation value is taken for Hamiltonians which are quadratic in $\widehat{A}$ and $\widehat{B}$ and if $\left[\widehat{A}, \left[\widehat{A}, \widehat{B}\right]\right]$. If and only if these two criteria are satisfied, then the above relation is true. Both criteria are satisfied for phonons.

$$\mathbf{u}(\mathbf{R}, t) = \sum_{\mathbf{q}} \frac{1}{\sqrt{2NM\omega_{\mathbf{q}}}} \left(a_{\mathbf{q}} \mathrm{e}^{\mathrm{i}(\mathbf{q}\cdot\mathbf{R} - \omega_{\mathbf{q}} t)} + a_{\mathbf{q}}^\dagger \mathrm{e}^{-\mathrm{i}(\mathbf{q}\cdot\mathbf{R} - \omega_{\mathbf{q}} t)} \right) \tag{3.24}$$

   We have to produce:

$$\mathbf{u}(\mathbf{R}, t) - \mathbf{u}(\mathbf{R}, 0) = \sum_{\mathbf{q}} \frac{1}{\sqrt{2NM\omega_{\mathbf{q}}}} \left[\widehat{a}_{\mathbf{q}} \left(\mathrm{e}^{\mathrm{i}(\mathbf{q}\cdot\mathbf{R}' - \omega_{\mathbf{q}} t)} - \mathrm{e}^{\mathrm{i}\mathbf{q}\cdot\mathbf{R}} \right) + \widehat{a}_{\mathbf{q}}^\dagger \left(\mathrm{e}^{\mathrm{i}(\mathbf{q}\cdot\mathbf{R} - \omega_{\mathbf{q}} t)} - \mathrm{e}^{-\mathrm{i}\mathbf{q}\cdot\mathbf{R}'} \right) \right] \tag{3.25}$$

$$[\mathbf{u}(\mathbf{R}, t) - \mathbf{u}(\mathbf{R}, 0)]^2 = \frac{1}{2NM} \sum_{\mathbf{q}} \frac{1}{\omega_{\mathbf{q}}} (2 - 2\cos\theta_{\mathbf{R}\mathbf{R}'}) (\widehat{a}_{\mathbf{q}}^\dagger \widehat{a}_{\mathbf{q}} + \widehat{a}_{\mathbf{q}} \widehat{a}_{\mathbf{q}}^\dagger) + \text{non-diag.} \tag{3.26}$$

$$\theta_{\mathbf{R}\mathbf{R}'} = \omega_{\mathbf{q}} t + \mathbf{q} \cdot (\mathbf{R} - \mathbf{R}') \tag{3.27}$$

Can ignore non-diagonal terms since we are taking an expectation value and

$$\widehat{H} = \sum_{\mathbf{q}} \omega_{\mathbf{q}} \widehat{a}^{\dagger}_{\mathbf{q}} \widehat{a}_{\mathbf{q}} \tag{3.28}$$

Thus, the expectation value of all non-diagonal terms is zero.

$$[\widehat{\mathbf{u}}(\mathbf{R}', t), \widehat{\mathbf{u}}(\mathbf{R}, 0)] = \frac{1}{2NM} \sum_{\mathbf{q}} \frac{1}{\omega_{\mathbf{q}}} \left\{ [\widehat{a}_{\mathbf{q}}, \widehat{a}^{\dagger}_{\mathbf{q}}] \mathrm{e}^{\mathrm{i}\theta_{\mathbf{R}\mathbf{R}'}} + \mathrm{h.c.} \right\} = \frac{2\mathrm{i}}{2NM} \sum_{\mathbf{q}} \frac{1}{\omega_{\mathbf{q}}} \sin\theta_{\mathbf{R}\mathbf{R}'} \tag{3.29}$$

Total exponent:

$$= \frac{k^2}{2NM} \sum_{\mathbf{q}} \frac{1}{\omega_{\mathbf{q}}} \left\{ (2\langle n_{\mathbf{q}} \rangle + 1)(1 - \cos\theta_{\mathbf{R}\mathbf{R}'}) - \mathrm{i}\sin\theta_{\mathbf{R}\mathbf{R}'} \right\} \tag{3.30}$$

The $\theta_{\mathbf{R}\mathbf{R}'}$ terms depend on time. We will expand the time dependent piece from the exponential. We will keep the 1 in the exponential and expand the cos and sin.

$$\begin{aligned} S(\mathbf{k}, t) = \sum_{\mathbf{R}\mathbf{R}'} \Bigg\{ & \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot(\mathbf{R}-\mathbf{R}')} + \frac{k^2}{2NM} \sum_{\mathbf{q}} \frac{1}{\omega_{\mathbf{q}}} \Big[\langle n_{\mathbf{q}} + 1 \rangle \, \mathrm{e}^{\mathrm{i}\omega_{\mathbf{q}} t} \mathrm{e}^{\mathrm{i}(\mathbf{q}-\mathbf{k})\cdot(\mathbf{R}-\mathbf{R}')} \\ & + \langle n_{\mathbf{q}} \rangle \, \mathrm{e}^{-\mathrm{i}\omega_{\mathbf{q}} t} \mathrm{e}^{-\mathrm{i}(\mathbf{q}+\mathbf{k})\cdot(\mathbf{R}-\mathbf{R}')} \Big] \Bigg\} \mathrm{e}^{-2W} \end{aligned} \tag{3.31}$$

where

$$\mathrm{e}^{-2W} = \exp\left\{ -\frac{k^2}{2NM} \sum_{\mathbf{q}} \frac{1}{\omega_{\mathbf{q}}} (2\langle n_{\mathbf{q}} \rangle + 1) \right\} \tag{3.32}$$

The Fourier Transform of the density autocorrelator factor is called the structure factor and it is given by

$$\begin{aligned} S(\mathbf{k}, \omega) = \mathrm{e}^{-2W} \Bigg\{ & \delta(\omega) \sum_{\mathbf{G}} \delta(\mathbf{k} - \mathbf{G}) \\ & + \frac{k^2}{2NM} \left[\sum_{\mathbf{q}} \frac{1}{\omega_{\mathbf{q}}} \delta(\omega - \omega_{\mathbf{q}}) \sum_{\mathbf{G}} \delta(\mathbf{k} - \mathbf{q} - \mathbf{G}) \langle n_{\mathbf{q}} + 1 \rangle \right. \\ & \left. + \frac{1}{\omega_{\mathbf{q}}} \delta(\omega + \omega_{\mathbf{q}}) \sum_{\mathbf{G}} \delta(\mathbf{k} + \mathbf{q} - \mathbf{G}) \langle n_{\mathbf{q}} \rangle \right] \Bigg\} + \text{two phonon processes} \end{aligned} \tag{3.33}$$

The first term yields Bragg peaks. The second term describes one phonon emission and absorption. e^{-2W} is the Debye-Waller factor. The zero-point fluctuations scatter the neutrons. The sum is logarithmically divergent in 2D. This suppresses the scattering correlation function to zero. Mermin-Wagner Theorem: In $d = 2$ the zero point fluctuations destroy the correlation function $S(\mathbf{k})$. NO LATTICE in $d = 2$. There are no elastic lattices in two dimensions.

Question

What happens if the magnetic susceptibility from the Stoner criterion becomes negative? We can only believe the Stoner criterion up to divergence. The system becomes unstable and develops a finite magnetization.

3.5 Neutron Scattering Experiment

Spallation Neutron Sources produce neutrons without radiation.

