Kinetic equations

Dyson equation: $\hat{=}$

"equation of motion" for $G(t,t')$ with memory kernel Σ

$\hat{=}$ spectrum $\otimes$ occupation

$\rightsquigarrow$

Goal: equation of motion for occupation function, without memory kernel?

(only approximate!)

Various strategies for derivation (almost equivalent):

"generalized Kadanoff Baym ansatz", equation of motion decoupling, here: Dyson equation

$\longrightarrow$ Wigner transformation + gradient approx.

$\longrightarrow$ Quasiparticle approximation

• (Based on Kamenev, Chapter 5)

STEP-1 Parametrization $G \hat{=}$ spectrum $\otimes$ occupation

In this section:

- arguments "1" $\hat{=} (t, \vec{r}, \sigma, \ldots)$

  t: real time, $t \in (-\infty, +\infty)$

  $\vec{r}, \sigma, \ldots$: orbital, spin, space

- convolution: as usual, just real time integral
  (may occasionally omit $*$, if context is clear)

  $$A * B(1,\bar{1}) = \underbrace{\int d\bar{1}}_{\int_{-\infty}^{+\infty} d\bar{t} \int d\bar{\vec{r}} \ldots} A(1,\bar{1})\, B(\bar{1},1')$$

Ansatz:

$$\boxed{G^K = G^R * F - F * G^A}$$

$F(1,1')$ hermitian : "distribution function"

- check that ansatz has correct symmetries:

  $(G^K)^\dagger \stackrel{!}{=} -(G^K)$ ("hermitian" property of $G^{\gtrless}$)

  use $(G^R)^\dagger = G^A$

  $$\big(G^{R\dagger}(1,1') = G^R(1',1)^* = $$
  $$= (G^> - G^<)(1',1)^* \, \Theta(t_1' - t_1)$$
  $$= (G^< - G^>)(1,1')\, \Theta(t_1' - t_1) =$$
  $$= G^A(1,1')$$

$$\Rightarrow \quad (G^R F - F G^A)^\dagger =$$

$$= -G^R F^\dagger + F^\dagger G^A \overset{F=F^\dagger}{=} -(G^R F - F G^A) \quad ✓$$

<u>motivation for ansatz:</u>

equilibrium, one orbital (orbital index omitted)

$\rightsquigarrow$ Fourier transform

$$G^K(\omega) = G^R(\omega+i0)\,F(\omega) - F(\omega)\,\underbrace{G^A(\omega-i0)}_{G^R(\omega+i0)^*}$$

Footnote (#)

$$= \left(G^R(\omega+i0) - G^R(\omega+i0)^*\right) F(\omega)$$

check!

$$= 2i\,\mathrm{Im}\,G^R(\omega+i0)\;F(\omega)$$

$$= -2\pi i\;A(\omega)\;F(\omega)$$

$\rightsquigarrow$ FT of $F(t-t') \hat{=}$ distribution function

$$F(\omega) = \begin{cases} \tanh\frac{\beta\omega}{2} & \text{Fermi} \\ \coth\frac{\beta\omega}{2} & \text{Bose} \end{cases}$$

(#) <u>Note:</u>

$$G^A(\omega-i0) = \int dt\, e^{+i(\omega-i0)t}\, G^A(t) =$$

$$= \int_{-\infty}^{\infty} dt\, \underbrace{G^A(t)}_{G^R(-t)^*}\, e^{i(\omega-i0)t} \underset{\uparrow}{=} \left[\int_0^\infty dt\, e^{i(\omega+i0)t}\, G^R(t)\right]^*$$

subst. $t \to -t$

Dyson equation for $F(1,1')$?

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I) $\underline{G_0^{-1}}\,\underline{G} - \underline{\Sigma}\,\underline{G} = \underline{1}$

II) $\underline{G}\,\underline{G_0^{-1}} - \underline{G}\,\underline{\Sigma} = \underline{1}$ $\rightsquigarrow$ Keldysh component.

