Boltzmann and kinetic equations

Boltzmann equation: semiclassical equation to describe nonequilibrium systems (e.g. transport)

Afterwards: derivation within NGF theory, and quantum generalisation

Distribution function $f(\vec{R}, \vec{P}, t)$

$f(\vec{R}, \vec{P}, t)\, \Delta^3 R\, \Delta^3 P =$ N. of particles in the corresponding phase space volume element at time t

(we can generalize considering band indices and crystal momentum)

in equilibrium for an homogenous system: $f = f_F(\mathcal{E}_P)$ Fermi func.

6.5.11A

For a quantum system, of course, $\Delta R, \Delta P$ cannot be infinitesimal but must be coarse grained $\Delta R \Delta P \gg h$

Consider now the action of an external field $\mathcal{U}(\vec{R}, t)$

$$\dot{\vec{P}} = \vec{F} = -\vec{\nabla}_R\, \mathcal{U}$$

$$\dot{\vec{R}} = \vec{v} = \vec{\nabla}_P\, \mathcal{E}(P)$$

semiclassical eq. of motion

In the absence of scattering between particles, thus

$$f(\vec{R}, \vec{P}, t) = f(\vec{R} - \vec{v}\Delta t, \vec{P} - \vec{F}\Delta t, t - \Delta t)$$

to linear order in Δt

$$\Delta t \left(\vec{v} \cdot \vec{\nabla}_R f + \vec{F} \cdot \vec{\nabla}_p f + \frac{\partial f}{\partial t} \right) = 0$$

if we assume a further modification of f due to scattering

$$(\Delta f)_s = \left(\frac{\partial f}{\partial t} \right)_s \Delta t$$

we get the Boltzmann equation

$$\vec{v} \cdot \vec{\nabla}_R f + \vec{F} \cdot \vec{\nabla}_p f + \frac{\partial f}{\partial t} = \left(\frac{\partial f}{\partial t} \right)_s \qquad (C0)$$

we will discuss the last term later

The treatment follows in general the Book by Haug and Jauho, although there are some small differences

Start from Dyson equation

$$G = G_0 + G_0 * (\Sigma + U) * G$$

for simplicity of notation, we now omit the "$*$"

we have separated the contr. from pure external potential U and the rest (Σ)

$$\left(G_0^{-1} - U\right) G = I + \Sigma G \qquad \text{(C1)}$$

The retarded (1,1) component of this equation gives (see "useful relations" on p. 35)

(cf.A9)

$$\left(G_{0r}^{-1} - U - \Sigma_r\right) G_r = I \qquad \text{(C1A)}$$

Similarly, the Keldysh (1,2) component gives (cf. A10)

$$\left(G_0^{-1} - U\right)_r G_K + \left(G_0^{-1} - U\right)_K G_a = 0 + \Sigma_r G_K + \Sigma_K G_a$$

we have already seen that (apart for singularities) $G_{0K}^{-1} = 0$

We have learned that it is justified to neglect these singularities when the free system is interacting with a continuum which provides a dissipation mechanism.

In the same spirit, we shall neglect the singularities in

G_{0r}^{-1}, G_{0a}^{-1} and we set them equal

we thus obtain

$$\left(G_{0r}^{-1} - U\right) G_K = \Sigma_r G_K + \Sigma_K G_a$$

similarly, the "right-hand" Dyson equation

$$G = G_0 + G \Sigma G_0$$

yields

$$G_K \left(G_{0a}^{-1} - U\right) = G_r \Sigma_K + G_K \Sigma_a$$

as discussed above, we set $G_{0a}^{-1} = G_{0r}^{-1}$

subtracting the two equations we obtain

$$\boxed{\left[G_{0r}^{-1} - U, G_K\right] = \Sigma_r G_K + \Sigma_K G_a - G_r \Sigma_K - G_K \Sigma_a} \tag{C2}$$

commutator

This is (essentially) the generalized Kadanoff-Baym (GKB) equation (to be precise one needs a further symmetrisation between r and a quantities), which is the im principle exact quantum kinetic equation.

Below, we will further transform the r.h.s. to obtain an expression similar to, .e.g. Haug-Jauho

Since there is no translation invariance neither in time nor in space, we should work in real time and space, so that all objects have to be interpreted as matrices in time and space, and the expressions above have to be interpreted as matrix products in time and real space, i. e. convolutions, for example

using the notation $X_i = (t_i, r_i)$

$C = AB$ has the meaning

$$C(X_1, X_2) = \int dX_3 \, A(X_1, X_3) B(X_3, X_2)$$

(C2B)

It is convenient to introduce Wigner coordinates

$$X = \frac{X_1 + X_2}{2} = (T, \vec{R}) \qquad x = X_1 - X_2 = (t, \vec{r})$$

and inverse

$$X_1 = X + \frac{x}{2} \qquad X_2 = X - \frac{x}{2}$$

(C3)

in general, one carries out a Fourier transform over the relative coordinates $x \rightarrow P = (\omega, \vec{p})$

$$C(P, X) = \int d^4x \, e^{iP\cdot x} \, C\Big(\overset{X_1}{\overset{''}{X + \frac{x}{2}}}, \overset{X_2}{\overset{''}{X - \frac{x}{2}}}\Big)$$

(C4)

we define for convenience a Minkowski-like scalar product

$$P\cdot x = \omega t - \vec{p}\cdot\vec{r}$$

(C4A)

We now quote without proof a useful relation for convolutions (see Haug - Jauho's book)

(cf. C2B)

$$C = A\,B$$

$$C(P,X) = A(P,X)\,\hat{G}(P,X)\,B(P,X)$$ (C5)

where $\hat{G}$ is an operator acting on left and right variables:

$$\hat{G}(P,X) = \exp\left(\frac{1}{2i}\left(\overleftarrow{\partial}_X\cdot\overrightarrow{\partial}_P - \overleftarrow{\partial}_P\cdot\overrightarrow{\partial}_X\right)\right)$$ (C6)

where the arrow indicate on which side the differential operator acts, and the scalar products are again Minkowski-like

$$\overleftarrow{\partial}_X\cdot\overrightarrow{\partial}_P \equiv \overleftarrow{\partial}_T\,\overrightarrow{\partial}_W - \overleftarrow{\partial}_{\vec{R}}\,\overrightarrow{\partial}_{\vec{P}}$$ (C7)

Of course, for translation invariance, the quantities do not depend on X , so that

$$\hat{G} = I$$

and one recovers the well-known result that

$$C(P) = A(P)\,B(P)$$

(Fourier transform of convolution)

Let us now apply this to the GKB equation (cf.C2)

$$\left[G_{0r}^{-1}-U,\, G_K\right] = \Sigma_r G_K + \Sigma_K G_a - G_r \Sigma_K - G_K \Sigma_a$$

The assumption for Boltzmann equation to be valid is that the fields change slowly as a function of time and space. This means that gradients and time derivatives are small and we can restrict to lowest order in those derivatives ("gradient expansion"), which amounts to using