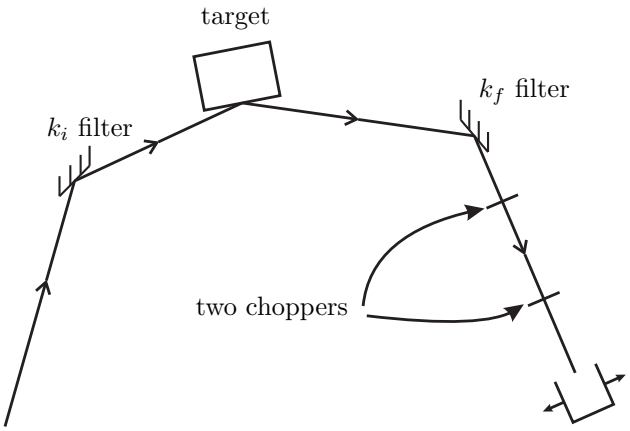
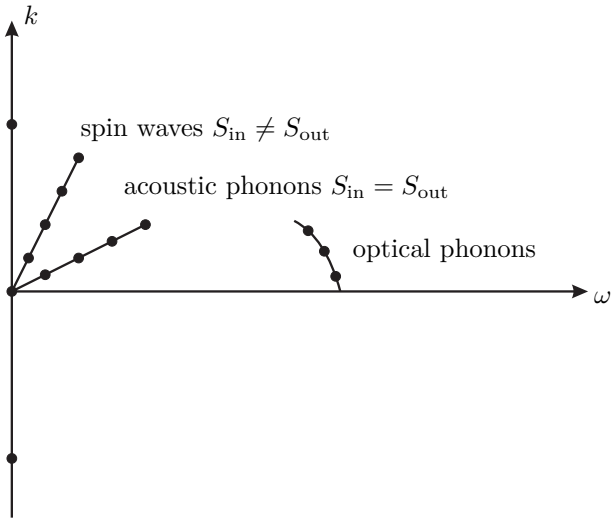


Figure 12: Schematic of a neutron scattering experiment where the energy is measured via the "time of flight" technique.

Scan for ω, $k(\equiv k_{\text{out}} - k_{\text{in}})$.



4 Total Energy of the Electron Gas

$$E = \langle \widehat{H} \rangle \tag{4.1}$$

Natural length scales:

$$r_s = \frac{\bar{r}_s}{a_0} \qquad a_0 = \frac{\hbar^2}{me^2} \qquad \frac{4}{3}\pi \bar{r}_s^3 = \frac{V}{N} \tag{4.2}$$

a_0 is the radius of s orbit in Hydrogen. $\bar{r}_s$ is the space per electron. When r_s is large, the system is dilute. When r_s is small, the system is dense. When r_s is large, the dominant contribution to come from the potential/interaction term. When r_s is small, the dominant term is from the kinetic term.

1. If there is no interaction, we have

$$E_{\text{kin}} = \sum_{\mathbf{k}} \frac{k^2}{2m} = 2\frac{V}{(2\pi)^3}\int \mathrm{d}^3k \frac{k^2}{2m} = \frac{V}{\pi^2}\frac{\hbar^2}{2m}\frac{k_F^5}{5} = N\frac{3}{5}\varepsilon_F \tag{4.3}$$

2. Hartree: cancels the electron-ion interaction

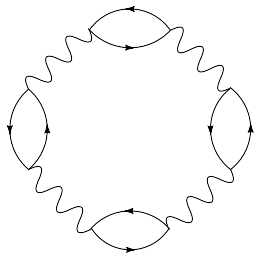
$$E_H = \frac{2.21}{r_s^2}\text{Ry} \tag{4.4}$$

3. Fock:

$$\varepsilon_{\mathbf{k}} \to \varepsilon_{\mathbf{k}} - \sum_{\mathbf{q}} U(\mathbf{q})\varepsilon_{\mathbf{k}-\mathbf{q}} \tag{4.5}$$

$$E_{HF} = \frac{2.21}{r_s^2} - \frac{0.91}{r_s} \tag{4.6}$$

4. RPA approximation singles out diagrams which form rings



   (a) Dense case, r_s small

$$E = \frac{2.21}{r_s^2} - \frac{0.91}{r_s} - 0.096 + 0.62\ln r_s + \mathcal{O}(r_s) \tag{4.7}$$

$$= \frac{2.21}{r_s^2}\left[1 + a_1 r_s + a_2 r_s^2 + a_3 r_s^2 \ln r_s \cdots\right] \tag{4.8}$$

   This is a power series in positive powers of r_s and is expected to be valid for small r_s

   (b) Dilute case, r_s large
   Start with interaction (put $\hbar = 0$). To optimize the repulsive energy, electrons will form a lattice. (Wigner crystal (WX))

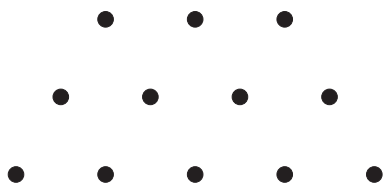


Figure 13: Optimal Wigner crystal, a triangular lattice.

$$E^{\text{WX}} = c\sum_{ij}\frac{1}{|\mathbf{r}_{ij}|} = -\frac{1.8}{r_s}\text{Ry} \tag{4.9}$$

$$\Rightarrow E^{\text{WX}} = -\frac{1.8}{r_s} + \frac{3.0}{r_s^{3/2}} = -\frac{1.8}{r_s}\left[1 + a_1 r^{-1/2} + a_2 r_s^{-1} + \cdots\right] \tag{4.10}$$

Expansion in negative increasing powers of r_s.
There is a phase transition when moving from small r_s to large r_s. The Wigner crystal is an insulator.

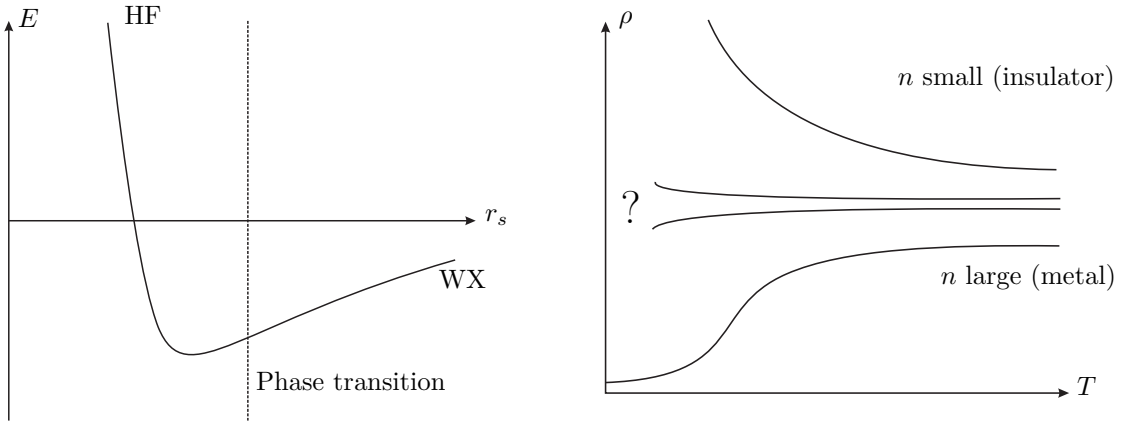


Figure 14: Left: Energy versus r_s. Right: Resistivity versus temperature.

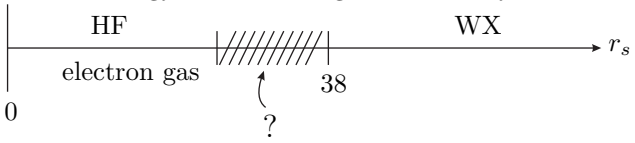


Figure 15: Phase diagram in 2D. Possibilities for the unknown phase in the middle include stripes or electronic microemulsions

Last Time

- Neutrons pick up the structure of the system and phonon peaks as well.
- Neutrons have a weight comparable to the ions. Electrons are so much lighter that you cannot simultaneously satisfy momentum and energy conservation with phonons.
- Acoustic phonons have no gap.
- Phonons in metals also have acoustic behavior.
- Energy of electron gas in small and high density limit.

5 Fermi Liquid Theory

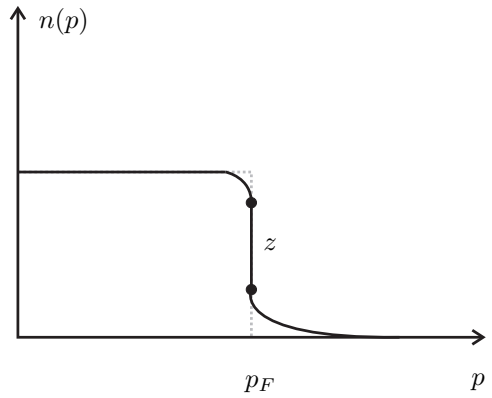
- Developed by Landau in the early forties.
- Started out as a phenomenology but became very powerful.
- Pursuit of a new type of small parameter in the problem of strong interactions.

Basic question: Why can the dense, strongly interacting fermion gas (like the electrons in metals) be described as more or less the free electrons only with changed mass, etc. ?
Phenomonology: We accept this fact as a basis.

