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Chapter 1

Electrons scattering by localized random impurities

The effect of impurity atoms on the properties of a metal is of considerable physical interest, because most real materials contain impurities which affect their physical properties. In this chapter, we consider electron scattering by impurity atoms. We assume the electrons to be non-interacting, but is perturbed by the potential due to the impurity atom. This problem can immediately be seen to be expressible in terms of the quantum mechanics of scattering of a single electron from the impurity potential. Thus in principle we donot need the mehtods of many-body theory to discuss the effect of impurities in metals. However, as soon as interactions between electrons are included, we obtain a true many-body problem. It is then no longer possible to treat the statistical mechanics separately from the determination of the energy levels, and we do need to use many-body theory to understand the physics of the situation. It is therefore helpful to formulate the initial problem of a potential acting on a non-interacting fermi gas in terms of Green's functions, so that one is later in a position to generalize to the case of interactions. It turns out that, this problem is a very nice illustration of many of the properties of Green's functions.

1.1 Diagram technique

Consider an electron moving in a random potential field, created by N_{imp} scatterers ("impurities"), which are randomly placed in space with a fixed density $n_i = N_{imp}/V$, where V is the system volume. The potential is taken as a summation of impurity potentials:

$$V(\mathbf{r}) = \sum_{j=1}^{N_{imp}} V(\mathbf{r} - \mathbf{R}_j) = \frac{1}{V}\sum_{\mathbf{p}}\sum_{j} v(\mathbf{p}) e^{i\mathbf{p}\cdot(\mathbf{r}-\mathbf{R}_j)} \tag{1.1}$$

where $v(p)$ is the Fourier transform of the potential of a single impurity. Here, we need distinguish two kinds of impurity potentials: one is like point-like consistent potential $v(\mathbf{q}) = v_0$ that is a constant, independent of momentum transfer $\mathbf{q}$; the other one is like the white noise: $\langle v(\mathbf{q} = 0)\rangle = 0, \langle v(\mathbf{q})v(\mathbf{q}')\rangle = u^2\delta(\mathbf{q} + \mathbf{q}' = 0)$.

Next we assume the scattering potential to be weak enough, we may develop perturbation theory, writing down the second-quantized Hamiltonian for electron interaction with random field as:

$$\begin{aligned}
H_{imp} &= \int d\mathbf{r}\psi^\dagger(\mathbf{r})V(\mathbf{r})\psi(\mathbf{r}) \\
&= \sum_{\mathbf{p},\mathbf{p}'} \langle \mathbf{p}|V|\mathbf{p}'\rangle a^\dagger_{\mathbf{p}} a_{\mathbf{p}'} = \sum_{\mathbf{p},\mathbf{p}'} \int d\mathbf{r} \langle p|r\rangle V(r) \langle r|p'\rangle a^\dagger_{\mathbf{p}} a_{\mathbf{p}'} \\
&= \sum_{\mathbf{p},\mathbf{p}'} \frac{1}{V} \int d\mathbf{r} e^{i\mathbf{p}\cdot\mathbf{r}} e^{-i\mathbf{p}'\cdot\mathbf{r}} \frac{1}{V} \sum_{\mathbf{q}}\sum_{j} v(\mathbf{q}) e^{i\mathbf{q}\cdot(\mathbf{r}-\mathbf{R}_j)} a^\dagger_{\mathbf{p}} a_{\mathbf{p}'} \\
&= \sum_{\mathbf{p},\mathbf{p}'} \frac{1}{V} \int d\mathbf{r} e^{i(\mathbf{p}-\mathbf{p}'+\mathbf{q})\cdot\mathbf{r}} v(\mathbf{q}) \frac{1}{V} \sum_{j} e^{-i\mathbf{q}\cdot\mathbf{R}_j} a^\dagger_{\mathbf{p}} a_{\mathbf{p}'} = \sum_{\mathbf{p},\mathbf{q}} v(\mathbf{q}) \frac{1}{V} \sum_{j} e^{-i\mathbf{q}\cdot\mathbf{R}_j} a^\dagger_{\mathbf{p}} a_{\mathbf{p}+\mathbf{q}} \\
&= \sum_{\mathbf{q}} v(\mathbf{q}) \rho_{imp}(\mathbf{q}) \rho(-\mathbf{q})
\end{aligned} \tag{1.2}$$

In the diagram language, the above scattering can be expressed as one electron scattering by a single impurity line with momentum transfer $\mathbf{q}$.

The full Green's function G can be understood as,

$$\begin{aligned} G(\mathbf{r}_b, \mathbf{r}_a) &= G_0(\mathbf{r}_b, \mathbf{r}_a) + \int d\mathbf{r}_1 G_0(\mathbf{r}_b, \mathbf{r}_1) V(\mathbf{r}_1) G(\mathbf{r}_1, \mathbf{r}_a) \\ &= G_0(\mathbf{r}_b, \mathbf{r}_a) + \int d\mathbf{r}_1 G_0(\mathbf{r}_b, \mathbf{r}_1) V(\mathbf{r}_1) G_0(\mathbf{r}_1, \mathbf{r}_a) + \int d\mathbf{r}_1 d\mathbf{r}_2 G_0(\mathbf{r}_b, \mathbf{r}_1) V(\mathbf{r}_1) G_0(\mathbf{r}_1, \mathbf{r}_2) V(\mathbf{r}_2) G_0(\mathbf{r}_2, \mathbf{r}_a \\ &= \sum_n G^{(n)}(\mathbf{r}_b, \mathbf{r}_a) \end{aligned} \tag{1.3}$$

i.e. the propagator of a fermion in an external potential is given as the sum of all possible processes involving unperturbed propagation (G_0) intersected by any number of scattering events V. Here we define

$$G^{(n)}(\mathbf{r}_b, \mathbf{r}_a) = \sum_{j_1=1}^{N_{imp}} ... \sum_{j_n=1}^{N_{imp}} \int d\mathbf{r}_1 ... \int d\mathbf{r}_n G_0(\mathbf{r}_b, \mathbf{r}_1) V(\mathbf{r}_1 - \mathbf{R}_{j_1}) G_0(\mathbf{r}_1, \mathbf{r}_2) V(\mathbf{r}_2 - \mathbf{R}_{j_2}) ... V(\mathbf{r}_n - \mathbf{R}_{j_n}) G_0(\mathbf{r}_n - \tag{1.4}$$

This n-th order contribution can be interpreted as the sum over all processes involving n scattering events in all possible combination of impurities. Using $G_0(\mathbf{r}, \mathbf{r}'; i\omega_n) = \frac{1}{V} \sum_{\mathbf{k}} G_0(\mathbf{k}, i\omega_n) e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')}$, we have

$$\begin{aligned} G^{(n)}(\mathbf{r}_b, \mathbf{r}_a) = \sum_{j_1,...j_n}^{N_{imp}} \frac{1}{V^n} \sum_{\mathbf{q}_1,...,\mathbf{q}_n} \frac{1}{V^{n+1}} \sum_{\mathbf{k_a},\mathbf{k_b},\mathbf{k_1},...,\mathbf{k_{n-1}}} \int d\mathbf{r}_1 ... \int d\mathbf{r}_n \\ G_0(\mathbf{k}_b) v(\mathbf{q}_1) G_0(\mathbf{k}_1) v(\mathbf{q}_2) ... v(\mathbf{q}_n) G_0(\mathbf{k}_a) \\ \times e^{i\mathbf{q}_1\cdot(\mathbf{r}_1-\mathbf{R}_{j_1})} e^{i\mathbf{q}_2\cdot(\mathbf{r}_2-\mathbf{R}_{j_2})} ... e^{i\mathbf{q}_n\cdot(\mathbf{r}_n-\mathbf{R}_{j_n})} e^{i\mathbf{k}_b\cdot(\mathbf{r}_b-\mathbf{r}_1)} e^{i\mathbf{k}_1\cdot(\mathbf{r}_1-\mathbf{r}_2)} ... e^{i\mathbf{k}_b\cdot(\mathbf{r}_n-\mathbf{r}_a)} \end{aligned} \tag{1.5}$$

$$\begin{aligned} = \frac{1}{V^2} \sum_{\mathbf{k}_a,\mathbf{k}_b} e^{i\mathbf{k}_b\cdot\mathbf{r}_b} e^{-i\mathbf{k}_a\cdot\mathbf{r}_a} \sum_{j_1,...j_n}^{N_{imp}} \frac{1}{V^{n-1}} \sum_{\mathbf{k_1},...,\mathbf{k_{n-1}}} \\ G_0(\mathbf{k}_b) v(\mathbf{k}_b - k_1) G_0(\mathbf{k}_1) v(\mathbf{k}_2 - \mathbf{k}_1) ... v(\mathbf{k}_n - \mathbf{k}_a) G_0(\mathbf{k}_a) e^{-i(\mathbf{k}_b-\mathbf{k}_1)\cdot\mathbf{R}_{j_1}} e^{-i(\mathbf{k}_2-\mathbf{k}_1)\cdot\mathbf{R}_{j_2}} ... e^{-i(\mathbf{k}_{n-1}-\mathbf{k}_a} \end{aligned} \tag{1.6}$$

$$\begin{aligned} \Rightarrow G^{(n)}(\mathbf{k}_b, \mathbf{k}_a) = \sum_{j_1,...j_n}^{N_{imp}} \frac{1}{V^{n-1}} \sum_{\mathbf{k_1},...,\mathbf{k_{n-1}}} G_0(\mathbf{k}_b) v(\mathbf{k}_b - \mathbf{k}_1) G_0(\mathbf{k}_1) v(\mathbf{k}_2 - \mathbf{k}_1) ... v(\mathbf{k}_n - \mathbf{k}_a) G_0(\mathbf{k}_a) \\ e^{-i(\mathbf{k}_b-\mathbf{k}_1)\cdot\mathbf{R}_{j_1}} e^{-i(\mathbf{k}_2-\mathbf{k}_1)\cdot\mathbf{R}_{j_2}} ... e^{-i(\mathbf{k}_{n-1}-\mathbf{k}_a)\cdot\mathbf{R}_{j_n}} \end{aligned} \tag{1.7}$$

