From Schrödinger to Boltzmann

Summary !

$$G_{11} = -i\langle T\psi(1)\psi^+(2)\rangle$$

$$G_{12} = G^< = i\langle \psi^+(2)\psi(1)\rangle$$

$$G_{21} = G^> = -i\langle \psi(1)\psi^+(2)\rangle$$

$$G_{22} = -i\langle \tilde{T}\psi(1)\psi^+(2)\rangle$$

$$G^R = -i\theta(t_1-t_2)\langle\{\psi(1), \psi^+(2)\}\rangle$$

$$G^A = i\theta(t_2-t_1)\langle\{\psi(1), \psi^+(2)\}\rangle$$

$$G^R - G^A = -i\langle\{\psi(1), \psi^+(2)\}\rangle$$

$$G^R - G^A = G^> - G^<$$

$$G^K = G^> + G^<$$

$\cancel{G^< G^<} \; t \; \cancel{2\pi i}$

Equilibrium Consider $H = \sum_p \varepsilon_p c_p^+ c_p$

$$\psi(r,t) = \frac{1}{\sqrt{V}}\sum_p e^{ipr - i\varepsilon_p t} c_p$$

$$\psi^+(r,t) = \frac{1}{\sqrt{V}}\sum_p e^{-ipr + i\varepsilon_p t} c_p^+$$

ε_p – dispersion

V – volume

$$\langle c_p^+ c_p\rangle = f(\varepsilon_p), \quad \langle c_p c_p^+\rangle = 1 - f(\varepsilon_p)$$

$$G^<(1,2) = i\frac{1}{V}\sum_{p_1 p_2} e^{-ip_2 r_2 + i\varepsilon_{p_2} t_2} e^{ip_1 r_1 - i\varepsilon_{p_1} t_1} \underbrace{\langle c_{p_2}^+ c_{p_1}\rangle}_{= f(\varepsilon_{p_1})\delta_{p_1 p_2}}$$

$$= i\frac{1}{V}\sum_p e^{ip(r_1-r_2) - i\varepsilon_p(t_1-t_2)} f(\varepsilon_p)$$

$\Downarrow$ Do Wigner transform with respect to time:

$$G^<(\varepsilon, r_1, r_2) = \int G^<(1,2)\, e^{i\varepsilon(t_1-t_2)}\, d(t_1-t_2) =$$

$$= 2\pi i\,\frac{1}{V}\sum_p e^{ip(r_1-r_2)}\,\delta(\varepsilon-\varepsilon_p)\, f(\varepsilon),$$

similarly

$$G^>(\varepsilon, r_1, r_2) = -2\pi i\,\frac{1}{V}\sum_p e^{ip(r_1-r_2)}\,\delta(\varepsilon-\varepsilon_p)\,(1 - f(\varepsilon))$$

So, indeed, according to general relations:

$$G^> - G^< = -2\pi i \frac{1}{V}\sum_p e^{ip(r_1-r_2)}\,\delta(\varepsilon-\varepsilon_p) \equiv G^R - G^A \quad (\varepsilon, r_1, r_2)$$

you may also check it directly:

$$G^R_p = \frac{1}{\varepsilon-\varepsilon_p+i0}, \quad G^A_p = \frac{1}{\varepsilon-\varepsilon_p-i0}$$

$$\Rightarrow \quad G^R_p - G^A_p = -2\pi i\,\delta(\varepsilon-\varepsilon_p)$$

$$G^R(\varepsilon, r_1, r_2) - G^A(\varepsilon, r_1, r_2) = \frac{1}{V}\sum_p e^{ip(r_1-r_2)}\left(-2\pi i\,\delta(\varepsilon-\varepsilon_p)\right) \quad \leftarrow \text{checked}$$

We have proven that

$$f(\varepsilon) = \frac{1}{e^{\frac{\varepsilon-\mu}{T}}+1}$$

$$G^<(\varepsilon, r_1, r_2) = -f(\varepsilon)\,(G^R - G^A)$$

$$G^> = (1-f(\varepsilon))\,(G^R - G^A)$$

$$\Rightarrow \quad G^K = G^> + G^< = \underbrace{(1-2f(\varepsilon))}_{\substack{\parallel \\ \tanh\frac{\varepsilon-\mu}{2T}}}(G^R - G^A)$$

