Lecture 9
Responses in Free Electron Gas. Electron Green's Function. Tunneling conductance. Friedel Oscillations. Migdal-Kohn Anomaly. Peierls Instability. Orthogonality Catastrophe.

Electron Green's Function

The electron Green's function at zero temperature is defined by the expression

$$G(t-t', \mathbf{r}-\mathbf{r}') = -i \begin{cases} <0|\psi^+(t,\mathbf{r})\psi(t',\mathbf{r}')|0>, & t<t' \\ -<0|\psi(t',\mathbf{r}')\psi^+(t,\mathbf{r})|0>, & t>t', \end{cases} \quad (1)$$

where $\psi(\mathbf{r},t)$ and $\psi+(\mathbf{r},t)$ are the Heisenberg operators of annihilation and creation of electrons respectively. In the energy-momentum representation the Green's function takes the form[1]:

$$G(\epsilon, \mathbf{p}') = \int d\mathbf{r}dtG(t, \mathbf{r})e^{i\epsilon t - i\mathbf{pr}} = \frac{1}{\epsilon - (\epsilon(\mathbf{p}) - \mu) + i\delta \mathrm{sgn}\, \epsilon}$$
$$= \frac{n(\mathbf{p})}{\epsilon - \epsilon(\mathbf{p}) + \mu - i\delta} + \frac{1 - n(\mathbf{p})}{\epsilon - \epsilon(\mathbf{p}) + \mu + i\delta}. \qquad (2)$$

Equation (2) shows that the electron Green's function consists of two parts, corresponding to the contributions of particles and holes respectively and its poles give to the energy spectrum $\epsilon = \epsilon(\mathbf{p})$.
For $|\epsilon(p) - \mu| \ll E_F$ this difference can be expanded about the Fermi momentum p_0:

$$\epsilon(\mathbf{p}) - \mu = v_F(p - p_0).$$

It can be shown that for a three-dimensional system of interacting electrons, the Green's function is dominated by a similar pole contribution in the vicinity of the Fermi surface $|\epsilon(p) - \mu| \ll E_F$.
Similar to the phonon Green's function, the electron Green's function $G(t, \mathbf{r})$ can be represented as a sum of the retarded and advanced functions G^R and G^A. Finally, one can define the Green's function for imaginary Matsubara times $0 < \tau < \beta$ with the boundary condition $G(0) = -G(\beta)$. This leads to the Matsubara energies $\epsilon_n = \pi T(2n + 1)$, which are related to the Fermi-Dirac distribution by the identity

$$T \sum_{n=-\infty}^{+\infty} \left(\frac{e^{-\epsilon_n \tau}}{i\epsilon_n - \epsilon(\mathbf{p}) + \mu} \right)_{\tau \to 0^+} = \frac{1}{2} \left(1 - \tanh \frac{\epsilon(\mathbf{p}) - \mu}{2T} \right) = n(\mathbf{p}).$$

[1]Everywhere below we assume that the zero of the energy ϵ coincides with the chemical potential.

Another representation of the Green's function (as a function of the Matsubara energy and the coordinate) will be useful for us in the future:

$$G(\epsilon_n, \mathbf{r}) = \int \frac{d\mathbf{p}}{(2\pi)^3} \frac{e^{i\mathbf{p}\mathbf{r}}}{i\epsilon_n - v_F(p - p_0)} = \frac{1}{2mr} \exp\left[ip_0 r \ \mathrm{sgn}\epsilon_n - \frac{|\epsilon_n| r}{v_F}\right] \tag{3}$$

Tunnelling Spectroscopy

The meaning of the Green's function $G(\epsilon, \mathbf{p})$ can be clearly seen if a complete set of intermediate states $|n>$ is introduced:

$$G(\epsilon, \mathbf{p}) = \sum_n \left\{ \frac{|<0|\psi_{\mathbf{p}}|n>|^2 n_{\mathbf{p}}}{\epsilon - v_F(p - p_0) + i\delta} - \frac{|<0|\psi_{\mathbf{p}}|n>|^2 (1 - n_{\mathbf{p}})}{\epsilon - v_F(p - p_0) - i\delta} \right\}. \tag{4}$$