We can now deduce the Feynman rules for the diagrams:

- Let the dashed line denote a scattering event $v(\mathbf{q})e^{-i\mathbf{q}\cdot\mathbf{R}_j}$; Draw n scattering events;

- Let solid line denote free Green's function for fermion $G_0(\mathbf{k})$; Draw $n+1$ Green's functions;
- Connect vertex with Green's function;
- Momentum conservation at each vertex;
- Perform the sums of momentum $\frac{1}{V^n}\sum_{k_j}$ and $\sum_{j_1,\ldots,j_n}^{N_{imp}}$ over $\mathbf{R}_j$.

The impurity scattering diagrams can be represented diagrammatically as shown in Fig. 1.1.

If the electron wavefunctions are completely coherent throughout the entire disordered metal each true electronic eigenfunction exhibit an extremely complex diffraction pattern spawned by the randomly positioned scatterers. In the following we average over all possible uncorrelated positions R_j of the N_{imp} impurities for the entire system. We will encounter products of the impurity density operator frequently:

$$f_n(\mathbf{q}_1, \mathbf{q}_2, ..., \mathbf{q}_n) = \langle \rho_{imp}(\mathbf{q}_1)\rho_{imp}(\mathbf{q}_2)...\rho_{imp}(\mathbf{q}_n)\rangle \tag{1.8}$$

This average is over the possible positions which the impurities may have in the solid.

Since the R_j is located randomly, the sum is zero unless $\mathbf{q} = 0$, so the first term is:

$$f_1(\mathbf{q}) = \langle \sum_j e^{i\mathbf{q}\cdot\mathbf{R}_j}\rangle = N_{imp}\delta_{\mathbf{q}=0} \tag{1.9}$$

The second term is

$$\begin{aligned} f_2(\mathbf{q}_1, \mathbf{q}_2) &= \langle \sum_{i,j} e^{i\mathbf{q}_1\cdot\mathbf{R}_i + i\mathbf{q}_2\cdot\mathbf{R}_j}\rangle = \langle \sum_{i=j} e^{i(\mathbf{q}_1+\mathbf{q}_2)\cdot\mathbf{R}_i} + \sum_{i\neq j} e^{i\mathbf{q}_1\cdot\mathbf{R}_i + i\mathbf{q}_2\cdot\mathbf{R}_j}\rangle \\ &= N_{imp}\delta_{\mathbf{q}_1+\mathbf{q}_2=0} + N_{imp}(N_{imp}-1)\delta_{\mathbf{q}_1=0}\delta_{\mathbf{q}_2=0} \end{aligned} \tag{1.10}$$

And generally, we have

$$f_n(\mathbf{q}_1, \mathbf{q}_2, ..., \mathbf{q}_n) = N_{imp}\delta_{\sum_i \mathbf{q}_i=0} + N_{imp}(N_{imp}-1)\sum_m \delta_{\sum_{i<m}\mathbf{q}_i=0}\delta_{\sum_{j>m}\mathbf{q}_j=0} + ... \tag{1.11}$$

where the factor $N_{imp}\delta_{\sum_i \mathbf{q}_i=0}$ is interpreted as the particle scattering from a single impurity, and summation zero means the momentum is conserved for this scattering. Nevertheless, the terms like $N_{imp}(N_{imp}-1)\delta_{q_1}\delta_{q_2}$ describes the scattering by two independent impurities. The general term in the series should include all possible repeated scattering events at all atoms. Clearly the general term will involve a very large number of possible diagrams. Next, we only consider the low-impurity density limit, where we just keep the scattering by a single impurities, for simplicity.

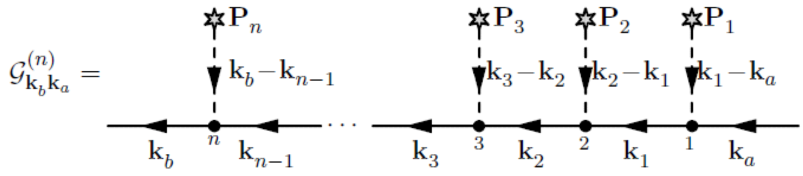

Figure 1.1: Diagrams representing different cumulants in the averaged perturbation series.

Moreover, we assume the potential is short-ranged white noise, or random Gaussian potentials, the odd products of impurity potential are zero. In this case,

$$\begin{aligned}
\overline{V(\mathbf{q})} &= \frac{1}{V}\langle v(\mathbf{q})\rangle\langle\sum_j e^{i\mathbf{q}\cdot\mathbf{R}_j}\rangle = 0 \\
\overline{V(\mathbf{q})V(\mathbf{q}')} &= \frac{1}{V^2}\langle v(\mathbf{q})v(\mathbf{q}')\rangle\langle\sum_i e^{i\mathbf{q}\cdot\mathbf{R}_i}\sum_j e^{i\mathbf{q}'\cdot\mathbf{R}_j}\rangle = n_i u^2\delta(\mathbf{q}+\mathbf{q}')\frac{1}{V}
\end{aligned}$$

This equivalently defines the vertex like Fig. 1.2.

With these preparation, next we can calculate the disorder induced the single-particle Green's function:

$$G(\mathbf{x},\mathbf{x}') = G^0(\mathbf{x},\mathbf{x}') + \int d\mathbf{r}d\mathbf{r}' G^0(\mathbf{x},\mathbf{r})\Sigma(\mathbf{r},\mathbf{r}')G(\mathbf{r}',\mathbf{x}') \tag{1.12}$$

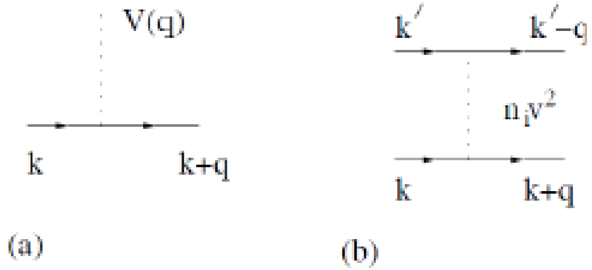

Figure 1.2: (a) The impurity vertex for a Gaussian-distributed potential $V(\mathbf{q})$. (b) The induced interaction which results from averaging over the probability distribution for $V(\mathbf{q})$.

or in momentum space

$$G(\mathbf{p},\epsilon_n)=G_0(\mathbf{p},\epsilon_n)+G_0(\mathbf{p},\epsilon_n)\Sigma(\mathbf{p}\epsilon_n)G(\mathbf{p},\epsilon_n) \tag{1.13}$$

where the full green's function and related self-energy is shown in Fig. 1.4. Consider the contribution of the first diagram of Fig. 1.4, corresponding, as we shall see shortly, to the first-order Born approximation for impurity scattering (1BA):

$$\begin{aligned}\Sigma^{1BA}(\mathbf{p},\epsilon_n) &= n_{imp}\frac{1}{V}\sum_{\mathbf{q}}|v(q)|^2\frac{1}{i\epsilon_n-\xi(\mathbf{p}-\mathbf{q})}=n_{imp}\frac{1}{V}\sum_{p'}|v(p-p')|^2\frac{1}{i\epsilon_n-\xi(p')}\\ &= n_{imp}\frac{1}{V}\sum_{p'}|v(p-p')|^2\frac{1}{\epsilon+isign(\epsilon_n)\delta-\xi(p')}\\ &= n_{imp}\int\frac{p'dp'd\theta}{(2\pi)^2}|v(p-p')|^2[\frac{\epsilon-\xi(p')}{(\epsilon-\xi(p'))^2+\delta^2}-isign(\epsilon_n)\pi\delta(\epsilon-\xi(p'))]\\ &\approx -isign(\epsilon_n)\pi n_{imp}\int\frac{p'dp'd\theta}{(2\pi)^2}|v(p-p')|^2\delta(\epsilon-\xi(p'))=-isign(\epsilon_n)\pi n_{imp}v^2\rho(\epsilon)\\ &= -isign(\epsilon_n)\frac{1}{2\tau_p}\end{aligned} \tag{1.14}$$

where $\xi(p)=E_p-\mu=v_F(p-p_F)$. When $v(q)$ is independent of q, the repeated summations over q can greatly simply this problem. If we assume $|v(p-p')|^2=const.$ and $\epsilon-\xi(p')$ is odd symmetric (like line dispersion), the real part of self-energy vanishes. The scattering rate (inverse of lifetime) of electrons due to impurities is $\gamma_p=1/\tau_p=\pi n_{imp}v^2\rho(\epsilon)$.