Towards Boltzmann Equation

We now separate the Hamiltonian to a non-interacting and interacting parts: $\mathcal{H} \Rightarrow \underbrace{\mathcal{H}_0}_{} + \mathcal{H}_{int}$

eigenstates can be found exactly

Quasiparticles that are described by the non-interacting part $\mathcal{H}_0$ will now aquire a finite life-time due to interactions.
This process is described in some desired approximation by the object called <u>Self-energy</u> Σ

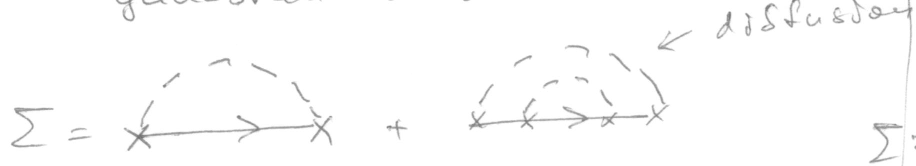
Interactions can be anything: Coulomb interactions between electrons, electron-phonon interactions, scattering of electrons on disorder potential, etc.

e-e interactions:

+ etc.

e-ph interactions

gaussian disorder



$\langle V(r) V(r') \rangle = 2\pi\alpha\, \delta(r-r')$

Strong disorder

weak localization

etc

Self-energy modifies G_0 in such a way that quasiparticles aquire a finite life time (spectrum also can change of course)

$$\boxed{G = G_0 + G_0 \circ \Sigma \circ G}$$ ← new Dyson equation

$$\cancel{G_0^{-1} \circ (G - \Sigma G) = 1}$$

$$\boxed{G_0^{-1} G = 1 + \Sigma \circ G}$$ ← convolution in space and time

$G_0^{-1} \equiv i\partial_t - H$, $1 = \delta(1,2)$ — in real space

We have seen already that $\hat{G}_0 = \begin{pmatrix} G_0^R & G_0^K \\ 0 & G_0^A \end{pmatrix}$ satisfies

$$\underbrace{\begin{pmatrix} i\partial_{t_1} - H_1^{(0)} + i0 & 0 \\ 0 & i\partial_{t_1} - H_1^{(0)} - i0 \end{pmatrix}}_{\substack{\parallel \\ \hat{G}_0^{-1}}} \begin{pmatrix} G_0^R(1,2) & G_0^K(1,2) \\ 0 & G_0^A(1,2) \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \delta(1,2)$$

$\hat{G}_0^{-1}$ - in operator sense

Now we have the following operator identities:

$$G_0^{-1} G = \hat{1} + \Sigma \circ G \qquad \Sigma = \begin{pmatrix} \Sigma^R & \Sigma^K \\ 0 & \Sigma^A \end{pmatrix}$$

$$G G_0^{-1} = \hat{1} + G \circ \Sigma$$

subtracting them we find

$$\Rightarrow \boxed{G_0^{-1} G - G G_0^{-1} = \Sigma \circ G - G \circ \Sigma}$$

← Keldysh component (or more precisely $\frac{1}{2}(K - R + A)$ - combination) of this equation is the Boltzmann equation!

Boltzmann Eq. is the equation on $\underset{\text{Wigner-transform}}{\underline{f(\varepsilon, p, R, T)}}$

G^K is often parameterized as

$$f = \frac{1-h}{2}$$

$$G^K = G^R \circ h - h \circ G^A \quad \text{convolution}$$

$$\left(G^< = \frac{1}{2}(G^K - G^R + G^A) \right)$$

$$\Rightarrow \boxed{G^< = - G^R \circ f + f \circ G^A}$$

f - non-equilibrium distribution function!

Before we consider examples we have to do one basic excercize that is central for treating the operator equation:

$$\boxed{G_0^{-1} G - G\, G_0^{-1} = \Sigma \circ G - G \circ \Sigma},$$

We have to write this equation in Wigner coordinates: $\underline{\varepsilon, p, R, t}$, since Boltzmann equation is the equation in Wigner coordinates!

