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Sheet 1

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1 Keldysh Green's function for noninteracting fermions

Consider a one-band model for noninteracting spinless fermions on a lattice with Hamiltonian

$$\hat{H} = \sum_{\boldsymbol{k}} \epsilon(\boldsymbol{k}) c_{\boldsymbol{k}}^{\dagger} c_{\boldsymbol{k}}, \tag{1}$$

with dispersion $\epsilon(\boldsymbol{k})$ and canonical second quantization fermionic operators with anticommutation relations $\{c_{\boldsymbol{k}}, c_{\boldsymbol{k}'}^{\dagger}\} = \delta_{\boldsymbol{k},\boldsymbol{k}'}$.

The single-particle Keldysh Green's function is defined as

$$G(\boldsymbol{k}, t, t') \equiv -i\mathcal{T}\langle c_{\boldsymbol{k}}(t) c_{\boldsymbol{k}}^{\dagger}(t')\rangle, \tag{2}$$

$$\langle ... \rangle \equiv \frac{\mathrm{Tr}\left[\exp(-\beta\hat{H})...\right]}{\mathrm{Tr}\left[\exp(-\beta\hat{H})\right]}, \tag{3}$$

with contour time-ordering operator $\mathcal{T}$ and time-dependent operators in the Heisenberg picture. The time arguments t and t' are on the 3-branch contour defined in the lecture. Here β is the inverse temperature.

(a) Compute the contour Green's function $G(\boldsymbol{k}, t, t')$. *Hint:* Use the fact that $c_{\boldsymbol{k}}^{\dagger} c_{\boldsymbol{k}} |n_k\rangle = n_k |n_k\rangle$ implies $\exp(i\epsilon(\boldsymbol{k}) c_{\boldsymbol{k}}^{\dagger} c_{\boldsymbol{k}} t)|n_k\rangle = \exp(i\epsilon(\boldsymbol{k}) n_k t)|n_k\rangle$ in particle-number notation.

(b) Extract specifically the imaginary-time Green's function. Convince yourself that the imaginary branch of the 3-branch contour can be attached in different ways. What is the periodicity of the imaginary-time Green's function? Compute the Matsubara frequency Green's function by Fourier transformation, $f(i\omega_n) \equiv \int_0^{\beta} d\tau \exp(i\omega_n\tau) f(\tau)$ with $\omega_n = (2n+1)\pi/\beta$.

(c) Extract the retarded Green's function and Fourier transform to real frequencies, $f(\omega) \equiv \int dt \exp(i\omega t) f(t)$. How is the spectral function obtained from this expression?

(d) How is the expression obtained in (a) modified in the presence of an electromagnetic vector potential field $\boldsymbol{A}(t)$ that is homogeneous in space, but time-dependent ("Peierls substitution"): $\epsilon(\boldsymbol{k}) \rightarrow \epsilon(\boldsymbol{k} - \boldsymbol{A}(t))$? Assume that $\boldsymbol{A}(0) = 0$ for the earliest time on the contour, i.e. the initial state is unaffected by the field.

Solution
Sheet 1 (28.10.14)

$$\hat{H} = \sum_{\vec{k}} \varepsilon(\vec{k})\, c^+_{\vec{k}} c_{\vec{k}} \qquad \{c_{\vec{k}}, c^+_{\vec{k}'}\} = \delta_{\vec{k}\vec{k}'}$$

$$G(\vec{k}, t, t') \equiv -i\,\mathcal{T} \langle c_{\vec{k}}(t)\; c^+_{\vec{k}}(t') \rangle$$

$$\langle \dots \rangle \equiv \frac{\mathrm{Tr}\left[e^{-\beta \hat{H}} \dots\right]}{\mathrm{Tr}\left[e^{-\beta \hat{H}}\right]}$$

