Keldysh Green Functions

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Abstract

A note on Keldysh Green functions, which are useful when dealing with non-equilibrium systems.

The Keldysh Green function is defined as follows:

$$G_{\alpha\beta}(1,2) = i\left\langle \hat{T}_c\left[\tilde{\psi}_\alpha(\vec{r}_1,t_1)\tilde{\psi}^\dagger_\beta(\vec{r}_2,t_2)\right]\right\rangle_{\rm st} \tag{1}$$

(The sign follows Kopnin. It's the opposite of AGD.) Each of the notations used here is explained. First, the statistical average $\langle\cdots\rangle_{\rm st}$ is defined as:

$$\mathrm{Tr}\left[\exp\left(\frac{\Omega+\mu\hat{N}-\hat{\mathcal{H}}(t_0)}{T}\right)\left(\tilde{\psi}_\alpha(1)\tilde{\psi}^\dagger_\beta(2)\right)\right] = \left\langle\tilde{\psi}_\alpha(1)\tilde{\psi}^\dagger_\beta(2)\right\rangle_{\rm st} \tag{2}$$

For variables, a short-hand notation like $1=(\vec{r}_1,t_1)$ was used. Also, $\tilde{\psi}_\alpha(1)$ is a Heisenberg operator and is defined as:

$$\tilde{\psi}_\alpha(\vec{r},t) = \hat{S}^{-1}(t,t_0)\tilde{\psi}_\alpha(\vec{r},t_0)\hat{S}(t,t_0) \tag{3}$$

The S-matrix is:

$$\hat{S}(t,t_0) = \hat{T}_t\exp\left[-i\int_{t_0}^{t}(\hat{\mathcal{H}}-\mu\hat{N})dt'\right] \tag{4}$$

Let's assume the temperature is T at time $t=t_0$. The time when the non-equilibrium interaction is applied is $t_0=-\infty$, and the interaction continues to be applied until $t_0=\max\{t_1,t_2\}$. The path running in the positive direction of the time axis is denoted by c_1. Conversely, the path running in the reverse direction from $t_0=\max\{t_1,t_2\}$ to $t_0=-\infty$ is denoted by c_2, and all paths are defined as $c=c_1+c_2$. (This is called the Keldysh contour, but it was originally devised by J. Schwinger.) Furthermore, we introduce inequalities $>_c$ and $<_c$ defined along the entire Keldysh contour c, and the time-ordering product $\hat{T}_c$ on the Keldysh contour is defined as:

$$\hat{T}_c\left[\tilde{\psi}_\alpha(1)\tilde{\psi}^\dagger_\beta(2)\right] = \begin{cases} \tilde{\psi}_\alpha(1)\tilde{\psi}^\dagger_\beta(2), & (t_1 >_c t_2) \\ \mp\tilde{\psi}^\dagger_\beta(2)\tilde{\psi}_\alpha(1), & (t_1 <_c t_2) \end{cases} \tag{5}$$

The upper sign is for fermions and the lower is for bosons.

We also define the following two new Green functions:

$$G^{>}_{\alpha\beta}(1,2) = i\Big\langle \tilde{\psi}_\alpha(1)\tilde{\psi}^\dagger_\beta(2)\Big\rangle_{\rm st} \tag{6}$$

$$G^{<}_{\alpha\beta}(1,2) = \mp i\Big\langle \tilde{\psi}^\dagger_\beta(2)\tilde{\psi}_\alpha(1)\Big\rangle_{\rm st} \tag{7}$$

Using these, we can write:

$$G_{\alpha\beta}(1,2) = \begin{cases} G^{>}_{\alpha\beta}(1,2), & (t_1 >_c t_2) \\ G^{<}_{\alpha\beta}(1,2), & (t_1 <_c t_2) \end{cases} \tag{8}$$

A function with these functions as matrix elements is defined as follows:

$$\underline{\check{\rm G}} = \begin{pmatrix} G^{11} & G^{12} \\ G^{21} & G^{22} \end{pmatrix} \tag{9}$$