I) $\Rightarrow (G_0^R)^{-1} * G^K - \Sigma^R * G^K - \Sigma^K * G^A = 0$

$\rightsquigarrow$ ansatz for G^K:

$$((G_0^R)^{-1} - \Sigma^R) * (G^R * F - F * G^A) - \Sigma^K * G^A = 0$$

$$F - ((G_0^R)^{-1} - \Sigma^R) * F * G^A - \Sigma^K * G^A = 0$$

use II) $\Rightarrow G^A \cdot ((G^A)^{-1} - \Sigma^A) = 1 \Rightarrow$

$$F\,((G_0^A)^{-1} - \Sigma^A) - ((G_0^R)^{-1} - \Sigma^R) * F = \Sigma^K$$

$\rightsquigarrow$

$$\boxed{-\underbrace{\left[(G_0^R)^{-1} \overset{*}{,} F\right]}_{\text{"kinetic term"}} = \underbrace{\Sigma^K - (\Sigma^R * F - F * \Sigma^A)}_{\text{"collision integral"}}}$$

(nomenclature clear only below)

$[A \overset{*}{,} B] = A * B - B * A$

explicit form of $[(G_0^R)^{-1} \overset{*}{;} F]$:

... for particles in potential $V(\vec{r})$, real-space basis, omit spin for simplicity:

$$(G_0^R)^{-1} = \left\{ i\partial_t + \frac{\hbar^2 \vec{\nabla}_r^2}{2m} - V(\vec{r}) \right\} \delta(t-t')\, \delta(\vec{r}-\vec{r}')$$

$$[i\partial_t \delta(t-t') \overset{*}{;} F] =$$

integrate by part

$$\int d\bar{t} \left\{ i\partial_{\bar{t}} \delta(t-\bar{t})\, F(\bar{t},t') - F(t,\bar{t})\, i\partial_{\bar{t}} \delta(\bar{t}-t') \right\}$$

$$= i(\partial_t + \partial_{t'})\, F(t,t')$$

$$\boxed{[(G_0^R)^{-1} \overset{*}{;} F] = \left\{ i(\partial_t + \partial_{t'}) + \frac{\hbar^2}{2m}\left(\nabla_r^2 - \nabla_{r'}^2\right) - \left(V(\vec{r}) - V(\vec{r}')\right) \right\} F(1,1')}$$

STEP - 2 Separation of "slow average time" vs. "fast relative time" dependence

consider space-time indices $x \equiv \vec{r}, t$

average / relative time for two-point correlation function $A(x,x')$

$$\boxed{\begin{array}{l} x_{av} = \dfrac{x+x'}{2} \qquad x_{rel} = x - x' \\[2ex] A(x,x') = A\left(x_{av} + \dfrac{x_{rel}}{2},\, x_{av} - \dfrac{x_{rel}}{2}\right) \end{array}}$$

(Note: all arguments below work also for lattice, just replace continuous $\vec{r}$ variable by disrete $\vec{r}$.)

equilibrium: no dependence of any $A(x,x')$ on $t_{av} = (t+t')/2$.

$\rightsquigarrow$ hope: non-equilibrium well described by "weak" x_{av} - dependence.

Example: Fermi gas

- x_{av} - dependence:

$$-i\, G^<(x,x') \underset{\text{e.g. } x_{rel}=0}{=} \langle \psi^+(x_{av})\, \psi(x_{av}) \rangle$$

$$= \rho(\vec{r}_{av}, t_{av}) \quad \text{density}$$

$\Rightarrow$ only (slow) variations due to external potential V

- x_{rel} - dependence

$$-i\, G^<(x,x') \underset{\text{e.g. } x_{av}=0}{=} \left\langle \psi^+(-x_{rel}/2)\; \psi(+x_{rel}/2) \right\rangle$$

$$= \frac{1}{Vol} \sum_{kk'} \langle c_k^+(-t_{av}/2)\; c_{k'}(t_{av}/2) \rangle \cdot$$

$$\cdot\, e^{-i\vec{k}(-\vec{r}_{av}/2)}\; e^{+i\vec{k}'\vec{r}_{av}/2}$$

... evaluate for non-interacting system in equilibrium

$$\ldots = \frac{1}{Vol} \sum_{kk'} \langle c_k^+ c_{k'} \rangle \, e^{+i \vec{k} r_{rel} \mp i \xi_k t_{rel}}$$

$$= \int \frac{d^3k}{(2\pi)^3} f(\xi_k - \mu) \, e^{i(\vec{k} \vec{r}_{rel} - \xi_k t_{rel})}$$

$f(\xi_k - \mu)$ varies on scale k_F, E_F

$\Rightarrow$ $G(x, x')$ has strong variations on scale $r_{rel} \sim 1/k_F$ $t_{rel} \sim 1/E_F$

(... won't be "better" in non-equilib., or interacting system)

e.g.: $T=0$, discontinuity at $\vec{k} = k_F$

$\Rightarrow$ $2k_F$-oscillations (Friedel-oscillations) in $\langle \psi^+(r/2) \, \psi(-\vec{r}/2) \rangle$