$$\begin{aligned}\Sigma(p,i\omega_n) &= n_i\sum_q|v(q)|^2\frac{1}{i\omega_n-\varepsilon(p-q)}=n_i\sum_{q'}|v(p-q')|^2\frac{1}{i\omega_n-\varepsilon(q')}\\ &= n_i\sum_{q'}|v(p-q')|^2\frac{1}{i\omega_n-\varepsilon(q')}=n_i\int\frac{q'dq'd\theta}{4\pi^2}|v(\theta)|^2\frac{1}{i\omega_n-\varepsilon(q')}\\ &= n_i\frac{m}{\hbar^2}\int\frac{d\varepsilon(q')d\theta}{4\pi^2}|v(\theta)|^2\frac{1}{i\omega_n-\varepsilon(q')}\\ &= n_i\frac{m}{\hbar^2}\int\frac{d\theta}{4\pi^2}|v(\theta)|^2\int_{-\infty}^{\infty}d\varepsilon\frac{-i\omega_n-\varepsilon}{\omega_n^2+\varepsilon^2}\\ &= n_i\frac{m}{\hbar^2}\int\frac{d\theta}{4\pi^2}|v(\theta)|^2\frac{-i\omega_n}{|\omega_n|}arctan(\frac{\varepsilon}{\omega_n})\Big|_{-\infty}^{\infty}\\ &= -\pi i n_i\rho sgn(\omega_n)\int\frac{d\theta}{2\pi}|v(\theta)|^2\end{aligned}$$

Or:

$$\begin{aligned}
\Sigma(p, i\omega_n \mapsto \omega + i0^+) &= n_i \frac{m}{\hbar^2} \int \frac{d\varepsilon(q')d\theta}{4\pi^2} |v(\theta)|^2 \frac{1}{\omega - \varepsilon(q') + i0^+} \\
&= n_i \frac{m}{\hbar^2} \int \frac{d\theta}{4\pi^2} |v(\theta)|^2 \int_{-\infty}^{\infty} d\varepsilon [P \frac{1}{\omega - \varepsilon} - i\pi\delta(\omega - \varepsilon)] \\
&= n_i \frac{m}{\hbar^2} \int \frac{d\theta}{4\pi^2} |v(\theta)|^2 [\int_{-\infty}^{\infty} d\varepsilon P \frac{1}{\omega - \varepsilon} - i\pi] \\
&= -\pi i n_i \rho \int \frac{d\theta}{2\pi} |v(\theta)|^2
\end{aligned}$$

Or, you can use the integral by contour methods. But NOTE that it can not use the $\int_R f(z)dz \mapsto 0$ to construct a closed region including a half plane, because here the power of denominator is only one larger than the power of numerator.

We can construct a contour as shown in Fig. 1.3, (if $\omega_n > 0$, $R \mapsto \infty$)

$$\begin{aligned}
I &= C_1 + C_2 + C_r + C_R + C_{-R} = 0 \\
C_1 &= \int_{-R}^{R} d\varepsilon \frac{1}{i\omega_n - \varepsilon} \\
C_R &= C_{-R} = 0 \\
C_r &= i(\pi - 2\pi) \cdot \frac{1}{i\omega_n - \varepsilon} (\varepsilon - i\omega_n) = i\pi \\
C_2 &= \int_{R}^{-R} d\varepsilon' \frac{1}{-\varepsilon'} = 0
\end{aligned}$$

So that $C_1 = -C_r = -i\pi$ and $\Sigma(i\omega_n) = -\pi i n_i \rho sgn(\omega_n) \overline{|v(\theta)|^2}$.

Some useful law in integral by contour methods

- For $\int_{-\infty}^{+\infty} R(x)dx$ and $R(x) = \frac{P(x)}{Q(x)}$, $P(x)(Q(x))$ is rational function with largest power of $p(q)$. IF $q > p + 2$ AND $R(z)$ has no singular point on real axis, $\int_{-\infty}^{+\infty} R(x)dx = 2\pi i \sum_k Res[R(z), z_k]$, where z_k are the singular points on the UP-half plane. Remember that if you choose the singular points on the LOW-half plane, the residue has a negative signal because the anti-clock direction is defined to be positive.
- For $\int_{-\infty}^{+\infty} R(x)e^{i\alpha x}dx$ $(\alpha > 0)$ and $R(x) = \frac{P(x)}{Q(x)}$, $P(x)(Q(x))$ is rational function with largest power of $p(q)$. IF $q > p + 1$ AND $R(z)$ has no singular point on real axis, $\int_{-\infty}^{+\infty} R(x)e^{i\alpha x}dx = 2\pi i \sum_k Res[R(z)e^{i\alpha x}, z_k]$, where z_k are the singular points on the

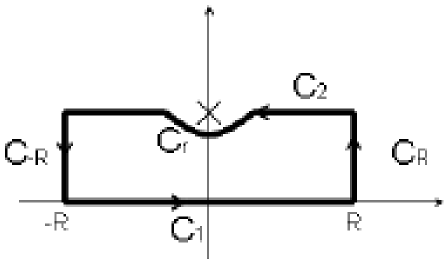

Figure 1.3: contour method for first-order Born approximation of self-energy.

UP-half plane. Remember that if $\alpha < 0$, one should choose the LOW-half plane due to the *Jordan-lemma*.

- (Small circle arc theorem) IF $f(z)$ is continuous on $0 < |z-a| < r$, $\theta_1 < arg(z-a) < \theta_2$, AND $lim_{z \mapsto a}(z-a)f(z) = A$, $lim_{r \mapsto 0} \int_{\Gamma_r} f(z)dz = i(\theta_2 - \theta_1)A$. This theorem can be used to calculate the integral on a line with some singular points. Remember that the arg is defined in anti-clock direction.

Or from Fermi Golden rule:

$$\begin{aligned} \tau^{-1} &= \frac{2\pi}{\hbar} n_i \int \frac{kdkd\theta}{4\pi^2} |v(k-k')|^2 \delta(\varepsilon(k) - \varepsilon(k')) \\ &= \frac{2\pi}{\hbar} n_i \rho \int \frac{d\theta}{2\pi} |v(\theta)|^2 = \frac{2\pi}{\hbar} n_i \rho \overline{|v(\theta)|^2} \end{aligned}$$

Finally, in this approximation, the averaged single-electron Green's function can be writtern as

$$G^{1BA}(\mathbf{p}, \epsilon_n) = \frac{1}{i\epsilon_n - \xi(p) + isign(\epsilon_n)\gamma_p} \tag{1.15}$$

$$G^R(p,t) = \int \frac{d\epsilon}{2\pi} \frac{e^{-i(\epsilon + i\delta)t}}{\epsilon - \xi(p) + i\gamma_p} = -i\Theta(t) e^{-i\xi(p)t} e^{-\gamma_p t} \tag{1.16}$$

So physically τ_p describes the damping of particle, by impurity. Spectral density, corresponding to the form of a simple Lorentzian:

$$A(\mathbf{p}, \epsilon) = -\frac{1}{\pi} Im G^R(\mathbf{p}, \epsilon) = \frac{1}{\pi} \frac{\gamma_p}{(\epsilon - \xi(\mathbf{p}))^2 + \gamma_p^2} \tag{1.17}$$

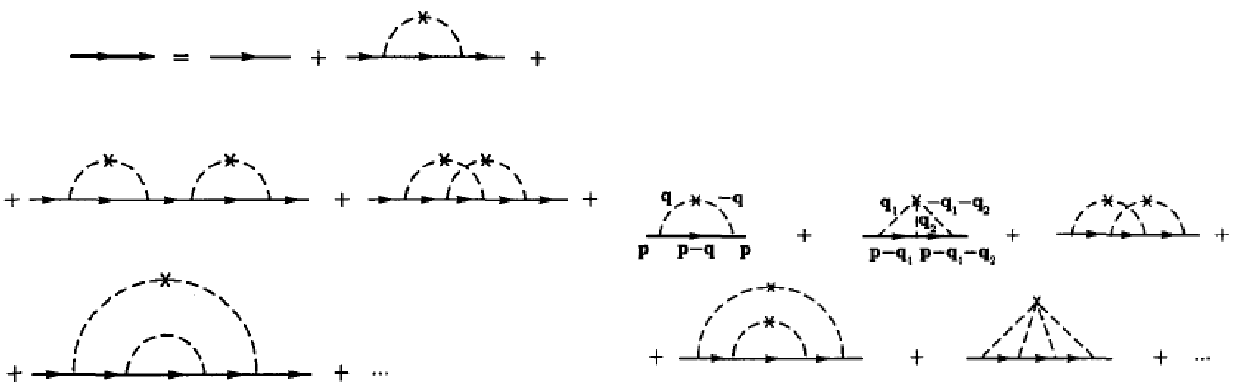

Figure 1.4: Diagrams representing different cumulants in the averaged perturbation series.