This allows us to consider the current-voltage characteristics of a tunnel junction. Let us assume that we have two metals A and B divided by a tunnel barrier. The Hamiltonian of such a system consists of the Hamiltonian $\mathcal{H}_{A(B)}$ of the electrodes and the tunnelling Hamiltonian $\mathcal{H}_T$:

$$\mathcal{H} = \mathcal{H}_A + \mathcal{H}_B + \mathcal{H}_T; \ H_{A(B)} = \sum_{\mathbf{p}} \epsilon_{A(B)}(\mathbf{p}) \psi^+_{A(B)}(\mathbf{p}) \psi_{A(B)}(\mathbf{p}); \tag{5}$$

$$\mathcal{H}_T = \sum_{\mathbf{p}\mathbf{p}'} T_{\mathbf{p}\mathbf{p}'} \left(\psi^+_A(\mathbf{p}) \psi_B(\mathbf{p}') + \psi^+_B(\mathbf{p}') \psi_A(\mathbf{p}) \right). \tag{6}$$

If these two metals are in contact, electrons can tunnel from A to B and back. In the case when there is a voltage V across the tunnel, and the chemical potentials of the electrodes are different, $\mu_A - \mu_B = eV$, a finite tunneling current I builds up:

$$I = e\int_{-\infty}^{+\infty} d\epsilon \sum_{\mathbf{pp}'} |T_{\mathbf{pp}'}|^2 \mathrm{Im}\ G_A\left(\mathbf{p}, \epsilon + \frac{eV}{2}\right) \mathrm{Im}\ G_B\left(\mathbf{p}', \epsilon - \frac{eV}{2}\right) \cdot \\ \cdot \left[n\left(\epsilon - \frac{eV}{2}\right) - n\left(\epsilon + \frac{eV}{2}\right)\right] \propto \\ \propto \int_{-\infty}^{+\infty} d\epsilon \nu_A \left(\epsilon + \frac{eV}{2}\right) \nu_B \left(\epsilon + \frac{eV}{2}\right) \left[n\left(\epsilon - \frac{eV}{2}\right) - n\left(\epsilon + \frac{eV}{2}\right)\right]. \quad (7)$$

This gives the opportunity to study the density of states of the material A if that of the material B is known.

Response to a static local perturbation at large distances

Consider a local perturbation, caused by an impurity which repels electrons. The relevant Hamiltonian has the following form [2]:

$$\mathcal{H}_{imp} = \int d\mathbf{r} V(\mathbf{r}_{imp} - \mathbf{r})\psi^+(\mathbf{r})\psi(\mathbf{r}) = \\ = \int (d\mathbf{p})(d\mathbf{p}')V(\mathbf{p} - \mathbf{p}')\psi^+_{\mathbf{p}}\psi_{\mathbf{p}'}e^{i(\mathbf{p}-\mathbf{p}')\mathbf{r}_{imp}} \quad (9)$$

Let us calculate the extra density $\delta n(\mathbf{r})$ at a point $\mathbf{r}$, such

[2] The perturbation is can be caused by a magnetic impurity, which has a free moving spin $\mathbf{S}$. The exchange interaction of the magnetic impurity with the conduction electrons has the form:

$$\mathcal{H}_{sd} = \int d\mathbf{r} J(\mathbf{r}_{imp} - \mathbf{r})\psi^+_\alpha(\mathbf{r})\sigma^i_{\alpha\beta}\psi_\beta(\mathbf{r})S^i. \quad (8)$$

The calculation of the spin polarization induced by the magnetic impurity is similar to that of the extra density given below.