1. The states are still characterized by a momentum quantum number $\mathbf{p}$.
2. The interaction only changes parameters: $m \to m^*$.

$$\varepsilon = \frac{p^2}{2m^*} \tag{5.1}$$

3. $n(\mathbf{p})$ still has a jump at the Fermi surface $\varepsilon = \varepsilon_F$.



   where z is the "pole strength of the Green's function." Also, the Fermi volume remains unchanged (Luttinger Theorem).

4. 1-4 define the Landau quasi-particles. The effect of strong interaction is captured through the parameters m^* and z. The remaining interaction is weak.
5. Lifetime of the quasi-particles is long.

$$\frac{1}{\tau(\varepsilon)} \sim \varepsilon^2 \qquad (\varepsilon = E - E_F) \tag{5.2}$$

6.

$$F = E - \mu N = F_0 + \sum_{\mathbf{p}} (\varepsilon_p - \mu)\delta n_{\mathbf{p}} + \frac{1}{2V}\sum_{\mathbf{p}\mathbf{p}'} f_{\mathbf{p}\sigma,\mathbf{p}'\sigma'}\delta n_{\mathbf{p}\sigma}\delta n_{\mathbf{p}'\sigma'} + \mathcal{O}((\delta n)^3) \tag{5.3}$$

F_0 results when the interaction is zero. $\delta n_{\mathbf{p}}$ is the small fluctuation or variations in occupation number of the quasi-particle caused by the interactions. The interaction is weak because the δn's are hypothesized to be small.

Parametrization:

1.

$$f_{\mathbf{p}\sigma,\mathbf{p}'\sigma'} = \delta_{\sigma\sigma'} f^s_{\mathbf{p}\mathbf{p}} + \boldsymbol{\sigma}_{\sigma\sigma''}\cdot\boldsymbol{\sigma}_{\sigma''\sigma'} f^a_{\mathbf{p}\mathbf{p}'} \tag{5.4}$$

s stands for symmetric. a stands for anti-symmetric.

- No spin-orbit interaction, would be relevant for heavy elements.
- No crystalline anisotropies

2. All $\mathbf{p}$, $\mathbf{p}'$ have a magnitude $\approx p_F$.

$$f^{s,a}_{\mathbf{p}\mathbf{p}'} = \frac{1}{N(0)}\sum_{\ell=0}^{\infty} F^{s,a}_{\ell} P_\ell(\cos\theta) \tag{5.5}$$

$$N(0) = \rho(\varepsilon_F) = \frac{m^* p_F}{\pi^2\hbar^3} \qquad \text{(3D)} \tag{5.6}$$

We want to calculate the particle current in two ways. Equating them will give a constraint on the F's. Continuity equation:

$$\frac{\mathrm{d}}{\mathrm{d}t} n_p = \frac{\partial n_p(\mathbf{r},t)}{\partial t} + \nabla_r n_p\cdot\dot{r} + \nabla_p n_p \dot{p} = 0 \qquad \dot{r} = v_p = \nabla_p \varepsilon_p \qquad \dot{p} = -\nabla_r \varepsilon_p \tag{5.7}$$

Last Time

- Knowing that the interactions between electrons are strong, we capture these strong interactions by forming quasi-particles (characterized by m^* and z).
- The quasi-particles interact weakly.

Fermi Liquid Theory Cont.

Recall

$$\frac{\mathrm{d}n_p}{\mathrm{d}t} = \frac{\partial n_p}{\partial t} + \nabla_r n_p \cdot \dot{\mathbf{r}} + \nabla_p n_p \cdot \dot{\mathbf{p}} = 0 \qquad \dot{\mathbf{r}} = \nabla_p \varepsilon_p \qquad \dot{\mathbf{p}} = -\nabla_r \varepsilon_p$$

Also

$$n_{\mathbf{p}}(\mathbf{r},t) = n^0_{\mathbf{p}} + \delta n_{\mathbf{p}}(\mathbf{r},t) \tag{5.8}$$

$$\partial_t \delta n_{\mathbf{p}}(\mathbf{r},t) + \mathbf{v}_{\mathbf{p}} \cdot \nabla_r \delta n_{\mathbf{p}}(\mathbf{r},t) - \nabla_{\mathbf{p}} n^0_{\mathbf{p}} \cdot \sum_{\mathbf{p}'} f_{\mathbf{p}\mathbf{p}'} \nabla_r \delta n_{\mathbf{p}'}(\mathbf{r},t) = 0 \tag{5.9}$$

Recall $\nabla n_{\mathbf{p}} = -\mathbf{v}_{\mathbf{p}} \frac{\partial n^0}{\partial \varepsilon}$. Thus, the last two terms can be written

$$\nabla_r \cdot \left\{ \mathbf{v}_{\mathbf{p}} \left(\delta n_{\mathbf{p}} - \sum_{\mathbf{p}'} f_{\mathbf{p}\mathbf{p}'} \frac{\partial n_0}{\partial \varepsilon_{\mathbf{p}}} \delta n_{\mathbf{p}'} \right) \right\} \tag{5.10}$$

The terms in the braces must be the current $\mathbf{j}_p$ since by the continuity equation $\partial_t \delta n_p + \nabla_r \cdot \mathbf{j} = 0$

$$\mathbf{J} = \sum_{\mathbf{p}} \tilde{\mathbf{j}}_{\mathbf{p}} = \sum_{\mathbf{p}} \delta n_{\mathbf{p}} \mathbf{v}_{\mathbf{p}} - \sum_{\mathbf{p}\mathbf{p}'} \mathbf{v}_{\mathbf{p}} f_{\mathbf{p}\mathbf{p}'} \frac{\partial n^0}{\partial \varepsilon_{\mathbf{p}}} \delta n_{\mathbf{p}'} \tag{5.11}$$

$$= \sum_{\mathbf{p}} \delta n_p \mathbf{v}_p - \sum_{\mathbf{p}\mathbf{p}'} \mathbf{v}_{p'} f_{pp'} \frac{\partial n^0}{\partial \varepsilon_{p'}} \delta n_p \tag{5.12}$$

$$= \sum_{\mathbf{p}} \delta n_{\mathbf{p}} \left(\mathbf{v}_p - \sum_{\mathbf{p}'} f_{pp'} \frac{\partial n^0}{\partial \varepsilon_{p'}} \mathbf{v}_{p'} \right) = \sum_{\mathbf{p}} \delta n_{\mathbf{p}} \mathbf{j}_{\mathbf{p}} \tag{5.13}$$

- Eqn. (5.10): $\delta n_{\mathbf{p}}$ induces other fluctuations with amplitude $\delta n_{\mathbf{p}'}$.
- Eqn. (5.13) $\mathbf{v}_{\mathbf{p}}$ current experiences/induces other current $\mathbf{v}_{\mathbf{p}'}$. The second term in (5.13) is called drag current or back flow.

5.1 Transport in Fermi Liquid

Insert an extra electron into the Fermi Liquid with momentum $\mathbf{p}$. We calculate the total current in two different ways.

1. If effects of the crystal are disregarded (i.e. the system is Galilean invariant), then

$$\mathbf{J} = \frac{\mathbf{p}}{m} \tag{5.14}$$

2. $\mathbf{J}$ after a while will be given by our $\mathbf{j}_{\mathbf{p}}$

$$\mathbf{J} = \frac{\mathbf{p}}{m} = \frac{\mathbf{p}}{m^*} - \sum_{\mathbf{p}'} f_{\mathbf{p}\mathbf{p}'} \frac{\partial n^0}{\partial \varepsilon_{\mathbf{p}'}} \frac{\mathbf{p}'}{m^*} \tag{5.15}$$

$$= \frac{\mathbf{p}}{m^*} + \frac{\mathbf{p}}{m^*} \sum_{\mathbf{p}'} f_{\mathbf{p}\mathbf{p}'} z \cdot \delta(\varepsilon_{\mathbf{p}} - \mu) \cos\vartheta \tag{5.16}$$

ϑ is the angle between $\mathbf{p}$ and $\mathbf{p}'$

$$\frac{\mathbf{p}}{m} = \frac{\mathbf{p}}{m^*}\left(1 - \int \mathrm{d}\Omega \cos\vartheta \sum_\ell F_\ell^s P_\ell(\cos\vartheta)\right) \qquad F = zN(0)f \tag{5.17}$$

$$= \frac{\mathbf{p}}{m^*}\left(1 + \frac{1}{3}F_1^s\right) \tag{5.18}$$

The $\delta(\varepsilon_{\mathbf{p}'} - \mu)$ forces the sum over $\mathbf{p}'$ to be an angular integral over the Fermi Surface. Thus, the effective mass ratio is

$$\boxed{\frac{m^*}{m} = 1 + \frac{1}{3}F_1^s} \tag{5.19}$$

Thus, a measurement of m^*/m gives F_1^s. This is a non-perturbative results. $F_\ell^{s,a}$ can be > 1, as long as the system is a Fermi-liquid. Formula will be true until we hit a phase transition!