1st Born approximation is the most simplest approximation.

Moreover, one can think about the higher-order corrections, or self-consistent Born approximation:

$$\Sigma^{SCBA}(\mathbf{p},\epsilon_n) = n_{imp}\sum_{p'}|v(p-p')|^2\frac{1}{i\epsilon_n - \xi(p') - \Sigma^{SCBA}(\mathbf{p},\epsilon_n)} \tag{1.18}$$

But the solution is not so straight-forward (in principal it works). We neglect the discussion here.

1.2 Diffusion correction in conductivity

A metallic state in a disordered system can be approached perturbatively from the clean metallic state. In order to do so, we will need to handle the perturbation caused by impurity scattering. Let us imagine breaking our system into a large number N cells, each of which is macroscopic. Then the configuration of impurities in each cell will be different. If we compute an extensive quantity, such as the free energy, then it will be essentially (up to boundary terms) the sum of the free energies of each of the cells. Since each cell will have a different impurity configuration, the sum over cells will be an average over impurity configurations. Hence, the free energy in a disordered system can be computed by computing the free energy for a fixed realization of the disorder and then averaging over all realizations of the disorder (with respect to some probability distribution for the disorder). Such an approximation (which we take to be exact in the thermodynamic limit) for the free energy is called the quenched approximation and such an average is called a quenched average.

Let us consider the impurity model like :

$$\begin{aligned}\overline{V(\mathbf{r})} &= 0\\ \overline{V(\mathbf{r})V(\mathbf{r}')} &= n_i u^2 \delta(\mathbf{r}-\mathbf{r}')\end{aligned}$$

Now suppose that we average over $V(\mathbf{q}) = V(\mathbf{q}=\mathbf{k}-\mathbf{k}') =<\mathbf{k}'|V(\mathbf{r})|\mathbf{k}>= \int V(r)\exp(-i(\mathbf{k}'-\mathbf{k})\cdot\mathbf{r})\frac{d\mathbf{r}}{L^2}$. Let us consider, for simplicity, a distribution for $V(\mathbf{q})$ of the form

$$\begin{aligned}\overline{V(\mathbf{q})} &= 0\\ \overline{V(\mathbf{q})V(\mathbf{q}')} &= n_i u^2 \delta(\mathbf{q}+\mathbf{q}')/V\end{aligned}$$

where $n_i = N_i/V$ is the impurity concentration (dimensionless) and u is a measure of the strength of the scattering potential due to each impurity. All higher moments are taken to be factorizable into products of $\overline{VV}$. In other words, the diagrams is shown in Fig. 1.2.

The zero-th order of conductivity has been calculated before. Here we consider the disorder corrections to the Drude formula. To improve our calculation, let us now examine the vertex corrections that we have so far neglected. Let us now re-introduce the ladder vertex corrections as shown in Fig. 1.6, where the vertex correction is approximated by a sum of ladder diagrams.

We shall re-write the vertex part as a self-consistent Dyson equation, as follows:

$$ev_F\Lambda(\omega_r,\nu_n) = ev_F + \frac{n_i}{L^2}\sum_{\mathbf{p}'}|u(\mathbf{p}-\mathbf{p}')|^2\mathcal{G}(\mathbf{p}',i\omega_r^+)\mathcal{G}(\mathbf{p}',i\omega_r)\Lambda(\omega_r,\nu_n)ev'_F(\hat{\mathbf{p}}\cdot\hat{\mathbf{p}}') \quad (1.19)$$

Here we assume that the vertex part only depends on frequencies, and has no momentum dependence (so that the momentum in Green's function is simple), we may then write

$$\Lambda(\omega_r,\nu_n) = 1+\Lambda(\omega_r,\nu_n)n_i\int\frac{p'dp'd\theta}{(2\pi)^2}[|u(\theta)|^2\cos\theta]\mathcal{G}(p',i\omega_r^+)\mathcal{G}(p',i\omega_r)$$

where we introduce an anisotropic scattering for the transport $|u(p-p')|^2 = |u(\theta)|^2$, and $\cos\theta$ comes from the angle between $\mathbf{p}$ and $\mathbf{p}'$.

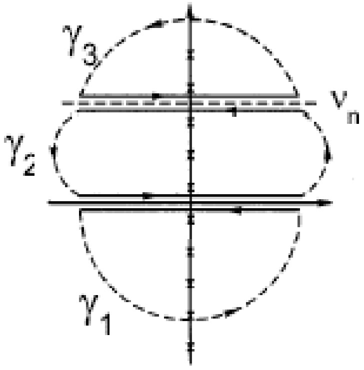

Figure 1.5: contour method for Duffsion mode.

Recall that, as shown in Fig. 1.2, (I neglect the $\hbar$ in all $\hbar/\tau$)

$$\begin{aligned}
&\int d\varepsilon \frac{1}{i\omega_r^+ - \varepsilon + isgn(\omega_r^+)/2\tau}\frac{1}{i\omega_r - \varepsilon + isgn(\omega_r)/2\tau} \\
&= Res[\frac{1}{i\omega_r^+ - \varepsilon + isgn(\omega_r^+)/2\tau}\frac{1}{i\omega_r - \varepsilon + isgn(\omega_r)/2\tau}, \varepsilon] \\
&= 2\pi i \left[\frac{1}{i\omega_r^+ - \varepsilon + isgn(\omega_r^+)/2\tau}\frac{1}{i\omega_r - \varepsilon + isgn(\omega_r)/2\tau}(\varepsilon - i\omega_r^+ - isgn(\omega_r^+)/2\tau)\right]\Big|_{\varepsilon = i\omega_r^+ + isgn(\omega_r^+)/2\tau} \\
&= -2\pi i \frac{1}{i\omega_r - i\omega_r^+ + isgn(\omega_r)/2\tau - isgn(\omega_r^+)/2\tau} \\
&= \frac{2\pi i}{i\nu_n + i\tau^{-1}} = \frac{2\pi i}{i\nu_n + i\hbar\tau^{-1}}
\end{aligned} \tag{1.20}$$

$$\begin{aligned}
\int \frac{p'dp'}{(2\pi)^2}\mathcal{G}(p', i\omega_r^+)\mathcal{G}(p', i\omega_r) &= \frac{m}{\hbar^2}\int \frac{d\varepsilon(p')}{4\pi^2}\frac{1}{i\omega_r^+ - \varepsilon}\frac{1}{i\omega_r - \varepsilon} \\
&= \frac{m}{4\pi^2\hbar^2}\frac{2\pi i}{i\nu_n + i\hbar\tau^{-1}} \\
&= \frac{m}{2\pi\hbar^2}\frac{1}{\nu_n + \tau^{-1}} = \rho\frac{1}{\nu_n + \hbar\tau^{-1}}
\end{aligned}$$

where $-\nu_n < \omega_r < 0$, otherwise is 0. Density of states in two-dimension is $\rho = \frac{m}{2\pi\hbar^2}$ (excluding spin degree). A simple proof is necessary ($\varepsilon = \frac{\hbar^2 k^2}{2m}$):

$$\begin{aligned}
dN &= V\rho(\varepsilon)d\varepsilon = \frac{V}{(2\pi)^2}2\pi k dk \\
\rho(\varepsilon) &= \frac{m}{2\pi\hbar^2}
\end{aligned}$$

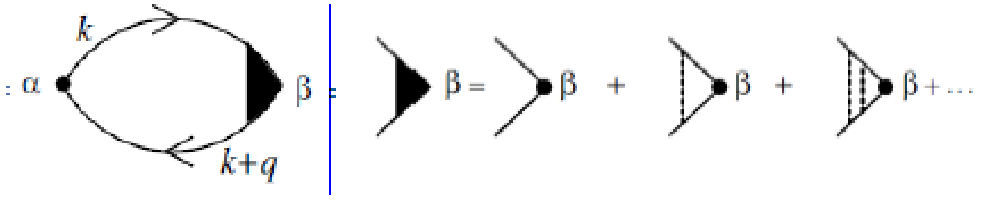

Figure 1.6: (a)Vertex correction to fermi-loop. (b) Ladder approximation of vertex diagram.

So, we obtain,

$$\Lambda \quad = \quad 1+\Lambda\frac{\hbar\tau_1^{-1}}{\nu_n+\hbar\tau^{-1}}\vartheta(-\nu_n<\omega_r<0)$$

where $\hbar\tau_1^{-1}=2\pi n_i\rho\overline{|u(\theta)|^2\cos\theta}$ and $\overline{|u(\theta)|^2}=\int\frac{d\theta}{2\pi}|u(\theta)|^2\cos\theta$.