(a) Compute $G(\vec{k}, t, t')$ for given $\hat{H}$

Case (i): $t > t'$

$$\Rightarrow \quad c_{\vec{k}}(t)\; c^+_{\vec{k}}(t')\, |\psi\rangle = e^{i\hat{H}t}\, c_{\vec{k}}\, e^{-i\hat{H}(t-t')}\, c^+_{\vec{k}}\, e^{-i\hat{H}t'} |\psi\rangle$$

with $|\psi\rangle = |n_{\vec{k}_1}, n_{\vec{k}_2}, \dots n_{\vec{k}_n}\rangle \longleftarrow$ occupation of $\vec{k}$ states (later: ensemble averages)

$$e^{-i\hat{H}t'} |\psi\rangle = e^{-i\left(\sum_{\vec{k}'} \varepsilon(\vec{k}')\, \hat{n}_{\vec{k}'}\right)t'} |n_{\vec{k}_1}, \dots, n_{\vec{k}_n}\rangle$$

$$= e^{-i\left(\sum_{\vec{k}'} \varepsilon(\vec{k}')\, n_{\vec{k}'}\right)t'} | \text{—}\,''\,\text{—} \rangle$$

$$c^+_{\vec{k}}\, e^{-i\hat{H}t'} |\psi\rangle = \underbrace{c^+_{\vec{k}} |\psi\rangle}_{= \begin{cases} 0 & \text{if } n_{\vec{k}} = 1 \text{ in } |\psi\rangle \\ |\psi; n_{\vec{k}} = 1\rangle & \text{if } n_{\vec{k}} = 0 \text{ in } |\psi\rangle \end{cases}} \underbrace{e^{-i\left(\sum_{\vec{k}'} \varepsilon(\vec{k}')\, n^{|\psi\rangle}_{\vec{k}'}\right)t'}}_{c\text{-number}}$$

$\longleftarrow$ Pauli blocking for fermions

$$\underbrace{e^{i\hat{H}(t'-t)}}_{e^{i\hat{H}t}\, c_{\vec{k}}}\, c^+_{\vec{k}}\, e^{-i\hat{H}t'} |\psi\rangle = c^+_{\vec{k}} |\psi\rangle\, e^{i\varepsilon_{\vec{k}}(t'-t)}\, e^{-i\sum_{\vec{k}'} \varepsilon(\vec{k}')\, n^{|\psi\rangle}_{\vec{k}'}}$$

$$\overset{\uparrow}{=} \cancel{e^{i\sum_{\vec{k}'} \varepsilon(\vec{k}')\, n^{|\psi\rangle}_{\vec{k}'}}}\; e^{i\varepsilon_{\vec{k}}(t'-t)}\; \cancel{e^{-i\sum_{\vec{k}'} \varepsilon(\vec{k}')\, n^{|\psi\rangle}_{\vec{k}'}}}$$

$c_{\vec{k}} c^+_{\vec{k}} |\psi\rangle = |\psi\rangle$ if $n_{\vec{k}} = 0$ in $|\psi\rangle$, 0 else

$$\Rightarrow \quad c_{\vec k}(t)\, c^+_{\vec k}(t')\,|\Psi\rangle = \begin{cases} e^{i\varepsilon(\vec k)(t'-t)}\,|\Psi\rangle & \text{if } n_{\vec k}=0 \text{ in } |\Psi\rangle \\ 0 & \text{else} \end{cases}$$

Ensemble average: the simplest way to obtain this is by noting that, for $t = t' = 0$ we can write

$$\langle c_{\vec k}\, c^+_{\vec k} \rangle \overset{\text{anticomm.}}{=} 1 - \underbrace{\langle c^+_{\vec k}\, c_{\vec k} \rangle}_{= n_{\vec k} \,\equiv\, n(\varepsilon(\vec k))} = 1 - f(\varepsilon(\vec k))$$

with the Fermi-Dirac function

$$f(\varepsilon(\vec k)) \equiv \frac{1}{e^{\beta \varepsilon(\vec k)} + 1}$$

which is obtained from the general expression

$$\frac{\mathrm{Tr}\left[e^{-\beta \hat H}\, c^+_{\vec k}\, c_{\vec k}\right]}{\mathrm{Tr}\left[e^{-\beta \hat H}\right]} = \frac{e^{-\beta \varepsilon(\vec k)}}{1 + e^{-\beta \varepsilon(\vec k)}} = f(\varepsilon(\vec k))$$

$$\Rightarrow \quad G(\vec k, t, t') = -i\,\left(1 - f(\varepsilon(\vec k))\right)\, e^{i\varepsilon(\vec k)(t'-t)} \qquad \text{for } t > t'$$