- Because of the interactions, the effective mass of the particles increases.

$$\frac{m^*}{m} = 1 + \frac{1}{3}F_1^s$$

- If the interaction is completely isotropic, $m^* = m$ ($F_1^s = 0$).
- In terms of momentum exchange, the Coulomb interaction is anisotropic.
- Effective mass can decrease (superconductivity)

Other similar calculations yield

$$\text{Compressibility} \qquad ? = \frac{1 + F_0^s}{1 + \frac{1}{3}F_1^s} \tag{5.20}$$

$$\text{Normal sound velocity} \qquad \left(\frac{c}{c_0}\right)^2 = \frac{1 + F_0^s}{1 + \frac{1}{3}F_1^s} \tag{5.21}$$

We have two equations and two unknowns (F_0^s and F_1^s). We have no predictive power yet. Landau predicted zero sound, which is related to F_0^s. Landau theory now has predictive power and is falsifiable.
Let us go back to the continuity equation (summing over all $\mathbf{p}$).

$$\frac{\partial \delta n}{\partial t} + \nabla_r \left\{ \sum_{\mathbf{p}} \mathbf{v}_{\mathbf{p}} \left(\delta n_{\mathbf{p}} - \frac{\partial n^0}{\partial \varepsilon_{\mathbf{p}}} \sum_{\mathbf{p}'} f_{\mathbf{p}\mathbf{p}'} \delta n_{\mathbf{p}'} \right) \right\} = 0 \tag{5.22}$$

In Fourier space

$$\delta n_{\mathbf{p}}(\mathbf{r}, t) = \delta n_{\mathbf{p}} \mathrm{e}^{\mathrm{i}(\mathbf{k}\cdot\mathbf{r} - \omega t)} \tag{5.23}$$

$$(\mathbf{v}\cdot\mathbf{k} - \omega)\delta n_{\mathbf{p}} - \mathbf{v}\cdot\mathbf{k}\frac{\partial n^0}{\partial \varepsilon_{\mathbf{p}}} \sum_{\mathbf{p}'} f_{\mathbf{p}\mathbf{p}'} \delta n_{\mathbf{p}'} = 0 \tag{5.24}$$

Recall $\dfrac{\partial n^0}{\partial \varepsilon_{\mathbf{p}}} = -z\delta(\varepsilon_{\mathbf{p}} - \mu)$. Let us consider the case when

$$\delta n_{\mathbf{p}} = -\delta(\varepsilon_{\mathbf{p}} - \mu)\nu(\vartheta, \varphi) \tag{5.25}$$

ϑ and φ describe the angle between $\mathbf{p}$ and $\mathbf{k}$. It follows that

$$(\mathbf{v}\cdot\mathbf{k} - \omega)\nu + \mathbf{v}\cdot\mathbf{k} \int \mathrm{d}\Omega \sum_{\ell} F_\ell^s(\vartheta')\nu(\vartheta') = 0 \tag{5.26}$$

The normal sound of the system is a density fluctuation.

$$\tilde{u} = \frac{\omega}{|\mathbf{k}|} \qquad \text{velocity of non-isotropic sound} \tag{5.27}$$

$|\mathbf{v}| = v_F$ is the Fermi velocity.

$$s = \frac{\tilde{u}}{v_F} \tag{5.28}$$

Let us rewrite our previous result in terms of s.

$$(s - \cos\vartheta)\nu(\vartheta) = \cos\vartheta \int \mathrm{d}\Omega \sum_{\ell} F_\ell^s(\vartheta')\nu(\vartheta') \tag{5.29}$$

$$v(\vartheta) \propto \frac{\cos\vartheta}{s - \cos\vartheta} \tag{5.30}$$

Question: Can s be chosen such that the LHS = RHS? We assume that only F_0^s is large, which yields

$$\frac{s}{2}\ln\frac{s+1}{s-1} - 1 = \frac{1}{F_0^s} \tag{5.31}$$

In ^{3}He this anisotropic sound "zero sound" was indeed observed. Normal sound $v_{\text{n.s.}} = \frac{1}{\sqrt{3}}v_F$. The experimental confirmation is that people in fermionic systems observed sound velocities that were profoundly different from the expected and Landau's prediction was the only "game in town" to account for the change in normal sound.

5.2 Spin-Dependent Case

$$\frac{\chi}{\chi_0} = \frac{1+\frac{1}{3}F_1^s}{1+F_0^a} \tag{5.32}$$

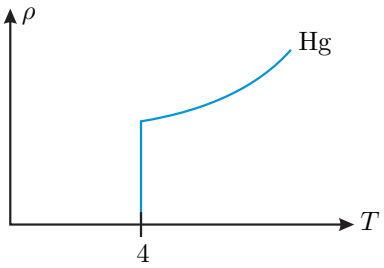
This formula is of analogous form as the Stoner criterion (RPA). $F_0^a \to -1$ is the equivalent of the Stoner criterion. This yields a magnetic instability (onset of ferromagnetism). K. Bedell (foremost expert in ferromagnetism) worked out the relationship between DMFT and Fermi-liquid theory (see Phys. Rev. Lett. from past few years). The numerator comes from the density of states. $\left(N(0) = m^* p_F/2\pi^2\right)$
Values for ^{3}He: $F_0^s \sim 10$, $F_1^s \sim 6$ and $F_0^a \sim -0.67$.

Question: How do we measure m^*?

1. $R_H = \dfrac{1}{nec}$ to get value for n
2. $\sigma = \dfrac{ne^2\tau}{m} \cdot \dfrac{1}{1+\omega^2\tau^2}$

6 Theory of Superconductivity

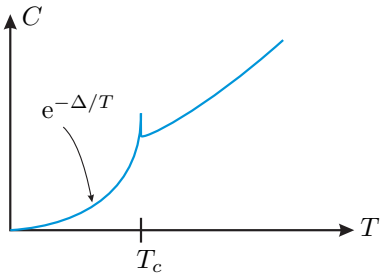
- Observed in 1911 by Kammerlimph Onnes (Leiden)



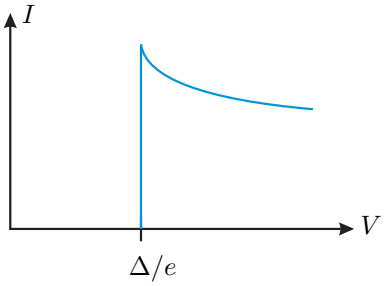
- 1957: Bardeen, Cooper and Schrieffer

6.1 Insights

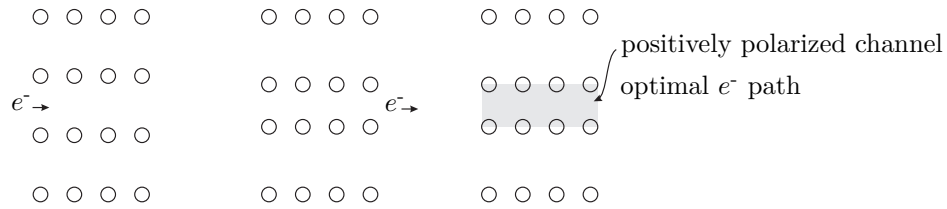
1. Isotope effect $T_c \sim \frac{1}{\sqrt{M}}$ (1952-3) Serin et. al.
2. Total absence of scattering: electrons formed single quantum state. Every classical liquid has a finite viscosity (resistivity). The effect that the electrons are showing no viscosity (resistivity) is an inherently quantum phenomena. Only a single quantum state is unable to scatter off itself.
3. Macroscopic (even double) occupation of a quantum state is prohibited by Pauli.
   Cooper: PAIR the electrons → form bosons.
4. Pairing explains
   - Gap in specific heat



   Δ: pair binding energy
   - Resistivity = 0 explained
     To make resistivity finite one has to BREAK the pair.
   - Tunneling



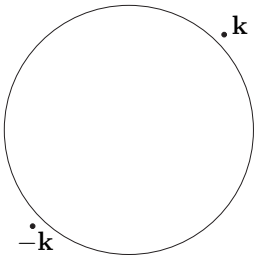
Question: How can phonons bind repulsive electrons?
The answer is retardation.