(cf.C6)

$$\mathcal{G}(P,X) \approx 1 + \frac{1}{2i}\left(\overleftarrow{\partial}_X \overrightarrow{\partial}_P - \overleftarrow{\partial}_P \overrightarrow{\partial}_X\right) \qquad \text{(C8)}$$

first observe that

$$G_{0r}^{-1}(P,X) = W - \varepsilon(\vec{p}) = G_{0r}^{-1}(P)$$

$$U(X_1,X_2) = U(X_1)\,\delta(X_1 - X_2)$$

(cf. C4) $\Rightarrow$ $$U(P,X) = U(X)$$

it is convenient to express the action of the "commutator" term (lhs of the GKB equation) on a generic function $\mathcal{F}$ in the form

(valid within the gradient expansion)

$$\left[G_{0r}^{-1}-U,\ \mathcal{F}\right] = i\hat{\mathcal{L}}\,\mathcal{F} \qquad \text{(C9)}$$

with the differential operator $\hat{\mathcal{L}}$

$$i\hat{\mathcal{L}} = i\left(\partial_T + \vec{v}\,\partial_{\vec{R}} + (\partial_x U)\cdot\partial_p\right)$$

$$v = v_{\vec{p}} = \frac{\partial \varepsilon(\vec{p})}{\partial \vec{p}}$$

(if not specified derivative apply to the righ)

Proof:

first of all the "1" term in C8 cancels in the commutator
the second term is already a commutator, and thus simply acquires a 2

$$\left[G_{0r}^{-1}-U,\ \mathcal{F}\right] = \frac{1}{i}\left(G_{0r}^{-1}-U\right)\left(\overleftarrow{\partial}_x\cdot\overrightarrow{\partial}_p - \underbrace{\overleftarrow{\partial}_p\cdot\overrightarrow{\partial}_x}_{\overleftarrow{\partial}_\omega\overrightarrow{\partial}_T - \overleftarrow{\partial}_{\vec{p}}\cdot\overrightarrow{\partial}_{\vec{R}}}\right)\mathcal{F} \qquad \text{(cf. C7)}$$

$$= -i\left(-(\partial_x U)\,\partial_p - \partial_T - \frac{\partial\varepsilon(\vec{p})}{\partial\vec{p}}\,\partial_{\vec{R}}\right)\mathcal{F}$$

explicitly, we can write, again using (C7):

$$i\hat{\mathcal{L}} = i\left(\partial_T + \vec{v}\,\partial_{\vec{R}} + \vec{F}\,\partial_{\vec{p}} + (\partial_T U)\,\partial_\omega\right) \qquad \text{(C10)}$$

$$\vec{F} = -\partial_{\vec{R}}U \qquad \text{(cf. C0)}$$

We need the following property:

if $\mathcal{F}$ is a function of $G_{0r}^{-1} - U$ only, we have

(cf. C10)

$$\mathcal{L}^{1}\mathcal{F}\left(G_{0r}^{-1} - U\right) = \mathcal{L}^{1}\mathcal{F}\left(W - \varepsilon(\vec{p}) - U\right) = 0$$

(C11)

which can be seen by explicit replacement, or by observing that in that case $\mathcal{F}$ commutes with $G_{0r}^{-1} - U$

Before going on, let us observe that in the lowest (nonzero) order of the
gradient expansion, the equation for the retarded Green's function

(cf. C1A)

$$\left(G_{0r}^{-1} - U - \Sigma_r \right) G_r = I$$

is quite simply obtained by setting $\xi = 1$, i. e.

$$G_r(P,X) = \left(w - \varepsilon(\vec{p}) - U(X) - \Sigma_r(P,X) \right)^{-1}$$

and similarly for the advanced

And indeed, it is sufficient to use the lowest order for G_r and G_a

in the GKB equation (C2), since there one has terms like $\Sigma_r G_a - G_r \Sigma_a$

which are already first order in the gradient expansion (commutators)

Quasiparticle Approximation

The Boltzmann equation relies on the "quasiparticle approximation"
according to which one neglects Σ in G_r and G_a
(in some cases one could also introduce a renormalisation of the
single-particle energy originating from Σ)

$$\Rightarrow \quad G_r(P,X) = \left(w - \varepsilon(\vec{p}) - U(x) + i 0^+ \right)^{-1}$$

(C12)

the spectral function reads

$$A(P,X) = \frac{i}{2\pi}\left(G_r - G_a \right) = \delta\left(w - \varepsilon(\vec{p}) - U \right)$$

(C13)

In order to make progress, we express the Keldysh Green's function in a form similar to equilibrium

$$G_K = \left(G_r - G_a\right) S(P,X)$$

$$= -2\pi i\, A(P,X)\, S(P,X) \qquad \text{(C14)}$$

$$S(P,X) = \left(1 - 2f(P,X)\right) \qquad \text{(fermions)}$$

Remember, in equilibrium $f(P,X) = n(\omega) = f_F(\omega)$

was the distribution function.
In this nonequilibrium case, we can interpret $f(P,X)$ as the nonequilibrium distribution function. The central quantity in Boltzmann's theory

In principle, $f(P,X) = f(\omega, \vec{p}, T, \vec{R})$

However, due to the δ originating from $A(P,X)$ (cf. C13), we can eliminate ω in favor of the other variables and write C14 as

$$G_K = -2\pi i\, \delta\left(\omega - \varepsilon(\vec{p}) - U\right)\left(1 - 2f(\vec{p}, X)\right)$$

Let us now apply the lhs of the GKB equation (C2 with C9)

$$\hat{\mathcal{L}} G_K = 4\pi i\, A(P,X)\, \hat{\mathcal{L}} f(\vec{P},X) \qquad \text{(C15)}$$

where we have used the fact that (cf. C11),

$\hat{\mathcal{L}} A = 0$ since A is a function of $G_{0r}^{-1} - U$

In the absence of scatterings, i. e. $\Sigma = 0$

the GKB equation (C2) without self-energy, thus reads

$$\delta\left(W - \varepsilon(\vec{P}) - U\right) \hat{\mathcal{L}} f(\vec{P},X) = 0$$

since f does not depend on W. We thus have:

$$\left(\partial_T + \vec{v}\,\partial_{\vec{R}} + \vec{F}\,\partial_{\vec{P}}\right) f(\vec{P},X) = 0$$

which is identical to the Boltzmann equation (C0) in absence of scattering

The scattering term can be then derived from the r.h.s. of the GKB equation (C2) upon setting $W = \varepsilon(\vec{P}) + U(X)$

(6.9.11 B)