In order to do that we have to know what is the Wigner transform of a convolution $A \circ B$ and how ~~does it~~ can it be expressed through the Wigner transforms of A & B individually. Example: (consider only time)

$$A \circ B\, (t_1, t_2) = \int_{-\infty}^{+\infty} dt_3\; A(t_1, t_3)\, B(t_3, t_2)$$

we have: $$A(t_1, t_2) = \int_{-\infty}^{+\infty} \frac{d\varepsilon}{2\pi}\, e^{-i\varepsilon(t_1 - t_2)} \underbrace{A\left(\varepsilon, \frac{t_1+t_2}{2}\right)}_{\text{Wigner transform}}$$

How do express $\underline{A \circ B\, (\varepsilon, t) \text{ through } A(\varepsilon, t) \text{ \& } B(\varepsilon, t)\ ?}$

introduce $\tau = t_1 - t_2$, $t = \dfrac{t_1 + t_2}{2}$ $\Rightarrow$ $(A \circ B)(\varepsilon, t) = \int_{-\infty}^{+\infty} d\tau\, e^{i\varepsilon\tau} \int_{-\infty}^{+\infty} dt_3\, A(t+\frac{\tau}{2}, t_3)\, B(t_3, t-\frac{\tau}{2}) =$

$$t_1 = t + \tau/2, \quad t_2 = t - \tau/2$$

$$= \int d\tau\, e^{i\varepsilon\tau} \int dt_3 \int \frac{d\varepsilon_1}{2\pi} \int \frac{d\varepsilon_2}{2\pi}\, e^{-i\varepsilon_1 (\underbrace{t+\frac{\tau}{2}-t_3}_{t_1 - t_3})}\, e^{-i\varepsilon_2 (\underbrace{t_3 - t + \frac{\tau}{2}}_{t_3 - t_2})}\, A\Big(\varepsilon_1, \frac{t+\frac{\tau}{2}+t_3}{2}\Big)\, B\Big(\varepsilon_2, \frac{t-\frac{\tau}{2}+t_3}{2}\Big)$$

Use $A(\varepsilon_1, \frac{t_1+t_3}{2}) = A(\varepsilon_1, \underbrace{\frac{t_1+t_2}{2}}_{\equiv\, t} + \frac{t_3 - t_2}{2}) = e^{\frac{t_3 - t_2}{2}\frac{\partial}{\partial t}} A(\varepsilon_1, t)$

Similarly $B(\varepsilon_2, \frac{t_3+t_2}{2}) = B(\varepsilon_2, \underbrace{\frac{t_1+t_2}{2}}_{t} + \frac{t_3 - t_1}{2}) = e^{\frac{t_3 - t_1}{2}\frac{\partial}{\partial t}} B(\varepsilon_2, t)$

$\Rightarrow$

$$(A \circ B)(\varepsilon, t) = \int d\tau\, e^{i\varepsilon\tau} \int dt_3 \int \frac{d\varepsilon_1}{2\pi} \int \frac{d\varepsilon_2}{2\pi}\, e^{-i\varepsilon_1 (t_1 - t_3)}\, e^{-i\varepsilon_2 (t_3 - t_2)} \Big(e^{\frac{t_3 - t_2}{2}\partial_t} A(\varepsilon_1, t)\Big) \Big(e^{\frac{t_3 - t_1}{2}\partial_t} B(\varepsilon_2, t)\Big)$$

powers of $(t_3 - t_2)$ can be obtained by differentiating the exponent $e^{-i\varepsilon_2 (t_3 - t_2)}$ over energy ε_2

These derivatives can be then passed by integration by parts on the function $B(\varepsilon_2, t)$ (and same with A)

$\Rightarrow \quad \frac{t_3 - t_2}{2} \Rightarrow -\frac{i}{2}\frac{\partial}{\partial \varepsilon_2} \leftarrow$ acting on B function

$\frac{t_3 - t_1}{2} \Rightarrow \frac{i}{2}\frac{\partial}{\partial \varepsilon_1} \leftarrow$ acting on A function

$\Rightarrow$

acting on A   acting on B

$$(A \circ B)(\varepsilon, t) = \underbrace{\int d\tau\, e^{i\varepsilon\tau}}_{\text{gives } 2\pi\,\delta\left(\varepsilon - \frac{\varepsilon_1+\varepsilon_2}{2}\right)} \underbrace{\int dt_3}_{\text{gives } 2\pi\,\delta(\varepsilon_1 - \varepsilon_2)} \int \frac{d\varepsilon_1}{2\pi} \int \frac{d\varepsilon_2}{2\pi}\, e^{-i\varepsilon_1(t_1 - t_3)}\, e^{-i\varepsilon_2(t_3 - t_2)} \left(e^{-\frac{i}{2}\frac{\partial}{\partial \varepsilon_2}\frac{\partial^{A}}{\partial t}}\, e^{\frac{i}{2}\frac{\partial}{\partial \varepsilon_1}\frac{\partial^{B}}{\partial t}} A B \right)$$