1. Electron 1 (e_1^-) positively polarizes the channel
2. Polarization remains long after electron 1 is gone.
3. Electron 2 (e_2^-) can lower its energy by retracing e_1^-'s channel.

6.2 Microscopic Theory

1. Two electrons (Cooper 1956) in the presence of a Fermi surface.



Only $\epsilon_k > 0$ states are available.

$$\psi(\mathbf{r}_1, \mathbf{r}_2) = \varphi_{\mathbf{q}}(\rho) \mathrm{e}^{\mathrm{i}\mathbf{q}\cdot\mathbf{R}} \tag{6.1}$$

$\mathbf{q} \equiv$ CM momentum. Let us consider only $\mathbf{q} = 0$.

$$\psi(\mathbf{r}_1, \mathbf{r}_2) = \sum_{\mathbf{k}} a_{\mathbf{k}} \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}_1} \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{r}_2} \tag{6.2}$$

The Hamiltonian is

$$\langle \psi | H | \psi \rangle = \sum_{\mathbf{k}} 2\epsilon_{\mathbf{k}} a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + \sum_{\mathbf{k}\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'} a_{\mathbf{k}}^\dagger a_{\mathbf{k}'} \tag{6.3}$$

The first term is the kinetic energy. The second describes an attractive interaction.

$$\widehat{H} |\psi\rangle = E |\psi\rangle \Rightarrow (E - 2\epsilon_{\mathbf{k}}) a_{\mathbf{k}} = \sum_{\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'} a_{\mathbf{k}'} \tag{6.4}$$

The interaction is

$$V_{\mathbf{k}\mathbf{k}'} = \begin{cases} -|V| & 0 < \epsilon_{\mathbf{k}}, \epsilon_{\mathbf{k}'} < \omega_D \\ 0 & \text{otherwise} \end{cases} \tag{6.5}$$

The coefficients are

$$a_{\mathbf{k}} = \frac{V \sum_{\mathbf{k}'} a_{\mathbf{k}'}}{E - 2\epsilon_{\mathbf{k}}} \tag{6.6}$$

$$\sum_{\mathbf{k}} a_{\mathbf{k}} = V \sum_{\mathbf{k}'} a_{\mathbf{k}'} \sum_{\mathbf{k}} \frac{1}{E - 2\epsilon_{\mathbf{k}}} \tag{6.7}$$

Since the sums over the $a_{\mathbf{k}}$'s are the same, we find

$$1 = V \sum_{\mathbf{k}} \frac{1}{E - 2\epsilon_{\mathbf{k}}} \equiv V \cdot \phi \tag{6.8}$$

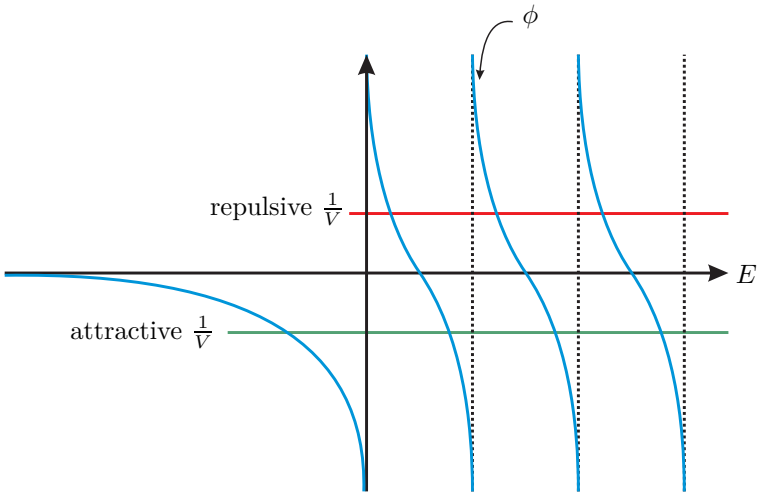


Figure 16: The red line indicates a positive or repulsive $\frac{1}{V}$. The green line indicates a negative or attractive $\frac{1}{V}$. The difference between dotted lines is $2\epsilon_{\mathbf{k}}$.

For attractive V, a single eigenvalue becomes negative. Thus, a BOUND state is present for arbitrary weak attraction.

$$\frac{1}{|V|} = -N(0) \int_0^{\omega_D} \mathrm{d}\epsilon \frac{1}{w - 2\epsilon} = \frac{N(0)}{2} \int_0^{2\omega_D} \mathrm{d}\epsilon \frac{1}{\epsilon + |w|} = \frac{N(0)}{2} \ln \frac{2\omega_D + |w|}{|w|} \approx \frac{N(0)}{2} \ln \frac{2\omega_D}{|w|} \tag{6.9}$$

$$\boxed{|w| = 2\omega_D \ \exp\left(\frac{-2}{N(0)V}\right)} \tag{6.10}$$

This is inherently non-perturbative since there is no Taylor expansion for $\mathrm{e}^{-1/x}$

Last Time

- From the isotope effect Bardin concluded that phonons play an important role in superconductivity.
- Since the resistivity is so low the electrons do not experience scattering and the electrons stay in a particular quantum state.
- How can many electrons stay in the same quantum state when this is forbidden by the Pauli principle? We pair the electrons and they become bosons!
- Arbitrarily weak attraction can form a bound state.

Microscopic Theory Cont.

We neglected exchange!

2. Full many body calculation (following Schrieffer)

$$\widehat{H}_{\text{red}} = \sum_{\mathbf{k}s} \epsilon_{\mathbf{k}s} \hat{n}^f_{\mathbf{k}s} + \sum_{\mathbf{k}\mathbf{k}'} \mathrm{v}_{\mathbf{k}\mathbf{k}'} \hat{b}^\dagger_{\mathbf{k}'} \hat{b}_{\mathbf{k}} \qquad b^\dagger_{\mathbf{k}'} = c^\dagger_{\mathbf{k}'\uparrow} c^\dagger_{-\mathbf{k}\downarrow} \qquad \epsilon_{\mathbf{k}} \equiv \varepsilon_{\mathbf{k}} - \mu \tag{6.11}$$

- $\widehat{H}_{\text{red}}$ keeps only $\mathbf{q} = 0$ in $U \sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} c^\dagger_{\mathbf{k}'-\mathbf{q}} c^\dagger_{\mathbf{k}+\mathbf{q}} c_{\mathbf{k}'} c_{\mathbf{k}}$. This is down by a factor of $1/N$ (bad).
- The ground state will be occupied by N bosons, $\hat{b}^\dagger \hat{b}$ will bring out a factor of N.

$$\widehat{H}_{\text{red}} = \sum_{\mathbf{k}} 2\epsilon_{\mathbf{k}} \hat{b}^\dagger_{\mathbf{k}} \hat{b}_{\mathbf{k}} + \sum_{\mathbf{k}\mathbf{k}'} \mathrm{v}_{\mathbf{k}\mathbf{k}'} \hat{b}^\dagger_{\mathbf{k}'} \hat{b}_{\mathbf{k}} \tag{6.12}$$

$\widehat{H}$ seems to be quadratic and hence diagonalizable. However, our bosons are hard core bosons.

$$\left[\hat{b}_{\mathbf{k}}, \hat{b}^\dagger_{\mathbf{k}'}\right] = \delta_{\mathbf{k}\mathbf{k}'} \left[1 - (n_{\mathbf{k}\uparrow} + n_{-\mathbf{k}\downarrow})\right] \tag{6.13}$$

$$\left(\hat{b}^\dagger_{\mathbf{k}}\right)^2 = 0 \tag{6.14}$$

The $\mathbf{k}$ is a quantum number, but it is not the momentum of the boson. The $\mathbf{k}$ reminds us that the boson is composed of two electrons with momentum $\mathbf{k}$ and $-\mathbf{k}$.

