Quantum Theory of Many-Body systems in Condensed Matter (4302112) 2020

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Today's class: *Equations of motion for Green's functions (Zubarev formalism)*

- Equations of motion for retarded Green's functions.
- Zubarev notation.
- Example: resonant level model.

Equation of motion for the R-GF

Retarded GF: $$G^R_{km}(t-t') = -i\theta(t-t')\left\langle\left[\hat{a}_k(t),\hat{a}^\dagger_m(t')\right]_\mp\right\rangle$$

$$\langle\ldots\rangle = \frac{1}{Z}\mathrm{Tr}\ (\hat{\rho}\ldots)$$

field operators

-: Bosons

+: Fermions

EOM:

$$i\frac{d}{dt}G^R_{km}(t-t') = \delta_{km}\delta(t-t') + D^R_{km}(t-t')$$

where

$$D^R_{km}(t-t') \equiv -i\theta(t-t')\left\langle\left[\left[\hat{a}_k(t),\hat{H}\right]_-,\hat{a}^\dagger_m(t')\right]_\mp\right\rangle$$

is also a retarded correlation function.

Fourier transform

$$\omega \to \omega^+ = \omega + i\eta$$

Retarded GFs:

$$\begin{cases} G^R_{km}(\omega^+) = \int_{-\infty}^{\infty} d(t-t')\; e^{i\omega^+(t-t')} G^R_{km}(t-t') \\ D^R_{km}(\omega^+) = \int_{-\infty}^{\infty} d(t-t')\; e^{i\omega^+(t-t')} D^R_{km}(t-t') \end{cases}$$

Now:

$$i\frac{d}{dt} G^R_{km}(t-t') \to \omega^+ G^R_{km}(\omega^+)$$

EOM:

$$\omega^+ G^R_{km}(\omega^+) = \delta_{km} + D^R_{km}(\omega^+)$$

Ok, fine. But how do I calculate these things?

Example 0: Free Hamiltonian

Step 1:
Commutator

$$\hat{H} = \sum_i \epsilon_i \hat{a}_i^\dagger \hat{a}_i \quad \Rightarrow \quad \left[\hat{a}_k, \hat{H}\right]_- = +\epsilon_k a_k$$

$$D^R_{km}(t-t') = -i\theta(t-t')\left\langle \left[\epsilon_k \hat{a}_k(t), \hat{a}^\dagger_m(t')\right]_\mp \right\rangle = \epsilon_k G^R_{km}(t-t')$$

Step 2:
EOM

$$\omega^+ G^R_{km}(\omega^+) = \delta_{km} + \epsilon_k G^R_{km}(\omega^+)$$

it “closes”!

$$\Rightarrow \quad G^R_{km}(\omega^+) = \frac{\delta_{km}}{\omega^+ - \epsilon_k}$$

EOM: Zubarev notation

$$\begin{cases} -i\theta(t-t')\left\langle \left[\hat{A}(t),\hat{B}(t')\right]_{\mp}\right\rangle \rightarrow \langle\langle \hat{A}:\hat{B}\rangle\rangle_{(t-t')} \\ \langle\langle \hat{A}:\hat{B}\rangle\rangle_{\omega} = \int_{-\infty}^{\infty} d(t-t')\, e^{i\omega^{+}(t-t')}\langle\langle \hat{A}:\hat{B}\rangle\rangle_{(t-t')} \end{cases}$$

-: Bosons

+: Fermions

EOM:

$$\omega^{+}\langle\langle \hat{A}:\hat{B}\rangle\rangle_{\omega} = \langle[\hat{A},\hat{B}]_{\mp}\rangle + \left\langle\left\langle \left[\hat{H},\hat{A}\right]_{-} : \hat{B}\right\rangle\right\rangle_{\omega}$$

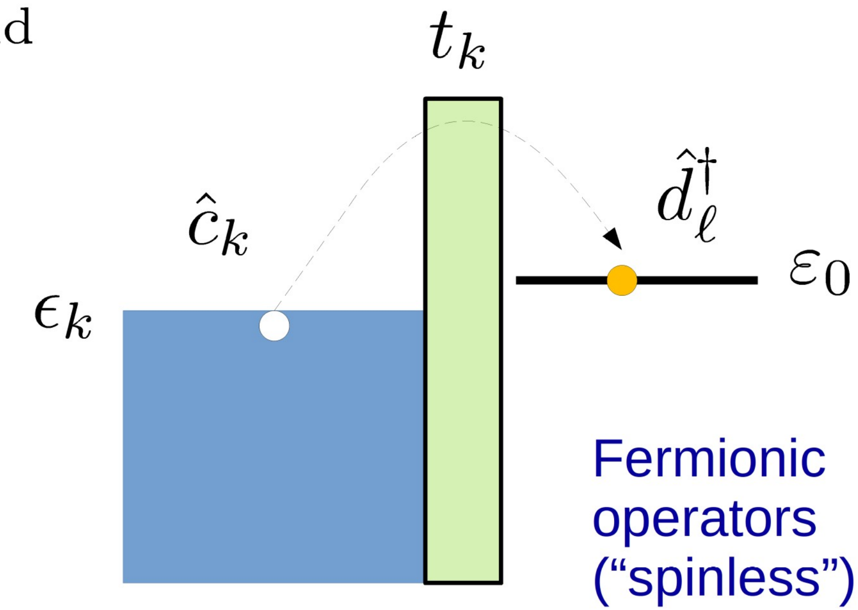
Zubarev, D. N.
Double-time Green functions in Statistical Physics
Soviet Phys. Usp, **3**, 320 (1960)