Self-energy term

We now work on the rhs of the GKB equation (C2) , we always restrict to the lowest order in the gradient expansion

$$\Sigma_r G_K - G_K \Sigma_a + \Sigma_K G_a - G_r \Sigma_K$$

we introduce

$$\Sigma = \frac{\Sigma_r + \Sigma_a}{2} = \mathrm{Re}\, \Sigma_r$$

$$\Sigma_- = \frac{\Sigma_r - \Sigma_a}{2}$$

$$\Rightarrow \quad \Sigma_{\substack{r \\ a}} = \Sigma \pm \Sigma_- \qquad \text{(C16)}$$

we obtain

$$\Sigma_r G_K - G_K \Sigma_a = [\Sigma, G_K] + \underset{\text{anticommutator}}{\{\Sigma_-, G_K\}}$$

similarly for G (with analogous definitions to C16)

$$G_r \Sigma_K - \Sigma_K G_a = [G, \Sigma_K] + \{G_-, \Sigma_K\}$$

inserting in the GKB equation (C2) yields

$$\left[G_{0r}^{-1} - U, G_K\right] = \left[\Sigma, G_K\right] - \left[G, \Sigma_K\right] + \left\{\Sigma_-, G_K\right\} - \left\{G_-, \Sigma_K\right\}$$

$$\left[G_{0r}^{-1} - U - \Sigma, G_K\right] + \left[G, \Sigma_K\right] = -i\pi\left(\left\{\Gamma, G_K\right\} - \left\{A, \Sigma_K\right\}\right)$$

where we have introduced the spectral functions

(C17)

$$-2i\pi A = G_r - G_a$$

$$-2i\pi\Gamma = \Sigma_r - \Sigma_a$$

(C17A)

This is actually the standard form of the GKB equation
so far this is exact, i. e. not restricted to the gradient expansion

remember, the "products" in this equation are convolutions
over internal variables

Scattering term in the Boltzmann equation

For the Boltzmann equation, we assume that gradients are small, and self energies are small.

In the GKB equation commutators [...] are proportional to gradients square (cf. C8), so that, at this order, we can neglect self-energies within [...]

Moreover, in the same approximation, we can replace anticommutators {...} by (twice) simple products.

In this way, (C17) with (C9) yields

$$i\hat{\mathcal{L}}\, G_\kappa(p,X) = 2i\pi\Big(A(p,X)\,\Sigma_\kappa(p,X) - \Gamma(p,X)\,G_\kappa(p,X)\Big) \tag{C18}$$

As discussed earlier (cf. C15), the left hand side produces the "flow" term of the Boltzmann equation (C0). The right h.s., is thus the scattering term.

We will evaluate this term, which is of course important, since it, ultimately, leads to equilibrium, for the simple case of scattering from impurities

Scattering from impurities

we evaluate this term for the case of
scattering from diluted random impurities

for this case the self-energy can be obtained within the
self-consisten Born approximation (we will show this later)

$$\Sigma_h(P,X) = c\int d_3p' \, |V(\vec{p}-\vec{p}')|^2 \, G_h(P',X) \tag{C19}$$

this equation holds for all three self energies $h = k, r, a$

Notation $\quad d_D q = \dfrac{d^D q}{(2\pi)^D} \qquad \delta_D(q \ldots) = (2\pi)^D \delta^D(q \ldots)$ (C19A)

D = dimension

To get Γ (C17A) one simply has to replace G with A in C19

c is the impurity concentration and V the potential

The rhs of the Boltzmann equation (C18) becomes

$$2i\pi c\int d_3p' |V(\vec{p}-\vec{p}')|^2 \Big(A(P,X)\, G_K(P',X) - A(P',X)\, G_K(P,X) \Big)$$

inserting the expression for G_K from the quasiparticle approxim. (C14):

$$= 4\pi^2 c\int d_3p' |V(\vec{p}-\vec{p}')|^2 \, A(P,X)\, A(P',X) \Big(S(P',X) - S(P,X) \Big)$$

$$= 8\pi^2 C\int d_3p'\,|V(\vec p-\vec p')|^2 A(p,x)A(p',x)\big(f(p,x)-f(p',x)\big)$$

(C20)

The lhs is (cf. C15)

$$i\hat{\mathcal{L}}\,G_K = -4\pi\,A(p,x)\,\hat{\mathcal{L}}\,f(\vec p,x)$$

using again $A(p,x) = \delta(w-\varepsilon(\vec p)-U)$

and integrating over w both sides (cf. C18,C20)
(leading to $w \to \varepsilon(\vec p)+U$)

and dividing both sides by $-4\pi\,A(p,x)$ yields:

this was the $A(\vec p',x)$

$$\hat{\mathcal{L}}\,f(\vec p,x) = 2\pi\,C\int d_3p'\,|V(\vec p-\vec p')|^2\,\delta(\varepsilon(\vec p)-\varepsilon(\vec p'))\big(f(\vec p',x)-f(\vec p,x)\big)$$

using (C10), and since f does not depend on w

$$\boxed{\begin{aligned}&(\partial_T+\vec v\,\partial_{\vec R}+\vec F\,\partial_{\vec p})\,f(\vec p,x) = \\ &\qquad = 2\pi\,C\int d_3p'\,|V(\vec p-\vec p')|^2\,\delta(\varepsilon(\vec p)-\varepsilon(\vec p'))\big(f(\vec p',x)-f(\vec p,x)\big)\end{aligned}}$$

(C21)

which identifies the scattering term (cf. C0) $\left(\frac{\partial f}{\partial t}\right)_s$

Interpretation: $f(p,x)$ decreases due to a scattering from p to p' with prob. $\propto f(p,x)$
and increases due to a scattering from p' to p with prob. $\propto f(\vec p',x)$

The delta enforces energy conservation

Random impurity potential

(see, e.g. Bruus-Flensberg)

We have impurities with concentration c at random positions $\vec{y}_n$

$$V(\vec{x}) = \sum_n v(\vec{x} - \vec{y}_n)$$

$$= \sum_n \int d_3 q \, e^{iqx} e^{-iqy_n} v(q) \tag{C22}$$

Notation $d_D q = \frac{d^D q}{(2\pi)^D}$ $\quad \delta_D(q\cdots) = (2\pi)^D \delta^D(q\cdots)$

D = dimension

$$V(\vec{q}) = \sum_n \int d\vec{x} \, e^{-i\vec{q}(\vec{x}+\vec{y}_n)} v(\vec{x})$$

$$= \sum_n e^{-i\vec{q}\vec{y}_n} v(\vec{q}) \tag{C23}$$

Impurity average: average over the positions y_n

$$\overline{V(\vec{q})} = \frac{1}{VOL} \sum_n \int dy_n \, e^{-i\vec{q}\vec{y}_n} v(\vec{q})$$

$$= c \, v(\vec{q}=0) \, \delta_D(q) \tag{C24}$$

$$\overline{V}(x) = c \, v(\vec{q}=0) \equiv \overline{V} \quad \text{independent of } x \tag{C25}$$

(cf. C22)