6.3 Variational Approach

Coherent state representation for bose-fields

$$|\psi\rangle = \prod_{\mathbf{k}} \mathrm{e}^{g_{\mathbf{k}}(\hat{a}^\dagger_{\mathbf{k}} + \hat{a}_{-\mathbf{k}})} |0\rangle \tag{6.15}$$

b is a hard core boson, thus we have

$$|\psi\rangle = N \prod_{\mathbf{k}} \left(1 + g_{\mathbf{k}} \hat{b}^\dagger_{\mathbf{k}}\right) |0\rangle \qquad \text{Variational wave function} \tag{6.16}$$

The normalization is given by

$$\langle\psi|\psi\rangle = N^2 \prod_{\mathbf{k}} (1 + g^2_{\mathbf{k}}) \tag{6.17}$$

Thus, the wave function becomes

$$|\psi_{\text{BCS}}\rangle = \prod_{\mathbf{k}} \frac{1 + g_{\mathbf{k}} \hat{b}^\dagger_{\mathbf{k}}}{(1 + g^2_{\mathbf{k}})^{1/2}} |0\rangle = \prod_{\mathbf{k}} (u_{\mathbf{k}} + v_{\mathbf{k}} \hat{b}^\dagger_{\mathbf{k}}) |0\rangle \tag{6.18}$$

where

$$u_{\mathbf{k}} = \frac{1}{(1+g_{\mathbf{k}}^2)^{1/2}} \qquad v_{\mathbf{k}} = \frac{g_{\mathbf{k}}}{(1+g_{\mathbf{k}}^2)^{1/2}} \qquad u_{\mathbf{k}}^2 + v_{\mathbf{k}}^2 = 1 \tag{6.19}$$

The ground state energy is

$$E_{\mathrm{GS}} = \langle \psi_{\mathrm{BCS}} | H_{\mathrm{red}} | \psi_{\mathrm{BCS}} \rangle = \sum_{\mathbf{k}} 2\epsilon_{\mathbf{k}} v_{\mathbf{k}}^2 + \sum_{\mathbf{k}\mathbf{k}'} \mathrm{v}_{\mathbf{k}\mathbf{k}'} u_{\mathbf{k}} v_{\mathbf{k}} u_{\mathbf{k}'} v_{\mathbf{k}'} \tag{6.20}$$

The second term is given by

$$\left\langle 0 \middle| (u_{\mathbf{k}'} + v_{\mathbf{k}'}\hat{b}_{\mathbf{k}'})(u_{\mathbf{k}} + v_{\mathbf{k}}\hat{b}_{\mathbf{k}}) \mathrm{v}_{\mathbf{k}\mathbf{k}'} \hat{b}_{\mathbf{k}'}^\dagger \hat{b}_{\mathbf{k}} (u_{\mathbf{k}'} + v_{\mathbf{k}'}\hat{b}_{\mathbf{k}'}^\dagger)(u_{\mathbf{k}} + v_{\mathbf{k}}\hat{b}_{\mathbf{k}}^\dagger) \middle| 0 \right\rangle \tag{6.21}$$

We have to assure that there are no electrons with momentum $\mathbf{k}'$. We wish to minimize the energy with respect to $g_{\mathbf{k}}$. Using $u_{\mathbf{k}}^2 + v_{\mathbf{k}}^2 = 1$

$$u_{\mathbf{k}}^2 = \frac{1}{2}(1 + a_{\mathbf{k}}) \tag{6.22}$$

$$v_{\mathbf{k}}^2 = \frac{1}{2}(1 - a_{\mathbf{k}}) \tag{6.23}$$

Minimizing with respect to a $\left(\frac{\partial E}{\partial a} = 0\right)$ and noting $u_{\mathbf{k}} v_{\mathbf{k}} = \frac{1}{2}(1 - a_{\mathbf{k}}^2)^{1/2}$, yields

$$E_{\mathrm{GS}} = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}}(1 - a_{\mathbf{k}}) + \sum_{\mathbf{k}\mathbf{k}'} \mathrm{v}_{\mathbf{k}\mathbf{k}'} \frac{1}{2}(1 - a_{\mathbf{k}}^2)^{1/2} \frac{1}{2}(1 - a_{\mathbf{k}'}^2)^{1/2} \tag{6.24}$$

$$\frac{\partial E_{\mathrm{GS}}}{\partial a_{\mathbf{k}}} = 0 = -\sum_{\mathbf{k}} \epsilon_{\mathbf{k}} + 2 \cdot \frac{1}{2} \sum_{\mathbf{k}'} \mathrm{v}_{\mathbf{k}\mathbf{k}'} \frac{1}{2}(1 - a_{\mathbf{k}'}^2)^{1/2} \cdot 2 \cdot \frac{1}{2} \frac{-a_{\mathbf{k}}}{(1 - a_{\mathbf{k}}^2)^{1/2}} \tag{6.25}$$

$$\Delta_{\mathbf{k}} \equiv \sum_{\mathbf{k}'} \mathrm{v}_{\mathbf{k}\mathbf{k}'} \frac{1}{2}(1 - a_{\mathbf{k}'}^2)^{1/2} \tag{6.26}$$

$$\epsilon_{\mathbf{k}} = \Delta_{\mathbf{k}} \frac{a_{\mathbf{k}}}{(1 - a_{\mathbf{k}}^2)^{1/2}} \tag{6.27}$$

$$(1 - a_{\mathbf{k}}^2) = \frac{\Delta_{\mathbf{k}}^2}{\epsilon_{\mathbf{k}}^2} a_{\mathbf{k}}^2 \tag{6.28}$$

$$a_{\mathbf{k}}^2 = \left(1 + \frac{\Delta_{\mathbf{k}}^2}{\epsilon_{\mathbf{k}}^2}\right)^{-1} \tag{6.29}$$

From this, we can get a self-consistent equation for $\Delta_{\mathbf{k}}$.

$$\Delta_{\mathbf{k}} = -\frac{1}{2} \sum_{\mathbf{k}'} \mathrm{v}_{\mathbf{k}\mathbf{k}'} (1 - a_{\mathbf{k}'}^2)^{1/2} \tag{6.30}$$

$$= -\frac{1}{2} \sum_{\mathbf{k}'} \mathrm{v}_{\mathbf{k}\mathbf{k}'} \left(1 - \frac{1}{1 + \frac{\Delta_{\mathbf{k}'}^2}{\epsilon_{\mathbf{k}'}^2}}\right)^{1/2} \tag{6.31}$$

$$= -\frac{1}{2} \sum_{\mathbf{k}'} \mathrm{v}_{\mathbf{k}\mathbf{k}'} \left(\frac{\Delta_{\mathbf{k}'}^2/\epsilon_{\mathbf{k}'}^2}{1 + \Delta_{\mathbf{k}'}^2/\epsilon_{\mathbf{k}'}^2}\right)^{1/2} \tag{6.32}$$

$$= -\frac{1}{2} \sum_{\mathbf{k}'} \mathrm{v}_{\mathbf{k}\mathbf{k}'} \frac{\Delta_{\mathbf{k}'}}{E_{\mathbf{k}'}} \qquad E_{\mathbf{k}} = \sqrt{\epsilon_{\mathbf{k}}^2 + \Delta_{\mathbf{k}}^2} \tag{6.33}$$

$$\mathrm{v}_{\mathbf{k}\mathbf{k}'} = \begin{cases} V & 0 < |\epsilon_{\mathbf{k}}|, |\epsilon_{\mathbf{k}'} < \omega_D \\ 0 & \text{otherwise} \end{cases} \tag{6.34}$$

$$\Delta_{\mathbf{k}\mathbf{k}'} = \begin{cases} \Delta & 0 < |\epsilon_{\mathbf{k}}|, |\epsilon_{\mathbf{k}'} < \omega_D \\ 0 & \text{otherwise} \end{cases} \tag{6.35}$$

$$\Delta = -V \sum_{\mathbf{k}'} \frac{\Delta}{2(\epsilon_{\mathbf{k}'}^2 + \Delta^2)^{1/2}} \tag{6.36}$$

$$1 = |V| \cdot N(0) \int_{-\omega_D}^{\omega_D} \frac{\mathrm{d}\epsilon}{2(\epsilon^2 + \Delta^2)^{1/2}} = |V| N(0) \ln \frac{2\omega_D}{\Delta} \tag{6.37}$$

$$\boxed{\Delta = 2\omega_D \ \exp\left(\frac{-1}{N(0)|V|}\right)} \tag{6.38}$$

This is similar to Cooper's formula, but the 2 is not there. This is a many body effect.