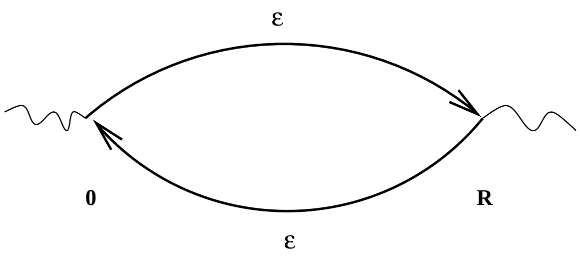

Figure 1: Feynman diagram for response of the electron gas to a local static perturbation

that $\mathbf{R} = \mathbf{r} - \mathbf{r}_{imp} \gg \hbar/p_F$. To a first order in $\mathcal{H}_{imp}$, given by the diagram in Fig 1, we obtain ($\mathbf{r}_{imp} = 0$):

$$\delta n(\mathbf{r}) = T \sum_{\epsilon_n} \delta G(\epsilon_n, \mathbf{r}, \mathbf{r}) = \int d\mathbf{r}' V(\mathbf{r}') \mathcal{R}(\mathbf{r} - \mathbf{r}'); \tag{10}$$

$$\mathcal{R}(\mathbf{R}) = \int \frac{\epsilon}{2\pi} \, G^2(\epsilon, \mathbf{R}) = \frac{v_F}{8\pi m^2} \, \frac{\cos 2p_F R}{R^3}, \tag{11}$$

where the expression (3) for the Green's function at large distances has been used to get the asymptotic (RKKY) form for the kernel $\mathcal{R}(\mathbf{R})$.

Migdal-Kohn anomaly

The power-law asymptote (11) means that the response function $\mathcal{R}(\omega, \mathbf{q})$ in the limit as $\omega \to 0$, has a singularity when the modulus of the wave vector $\mathbf{q}$ approaches the real value $2p_F$. In order to clarify the origin of this singularity, let us consider the interaction of electrons with acoustic phonons. The relevant Hamiltonian has the form:

$$\mathcal{H}_{e-ph} = \alpha \int \frac{(d\mathbf{p})(d\mathbf{p}')(d\mathbf{q})}{\sqrt{2m\omega(\mathbf{q})}} \psi^+(\mathbf{p})\psi(\mathbf{p}')[b^+(\mathbf{q})+b(-\mathbf{q})]\delta(\mathbf{p}'-\mathbf{p}-\mathbf{q}), \tag{12}$$

where b and b^+ are the annihilation and creation operators for the phonons. The probability W_q of absorbing a phonon with the wave vector $\mathbf{q}$ and frequency $\omega(\mathbf{q}) = sq$ is given by the Fermi golden rule:

$$W_q = 2\pi \frac{\alpha^2}{2m\omega(q)} \int (d\mathbf{p}) n(\mathbf{p}+\mathbf{q})[1-n(\mathbf{p})]\delta(\epsilon(\mathbf{p}+\mathbf{q})-\epsilon(\mathbf{p})-\omega(\mathbf{q})). \tag{13}$$

Since

$$\epsilon(p) = \mu + v_F(p - p_F), \qquad \omega(q) = sq, \qquad s \ll v_F,$$

one can neglect $\omega(q)$ in the argument of the δ-function in Eq (13).The regions in the $\mathbf{p}$-space, where the energy and momentum conservation laws hold for the sound adsorption and the Pauli exclusion principle does not restrict it, are shown in Fig. 2. It is clear, that there are no permitted processes for $q > 2p_F$ and therefore $W_q \propto \theta(2p_F - q)$. An accurate calculation of W_q gives a threshold singularity:

$$W_q \propto \alpha^2 \frac{4p_F^2 - q^2}{q^2} \theta(2p_F - q) \tag{14}$$

The probability of the sound absorption corresponds to the imaginary part of the electron susceptibility $\mathrm{Im}\mathcal{R}(\omega, q)|_{\omega\to 0}$. Its real part also has a singularity:

$$\mathrm{Re}\mathcal{R}(0, q) \propto \frac{4p_F^2 - q^2}{q^2} \ln \frac{2p_F + q}{2p_F - q}. \tag{15}$$

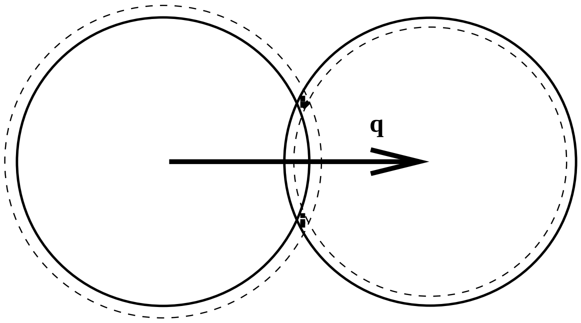

Figure 2: The phase volume for sound adsorption

This singularity is responsible for the RKKY interaction. It also leads to a strong anomaly in the electron renormalization of the sound velocity in metals near $q = 2p_F$ (the Migdal-Kohn anomaly).