Second-order term:

$$\overline{V(\vec{q}_1)V(\vec{q}_2)} = \frac{1}{\mathrm{vol}^2}\sum_{n\neq m}\int dy_n\, dy_m\, e^{-iq_1 y_n}\, e^{-iq_2 y_m}\, v(\vec{q}_1)\, v(\vec{q}_2)$$

$$+ \frac{1}{\mathrm{vol}}\sum_{n}\int dy_n\, e^{-i(q_1+q_2)y_n}\, v(q_1)\, v(q_2)$$

$$= c^2\, \delta_3(q_1)\,\delta_3(q_2)\, v(0)^2$$

$$+ c\, \delta_3(\vec{q}_1+\vec{q}_2)\, v(q_1)\, v(q_2) \qquad \text{(C26)}$$

in real space

$$\overline{V(x)V(y)} = \int \frac{dq_1}{(2\pi)^3}\frac{dq_2}{(2\pi)^3}\, e^{iq_1 x}\, e^{iq_2 y}\, \overline{V(q_1)V(q_2)}$$

$$= \underbrace{c\int \frac{dq}{(2\pi)^3}\, e^{iq(x-y)}\, |v(q)|^2}_{} + \bar{V}^2$$

$$\equiv \overline{V^2}(x-y) \qquad \text{(C27)}$$

In general, one can write , e.g.

$$\overline{V(q_1)V(q_2)V(q_3)} = \overline{V(q_1)}\;\overline{V(q_2)V(q_3)}^{c} + \overline{V(q_1)V(q_3)}^{c}\;\overline{V(q_2)} + \overline{V(q_1)V(q_2)}^{c}\;\overline{V(q_3)} + \overline{V(q_1)}\;\overline{V(q_2)}\;\overline{V(q_3)} + \overline{V(q_1)V(q_2)V(q_3)}^{c}$$

Sum over connected terms

$\overline{V\cdots V}^{c}$ = connected average

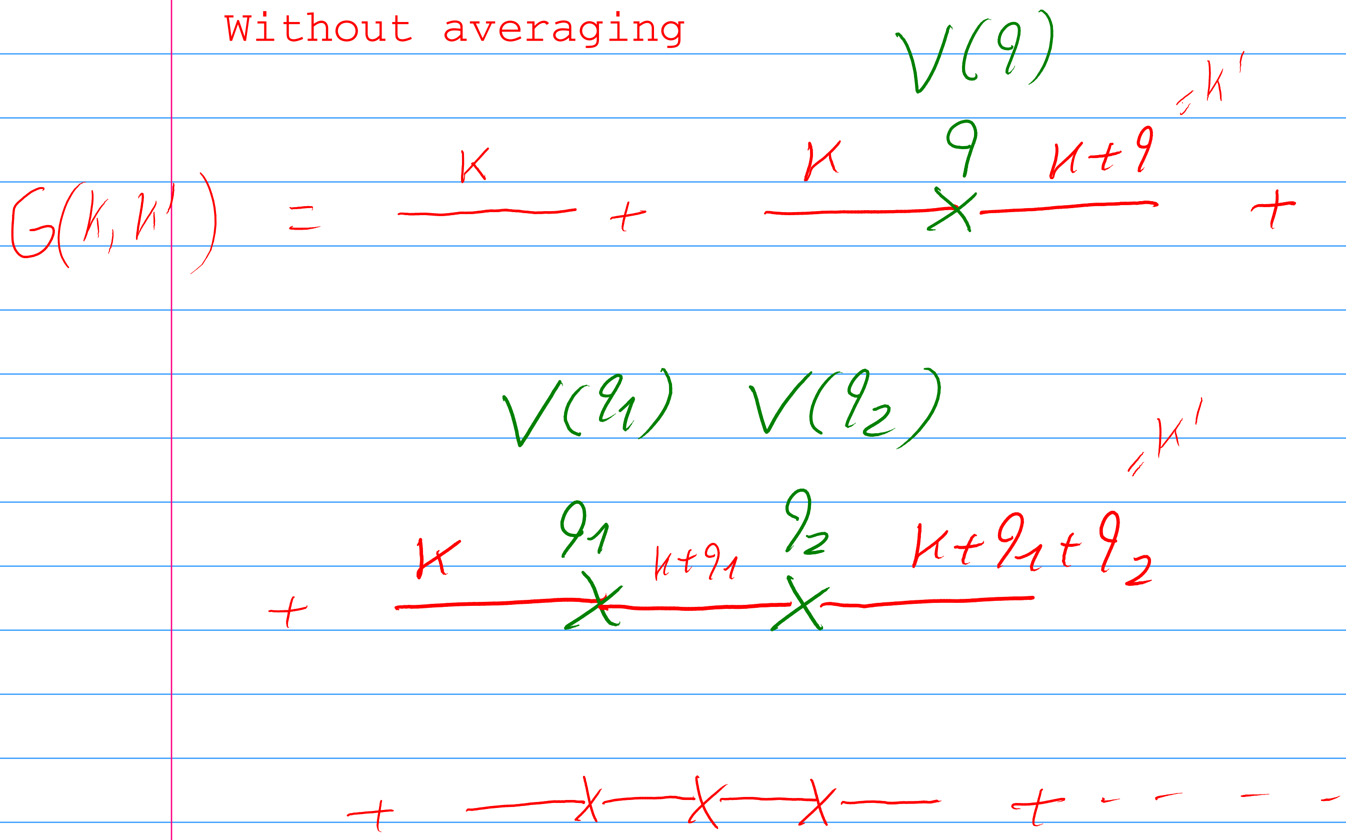
In this case, the connected average in the sum above runs over just one impurity index, e.g.

$$\overline{V(q_1)V(q_2)V(q_3)}^{C} = \frac{1}{Vol}\sum_n \int dy_n\, e^{-i(q_1+q_2+q_3)y_n}\, v(q_1)\, v(q_2)\, v(q_3)$$

$$= C\,\delta_D(q_1+q_2+q_3)\, v(q_1)\, v(q_2)\, v(q_3) \qquad \text{(C28)}$$

Diagrams

Without averaging

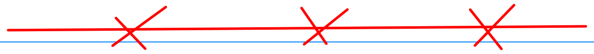


Momentum is obviously not conserved

Impurity averaging

consider one contribution

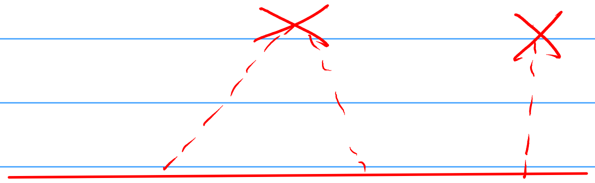
$$\overline{V(q_1)\quad V(q_2)\quad V(q_3)}$$ averaging