So that,

$$\Lambda=\begin{cases}\frac{\nu_n+\hbar\tau^{-1}}{\nu_n+\hbar\tau_{tr}^{-1}}\vartheta(-\nu_n<\omega_r<0)\\ \qquad 0, otherwise.\end{cases} \tag{1.21}$$

where $\hbar\tau_{tr}^{-1}=\hbar\tau^{-1}-\hbar\tau_1^{-1}=2\pi n_i\rho\overline{(1-cos\theta)|u(\theta)|^2}$ is the transport scattering time (Please distinguish it from $\hbar/\tau$). For the isotropic scattering, the correction vanishes because of $cos\theta\mapsto 1$. Here τ is elastic scattering time, as obtained from self-energy calculation ($\frac{\hbar}{2\tau}=-Im\Sigma$).

Go to linear response theory and insert our vertex correction:

$$\begin{aligned}&\Pi_{xx}(q=0,i\nu_n)\\&=2e^2T\frac{k_F^2}{m}\sum_{i\omega_r}\int\frac{d\varepsilon(k)}{4\pi}\left[\frac{1}{i\omega_r^+-\varepsilon+isgn(\omega_r^+)\hbar/2\tau}\frac{1}{i\omega_r-\varepsilon+isgn(\omega_r)\hbar/2\tau}-(i\nu_n\mapsto 0)\right]\Lambda(i\omega_r,i\nu_n)\\&=\frac{2e^2k_F^2}{4\pi m}T\sum_{0>i\omega_r>-i\nu_n}\frac{2\pi i}{i\nu_n+i\hbar\tau^{-1}}\frac{\nu_n+\hbar\tau^{-1}}{\nu_n+\hbar\tau_{tr}^{-1}}\\&=\frac{n_se^2}{m}\frac{\nu_n}{\nu_n+\hbar\tau_{tr}^{-1}}\end{aligned} \tag{1.22}$$

The difference between zero-th order result (see previous chapter) and Eq. 1.22 is $\tau^{-1}\mapsto\tau_{tr}^{-1}$ (Note that $\hbar$ has been canceled by $i\nu_n\mapsto\hbar\nu+i0^+$).

$$\begin{aligned}\sigma_{xx}(\nu+i0^+)\quad&=\quad-\lim_{\nu\mapsto 0}\frac{Im\Pi_{xx}(q=0,i\nu_n\mapsto\nu+i0^+)}{\nu}\\&=\quad-\frac{n_se^2}{m}\lim_{\nu\mapsto 0}\frac{1}{\nu}Im\frac{-i\nu}{-i\nu+\tau_{tr}^{-1}}=\frac{n_se^2}{m}\tau_{tr}\end{aligned} \tag{1.23}$$

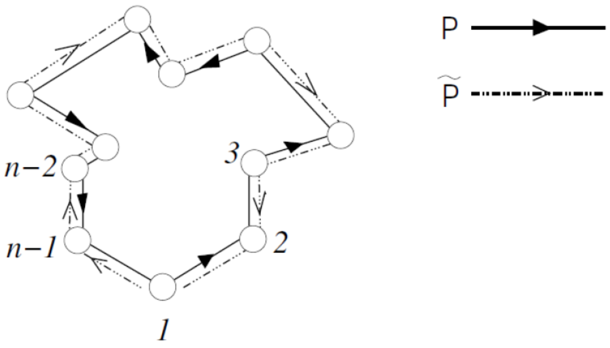

Figure 1.7: Scattering of an electron around two time-reversed paths.

1.3 Localization

We would like to finish our introduction to random impurities by touching on the concept of electron localization. In fact, disorder actually gives rise to collective interference effects within the electron gas, which ultimately lead to the localization of the electron wavefunction. This idea was proposed in 1958 by Philip W. Anderson, and subsequently named after him. Our modern understanding of electron localization was greatly aided by a conceptual breakthrough on this problem made by Don Liciardello and David Thouless, who proposed that the resistance of a material, or rather the inverse resistance, the conductance $G = 1/R$, is a function of scale. Thouless idea, initially proposed for one dimension, was taken up by the "Gang of Four", Elihu Abrahams, Philip W. Anderson, Don Licciardello, and Tirupattur Ramakrishnan, and extended to higher dimensions, leading to the modern scaling theory of localization.

To develop a rudimentary conceptual understanding of electron localization, we shall follow a heuristic argument by Altshuler, Aronov, Larkin and Khmelnitskii, (see also Bergman) who pointed out that weak localization results from the constructive interference between electrons passing along time-reversed paths. Weak localization is an interesting and rich phenomena that can arise from the nonclassical character of wave transport.

Consider the amplitude for an electron to return to its starting point. In general, it can do this by passing around a a sequence of scattering sites labelled 1 through n, as shown in Fig. 1.7,

$$\begin{aligned} A_P &= t_1 G(1,2) t_2 G(2,3) t_3 ... t_{n-1} G(n-1, n=1) t_n \\ &= A_0 \exp[i\mathbf{k}_i \cdot (\mathbf{r}_1 - \mathbf{r}) + i\mathbf{k}_{1,2} \cdot (\mathbf{r}_2 - \mathbf{r}_1) + ... + i\mathbf{k}_{n-1,n} \cdot (\mathbf{r}_n - \mathbf{r}_{n-1}) + i\mathbf{k}_f \cdot (\mathbf{r}' - \mathbf{r}_n)] \\ &\equiv \exp[i\mathbf{k}_i \cdot (\mathbf{r}_1 - \mathbf{r}) + i\mathbf{k}_f \cdot (\mathbf{r}' - \mathbf{r}_n)] \Pi_n A_n \end{aligned} \tag{1.24}$$

where $G(x_1, x_2)$ is the retarded propagator describing the amplitude for an electron of frequency to propagate between two sites.

Now for each path P, there is a corresponding time-reversed path $\widetilde{P}$ (at the same source point $\mathbf{r}$ and the same incident and exit wave vectors k_i, k_f as P. The amplitude for the same electron to follow $\widetilde{P}$ is

$$\begin{aligned} A_{\widetilde{P}} &= t_n G(n=1, n-1) t_{n-1} G(n-1, n-2) t_{n-2} ... t_2 G(2,1) t_1 \\ &= A_0 \exp[i\mathbf{k}_i \cdot (\mathbf{r}_n - \mathbf{r}) + i\mathbf{k}_{n,n-1} \cdot (\mathbf{r}_{n-1} - \mathbf{r}_n) + ... + i\mathbf{k}_{2,1} \cdot (\mathbf{r}_1 - \mathbf{r}_2) + i\mathbf{k}_f \cdot (\mathbf{r} - \mathbf{r}_1)] \\ &\equiv \exp[i\mathbf{k}_i \cdot (\mathbf{r}_n - \mathbf{r}) + i\mathbf{k}_f \cdot (\mathbf{r}' - \mathbf{r}_1)] \Pi_n A_n \end{aligned} \tag{1.25}$$

For time-reversal path, $\mathbf{k}_{i,i-1} = -\mathbf{k}_{i-1,i}$, so we find that the phase accumulated in the loop from $1 \rightarrow n$ and $n \rightarrow 1$ are identical.

The total probability associated with passage along both paths is given by

$$P = |A_P + A_{\widetilde{P}}|^2 = |A_P|^2 + |A_{\widetilde{P}}|^2 + 2Re[A_P A_{\widetilde{P}}] = p_1^2 + p_2^2 + 2p_1 p_2 cos(\phi_1 - \phi_2) \tag{1.26}$$

where $A_P = p_1 e^{i\phi_1}$ and $A_{\widetilde{P}} = p_2 e^{i\phi_2}$.

If the two paths were unrelated, then the impurity average of interference term would be zero, and we would expect $P = p_1 + p_2$. However, if the two paths are related by time-reversal, $A_{\widetilde{P}} = A_P$, with precisely the same magnitude and phase, and so the two processes always constructively interfere,

$$P = 4p_1^2$$

where we see that constructive interference between time-reversed paths doubles the return probability.

This means that an electron that enters into a random medium has an quantum mechanically

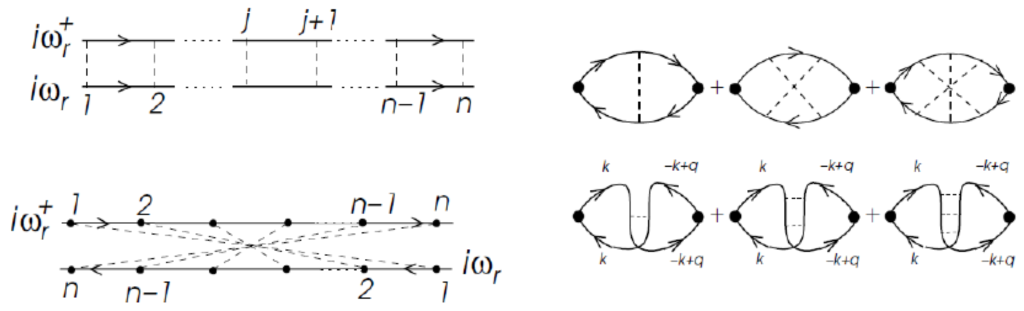

Figure 1.8: (a)n-th order contribution to the "Cooperon" (b)A twisted cooper diagram forms a maximally crossed diagram. (c) the maximally crossed contributions to the conductivity.

enhanced probability of returning to its starting point - quantum electrons "bounce back" twice as often as classical electrons in a a random medium! The same phenomenon causes the light from a car's headlamps to reflect backwards in a Fog. These effects tend to localize waves - causing light localization in the case of fog - and electron localization in disordered conductors. We shall see that the return probability is enhanced in lower dimensions, and in one, or two dimensions, these effects inevitably lead to the localization of electrons, for arbitrarily small amounts of disorder.