$\Rightarrow$ In general, we have to try to make use of assumption

$$\boxed{\underbrace{\delta x_{av}}_{\text{scale on}} \ll \underbrace{\delta x_{rel}}_{\text{while } x_{av}\,(x_{rel}) \text{ varies}}}$$

$\Rightarrow$ introduce Fourier transform with respect to fast variable: <u>Wigner-transform</u>

$$\underline{p \equiv \omega, \vec{k}} \quad ; \quad \underline{x \cdot p = -\omega t + \vec{k}\vec{r}}$$

$$\int dx = \int dt \int d^3 r \quad ; \quad \sum_p = \sum_k \int \frac{d\omega}{2\pi}$$

$$\boxed{\begin{aligned} \tilde{A}(x_{av}, p) &:= \int dx_{rel}\, e^{-ipx_{rel}} A\left(x_{av} + \frac{x_{rel}}{2}, x_{av} - \frac{x_{rel}}{2}\right) \\ A(x,x') &= \sum_p e^{ip(x-x')} \tilde{A}\left(\frac{x+x'}{2}, p\right) \end{aligned}}$$

... have to express convolution in terms of Wigner transform: $\quad C = A * B$

<u>Claim</u>:
$$\boxed{\tilde{C}(x,p) = \tilde{A}(x,p)\, e^{\frac{i}{2}\left(\overleftarrow{\partial}_x \overrightarrow{\partial}_p - \overleftarrow{\partial}_p \overrightarrow{\partial}_x\right)} \tilde{B}(x,p)}$$

$$\partial_x \partial_p = \vec{\nabla}_r \vec{\nabla}_k - \partial_t \partial_\varepsilon$$

<u>proof</u>:

$$\tilde{C}(x,p) = \int dx'\, e^{-ipx'} \underbrace{(A * B)}_{\int dx_3 A(x+\frac{x'}{2}, x_3) B(x_3, x-\frac{x'}{2})}\left(x + \frac{x'}{2}, x - \frac{x'}{2}\right)$$

$$= \int dx' \, e^{-ipx} \sum_{p_1 p_2} \int dx_3 \, e^{ip_1(x+\frac{x'}{2}-x_3)} \, e^{ip_2(x_3-x+\frac{x'}{2})} \cdot$$

$$\tilde{A}\left(\frac{x+x'/2+x_3}{2}, p_1\right) \tilde{B}\left(\frac{x-x'/2+x_3}{2}, p_2\right)$$

substitution: $x_{a,b} = x_3 - x \pm x'/2$

$p_{a,b} = p_{1/2} - p$

$$\tilde{C}(x,p) = \int dx_a \, dx_b \sum_{p_a p_b} e^{i(p_b x_a - p_a x_b)} \cdot$$

$$\cdot \; \tilde{A}\left(x+\frac{x_a}{2}, p+p_a\right) \tilde{B}\left(x+\frac{x_b}{2}, p+p_b\right)$$

- Taylor expansion:

a bit sloppy notation, as $p = (\vec{p}, \omega)$ etc...

$$\tilde{A}\left(x+\frac{x_a}{2}, p+p_a\right) = \sum_{n=0}^{\infty} \frac{p_a^n}{n!} \partial_p^n \tilde{A}\left(x+\frac{x_a}{2}, p\right)$$

analog. for $\tilde{B}$

- $\int dx_b \; \cancel{\sum_{p_a}} \; e^{-ip_a x_b} \, p_a^n \ldots$

$$= \int dx_b \, (+i)^n \left(\frac{\partial^n}{\partial x_b^n} e^{ip_a x_b}\right) \ldots \stackrel{\text{part int.}}{=}$$

$$= \int dx_b \, (-i)^n \, e^{ip_a x_b} \left(\frac{\partial}{\partial x_b}\right)^n \ldots$$

analog $a \leftrightarrow b$ with $i \to -i$

$$\tilde{C}(x,p) = \int dx_a \int dx_b \sum_{p_a p_b} e^{i(p_b x_a - p_a x_b)} \sum_{nm} (-i)^n (+i)^m$$

$$\cdot \Big[\underbrace{\partial_p^n \partial_{x_a}^m \tilde{A}(x+\tfrac{x_a}{2},p)}_{(\frac{1}{2})^m \partial_x \tilde{A}}\Big]\Big[\underbrace{\partial_p^m \partial_{x_b}^n \tilde{B}(x+\tfrac{x_b}{2},p)}_{(\frac{1}{2})^n \partial_x \tilde{B}}\Big]$$

use $\sum_{p_b} \int dx_a \, e^{i p_b x_a} = \int dx_a \, \delta(x_a) \ldots$

$$\tilde{C}(x,p) = \sum_{nm} \left(\frac{-i}{2}\right)^n \left(\frac{i}{2}\right)^m \left[\partial_p^n \partial_x^m \tilde{A}(x,p)\right] \cdot \left[\partial_p^m \partial_x^n \tilde{B}(x,p)\right]$$

$$= \tilde{A}(x,p) \, e^{\frac{i}{2}(\overleftarrow{\partial}_x \overrightarrow{\partial}_p - \overleftarrow{\partial}_p \overrightarrow{\partial}_x)} \tilde{B}(x,p) \quad \checkmark$$