average: sum over connected contributions

we indicate the connected terms by linking the X together

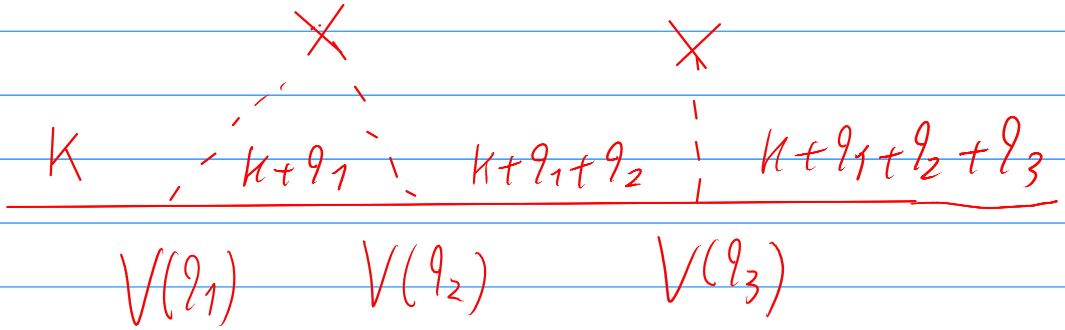
Example



$V(q_1)\quad V(q_2)\quad V(q_3)$

$$\to \overline{V(q_1)V(q_2)}^{c}\;\overline{V(q_3)}$$

let us introduce the momenta of the Green's functions

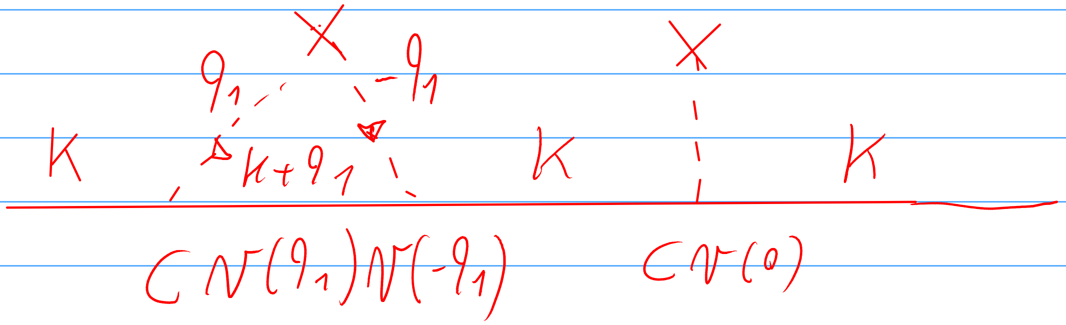


Using the expressions for the averages

$$\overline{V(q_1)V(q_2)} = C\,\nu(q_1)\,\nu(q_2)\;\delta_D(q_1+q_2)$$

$$\overline{V(q_3)} = C\,\nu(0)\;\delta_D(q_3)$$

we can represent schematically the diagram as



(C29)

we can thus interpret the dashed line as carrying momentum,

the nice things (however expected) is that momentum conservation is restored!

The total contribution to the diagram C(29) is, thus

$$G_0(k)\left[C\int N(q_1)N(-q_1)\,G_0(k+q_1)\,d_3\,q_1\right]G_0(k)$$

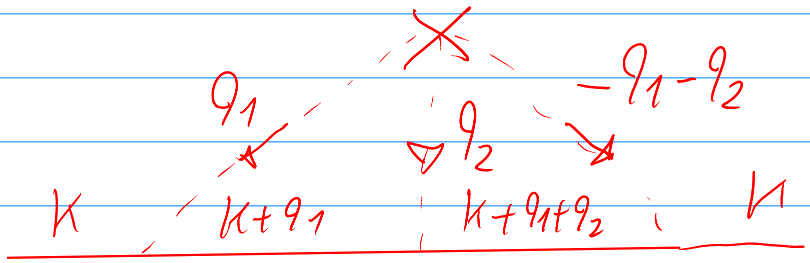
$$\times\, C\,N(0)\,G_0(k)$$

It is an independent product of terms

In Keldysh notation one should remember that a solid line corresponds to a 2x2 matrix in Keldysh space, and an impurity potential termis proportional to the identity in 2x2 Keldysh space

The order of the product is, thus, important

Let us consider a term with three connected potentials



$$\overline{V(q_1)\,V(q_2)\,V(q_3)}^{\,C} = C\,\delta_3(q_1+q_2+q_3)\,v(q_1)v(q_2)\,v(q_3)$$

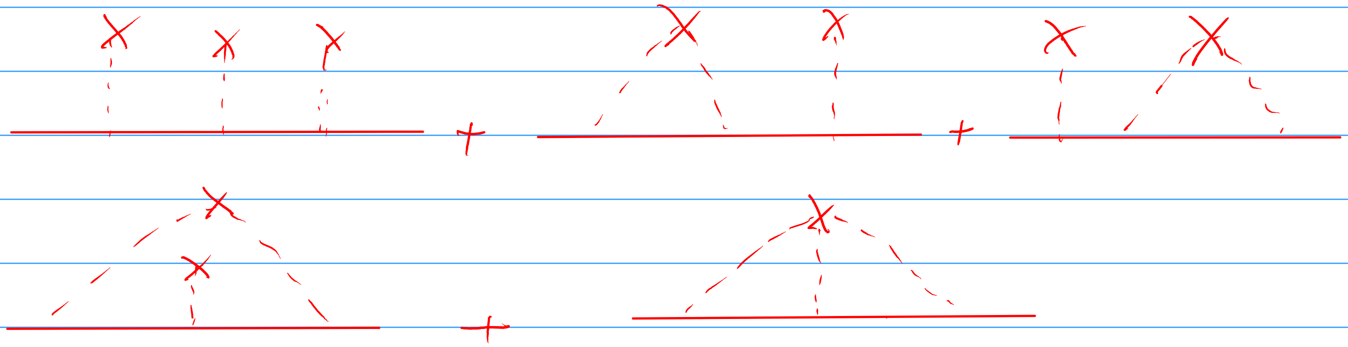
Total contribution

$$G_0(K)\cdot$$

$$\cdot\, C\int v(q_1)\,v(q_2)\,v(-q_1-q_2)\,G_0(k+q_1)\;G_0(k+q_1+q_2)\,d_3q_1\,d_3q_2$$

$$\cdot\; G_0(k)$$

For a term at a certain order in V one has to sum over all connected possibilities. For example, at third order one has



The rules consist then in associating to each dashed line a term

$V(q) I_{2x2}$ and each vertex conserves momentum (both the $\times$ as well as the vertices where dashed and solid line meet)

Notice that since impurity potentials are time-independent, this means that in frequency space, each dashed line carries frequency $\nu = 0$