Peierls instability

The Migdal-Kohn anomaly has a striking form in one dimension. Consider a one-dimensional chain of atoms with one free electron per atom. The electron energy spectrum for such a metal is shown in Fig 3. Since the electron concentration is exactly half of the capacity of the energy band, the Fermi momentum is equal to the half of the value of quasi-momentum, which corresponds to the boundary of the Brillouin zone $p_F = \pi/2a$ and the energy spectrum is $\epsilon_0(p) = v_F(p - p_F)$. If every second atom is displaced by u from its position of equilibrium, the period of the chain gets doubled and the size of the Brillouin zone shrinks by a factor of two. This brings about another branch of the electron spectrum, shown in Fig. 3 by the dashed line. The hybridization of these branches leads to their repulsion, as shown in Fig. 3, and the transformation of the metal into the Peierls dielectric. For the quasi-momentum p close to the Fermi momentum, the spectra has the form

$$\epsilon_\pm = \pm\sqrt{\Delta^2 + v_F^2(p-p_F)^2}, \qquad \Delta = \alpha u. \tag{16}$$

The total energy of deformation $E(u)$ consists of the energy loss $Ku^2/2$ due to the elasticity and the energy gain due to the electron redistribution:

$$E(u) = \frac{Ku^2}{2} - 2\cdot 2\int_0^{p_F}\frac{2dp}{2\pi\hbar}[\epsilon_0(p) - \epsilon(p)] =$$

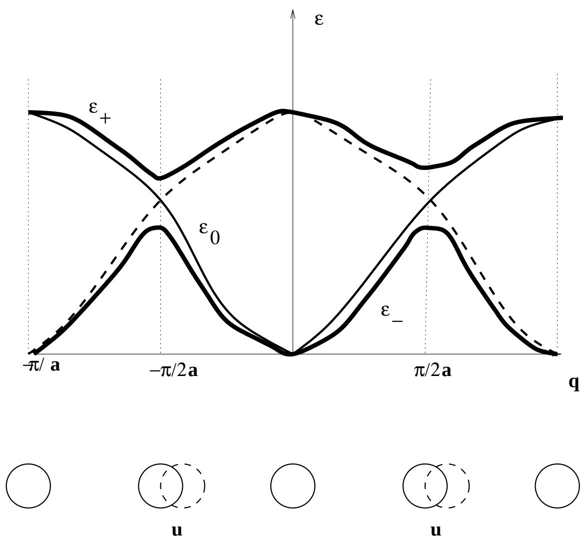

Figure 3: Electron spectrum in one-dimensional chain and its transformation due to deformation u of the period doubling.

$$= \frac{Ku^2}{2} - \frac{4\alpha^2}{\pi\hbar}u^2\int_0^{p_F}\frac{dp}{v_F p} = \left(\frac{K}{2} - \frac{4\alpha^2}{\pi\hbar v_F}\ln\frac{\epsilon_F}{\alpha u}\right)u^2 \quad (17)$$

Equation (17) shows that no matter how weak is the coupling α of the electrons with the lattice, for small enough deformations u of the period doubling, the compressibility d^2E/du^2 changes its sign, which signifies an instability (the Peierls instability)[3].

Orthogonality catastrophe

We consider here the reaction of the electron gas to a sudden local perturbation. For instance, if the atomic core undergoes a quick change due to recharging, nuclear reaction, interaction with the X-rays, etc, the core potential changes abruptly:

$$V(t) = V_0(r)\ \theta(t)$$

It is obvious that, even if the electron system was in its ground state $\mid 0 >$ at $t < 0$, such a time-dependent perturbation may create excitations of the electron gas. What is the probability that a finite size sample finds itself in a new ground state $\mid \tilde{0} >$? To answer this question, we have to calculate the orthogonality factor $Q = \mid < 0 \mid \tilde{0} > \mid^2$.