The space formed by this four-component function is called the Keldysh space. The components are, respectively:

$$\begin{cases} G^{11}(1,2) &=& i\Big\langle \hat{T}_t\Big[\tilde{\psi}_\alpha(1)\tilde{\psi}^\dagger_\beta(2)\Big]\Big\rangle_{\rm st} \\ G^{12}(1,2) &=& G^{<}_{\alpha\beta}(1,2) \\ G^{21}(1,2) &=& G^{>}_{\alpha\beta}(1,2) \\ G^{22}(1,2) &=& i\Big\langle \hat{\bar{T}}_t\Big[\tilde{\psi}_\alpha(1)\tilde{\psi}^\dagger_\beta(2)\Big]\Big\rangle_{\rm st} \end{cases} \tag{10}$$

The $\hat{\bar{T}}_t$ in the (2,2) component is the anti-time-ordering product, and is defined as:

$$\hat{\bar{T}}_t\Big[\tilde{\psi}_\alpha(1)\tilde{\psi}^\dagger_\beta(2)\Big] = \begin{cases} \tilde{\psi}_\alpha(1)\tilde{\psi}^\dagger_\beta(2), & (t_1 < t_2) \\ \mp\tilde{\psi}^\dagger_\beta(2)\tilde{\psi}_\alpha(1), & (t_1 > t_2) \end{cases} \tag{11}$$

Similar to the conventional Green function method, we define the retarded Green function and the advanced Green function as follows:

$$G^{R}_{\alpha\beta}(1,2) = i\theta(t_1-t_2)\Big\langle \tilde{\psi}_\alpha(1)\tilde{\psi}^\dagger_\beta(2) \pm \tilde{\psi}^\dagger_\beta(2)\tilde{\psi}_\alpha(1)\Big\rangle_{\rm st} \tag{12}$$

$$G^{A}_{\alpha\beta}(1,2) = -i\theta(t_2-t_1)\Big\langle \tilde{\psi}_\alpha(1)\tilde{\psi}^\dagger_\beta(2) \pm \tilde{\psi}^\dagger_\beta(2)\tilde{\psi}_\alpha(1)\Big\rangle_{\rm st} \tag{13}$$

In addition to these, we also define the Keldysh Green function:

$$G^{K}_{\alpha\beta}(1,2) = G^{<}_{\alpha\beta}(1,2) + G^{>}_{\alpha\beta}(1,2) \tag{14}$$

Using these, the components of the matrix $\underline{\check{\rm G}}$ in Keldysh space can be expressed as:

$$G^R = G_{11} - G_{12} = G_{21} - G_{22} \tag{15}$$
$$G^A = G_{11} - G_{21} = G_{12} - G_{22} \tag{16}$$
$$G^K = G_{12} + G_{21} = G_{11} + G_{22} \tag{17}$$

Therefore, by performing an operation called the Keldysh transformation (Keldysh rotation) as follows:

$$\check{G} = \check{L}\check{\tau}_3\underline{\check{G}}\check{L}^{\mathrm{T}} = \begin{pmatrix} G^R & G^K \\ 0 & G^A \end{pmatrix} \tag{18}$$

we can obtain an expression like this. However, we have set:

$$\check{L} = \frac{1}{\sqrt{2}}(\check{1} - i\check{\tau}_2) \tag{19}$$

While the G^{ij} (where $i, j = 1, 2$) are dependent on each other, these G^R, G^A, and G^K are mutually independent. When dealing with non-equilibrium Green functions, this choice of basis for the matrix $\check{G}$ is convenient and standard.