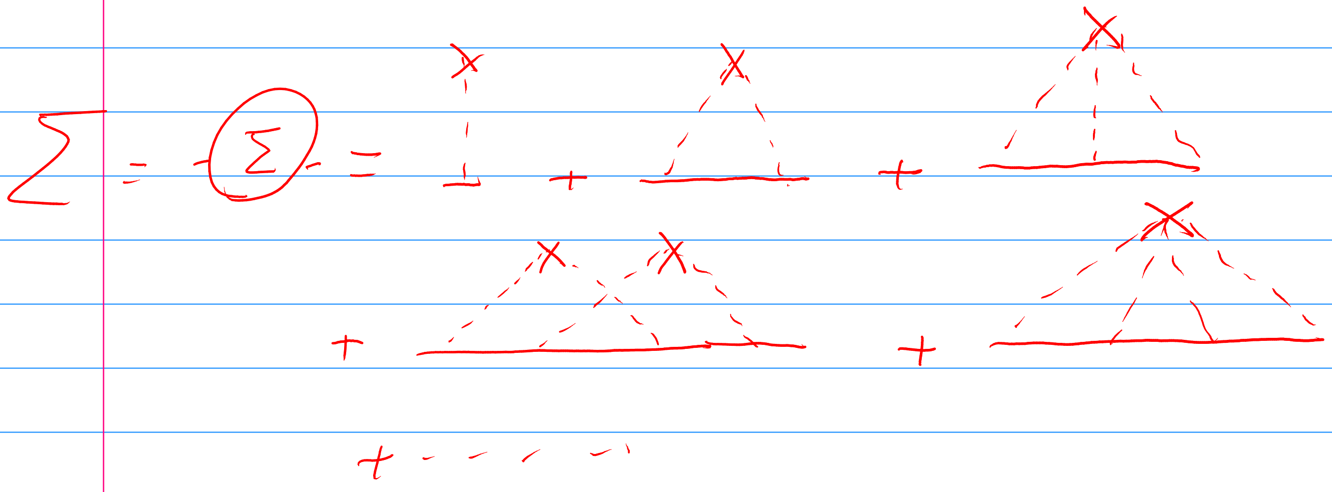
Moreover, each $\times$ contributes c (concentration)

And as usually, each solid line contributes $G(k)$

which is a 2x2 matrix

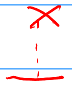
Self-energy

One can define a self-energy in the usual way, as the sum of all single-particle connected diagrams



and of course we have Dyson's equation

$$G = G_0 + G_0 \Sigma G$$

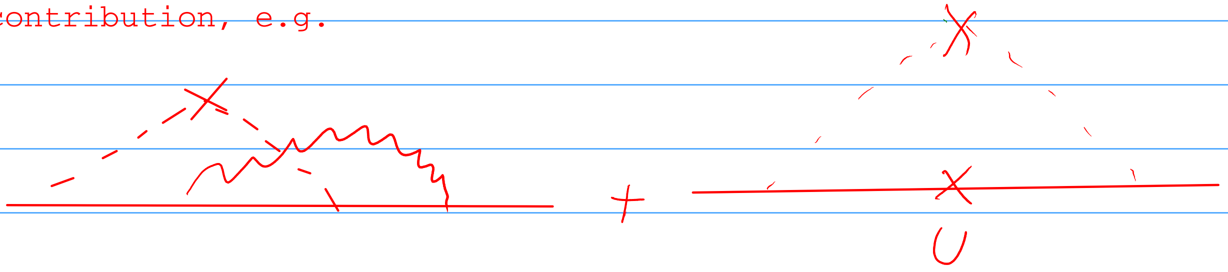
The lowest order term  $= cN(0)$

is just a constant, and can be absorbed in the single-particle energy

i.e. replacing $\varepsilon(\vec{p}) \to \varepsilon(\vec{p}) + cN(0)$

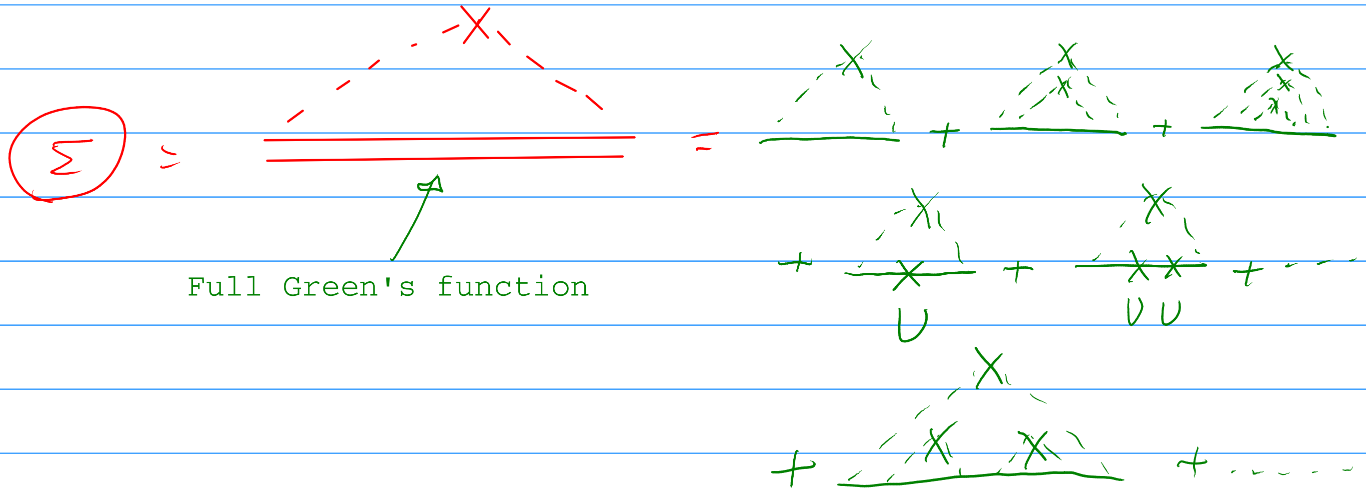
we can omit that term

when there are other perturbations, like, el.-el., el.-phonon, or external potential U) one in principle should consider all mixed contribution, e.g.

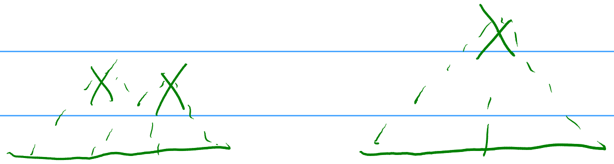


at the lowest order we take for the self energy

Self-consistent Born approximation



possible terms
not considered



it can be shown that this is the dominant term in the
low impurity concentration limit

$$\Sigma(K|W) = C\int d_3q\, \mathcal{V}(q)\, G(K+q|W)\, \mathcal{V}(-q)$$

$$= C\int d_3q\, |\mathcal{V}(q)|^2\, G(k+q|w) \qquad \text{(C30)}$$

since the $\mathcal{V}$ are proportional to the identity

this is an equation for each component (r,a,k)

It's the equation we have used above in (C19)

Useful relation

In solid state physics it is more common to consider a finite volume and replacing the integral over q with a sum