Let us now make a diagramatic identification of these interference terms. The complex conjugate of the retarded propagator is the advanced propagator

$$G^R(2-1,E)^* = G(2-1,E+i0^+)^* = G(1-2,E-i0^+) = G^A(1-2,E)$$

So the interference term

$$A_P^* A_P = \prod_{j=1}^{j=n-1} G^R(j+1,j)G^A(j+1,j) \tag{1.27}$$

which is represented by a "ladder diagram" for repeated scattering of electron pairs as shown in Fig. 1.8(a). The sum of all such diagrams is called a "Cooperon", because of its similarity to the pair susceptibility in superconductivity. Now if we twist the Cooperon around, we see that it is equivalent to a maximally crossed or "Langer-Neal" diagram, as shown in Fig. 1.8.

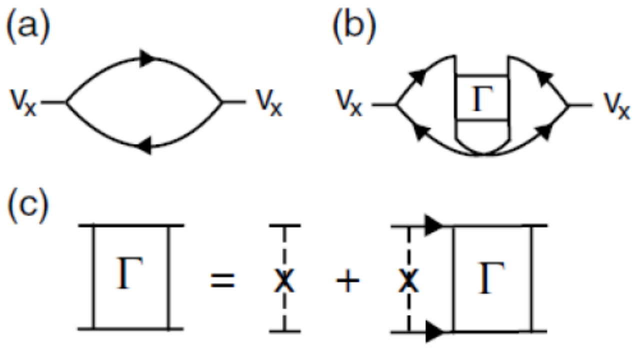

Figure 1.9: Diagrams for calculations of conductivity by Kubo formula: (a) Boltzmann conductivity, (b) weak-localization correction, and (c) Bethe-Salpeter equation for vertex function Γ. A line with an arrow represents an impurity-averaged Green function. A dashed line with a cross shows an averaged product of two impurity potentials, or a bare vertex function.

1.3.1 Weak localization

For quantum corrections to the Boltzmann conductivity we collect what is called maximally crossed diagrams. As shown in Fig. 1.9(b) the sum of them is expressed as (spin degree has not been included here: note that the conductivity is expressed by G^R and G^A):

$$\Delta\sigma_{xx} = \frac{e^2\hbar}{2\pi L^2}\sum_{\alpha,\beta} v^x_\alpha G^R_\alpha G^A_\alpha \Gamma_{\alpha\beta\beta\alpha} G^R_\beta G^A_\beta v^x_\beta \tag{1.28}$$

using the vertex function $\Gamma_{\alpha\beta\beta\alpha}$, where the dependence on E_F is not explicitly shown. Fig. 1.9(c) graphically shows the Bethe-Salpeter equation for $\Gamma_{\alpha\beta\beta\alpha}$:

$$\Gamma_{\beta\beta'\alpha\alpha'} = \Gamma^0_{\beta\beta'\alpha\alpha'} + \sum_{\mu,\mu'} \Gamma^0_{\beta\beta'\mu\mu'} G^R_\mu G^A_{\mu'} \Gamma_{\mu\mu'\alpha\alpha'} \tag{1.29}$$

where the bare vertex $\Gamma^0_{\beta\beta'\alpha\alpha'} =< U_{\beta\alpha}U_{\beta'\alpha'} >_{imp}$. Owing to the momentum conversation, we have,

$$q = k_\alpha + k_{\alpha'} = k_\beta + k_{\beta'} = k_\mu + k_{\mu'} \tag{1.30}$$

So as the zeroth order vertex, as shown in Fig. 1.2:

$$\begin{aligned} \Gamma^0_{\beta\beta'\alpha\alpha'} &= < U_{\beta\alpha}U_{\beta'\alpha'} >_{imp} \\ &= < U(q)U(-q) >_{imp} = n_i u^2/L^2 \end{aligned} \tag{1.31}$$

The quantity is important:

$$\begin{aligned}
&\Lambda(\mathbf{k},\mathbf{k}') = \frac{n_i u^2}{L^2}\sum_p G^R(\mathbf{k}-\mathbf{p})G^A(\mathbf{k}'+\mathbf{p}) = \frac{n_i u^2}{L^2}\sum_k G^R(\mathbf{k})G^A(\mathbf{q}-\mathbf{k})\\
&= n_i u^2 \int \frac{kdkd\theta}{4\pi^2}\frac{1}{E-\varepsilon(k)+i\frac{\hbar}{2\tau}}\frac{1}{E-\varepsilon(q-k)-i\frac{\hbar}{2\tau}}\\
&= n_i u^2 \int \frac{md\varepsilon(k)d\theta}{4\pi^2\hbar^2}\frac{1}{E-\varepsilon(k)-(\hbar^2q^2/2m)+(\hbar^2kqcos\theta/m)-i\frac{\hbar}{2\tau}}\frac{1}{E-\varepsilon(k)+i\frac{\hbar}{2\tau}}\\
&= \frac{mn_iu^2}{4\pi^2\hbar^2}\int d\theta 2\pi i\left[\frac{1}{\varepsilon(k)-E+(\hbar^2q^2/2m)-(\hbar^2kqcos\theta/m)+i\frac{\hbar}{2\tau}}\right]\Big|_{\varepsilon(k)=E+i\frac{\hbar}{2\tau}}\\
&= \frac{mn_iu^2\tau}{\hbar^3}\int\frac{d\theta}{2\pi}\frac{1}{1+i(\hbar vq\cos\theta\tau)}
\end{aligned} \tag{1.32}$$

Here we find the importance of the maximally crossed diagrams arises from the fact that

$$\Lambda(\mathbf{k},\mathbf{k}') = \frac{mn_iu^2\tau}{\hbar^3} \approx 1,\ if\ \mathbf{q} = \mathbf{k}+\mathbf{k}' = 0 \tag{1.33}$$

leading to a large contribution for $\mathbf{k}+\mathbf{k}'=0$. This is a manifestation of the enhanced backscattering that leads to phenomenon of weak localization. The conductivity correction due to WL arises primarily from a small angle of wavevectors around the backscattering direction defined by $q=0$, so we can expand Λ for small q:

$$\begin{aligned}
\Lambda(\mathbf{k},\mathbf{k}') &\approx \frac{mn_iu^2\tau}{\hbar^3}\int\frac{d\theta}{2\pi}\frac{1}{1+i(\hbar vqcos\theta\tau)}\\
&= \frac{mn_iu^2\tau}{\hbar^3}\int\frac{d\theta}{2\pi}\left(1-i\hbar vqcos\theta\tau-\hbar^2v^2q^2cos^2\theta\tau^2+...\right)\\
&\approx \frac{mn_iu^2\tau}{\hbar^3}\left(1-\frac{\hbar^2v^2q^2\tau^2}{2}\right)\\
&= \frac{mn_iu^2\tau}{\hbar^3}(1-\frac{\hbar^2v^2\tau^2q^2}{2}) \approx (1-\frac{\hbar^2v^2\tau^2q^2}{2}) = (1-D\tau q^2)
\end{aligned} \tag{1.34}$$

where $D = v^2\tau/d$ is the diffusion coefficient (d is the spatial dimension).