Using the Keldysh Green function, we count the number of fermions N when an interaction is applied.

$$N = \sum_\alpha \left\langle \tilde{\psi}^\dagger_\alpha(1)\tilde{\psi}_\alpha(1) \right\rangle_{\mathrm{st}}$$
$$= i\sum_\alpha G^<_{\alpha\alpha}(1,1) \tag{20}$$

Using the following identity:

$$\lim_{t_1 \to t_2} \left[G^>_{\alpha\beta}(1,2) - G^<_{\alpha\beta}(1,2) \right] = i\delta(\vec{r}_1 - \vec{r}_2)\delta_{\alpha\beta} \tag{21}$$

and equation (14), we get:

$$\lim_{t_1 \to t_2} G^<_{\alpha\beta}(1,2) = \frac{1}{2}\lim_{t_1 \to t_2} G^K_{\alpha\beta}(1,2) - i\delta(\vec{r}_1 - \vec{r}_2)\delta_{\alpha\beta} \tag{22}$$

Using this, if we write the number of particles without interaction as N_0 and $N = N_0 + \delta N$, then:

$$N = N_0 + \frac{i}{2}\lim_{(\vec{r}_1,t_1)\to(\vec{r}_2,t_2)} \sum_\alpha \delta G^K_{\alpha\alpha}(1,2) \tag{23}$$

Here, δG^K represents the jump of the Green function at the same time, and can be replaced with:

$$\delta G^K = G^R - G^A = G^> - G^< \tag{24}$$

Furthermore, by performing a Fourier transform as follows:

$$G^K(1,2) = \int \frac{d\varepsilon\ d\omega}{(2\pi)^2} \frac{d^3\vec{p}\ d^3\vec{k}}{(2\pi)^6} e^{-i\varepsilon(t_1-t_2)} e^{-i\omega(t_1+t_2)} e^{i\vec{p}(\vec{r}_1-\vec{r}_2)} e^{i\vec{k}(\vec{r}_1+\vec{r}_2)/2}\ \ G^K_{\varepsilon_+,\varepsilon_-}(\vec{p}_+,\vec{p}_-) \tag{25}$$

we can also express it as:

$$N(\omega,\vec{k}) = N_0 - \frac{i}{2}\sum_\alpha \int \frac{d\varepsilon}{2\pi} \frac{d^3\vec{k}}{(2\pi)^3} G^K_{\varepsilon_+,\varepsilon_-}(\vec{p}_+,\vec{p}_-) \tag{26}$$

For the sake of notational simplicity, we have written $\vec{p}_\pm = \vec{p} \pm \dfrac{\vec{k}}{2}$ and $\varepsilon_\pm = \varepsilon \pm \dfrac{\omega}{2}$ here.

Similar to the conventional Green function method, the Dyson equation can also be constructed. We define the unperturbed Green function as $G^{(0)}_\varepsilon$:

$$G^{(0)}_\varepsilon = \frac{1}{\xi_{\vec{p}} - \varepsilon} \tag{27}$$

$\xi_{\vec{p}}$ represents the one-particle band dispersion. When an external potential $\check{U}(\vec{r},t)$ is applied, to the first order of $\check{U}$:

$$G^{ik\,(1)}(1,1') = -\int d^3\vec{r}_2 \int_{-\infty}^{\infty} dt_2\ G^{ij\,(0)}(1,2) U^{jl}(2) G^{lk\,(0)}(2,1') \tag{28}$$

[*1]

Here, $i,j,k = 1,2$. We assumed that the external potential has a structure like this, using the Pauli matrix $\check{\tau}_i$:

$$\check{U} = U\check{\tau}_3 \ \ = \ \ \begin{pmatrix} U & 0 \\ 0 & -U \end{pmatrix} \tag{29}$$

Omitting the matrix component indices and the integral sign, we write:

$$\underline{\check{\mathrm{G}}}^{(1)} = -\underline{\check{\mathrm{G}}}^{(0)} \check{U} \underline{\check{\mathrm{G}}}^{(0)} \tag{30}$$

By continuing to the second, third, $\cdots$ order, we can see that for all orders:

$$\underline{\check{\mathrm{G}}} = \underline{\check{\mathrm{G}}}^{(0)} - \underline{\check{\mathrm{G}}}^{(0)} \check{U} \underline{\check{\mathrm{G}}} \tag{31}$$