Rules to transform from continuum to discrete momenta

$$\int \frac{d^D q}{(2\pi)^D} = \int d_D q \Leftrightarrow \frac{1}{Vol} \sum_q$$

$$(2\pi)^D \delta(k_1 - k_2) = \delta_D(k_1 - k_2) \Leftrightarrow Vol\, \delta_{k_1, k_2} \qquad \text{(C31)}$$

Discussion about validity of gradient expansion in the scattering term

First point: we always consider impurity average quantities. (otherwise quantities would be strongly variing)

This includes G, which means f is the impurity averaged one

Impurity averaged means that $f(\vec{R},\vec{p},t)$ is coarse grained in the variable R, so R includes a "small volume" ΔV around R. ΔV contains a large number of impurities so that averaging is justified. Since we are considering the low-impurity density limit (Born approximation), we require

$$d \gg \frac{1}{k_F}$$ where d = interimpurity distance

this condition gives $$\Delta V \gg d^3 \gg (k_F)^{-3}$$ (C32)

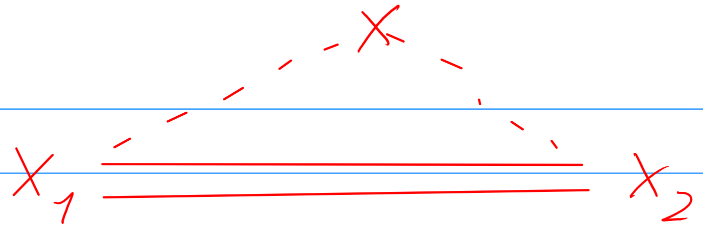
Giving this, we are allowed to average over impurities.

Σ is thus understood as being the one associated with the averaged G

(of course Σ is not the impurity averaged Σ as it appears the denominator)

Consider now the Born approximation,
we write the expression in real space

$$\Sigma(x_1, x_2) =$$



$$= \overline{V(x_1)V(x_2)}\; G(x_1, x_2)$$

$$= \overline{V^2}(x_1 - x_2)\; G(x_1, x_2)$$

There is no gradient approximation yet. Notice that the full G contains the external potential U, thus it depends on the center-of-mass coordinate X as well.

On the other hand, the important point is that the second order impurity averaged term $\overline{V^2}$, only depends on the difference coordinates. This is exact.

Already from this expression one can intuitively understand that

$\overline{V^2}(p)$ is a function of p and $G(p, X)$ of p, X

and we can estimate $\frac{\partial}{\partial p} \sim \frac{1}{k_F}, a$

a = interatomic distances. (Quite generally we can take $\frac{1}{k_F} \gtrsim a$)

$\frac{\partial}{\partial X} \sim \frac{1}{\lambda}$ λ = wavelength of U

The gradient term $\frac{\partial}{\partial X}\frac{\partial}{\partial p} \sim \frac{1}{\lambda k_F} << 1$ is required to be small

Consistent with C(32), we need $\lambda >> \Delta V >> d^3 >> (k_F)^{-3}$ (C33)

Let us try to be more precise

$$\Sigma(X_1,X_2) = \overline{V^2}(X_1-X_2)\; G(X_1,X_2)$$

we go over to the Wigner coordinates

$$\Sigma(P,X) = \int d^4x\, e^{iP.x}\, \overline{V^2}(x)\, G(x,X)$$

from usual Fourier transform rules:

$$= \int d_4 q\; \overline{V^2}(q)\, G(P-q, X)$$

Since V does not depend on time $\overline{V^2}(x) = \overline{V^2}(\vec{r})$

$$\overline{V^2}(q) = \overline{V^2}(\vec{q})\, \delta_1(w)$$

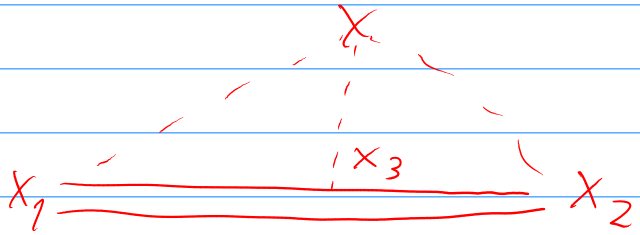
$$= \int d_3\vec{q}\; \overline{V^2}(\vec{q})\, G(\vec{P}-\vec{q}, w, X)$$

This is the expression we have in fact used

There is no gradient approximation here

INSERTION: check that the third-order term is also small in the sense of the gradient expansion

$$\Sigma^{(3)}(x_1,x_2) =$$



define $$\bar{V}^3(x_1-x_3,x_1-x_2) \equiv \overline{V(x_1)V(x_2)V(x_3)}^{\,c}$$

$$\int dx_3 \underbrace{\bar{V}^3(x_1-x_3,x_1-x_2)\,G(x_1,x_3)}_{\substack{\parallel \\ W(x_1,x_3|x_1-x_2)}}G(x_3,x_2)$$

Now define

$$\tilde{\Sigma}^{(3)}(x_1,x_2|\bar{x}) \equiv \int dx_3\, W(x_1,x_3|\bar{x})\,G(x_3,x_2)$$

obviously we eventually need

$$\Sigma^{(3)}(x_1,x_2) = \tilde{\Sigma}^{(3)}(x_1,x_2|x_1-x_2)$$

in Wigner coordinates

$$\Sigma^{(3)}(P,X) = \int \tilde{\Sigma}^{(3)}(x,X|x)\,dx\,e^{iPx}$$

$$= \int dx\,d\bar{x}\,\delta(x-\bar{x})\,e^{ipx}\,\tilde{\Sigma}^{(3)}(x,X|\bar{x})$$

$$= \int dx\,d\bar{x}\,dq\,e^{i(p+q)x}\,e^{-iq\bar{x}}\,\tilde{\Sigma}^{(3)}(x,X|\bar{x})$$

$$= \int dq\,\tilde{\Sigma}^{(3)}(p+q,X|q)$$

(notice: 2π have to be inserted wherever appropriate)

To evaluate $\tilde{\Sigma}^{(3)}$ we proceed by first

evaluating W in Wigner coordinates w.r. to X_1, X_3

where X_1-X_2 is an external variable

$$W(x,X|X_1-X_2) = V^3(x|X_1-X_2)\,G(x,X)$$

to carry out the convolution, i. e. the integral over X_3

we can use the gradient approximation

indeed for both W and G we have

$$\frac{\partial}{\partial P} \sim \frac{1}{K_F} \qquad \frac{\partial}{\partial X} \sim \frac{1}{\lambda}$$ as there is no q here!