$\tau = t_1 - t_2$

$t_1 = t + \frac{\tau}{2}, \quad t_2 = t - \frac{\tau}{2}$

Eventually

$$\boxed{(A \circ B)(\varepsilon, t) = e^{\frac{i}{2}\left(\frac{\partial^{A}}{\partial \varepsilon}\frac{\partial^{B}}{\partial t} - \frac{\partial^{A}}{\partial t}\frac{\partial^{B}}{\partial \varepsilon}\right)} A(\varepsilon, t)\; B(\varepsilon, t)}$$

acting on A   acting on B   acting on A   acting on B

Gradient expansion

$A(\varepsilon,t)$, $B(\varepsilon,t)$ – smooth functions of both ε, and t

$$\Rightarrow \quad (A\circ B)(\varepsilon,t) = A(\varepsilon,t)\,B(\varepsilon,t) + \frac{i}{2}\underbrace{\left(\frac{\partial A}{\partial \varepsilon}\frac{\partial B}{\partial t} - \frac{\partial A}{\partial t}\frac{\partial B}{\partial \varepsilon}\right)}_{\text{Poisson bracket}} + \ldots$$

Same for the Wigner transform in $\tau_1 - \tau_2$

$$(A\circ B)(R,p) = A(R,p)\,B(R,p) - \frac{i}{2}\left(\frac{\partial A}{\partial p}\frac{\partial B}{\partial R} - \frac{\partial A}{\partial R}\frac{\partial B}{\partial p}\right)$$

different sign due to convention

Now we shall return back to our Boltzmann equation!

$$G_0^{-1}G - G\,G_0^{-1} = \Sigma\circ G - G\circ\Sigma$$

$$\underbrace{G_0^{-1}G - GG_0^{-1}}_{} = [\Sigma ; G]$$

Let us first consider the left-hand part:

inverse direction by integration by parts

$$G_0^{-1}G - GG_0^{-1} = (i\partial_{t_1} - \mathcal{H}_1)\, G(1,2) - G(1,2)(-i\partial_{t_2} - \mathcal{H}_2)$$

$\Downarrow$

go to Wigner coordinates: $t = \dfrac{t_1 + t_2}{2}$, $\tau = t_1 - t_2$

$$\frac{\partial}{\partial t_1} = \frac{1}{2}\frac{\partial}{\partial t} + \frac{\partial}{\partial \tau} \qquad \Rightarrow \qquad \frac{\partial}{\partial t_1} + \frac{\partial}{\partial t_2} = \frac{\partial}{\partial t}$$

$$\frac{\partial}{\partial t_2} = \frac{1}{2}\frac{\partial}{\partial t} - \frac{\partial}{\partial \tau}$$

unit matrix in Keldysh

$$\mathcal{H}(\varepsilon, p, R, t) \sim \mathbb{1}$$

in gradient expansion

Consider $[\mathcal{H}, G] \cong i(\nabla_R H \nabla_p G - \nabla_p H \nabla_R G)$ ← (here we take the leading contribution with respect to ε, t)

Wigner transform of $\mathcal{H}$ is just a classical Hamiltonian like: $\mathcal{H} = \underline{\dfrac{p^2}{2m} + U(R, t)}$ ← external perturbation!

$\nabla_R H = \nabla_R U(R) = -\vec{F}$ ← force

$\nabla_p H = \vec{v}$ – velocity $\Rightarrow$ $[\mathcal{H}, G] = -i(\vec{F}\vec{\nabla}_p + \vec{v}\cdot\nabla_R)\, G$

$$\Rightarrow \quad G_0^{-1}G - GG_0^{-1} \cong i\,\underline{(\partial_t + \vec{F}\vec{\nabla}_p + \vec{v}\cdot\vec{\nabla}_R)}\, G \leftarrow \text{typical Boltzmann operator}$$

leading order in gradients

~~Thus we~~

For $[\Sigma \circ, G]$ we take the leading term in the gradient expansion, i.e. replace the Wigner transform of the product by the product of Wigner transforms:

$$\Rightarrow \quad \underbrace{(\partial_t + \bar{F}\bar{\nabla}_p + \bar{v}\cdot\bar{\nabla}_R)}_{\hat{L}\text{ - notation}} \hat{G}(\varepsilon, t, R, p) = i[\hat{\Sigma}, \hat{G}]$$

All matrices in rotated Keldysh space

$$G^R = \frac{1}{\varepsilon - \varepsilon_p - U(R,t) + i0} \quad ; \quad (F = -\nabla_R U)$$

external force!