Using the self-consistent form:

$$\begin{aligned}
\Gamma_{\beta\beta'\alpha\alpha'} &= \Gamma^0_{\beta\beta'\alpha\alpha'} + \sum_{\mu,\mu'}\Gamma^0_{\beta\beta'\mu\mu'}G^R_\mu G^A_{\mu'}\Gamma_{\mu\mu'\alpha\alpha'} \\
\Gamma_{k,k'} &= \frac{n_iu^2}{L^2} + \sum_p \frac{n_iu^2}{L^2}G^R(k-p)G^A(k'+p)\Gamma_{k,k'} \\
&= \frac{n_iu^2}{L^2} + \Lambda(k,k')\Gamma_{k,k'} \\
\Rightarrow \Gamma_{k,k'} &= \frac{n_iu^2}{L^2}\frac{1}{1-\Lambda(k,k')} = \frac{n_iu^2}{L^2}\frac{1}{D\tau q^2}. \qquad (1.35)
\end{aligned}$$

So

$$\begin{aligned}
\Delta\sigma_{xx} &= \frac{e^2\hbar}{2\pi L^2}\sum_{\alpha,\beta}v^x_\alpha G^R_\alpha G^A_\alpha \Gamma_{\alpha\beta\beta\alpha}G^R_\beta G^A_\beta v^x_\beta \\
&= \frac{e^2\hbar}{2\pi L^2}\sum_{k,q}v^x_k v^x_{q-k}G^R_k G^A_k \Gamma_{k,k,q-k,q-k}G^R_{q-k}G^A_{q-k} \\
&\approx \frac{e^2\hbar}{2\pi L^2}\sum_q \Gamma(q)\sum_k v^x_k v^x_{-k}G^R_k G^A_k G^R_{-k}G^A_{-k} \\
&= \frac{e^2\hbar}{2\pi L^2}S\int\frac{qdqd\phi}{4\pi^2}\left(\frac{n_iu^2}{L^2}\frac{2}{(v_Fq\tau)^2}\right)S\int\frac{kdkd\theta}{4\pi^2}\left(-\frac{\hbar^2k^2cos^2\theta}{m^2}G^R_kG^A_kG^R_{-k}G^A_{-k}\right) \\
&= \frac{e^2\hbar}{2\pi}\int\frac{qdq}{2\pi}\left(\frac{n_iu^2}{1}\frac{2}{(v_Fq\tau)^2}\right)\int\frac{\varepsilon(k)d\varepsilon(k)}{2\pi\hbar^2}\left(-\frac{1}{(E-\varepsilon(k)+i\eta)^2(E-\varepsilon(k)-i\eta)^2}\right) \\
&= \frac{e^2\hbar}{2\pi}\left[\frac{-1}{2\pi\hbar^2}2\pi i\frac{d}{d\varepsilon}\frac{\varepsilon}{(\varepsilon-E+i\eta)^2}\right]\Big|_{\varepsilon=E+i\eta}\int_{l_\phi^{-1}}^{l^{-1}}\frac{dq^2}{4\pi}\left(\frac{n_iu^2}{1}\frac{2}{(v_Fq\tau)^2}\right) \\
&= \frac{e^2\hbar}{2\pi}\left[\frac{-1}{2\pi\hbar^2}\frac{2\pi E}{4\eta^3}\right]\frac{n_iu^2}{2\pi v_F^2\tau^2}ln\frac{l_\phi^2}{l^2} \\
&= -\frac{e^2}{\pi h}ln\frac{l_\phi}{l} \qquad (1.36)
\end{aligned}$$

where we have used that $E = mv^2/2$ and $\hbar/\tau = 2\pi n_iu^2\rho = n_iu^2m/\hbar^2$. In this calculation, the spin degree has not been included. Here we introduce two length scales: l_ϕ is phase coherence length and l is mean free path.

1.3.2 Anderson Localization

If we consider the case where inelastic scattering is negligible, the electrical conductivity is

$$\sigma = \sigma_0 - \delta\sigma$$
$$\delta\sigma = \frac{e^2}{2\pi h}\begin{cases}\frac{1}{\pi}(\frac{1}{l}-\frac{1}{L}), 3D\\ \ln\frac{L}{l}, 2D\\ 2(L-l), 1D\end{cases} \tag{1.37}$$

In 1D and 2D, one sees that the conductivity drops gradually to zero as the size of the sample increases. The conductivity becomes of order e^2/h at the localization length

$$L_c \sim le^{const.} \equiv \xi, 2D \tag{1.38}$$
$$L_c \sim l + \sigma_0\pi, 1D \tag{1.39}$$

At longer length scales, the material evolves into an insulator.

In 3D, the correction term doesnot diverge as $L \to \infty$. But it still has some condition for localization. Let us consider $\sigma = 0$ in the case of $L = \infty$ in 3D, which gives the localization condition:

$$1 > n_s h 2\pi/ml\tau = \frac{2\pi^3}{3}\rho v l^2 \tag{1.40}$$

Since ρ can become very small near the band edge (if vl^2 does not diverge), it is easily to see localization near the band edge. Moreover, taking $\rho = \frac{mk}{\hbar 2\pi^2}$ and $v = \frac{\hbar k}{m}$, the criterion for the localization becomes

$$kl \leq \sqrt{3/\pi} \sim 1. \tag{1.41}$$

This inequality is known as the Ioffe-Regel criterion for localization (Ioffe and Regel, 1960). The physical meaning is, on the simple physical notion that if the mean free path becomes comparable to the effective wavelength, then a wave can no longer be plane wave-like, and wave localization is postulated to occur.

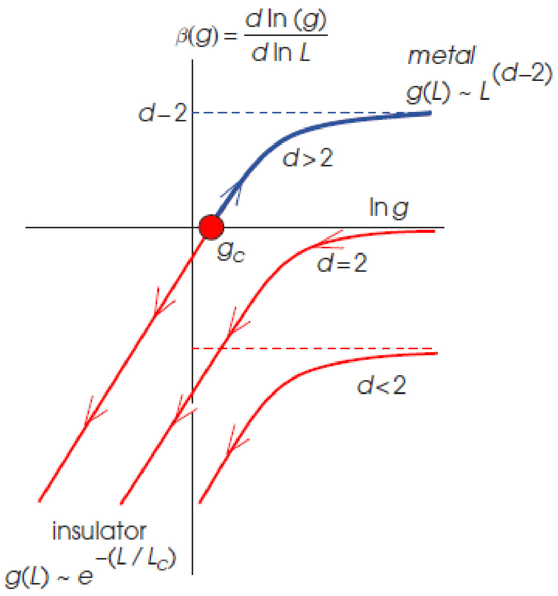

Figure 1.10: The scaling function $\beta(g)$ deduced by Abrahams et al. for a non-interacting metal. For $d > 2$ there is critical conductance g_c which gives rise to a disorder-driven metalinsulator transition. For $d \leq 2$ disorder always gives rise to localization and the formation of an insulator.

We shall end this section with a brief remark about the scaling theory of localization. Stimulated by the results in two dimensions, Abrahams et al. were led to propose that, in any dimension, conductance or inverse resistance $G = 1/R$ could always be normalized to form a dimensionless parameter

$$g(L) = \frac{G(L)}{e^2/h} \tag{1.42}$$

which satisfies a one-parameter scaling equation:

$$\frac{d \ln g(L)}{d \ln L} = \beta(g) \tag{1.43}$$

When conductivity is large we expect semi-classical approach in metal is valid, so we may use the Drude model, so that $g(L) = \frac{ne^2\tau}{m} L^{d-2}$ and

$$\beta(g) = d - 2, g \to \infty \tag{1.44}$$

When the conductance was small $g \to 0$ on scales longer than the localization length L_c, they argued that $g(L)$ would decay exponentially, $g(L) \approx \exp(-L/\xi)$, so

$$\beta(g) \sim \ln g, g \to 0 \tag{1.45}$$

By connecting these two asymptotic limits, "Gang of Four" reasoned that the beta function for conductance would take the form shown in Figure 1.10. In dimensions $d \leq 2$, $\beta(g)$ is always negative, so the conductance always scales to zero and electrons are always localized. However, in dimensions $d > 2$ there is a disorder-driven metalinsulator transition at the critical conductance $g = g_c$. As the amount of disorder is increased when the short-distance conductance g passes below g_c, the material becomes an insulator in the thermodynamic limit.

In 2D, from $\delta\sigma = -\frac{1}{\pi}\ln\frac{L}{l}$, we have

$$\frac{d\ln g}{d\ln L} = -\frac{1}{\pi g} \tag{1.46}$$

That means the β is always negative, so that all states in 2D are localized, no matter how weak the randomness. However, in some special system, like graphene, the delocalization is possible.

In 3D, g_c is usually non-zero, which leads to the "minimal conductance" as first proposed by Mott (Mott, 1975), i.e. the electrically conducting materials all have 3D conductivities larger than a certain minimum value.

In 3D, near g_c, we discuss the critical behavior

$$\beta(g) \sim s[\ln g - \ln g_c] = s\ln\frac{g}{g_c} \tag{1.47}$$

where s is the slope of the β function when it crosses zero at $\ln g_c$. From the definition

$$\frac{d\ln g}{\ln\frac{g}{g_c}} = sd\ln L \overset{integration}{\to} \frac{\ln(g/g_c)}{\ln g_0/g_c} = (L/l)^s, \tag{1.48}$$

where g_0 is the value of g at $L = l$. Let us define $\epsilon = \ln g_0 - \ln g_c$, so

$$\ln\frac{g}{g_c} = \epsilon(L/l)^s \to s^{-1} = \epsilon(\zeta/l)^s \to \zeta \sim l(s\epsilon)^{-1/s}, \tag{1.49}$$

since $\epsilon >> 1$, we have $\beta = d - 2 = 1 = s\ln(g/g_c)$ (by definition). Therefore, in 3D there is a length scale ζ, dubbed as correlation length, which defines the property of wave field in the extended regime. Close to the mobility edge $\epsilon \to 0$, we see $\zeta \to \infty$.

In the case of $\beta < 0$ or $\epsilon < 0$,

$$\ln \frac{g}{g_c} = -|\epsilon|(L/l)^s \to \ln \frac{g}{g_c} = -(L/(l|\epsilon|^{-1/s}))^s = -L/\xi, \tag{1.50}$$

because we know in the limit of $L \to \infty$, $\beta \propto \ln g \to s = 1$ (by assumption). So localization length ξ is determined by

$$\xi \sim l|\epsilon|^{-1/s} \sim l|\epsilon|^{-1} \tag{1.51}$$

which is divergent near the mobility edge (criticality).