Here we take the LOWEST order gradient approximation $g = 1$ since

there is always the small parameter V

In this approximation we get

$$\tilde{\Sigma}^{(3)}(P+q, X | q) = \tilde{W}(P+q, X | q)\, G(P+q, X)$$

we have

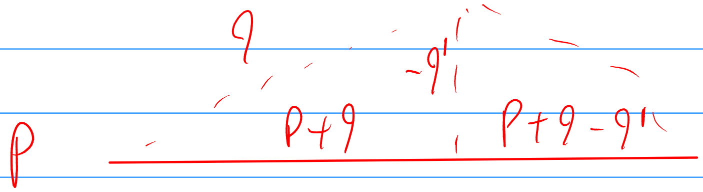
$$\tilde{W}(\bar{P}, X | q) = \int \bar{V}^3(q' | q)\, G(\bar{P}-q', X)\, dq'$$

which finally gives

$$\Sigma^{(3)}(P, X) = \int dq\, \tilde{\Sigma}^{(3)}(P+q, X | q) =$$

$$= \int dq\, dq'\, \bar{V}^3(q' | q)\, G(P+q-q', X)\, G(P+q, X)$$

which is the expected expression



END INSERTION

Evaluation of scattering term for a simple case

We evaluate the scattering term for an isotropic system (constant force) assuming that the deviation from equilibrium is small, i.e. we write

$$f(\vec{p},x) = f_F(\mathcal{E}(\vec{p})) + f_1(\vec{p},x)$$

for the small deviation f_1 we can assume, 1) that it only changes in the vicinity of the Fermi surface, so we can take it to depend only on an angle. Since the preferred direction is the force F, we take it (at lowest order) to be

$$f_1(\vec{p},x) \approx \hat{p}\cdot\hat{F}\,\alpha(p_F)$$

The scattering integral (C21), thus, becomes

$$\left(\frac{\partial f}{\partial t}\right)_S = 2\pi C\int d_D p' \left|\mathcal{V}(\vec{p}-\vec{p}\,')\right|^2 \delta(\mathcal{E}(p)-\mathcal{E}(p'))(\hat{p}'-\hat{p})\cdot\hat{F}\,\alpha(p_F) \tag{C34}$$

$$\boxed{\text{Useful expression} \quad 4\pi \int p'^2 dp' = \int N(\xi)\, d\xi}$$

Close to the Fermi surface we can replace

$$\int d_0 p' \rightarrow \frac{N(\mathcal{E}_F)}{4\pi} \int d\mathcal{E}'\, d\varphi'\, d\cos\theta'$$

We choose the directions of the vectors:

$$\hat{p} = (0,0,1) \qquad \hat{F} = (\sin\theta, 0, \cos\theta)$$

so we have $\hat{p}\cdot\hat{p}' = \cos\theta'$

$$\hat{p}\cdot\hat{F} = \cos\theta$$

$$\hat{p}'\cdot\hat{F} = \cos\theta\cos\theta' + \sin\theta\sin\theta'\cos\varphi'$$

again, close to the Fermi surface we can take the impurity potential to depend only on the angle between the p's

$$V(\vec{p}-\vec{p}') \rightarrow V(\cos\theta')$$

The scattering integral (C34) becomes

$$\left(\frac{\partial f}{\partial t}\right)_S = c\,\frac{N(\mathcal{E}_F)}{2}\,\alpha(p_F) \int d\varphi'\, d\cos\theta'\, V(\cos\theta') \times$$

$$\times \left(\hat{p}'\cdot\hat{F} - \cos\theta\right) \qquad \text{(C35)}$$

$$\cos\theta\cos\theta' + \sin\theta\sin\theta'\cos\varphi'$$

the integral over φ' can be easily done, removing the term $\cos\varphi'$

$$= \pi c N(\varepsilon_F)\, \alpha(p_F) \int d\cos\theta' \, \nu(\cos\theta') \times \cos\theta \left(\cos\theta' - 1\right)$$

$$= -\underbrace{\alpha(p_F)\cos\theta}_{f_1(\vec{p}, x) \,=\, f(\vec{p}, x) - f_F(\varepsilon_p)} \pi c N(\varepsilon_F) \int d\cos\theta' \, \nu(\cos\theta')(1-\cos\theta')$$

so that we can write

$$\left(\frac{\partial f}{\partial t}\right)_s = -\frac{f(\vec{p}, x) - f_F(\varepsilon(\vec{p}))}{\tau_1}$$

with the (inverse) relaxation time

$$\frac{1}{\tau_1} = \pi c N(\varepsilon_F) \int d\cos\theta' \, \nu(\cos\theta')(1-\cos\theta') \tag{C36}$$

This justifies the often adopted relaxation time approximation. However, notice that this form depends on the fact that we have an external force.

Proof that the equilibrium form is a solution of the GKB kinetic equation

We show that in equilibrium the time-independent form

$$G_K = \left(G_r - G_a\right) S(\omega)$$

is a solution of the exact kintetic equation (C17)

indeed from this we have

$$\Sigma_k = -\left(G^{-1}\right)_K = G_r^{-1} G_K G_a^{-1} = \left(G_a^{-1} - G_r^{-1}\right) S(\omega)$$

$$= \left(\Sigma_r - \Sigma_a\right) S(\omega)$$

In this way, the RHS of the kinetic equation (C17,C17A) yields

$$\frac{1}{2}\left(\left\{\Sigma_r - \Sigma_a, G_r - G_a\right\} S(\omega) - \left\{G_r - G_a, \Sigma_r - \Sigma_a\right\} S(\omega)\right) = 0$$

LHS: Since we are at equilibrium, there is no dependence on T. We assume that the system is homogeneous (I don't know how it works if one relaxes this hypothesis), so there is no dependence on $\vec{R}$

Therefore convolution are replaced by products , and commutators vanishes, so the LHS vanishes as well.

Useful observables

Single particle observables can be determined from

$$G^<(x_1,x_2) = i\langle \psi^\dagger(x_2)\,\psi(x_1)\rangle$$

It is convenient to express it in terms of the Keldysh GF
we use the relations on page 25 to get

$$G^< = G^K - G^>$$

$$G^r - G^a = G^> - G^<$$

$$G^< = G^K - (G^r - G^a) - G^<$$

$$\Rightarrow \boxed{G^< = \frac{1}{2} G^K + \pi i A} \tag{C37}$$

Particle density

$$\rho(X_1) = -i\, G^{<}(X_1, X_1)$$

$$= -i\, G^{<}(x=0, X=X_1)$$

$$= -i \int d_4 P\, G^{<}(P, X=X_1) \qquad \text{(C38)}$$

Particle current

$$J(X_1) = \mathrm{Re}\, \frac{1}{i} \left\langle \psi^{+}(X_1)\, \nabla_1 \psi(X_1) \right\rangle$$

$$= \mathrm{Im} \left\langle \psi^{+}(X_1)\, \nabla_1 \psi(X_1) \right\rangle$$

$$= \mathrm{Im} \left(-i\, \nabla_1\, G^{<}(X_1, X_2) \right) \Big|_{X_2 \to X_1}$$

$$= -\mathrm{Re}\, \nabla_1\, G^{<}(X_1, X_2) \Big|_{X_2 \to X_1} \qquad \text{(C39)}$$