[3]The Peierls instability exists in one dimension for any filling factor and manifests the Migdal-Kohn anomaly. Indeed, the sound absorption W_q is proportional to $\theta(2p - F - q)$, which immediately leads to succeptibility $\mathcal{R}(q) \propto \ln(2p_F - q)$ with infinity at $q = 2p_F$. As a result, an infinitesimal coupling of electrons with phonons leads to the $2p_F$-instability.(See further in Lecture 16)

Let us consider a sphere of radius R with the boundary condition $\psi(R)=0$. At $t<0$, the solutions of the Schrödinger equation for the electrons in the box have the form:

$$\psi_0^n(r)=N_n\frac{\sin k_n r}{r},\quad k_n=\frac{\pi n}{R},\ E_n=\frac{\hbar^2 k_n^2}{2m}<\epsilon_F \tag{18}$$

Let us assume that we can solve the Schrödinger equation for the electron in the presence of the potential $V_0(r)$ and find the stationary wave functions $\psi^n(r)$, which have the following form at large distance r:

$$\psi^n(r)=N_n'\frac{\sin(k_n' r-\delta(E_n'))}{r},\quad k_n'=\frac{\pi n}{R}+\frac{\delta(E_n')}{R}=k_n+\frac{\delta(E_n')}{R}. \tag{19}$$

The wave functions of the ground states are, respectively:

$$\mid 0\ >=\prod_{E_n<\epsilon_F}\psi_0^n(r);\quad \mid\tilde{0}\ >=\prod_{E_n<\epsilon_F}\psi^n(r). \tag{20}$$

The orthogonality factor

$$Q=\mid<0\mid\tilde{0}>\mid^2=\prod_{E_n<\epsilon_F,E_{n'}<\epsilon_F}A^2_{nn'},$$

$$A_{nn'}=4\pi\int_0^R r^2 dr\psi_0^n(r)\psi^{n'}(r)=\frac{2\pi N_n N_{n'}'}{k_n k_{n'}'}\ \frac{\sin\delta_{n'}}{k_n-k_{n'}} \tag{21}$$

Considering $A_{nn'}$ as a matrix, we arrive at the obvious expression:

$$Q=\det A^2 y=e^{\ln\det A^2}=\exp[\mathrm{tr}\ \ln A^2]. \tag{22}$$

Since

$$\psi^n(r)=\sum_{E_n<\epsilon_F}A_{nn'}\psi_0^{n'}(r)+\sum_{E_n>\epsilon_F}A_{nn'}\psi_0^{n'}(r),$$

and

$$\sum_{n'} A_{nn'}A_{n'n} = 1$$

we can re-write Eq (22) in the following form

$$Q = \exp\left\{\sum_{E_n<\epsilon_F}\left(\ln\left[1-\sum_{E'_n>\epsilon_F}\hat{A}^2\right]\right)_{nn'}\right\} =$$
$$= \exp\left\{-\sum_{E_n<\epsilon_F, E'_n>\epsilon_F} A^2_{nn'}\right\}. \qquad (23)$$

Direct calculation gives

$$\sum_{E_n<\epsilon_F, E'_n>\epsilon_F} A^2_{nn'} = \sum_{E_n<\epsilon_F, E'_n>\epsilon_F} \frac{\sin^2\delta}{(\pi n' - \pi n + \delta)^2} =$$
$$= \frac{\sin^2\delta}{\pi^2}\ \ln\left(\frac{p_F R}{\hbar}\right). \qquad (24)$$

Since the number of atoms N in the sphere of the radius R is

$$N = \frac{4\pi}{3v_0}R^3,$$

the orthogonality factor Q equals to

$$Q \propto N^{\sin^3\delta/3\pi^2} \qquad (25)$$

and vanishes if $N \to \infty$. This vanishing of Q is called the Anderson's orthogonality catastrophe.