We found

$$u_{\mathbf{k}}^2 = \frac{1}{2}\left(1 + \frac{\epsilon_{\mathbf{k}}}{\sqrt{\epsilon_{\mathbf{k}}^2 + \Delta^2}}\right) \qquad v_{\mathbf{k}}^2 = \frac{1}{2}\left(1 - \frac{\epsilon_{\mathbf{k}}}{\sqrt{\epsilon_{\mathbf{k}}^2 + \Delta^2}}\right) \tag{6.39}$$

Thus the energy difference is

$$\Delta E_{\rm GS} = \frac{1}{2}N(0)\Delta^2 = -\frac{1}{2}N(0)\omega_D^2 \exp\left(-\frac{2}{N(0)|V|}\right) \tag{6.40}$$

$\Delta \sim 1$ K, $N(0) \sim \frac{1}{\epsilon_F} \sim \frac{1}{10^4\ \rm K}$. Thus, $\Delta E_{\rm GS} \sim 10^{-3}$ K. $\Delta E_{\rm GS} \sim 10^{-7} E_F$. First principles calculations cannot pick up such minute differences.

$$\Delta E_{\rm GS} = \frac{1}{8\pi}H_c^2 \qquad H_c = 2[\pi N(0)]^{1/2}\Delta \tag{6.41}$$

6.4 Quasi-particle Excitations

How do we create an excitation?

1. Take away a Cooper pair with $(\mathbf{p}, -\mathbf{p})$.

$$\Delta E^1 = -2\epsilon_{\mathbf{p}}v_{\mathbf{p}}^2 - 2\left[\sum_{\mathbf{k}} v_{\mathbf{pk}}u_{\mathbf{k}}v_{\mathbf{k}}\right]u_{\mathbf{p}}v_{\mathbf{p}} = -2\epsilon_{\mathbf{p}}v_{\mathbf{p}}^2 + 2\Delta u_{\mathbf{p}}v_{\mathbf{p}} \tag{6.42}$$

2. Add electron with $\mathbf{p}$.

$$\Delta E^2 = \epsilon_{\mathbf{p}} \tag{6.43}$$

The total energy change is

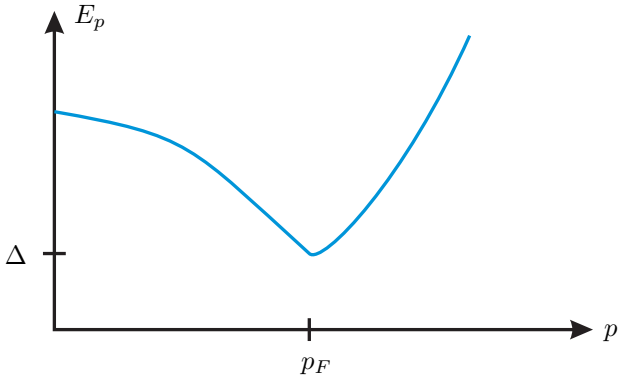
$$\Delta E^1 + \Delta E^2 = \epsilon_{\mathbf{p}}(1 - 2v_{\mathbf{p}}^2) + 2\Delta u_{\mathbf{p}}v_{\mathbf{p}} \tag{6.44}$$

$$u^2v^2 = \frac{1}{4}\left(1 - \frac{\epsilon^2}{\epsilon^2 + \Delta^2}\right) = \frac{1}{4}\frac{\Delta^2}{E^2} \tag{6.45}$$

$$u_{\mathbf{k}}v_{\mathbf{k}} = \frac{1}{2}\frac{\Delta_{\mathbf{k}}}{E_{\mathbf{k}}} \tag{6.46}$$

$$\Delta E^1 + \Delta E^2 = \epsilon_{\mathbf{p}} \cdot \frac{\epsilon_{\mathbf{p}}}{E_{\mathbf{p}}} + \Delta \cdot \frac{\Delta}{E_{\mathbf{p}}} \tag{6.47}$$

$$\boxed{\Delta E^1 + \Delta E_2 = E_{\mathbf{p}} = \sqrt{\epsilon_{\mathbf{p}}^2 + \Delta^2}} \tag{6.48}$$



When we break a Cooper pair, we create a particle with $\mathbf{p}$ and a second one with $-\mathbf{p}$ and the creation energy for each is Δ. Thus, the energy for breaking a pair is 2Δ. From this we see that the binding energy of a Cooper pair is 2Δ.

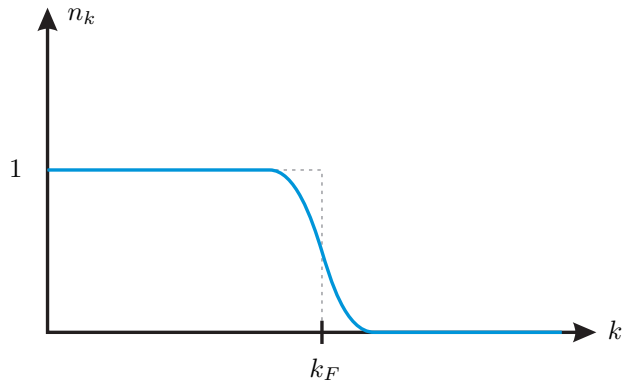
6.4.1 Particle number expectation value

$$\langle n_{\mathbf{k}} \rangle \equiv v_{\mathbf{k}}^2 \tag{6.49}$$

$$= \langle \psi_{\rm BCS} | n_{\mathbf{k}} | \psi_{\rm BCS} \rangle = \left\langle 0 \middle| (u_{\mathbf{k}} + v_{\mathbf{k}} \hat{b}_{\mathbf{k}}) \hat{b}_{\mathbf{k}}^\dagger \hat{b}_{\mathbf{k}} (u_{\mathbf{k}} + v_{\mathbf{k}} \hat{b}_{\mathbf{k}}^\dagger) \middle| 0 \right\rangle \tag{6.50}$$

$$v_{\mathbf{k}}^2 = \frac{1}{2}\left(1 - \frac{\epsilon_{\mathbf{k}}}{E_{\mathbf{k}}}\right) \tag{6.51}$$

$n_{\mathbf{k}}$ is smooth. There is no jump at the Fermi surface ($z = 0$). This a non-Fermi liquid system.



6.4.2 One particle (quasi-particle) states

$$\hat{c}_{\mathbf{p}\uparrow}^\dagger |\psi_{\rm BCS}\rangle = \hat{c}_{\mathbf{p}\uparrow}^\dagger \prod_{\mathbf{k}} (u_{\mathbf{k}} + v_{\mathbf{k}} \hat{b}_{\mathbf{k}}^\dagger) |0\rangle \tag{6.52}$$

$$= u_{\mathbf{p}} \hat{c}_{\mathbf{p}\uparrow}^\dagger \prod_{\mathbf{k}\neq\mathbf{p}} (u_{\mathbf{k}} + v_{\mathbf{k}} \hat{b}_{\mathbf{k}}^\dagger) |0\rangle \equiv u_{\mathbf{p}} |\psi_{\mathbf{p}\uparrow}^\dagger\rangle \tag{6.53}$$

$$\hat{c}_{-\mathbf{p}\downarrow} |\psi_{\rm BCS}\rangle = -v_{\mathbf{p}} \hat{c}_{\mathbf{p}\uparrow}^\dagger \prod_{\mathbf{k}\neq\mathbf{p}} (u_{\mathbf{k}} + v_{\mathbf{k}} \hat{b}_{\mathbf{k}}^\dagger) = -v_{\mathbf{p}} |\psi_{\mathbf{p}\uparrow}^\dagger\rangle \tag{6.54}$$

Two different ways of creating a quasi-particle with momentum $\mathbf{p}$ that are spin-up. Both require energy $E_{\mathbf{p}}$. The Hilbert space of BCS Hamiltonian consists of 2D degenerate subspaces. Small perturbations will couple to a linear combination of these eigenstates. (= "diagonalize H")

6.4.3 Bogoliubov-Valatin Transformation

$$\hat{\gamma}_{\mathbf{p}\uparrow}^\dagger = u_{\mathbf{p}} \hat{c}_{\mathbf{p}\uparrow}^\dagger - v_{\mathbf{p}} \hat{c}_{\mathbf{p}\downarrow} \qquad\qquad \hat{\gamma}_{\mathbf{p}\uparrow}^\dagger |\psi_{\rm BCS}\rangle = |\psi_{\mathbf{p}\uparrow}^\dagger\rangle \tag{6.55}$$