$$\omega^{+}\langle\langle \hat{A}:\hat{B}\rangle\rangle_{\omega} = \langle[\hat{A},\hat{B}]_{\mp}\rangle + \left\langle\left\langle \left[\hat{H},\hat{A}\right]_{-} : \hat{B}\right\rangle\right\rangle_{\omega}$$

Example 1: Resonant level model

$$\hat{H} = \hat{H}_{\text{level}} + \hat{H}_{\text{coup}} + \hat{H}_{\text{band}}$$

$$\left\{ \begin{aligned} \hat{H}_{\text{level}} &= \varepsilon_0 \hat{d}_\ell^\dagger \hat{d}_\ell \\ \hat{H}_{\text{coup}} &= \sum_k t_k \hat{d}_\ell^\dagger \hat{c}_k + t_k^* \hat{c}_k^\dagger \hat{d}_\ell \\ \hat{H}_{\text{band}} &= \sum_k \epsilon_k \hat{c}_k^\dagger \hat{c}_k \end{aligned} \right.$$



Fermionic operators (“spinless”):

We want to calculate the *spectral function* of the level:

$$A_\ell(\omega) = \frac{\text{- Im } G_\ell^R(\omega)}{\pi} \qquad G_\ell^R(\omega^+) = \langle\langle \hat{d}_\ell : \hat{d}_\ell^\dagger \rangle\rangle_\omega$$

Example 1: Resonant level model

Step 1: Commutators [redacted]

$$\begin{cases} \left[\hat{d}_\ell, \hat{H}\right]_- = +\varepsilon_0 \hat{d}_\ell + \sum_k t_k \hat{c}_k \\ \left[\hat{c}_k, \hat{H}\right]_- = +\epsilon_k \hat{c}_k + t_k^* \hat{d}_\ell \end{cases}$$

They "close"!

GFs:

$$\begin{cases} G_\ell^R(\omega^+) = \langle\langle \hat{d}_\ell : \hat{d}_\ell^\dagger \rangle\rangle_\omega \\ G_{k\ell}^R(\omega^+) = \langle\langle \hat{c}_k : \hat{d}_\ell^\dagger \rangle\rangle_\omega \\ G_{kk'}^R(\omega^+) = \langle\langle \hat{c}_k : \hat{c}_{k'}^\dagger \rangle\rangle_\omega \end{cases}$$

EOMs: [redacted]

$$\begin{cases} G_\ell^R(\omega^+) = \dfrac{1}{\omega^+ - \varepsilon_0 - \Sigma(\omega^+)} \\ \Sigma(\omega^+) = \sum_k \dfrac{|t_k|^2}{\omega^+ - \epsilon_k} \end{cases}$$

"Self energy"

Spectral function

Let's assume:

$$\Sigma(\omega^+) \approx \Lambda - i\Delta$$

$$A_\ell(\omega) = \frac{\Delta/\pi}{(\omega - \tilde{\varepsilon_0})^2 + \Delta^2}$$

Fluctuation-dissipation theorem

$$\begin{cases} -iG_\ell^<(\omega) = 2\pi A_\ell(\omega) n_F(\omega) \\ n_F(\omega) = (1 + e^{\beta\omega})^{-1} \end{cases}$$

Level occupation:

$$\langle \hat{n}_\ell \rangle = \langle c_\ell^\dagger c_\ell \rangle = -iG^<(t = t' = 0) = \frac{-i}{2\pi} \int_{-\infty}^{\infty} d\omega G_\ell^<(\omega) e^{i\omega(0)}$$

$$\langle \hat{n}_\ell \rangle = \int_{-\infty}^{\infty} A_\ell(\omega) n_F(\omega) d\omega$$

T=0: $\langle \hat{n}_\ell \rangle = \int_{-\infty}^{\epsilon_F} A_\ell(\omega) d\omega$