■

weak-dependence on "average" variables:

$\Rightarrow$ <u>gradient expansion</u> $\qquad \delta x_{av} \ll \frac{1}{\delta p} \sim \delta x_{rel}$

see p. 129 !!

$$\boxed{\tilde{C} = \tilde{A} \cdot \tilde{B} + \frac{i}{2}(\partial_x A)(\partial_p B) - \frac{i}{2}(\partial_p A)\,\partial_x B + \ldots}$$

WT of kinetic term:

$$\left\{ \left(i\partial_t + i\partial_{t'} \right) + \left(\nabla_r^2 - \vec{\nabla}_{r'}^2 \right) \frac{\hbar^2}{2m} - \left(V(\bar{r},t) - V(\bar{r}',t') \right) \right\} F(x,x')$$

1) $$(i\partial_t + i\partial_{t'}) F(x,x') = i\partial_{t_{av}} F \xrightarrow{WT} \underline{\underline{i\partial_{t_{av}} \tilde{F}(x_{av}, p)}}$$

2) $$\vec{\nabla}_r^2 F(x,x') = \vec{\nabla}_r^2 \sum_p e^{ip(x-x')} F(\overbrace{\frac{x+x'}{2}}^{x_{av}}, p)$$

$px = \bar{k}\bar{r} - \omega t$

$$= \sum_p e^{ip(x-x')} \left\{ (ik)^2 + i\vec{k} \cdot \vec{\nabla}_{r_{av}} + \frac{1}{4} \vec{\nabla}_{r_{av}}^2 \right\} F$$

$$\vec{\nabla}_{r'}^2 F(x,x') = \sum_p e^{ip(x-x')} \left\{ (-ik)^2 - i\vec{k}\vec{\nabla}_{r_{av}} + \frac{1}{4} \vec{\nabla}_{r_{av}}^2 \right\} F$$

$$\Rightarrow (\nabla_r^2 - \nabla_{r'}^2) F \xrightarrow{WT} \underline{\underline{2i\vec{k} \cdot \vec{\nabla}_{r_{av}} \tilde{F}(x_{av}, p)}}$$

3) $$[V(r,t) - V(r',t')] F(x,x') =$$

$$= [\underbrace{V(x)\,\delta(x-x')}_{\xrightarrow{WT} V(x_{av}) \text{ (independent of } p)} \stackrel{*}{,} F] = \# \xrightarrow{WT} \#$$

$$\# = \tilde{V}\tilde{F} + \frac{i}{2}\left(\partial_{x_{av}} \tilde{V} \partial_p \tilde{F} - \partial_p \tilde{V} \partial_{x_{av}} \tilde{F} \right) - \tilde{F}\tilde{V} -$$

gradient expansion

$$- \frac{i}{2} \left(\partial_{x_{av}} \tilde{F} \partial_p \tilde{V} - \partial_p \tilde{F} \partial_{x_{av}} \tilde{V} \right) =$$

$$= i\,\partial_{x_{av}} V(x_{av})\ \partial_p \tilde{F}(x_{av}, p)$$

$$= i\left\{ \left(\vec{\nabla}_{r_{av}} V(x_{av})\right)\cdot \vec{\nabla}_k \tilde{F}(x_{av}, p) - \left(\partial_{t_{av}} V(x_{av})\right)\partial_\varepsilon \tilde{F} \right\}$$

$$\Rightarrow \left[(G_0^R)^{-1} \overset{*}{,} F \right] \xrightarrow{WT}$$

$$\underline{\underline{\left\{ i\,\partial_{t_{av}} + i\,\frac{\hbar^2 \vec{k}}{2m}\cdot\vec{\nabla}_{r_{av}} \cancel{\pm}\ i\left(\vec{\nabla}_{r_{av}} V(x_{av})\right)\vec{\nabla}_k + i\left(\partial_{t_{av}} V\right)\partial_\varepsilon \right\} F(x_{av},}}$$

__Note:__ for a general dispersion, we should have

$\hbar^2 k/2m \longrightarrow \hbar v_k$, $v_k = \frac{1}{\hbar}\frac{\partial \varepsilon_k}{\partial k}$ band velocity.