Applying the Keldysh rotation, we get:

$$\check{G} = \check{G}^{(0)} - \check{G}^{(0)} (U\check{1}) \check{G} \tag{32}$$

Using the inverse operator of the Green function for the non-interacting case:

[*1] However, this time runs from negative to positive, similar to the usual time evolution, not along the Keldysh contour.

$$\check{G}^{(0)^{-1}} = -i\partial_t + \xi_{\vec{p}} \tag{33}$$

we can write:

$$(\check{G}^{(0)^{-1}} + U)\check{G} = \check{1} \tag{34}$$

which is similar to the conventional method. The above framework can be applied to, for example, impurity scattering, but even when interactions with phonons and/or electron-electron interactions are applied, the self-energy can be introduced in the Keldysh formalism in the same way and rewritten as follows. (The case for phonons will be summarized in a separate note.) [Rammer and Smith(1986)]

$$(\check{G}^{(0)^{-1}} + \check{\Sigma})\check{G} = \check{1}, \qquad \check{\Sigma} = \begin{pmatrix} \Sigma^R & \Sigma^K \\ 0 & \Sigma^A \end{pmatrix} \tag{35}$$

As an appendix, here are the expressions for the unperturbed Green functions. (Note that the sign definition is the opposite of AGD.)

$$\begin{pmatrix} G^{11}{}^{(0)}_{\varepsilon}(\vec{p}) & G^{12}{}^{(0)}_{\varepsilon}(\vec{p}) \\ G^{21}{}^{(0)}_{\varepsilon}(\vec{p}) & G^{22}{}^{(0)}_{\varepsilon}(\vec{p}) \end{pmatrix} \tag{36}$$

$$= \begin{pmatrix} \dfrac{1}{\xi_{\vec{p}} - (\varepsilon + i0)} \mp 2\pi i n_{\vec{p}} \delta(\xi_{\vec{p}} - \varepsilon) & \pm 2\pi i n_{\vec{p}} \delta(\xi_{\vec{p}} - \varepsilon) \\ -2\pi i(1 \mp n_{\vec{p}})\delta(\xi_{\vec{p}} - \varepsilon) & -\dfrac{1}{\xi_{\vec{p}} - (\varepsilon - i0)} \mp 2\pi i n_{\vec{p}} \delta(\xi_{\vec{p}} - \varepsilon) \end{pmatrix} \tag{37}$$

$$\begin{pmatrix} G^{R}{}^{(0)}_{\varepsilon}(\vec{p}) & G^{K}{}^{(0)}_{\varepsilon}(\vec{p}) \\ G^{A}{}^{(0)}_{\varepsilon}(\vec{p}) & 0 \end{pmatrix} = \begin{pmatrix} \dfrac{1}{\xi_{\vec{p}} - (\varepsilon + i0)} & -2\pi i n_{\vec{p}} \delta(\xi_{\vec{p}} - \varepsilon) \\ \dfrac{1}{\xi_{\vec{p}} - (\varepsilon - i0)} & 0 \end{pmatrix} \tag{38}$$

Furthermore, it can be extended to the BCS superconducting state. We just need to define the inverse Green operator as follows:

$$\check{G}^{-1}_{\varepsilon}(\vec{p} - \vec{k}_1, \varepsilon_1) = \begin{pmatrix} \xi_{\vec{p}} - \varepsilon & 0 \\ 0 & \xi_{\vec{p}} + \varepsilon \end{pmatrix} (2\pi)^4 \delta(\varepsilon_1)\delta(\vec{k}_1) + \check{H}_{\varepsilon_1} \tag{39}$$

$$\check{H}_{\varepsilon_1} = \begin{pmatrix} -\dfrac{e}{c}\vec{v}_{\mathrm{F}}\vec{A}(\vec{k}) + e\phi & -\Delta(\vec{k}) \\ \Delta^*(\vec{k}) & \dfrac{e}{c}\vec{v}_{\mathrm{F}}\vec{A}(\vec{k}) + e\phi \end{pmatrix} \tag{40}$$