The scaling law shown in Figure 1.10 can be verified numerically.

1.4 The coherent potential approximation for alloys

We consider a lattice system with the randomly distributed potentials:

$$H = \sum_{i,j} W_{ij} a_i^+ a_j + \sum_i V_i a_i^+ a_i \tag{1.52}$$

Here W_{ij} is the nearest-neighbor hoppings, and random potential V_i takes binary values: V_A on some lattice sites with possibility c while V_B on the other lattice site with possibility $1-c$. This type of discrete distribution mimics electrons in alloys, or electrons in amorphous semiconductors and in semiconductors containing high concentrations of impurities.

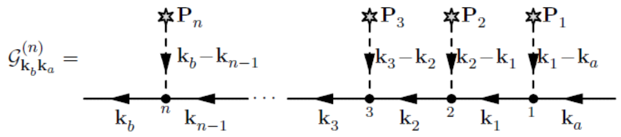

Figure 1.11: Diagrams scattering by (point-like) impurities.

1.4.1 Single-impurity T-matrix

We start this section by discussing the iterative solution in powers of U (the Born series). This series solution is defined by (see Fig. 1.11)

$$G(\mathbf{p}) = G^0(\mathbf{p}) + G^0(\mathbf{p})U(\mathbf{q}=0)G^0(\mathbf{p}) + G^0(\mathbf{p})\sum_{\mathbf{q}} U(\mathbf{q})G^0(\mathbf{p}+\mathbf{q})U(-\mathbf{q})G^0(\mathbf{p}) + \\ + G^0(\mathbf{p})\sum_{q,q'} U(\mathbf{q})G^0(\mathbf{p}+\mathbf{q})U(\mathbf{q}')G^0(\mathbf{p}+\mathbf{q}+\mathbf{q}')G^0(\mathbf{p}) + ... \tag{1.53}$$

The terms in this series can be represented by diagrams, describing multiple scattering processes of successively higher orders. An equivalent expansion is called the T-matrix:

$$\langle \mathbf{p}|t|\mathbf{p}\rangle = \langle \mathbf{p}|U|\mathbf{p}\rangle + \langle \mathbf{p}|U\frac{1}{E-H_0+i\eta}U|\mathbf{p}\rangle + \langle \mathbf{p}|U\frac{1}{E-H_0+i\eta}U\frac{1}{E-H_0+i\eta}U|\mathbf{p}\rangle + ... \tag{1.54}$$

In fact G and t are connected by the general operator relation

$$G = G^0 + G^0 t G^0 \tag{1.55}$$

Let us further define the self-energy function using Dyson equation $G = G^0 + G^0\Sigma G$, then one will get the relation between self-energy and T-matrix:

$$\Sigma = \frac{t}{1+G^0 t} \tag{1.56}$$

1.4.2 Average T-matrix approximation

To focus on the different impurities we write the operator V as a sum of contributions from the different sites:

$$T = V + VG_0V + VG_0VG_0V + ... = \frac{V}{1-G_0V} \tag{1.57}$$

where we define $V = \sum_i V_i$ (Please note that, this is not a single-impurity problem.)

Now we collect terms where consecutive scatterings take place at the same site and write

$$T = \sum_i V_i + \sum_i V_i G_0 \sum_j V_j + \sum_i V_i G_0 \sum_j V_j G_0 \sum_k V_k + ... \tag{1.58}$$

$$\begin{aligned} &= \sum_i [V_i + V_i G_0 V_i + V_i G_0 V_i G_0 V_i + ...] \\ &+ \sum_i [V_i + V_i G_0 V_i + V_i G_0 V_i G_0 V_i + ...] G_0 \sum_{j \neq i} [V_j + V_j G_0 V_j + V_j G_0 V_j G_0 V_j + ...] \\ &+ \sum_i [V_i + V_i G_0 V_i + ...] G_0 \sum_{j \neq i} [V_j + V_j G_0 V_j + ...] G_0 \sum_{k \neq i,j} [V_k + V_k G_0 V_k + ...] + ... \end{aligned} \tag{1.59}$$

In the above formula, the Green's function within the brackets always involves the propagation from one site back to the same site. (recall many results from the single-impurity T-matrix results)

Next we separate the Green's function to diagnoal part (proportional to the unit operator) and non-diagnoal part:

$$G_0 = G_D + G_0' \tag{1.60}$$

Using the definition of T-matrix, we have

$$\begin{aligned} T = \frac{V}{1 - G_0 V} &\to T(1 - G_0 V) = V \\ &\to T(1 - G_D V) - T G_0' V = V \\ &\to T = V(1 - G_D V)^{-1} + T G_0' V (1 - G_D V)^{-1} \end{aligned} \tag{1.61}$$

Next we denote the single-impurity T-matrix as t_i:

$$t_i = V_i [1 - G_D V_i]^{-1} \to V[1 - G_D V]^{-1} = \sum_i t_i \tag{1.62}$$

where we used the relation

$$\begin{aligned} t_i(1-G_DV_i) &= V_i \\ \rightarrow t_i &= V_i + t_iG_DV_i = V_i(V_i+t_iG_DV_i)G_DV_i = ... \\ t_i &= V_i + V_iG_DV_i + V_iG_DV_iG_DV_i + ... \\ \sum_i t_i &= \sum_i V_i + \sum_i V_iG_DV_i + ... \\ T &= = V(1-G_DV)^{-1} \end{aligned} \tag{1.63}$$

At last, if we assume the averaged T is independent of $V[1-G_DV]^{-1}$ (scattering by different impurity sites are independent), Eq. 1.61 will be simplified

$$\begin{aligned} &< T >=< \sum_i t_i > + < TG_0' \sum_i t_i > \approx < \sum_i t_i > + < T > G_0' < \sum_i t_i > \\ &\Rightarrow < T >= \frac{< \sum_i t_i >}{1 - G_0' < \sum_i t_i >} \end{aligned} \tag{1.64}$$

Especially, for the binary alloy disorder, the averaged single-impurity T-matrix is

$$< \sum_i t_i >= (1-c)t_A + ct_B \tag{1.65}$$

By further connecting the self-energy with T-matrix, we obtain

$$< \Sigma >= \frac{< T >}{1 + G^0 < T >} = \frac{< \sum_i t_i >}{1 + G_D < \sum_i t_i >} \tag{1.66}$$

1.4.3 Coherent potential approximation

The averaged T-matrix approximation ensures that we get the single-site scattering correct, but the scatterings from different impurities are ignored. The coherent potential approximation takes one step forward and use the average Green's function as the zeroth approximation, so some part of multi-scatterings can be accounted.

Based on the equation for G, we can induce the relations below:

$$\begin{aligned} & G = G_0 + G_0 V G = G_0 + G_0 V G_0 + ... \\ & \rightarrow G_0^{-1} G = 1 + V G \\ & \rightarrow (G_0^{-1} - \Sigma) G = 1 + (V - \Sigma) G \end{aligned} \tag{1.67}$$

Here the self-energy function Σ is to be determined. Accordingly to the Dyson equation, we have the averaged Green's function as

$$G_0^{-1} - \Sigma =< G^{-1} >\equiv G_M^{-1} \tag{1.68}$$

where $G_M \equiv< G >$ is the averaged Green's function of a new "medium" or mean-field solution.

By combining the above two equations Eq. 1.67 1.68, we have

$$G = G_M + G_M (V - \Sigma) G \equiv G_M + G_M T_M G_M \tag{1.69}$$

where $V - \Sigma$ is the perturbation and T_M is the T-matrix resulting from the this perturbation. We immediately have the relation:

$$G_M =< G >= G_M + G_M < T_M > G_M \Rightarrow< T_M >= 0 \tag{1.70}$$

which can be viewed as the self-consistent equation for Σ. If we could solve it exactly, the problem would be solved.

The coherent potential approximation is to replace the condition $< T_M >= 0$ by (see Eq. 1.64)

$$< t_i >= 0 \tag{1.71}$$

This means that we assume that in the medium the average scattering by a single impurity is zero.

For binary alloy,

$$
\begin{aligned}
< t_i >= 0 \rightarrow (1-c)t_A + ct_B = 0 \\
t_{A/B} = \frac{V_{A/B} - \Sigma(\omega)}{1 - G_M(\omega)(V_{A/B} - \Sigma(\omega))} \\
\Rightarrow \Sigma(\omega) - V_A = \frac{c(V_B - V_A)}{1 - G_M(\omega)[V_B - \Sigma(\omega)]}
\end{aligned}
\tag{1.72}
$$

At each site, we therefore have a potential $V_A - \Sigma(\omega)$ or $V_B - \Sigma(\omega)$ which now depends on energy. For a given host band structure, Eq. 1.72 and Eq. 1.68 form a closed loop to determine Σ for the medium and hence the average band structure for the disordered system.