WT of collision term (in gradient approx.)

$$\Sigma^K - \left(\Sigma^R * F - F * \Sigma^A\right) \xrightarrow{WT,\ \text{gradient exp.}}$$

$$\tilde{\Sigma}^K - (\tilde{\Sigma}^R - \tilde{\Sigma}^A)\tilde{F} -$$

$$-\frac{i}{2}\left(\partial_x \tilde{\Sigma}^R \partial_p \tilde{F} - \partial_p \Sigma^R \partial_x \tilde{F} - \partial_x \tilde{F}\partial_p \tilde{\Sigma}^A + \partial_p \tilde{F}\partial_x \tilde{\Sigma}^A\right)$$

$$= \tilde{\Sigma}^K - (\tilde{\Sigma}^R - \tilde{\Sigma}^A)\tilde{F} - \frac{i}{2}\left\{ \partial_p \tilde{F}\,\partial_x(\tilde{\Sigma}^R + \tilde{\Sigma}^A) - \partial_x \tilde{F}\,\partial_p(\tilde{\Sigma}^R - \tilde{\Sigma}^A)\right\}$$

use.

hermitian symmetry of $\Sigma \Rightarrow (\tilde{\Sigma}^R)^* = \tilde{\Sigma}^A$ check!

$\Rightarrow$ collision term $\overset{WT}{=}$ $\tilde{\Sigma}^K - 2i\tilde{F}\,\mathrm{Im}\,\tilde{\Sigma}^R -$

$$- i\,\partial_p\tilde{F}\,\partial_x \mathrm{Re}\,\tilde{\Sigma}^R + i\,\partial_x\tilde{F}\,\partial_p\,\mathrm{Re}\,\tilde{\Sigma}^R$$

$\Rightarrow$ full Dyson equation in WT + gradient approximation:

(multiply both sides with i), Notation $t_{av} \to t$, $r_{av} \to r$

$$-i\left[(G_0^R)^{-1} \overset{*}{,} F\right] = i\left(\Sigma^K - \Sigma^R * F + F * \Sigma^A\right) \longrightarrow$$

$$\left\{\partial_t + \hbar\vec{\nabla}_k\,\vec{\nabla}_{\vec{r}} + (\vec{\nabla}_r V)\cdot\vec{\nabla}_k - (\partial_t V)\partial_\varepsilon\right\}\tilde{F}$$

$$= i\tilde{\Sigma}_K + 2\tilde{F}\,\mathrm{Im}\,\tilde{\Sigma}^R +$$

$$+ (\vec{\nabla}_k\tilde{F})(\vec{\nabla}_{\vec{r}}\,\mathrm{Re}\,\tilde{\Sigma}^R) - \partial_\omega\tilde{F}\,\partial_t\,\mathrm{Re}\,\tilde{\Sigma}^R$$

$$- (\vec{\nabla}_r\tilde{F})(\vec{\nabla}_k\,\mathrm{Re}\,\Sigma^R) + \partial_t\tilde{F}\,\partial_\omega\,\mathrm{Re}\,\tilde{\Sigma}^R$$

Dyson in WT + gradient approx :

$$\boxed{\begin{aligned}&\left\{\left(1-\partial_\omega \mathrm{Re}\,\tilde\Sigma^R\right)\partial_t + (\partial_t V)\,\partial_\omega + \hbar\tilde{\vec v}_k\cdot\vec\nabla_r - (\vec\nabla_r\tilde V)\,\vec\nabla_k\right\}\tilde F \\ &= I^{coll}[\tilde F] \\ &\tilde{\vec v}_k = \frac{1}{\hbar}\vec\nabla_k\big(\overbrace{\varepsilon_k + \mathrm{Re}\,\tilde\Sigma^R}^{*}\big) \qquad * \\ &\tilde V(x,p) = V(x) + \mathrm{Re}\,\Sigma^R(x,p) \\ &I^{coll}[F] = i\,\tilde\Sigma^K + 2F\cdot \mathrm{Im}\,\tilde\Sigma^R\end{aligned}}$$

QBE : <u>Quantum</u> <u>Boltzmann</u> <u>equation</u>

partial differential equation, depending on 4 variables : $\vec r, t, \vec k, \omega$ (8-dimensional ?!)

<u>But:</u> No memory kernel as in original Dyson equation! $\rightsquigarrow$ this was dropped by making the gradient approximation in time.