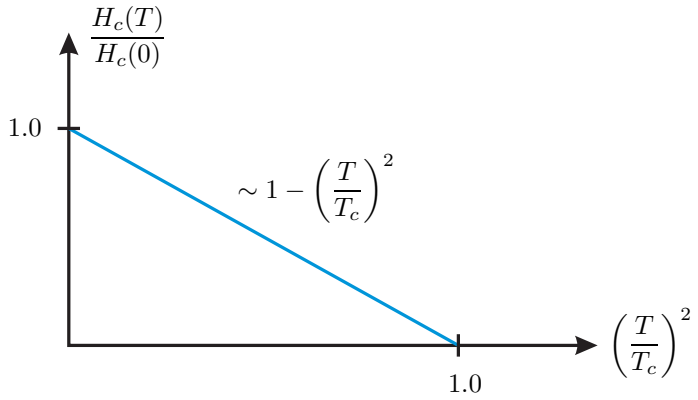
The reverse transformation is

$$\hat{c}_{\mathbf{p}\uparrow}^\dagger = u_{\mathbf{p}} \hat{\gamma}_{\mathbf{p}\uparrow}^\dagger + v_{\mathbf{p}} \hat{\gamma}_{-\mathbf{p}\downarrow} \tag{6.56}$$

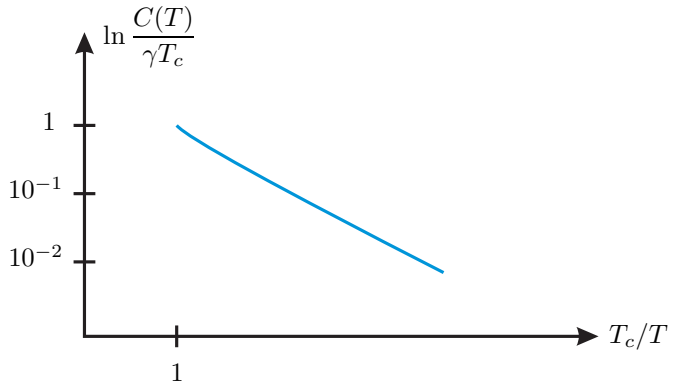
6.4.4 Calculation of Measurable Quantities

1. $H_c(T)$ Critical Field

$$\frac{H_c^2(T)}{8\pi} = F_N(T) - F_{\text{s.c.}}(T) \tag{6.57}$$



2. Specific heat



The specific heat is gapped, as expected.

For $T > 0$, we assumed

$$f_{\mathbf{k}} = \frac{1}{e^{\beta E_{\mathbf{k}}} + 1} \Rightarrow \Delta(T) \tag{6.58}$$

3. NMR relaxation rate

$$H_{I\cdot S} = A\sum_{\mathbf{k}\mathbf{k}'} a^*_{\mathbf{k}'} a_k \left\{ I_z \left(c^\dagger_{k'\uparrow} c_{k\uparrow} - c^\dagger_{k'\downarrow} c_{k\downarrow} \right) + I_+ c^\dagger_{k'\downarrow} c_{k\uparrow} + I_- c^\dagger_{k'\uparrow} c_{k\downarrow} \right\} \tag{6.59}$$

The term in the braces is $\{\cdots\} = \widehat{\mathbf{I}} \cdot \widehat{\mathbf{S}}$. For the specific case of superconductivity

$$c^\dagger_{k'\uparrow} c_{k\downarrow} + c^\dagger_{-k\uparrow} c_{-k'\downarrow} = (u_k u_{k'} + v_k v_{k'}) \left[\gamma_{k'\uparrow} \gamma_{k\downarrow} + \gamma^\dagger_{-k\uparrow} \gamma_{-k'\downarrow} \right] + (u_k u_{k'} - v_k v_{k'}) \left[\gamma_{k'\uparrow} \gamma_{-k\uparrow} + \gamma^\dagger_{k\downarrow} \gamma_{-k'\downarrow} \right] \tag{6.60}$$

The second term is called a pair breaking term. It does not contribute below energies $< \Delta$ ($\omega_{\rm NMR} \ll 2\Delta$). The transition rate is from Fermi's Golden rule

$$\begin{aligned} \frac{1}{T_1(s)} &= 2\pi |A|^2 |a|^4 \sum_{kk'} \left[f_k (1 - f_{k'}) - f_{k'} (1 - f_k) \right] \delta(E_{k'} - E_k - \omega) \cdot \\ &\qquad \frac{1}{2} \left(1 + \frac{\epsilon_k \epsilon_{k'} + \Delta_k \Delta_{k'}}{E_k E_{k'}} \right) \\ &= 2\pi |A|^2 |a|^4 N^2(0) \int_\Delta^\infty \mathrm{d}E \, \left(1 + \frac{\Delta^2}{E(E+\omega)} \right) \frac{E(E+\omega)\omega \cdot \left(-\frac{\partial f}{\partial E} \right)}{(E^2 - \Delta^2)^{1/2} [(E+\omega)^2 - \Delta^2]^{1/2}} \end{aligned} \tag{6.61}$$

For the normal state, we have

$$\frac{1}{T_1(n)} = \frac{1}{T_1(s, \Delta = 0)} = \# \int_0^\infty \mathrm{d}E \, \omega \left(-\frac{\partial f}{\partial E} \right) = \omega \cdot \# f(0) = \omega \cdot \# \frac{1}{2} \tag{6.62}$$

The ratio is

$$\frac{T_1(n)}{T_1(s)} = 2 \int_\Delta^\infty \mathrm{d}E \, \frac{(E(E+\omega) + \Delta)^2 \left(-\frac{\partial f}{\partial E} \right)}{(E^2 - \Delta^2)^{1/2} ((E+\omega)^2 - \Delta^2)^{1/2}} \tag{6.63}$$

In the limit as $\omega \to 0$, we have

$$\frac{T_1(n)}{T_1(s)} = 2 \int_\Delta^\infty \mathrm{d}E \, \frac{E^2 + \Delta^2}{E^2 - \Delta^2} \left(-\frac{\partial f}{\partial E} \right) \tag{6.64}$$

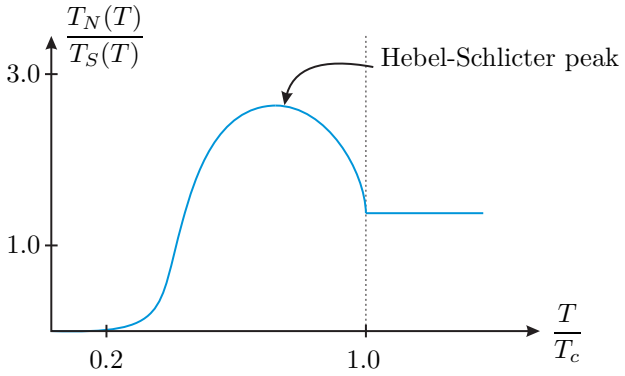
Factors:

(a) DOS $\to \frac{1}{E^2 - \Delta^2}$

(b) Coherence terms $\to 2$

DOS $\to$ ln divergence of integral. $\omega_{\rm NMR}$ cuts it off.

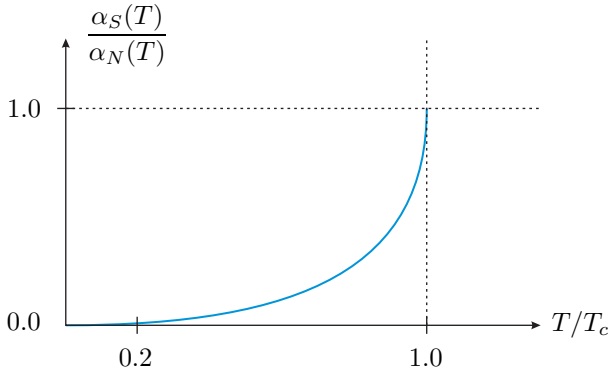
$$\frac{1}{T_1} \sim \ln \frac{\Delta}{\max(\omega_{\rm NMR}, \omega_{\rm Zeeman})} \tag{6.65}$$



4. Ultrasonic attenuation

Basic process: the phonons are absorbed by the electrons of the matrial.

$$\frac{\alpha(s)}{\alpha(n)} = \int_{\Delta}^{\infty} \mathrm{d}E \, \frac{E^2 - \Delta^2}{E^2 - \Delta^2} \left(-\frac{\partial f}{\partial E} \right) \tag{6.66}$$



The coherence factors eliminate the DOS log singularity.