In components:

$$\hat{L} = \frac{\partial}{\partial t} + \bar{F}\cdot\bar{\nabla}_p + \bar{v}\cdot\bar{\nabla}_R$$

$$\hat{L}\, G^R = 0$$

$$\hat{L}\, G^A = 0$$

$$\hat{L}\, G^K = -i\left(\underbrace{\Sigma^R G^K + \Sigma^K G^A - G^R\Sigma^K}_{\text{those are now usual products of Wigner transforms}} - G^K \Sigma^A\right)$$

$$\Rightarrow \quad \hat{L}\, G^K = i\left(\Sigma^K (G^R - G^A) - G^K(\Sigma^R - \Sigma^A)\right)$$

Let us now use the definition of the distribution function:

$$G^K = G^R \circ h - h \circ G^A$$

In Wigner transform (leading order):

$$G^K = (G^R - G^A)\, h \qquad \text{note that } \hat{L} G^{R,A} = 0$$

$$\Rightarrow \quad (G^R - G^A)\, \hat{L} h = i\left(\Sigma^K - h(\Sigma^R - \Sigma^A)\right)(G^R - G^A) \qquad (*)$$

It looks like we can cancel $G^R - G^A$, but remember that in equilibrium $\underbrace{G^R - G^A = -2\pi i\, \delta(\varepsilon - \varepsilon_p - U)}$

Therefore Eq. (*) has little or no sense outside the mass shell $\varepsilon = \varepsilon_p$ (if U is small!!!)

We shall integrate Eq. (*) over ε instead:

$$\Rightarrow \boxed{\left(\frac{\partial}{\partial t} + \vec{F}\cdot\vec{\nabla}_p + \vec{v}\cdot\vec{\nabla}_R\right) h_p = i\left(\Sigma^K(\varepsilon_p, p, R, t) - h_p\left(\Sigma^R - \Sigma^A\right)\right)}$$

Introduce $h_p(R,t) = -\frac{1}{2\pi i}\int d\varepsilon\, G^K(\varepsilon, p, R, t)$

(Note that $\vec{v} = \vec{\nabla}_p \varepsilon_p$ - group velocity)

Classical Boltzmann equation!

Note that Σ^K depends on h_p in the integral way, so the equation is actually <u>integro-differential</u>

In equilibrium one must find $\Sigma^K = h\left(\Sigma^R - \Sigma^A\right)$ that is also a test for your calculation of Σ

<u>Exercize!</u> Do a bit better by considering better approximation for $[\Sigma \circ, G]$ that includes Poisson bracket term, Take all terms with the gradients to the left-hand side of the equation!

Most of success of this approach goes in the following directions:

1) Situations when $\hat{H}$ and $\hat{G}$ have additional matrix structure apart from Keldysh

a) due to spin (spin-orbit, magnetism)

b) due to superconductivity (electron-hole basis)

c) due to pseudo-spin (valleys + sublattices, Kane-Mele models)

2) ~~Qu~~ Quasiclassical approximation

$$\hat{g}(p, R, t) = \frac{i}{\pi} \int_{-\infty}^{+\infty} d\varepsilon \, \hat{G}(\varepsilon, p, R, t) \quad \leftarrow \text{quasiclassical Green's function!}$$

for a metal $g^R = 1$, $g^A = -1$ $\Rightarrow$ $\hat{g} = \begin{pmatrix} 1 & 2h \\ 0 & -1 \end{pmatrix}$

note that $\hat{g}^2 = 1$

for superconductor: $\hat{g}$ is a bit more complex (see Usádel equation)

but the non-linear constraint $\underline{\hat{g}^2 = 1}$ remains

This defines non-linear theory of non-equilibrium superconductivity!!