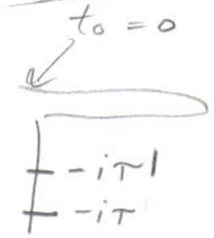
For the other case $t < t'$ we have to anticommute first:

$$G(\vec k, t, t')\Big|_{t<t'} = +i \left\langle c^+_{\vec k}(t')\, c_{\vec k}(t) \right\rangle = i\, f(\varepsilon(\vec k)) \text{ for } t' = t = 0$$

Together:

$$\boxed{G(\vec k, t, t') = i\left(f(\varepsilon(\vec k)) - \underbrace{\Theta(t > t')}_{\text{"contour theta function"}}\right) e^{i\varepsilon(\vec k)(t'-t)}}$$

· [later: the same result can be derived from an equation of motion, see Chapter IV.]



(b) imaginary times: $t \to -i\tau$

$t' \to -i\tau'$

$$G(\vec{k}, -i\tau, -i\tau') = i\left(f(\varepsilon(\vec{k})) - \Theta(\tau > \tau')\right)\underbrace{e^{i\varepsilon(\vec{k})(-i\tau' + i\tau)}}_{e^{\varepsilon(\vec{k})(\tau' - \tau)}}$$

Attach imaginary branch differently: Any shift leaves G invariant as long $\tau' - \tau$ stays the same.

For the perturbation theory (equation of motion, Ch. IV) it will be important to have a continuous contour – otherwise, the solutions on the imag. and real branches need not be smoothly connected.

Matsubara: we usually choose $G^M(\vec{k}, \tau) = -T_\tau \langle c_{\vec{k}}(\tau) c^\dagger_{\vec{k}} \rangle$

i.e. $\tau > \tau' = 0$ and without the "i".

$$\Rightarrow G^M(\vec{k}, \tau) = \underbrace{(f(\varepsilon(\vec{k})) - 1)}_{\frac{1 - (1 + e^{\beta\varepsilon(\vec{k})})}{1 + e^{\beta\varepsilon(\vec{k})}}} e^{-\varepsilon(\vec{k})\tau} = \frac{-e^{(\beta - \tau)\varepsilon(\vec{k})}}{1 + e^{\beta\varepsilon(\vec{k})}}$$

$$\int_0^\beta d\tau \, e^{(i\omega_n - \varepsilon(\vec{k}))\tau} = \frac{e^{(i\omega_n - \varepsilon(\vec{k}))\beta} - 1}{i\omega_n - \varepsilon(\vec{k})}$$

Fourier:

$$G^M(\vec{k}, i\omega_n) = \int_0^\beta d\tau \, G^M(\vec{k}, i\omega_n) e^{i\omega_n \tau} = \frac{1 - e^{i\omega_n\beta - \varepsilon(\vec{k})\beta}}{i\omega_n - \varepsilon(\vec{k})} \frac{e^{\beta(\varepsilon(\vec{k}))}}{1 + e^{\beta\varepsilon(\vec{k})}}$$

$$i\omega_n\beta = i(2n+1)\frac{\pi}{\beta}\beta = i(2n+1)\pi \Rightarrow e^{i\omega_n\beta} = e^{i\pi} = -1$$

$$\ldots \overset{\shortparallel}{=} \frac{1+e^{-\beta\varepsilon(\vec{k})}}{i\omega_n - \varepsilon(\vec{k})} \frac{1}{1+e^{-\beta\varepsilon(\vec{k})}} \Rightarrow$$

$$\Rightarrow \boxed{G^M(\vec{k}, i\omega_n) = \frac{1}{i\omega_n - \varepsilon(\vec{k})}}$$

periodicity:

$$G^M(\vec{k}, \tau-\beta) = -G^M(\vec{k}, \tau)$$

$\shortparallel \leftarrow$ now Θ-fct. $=0$ $\qquad \shortparallel$

$$f(\varepsilon(\vec{k}))\, e^{-\varepsilon(\vec{k})(\tau-\beta)} = \frac{e^{-\varepsilon(\vec{k})(\tau-\beta)}}{1+e^{\beta\varepsilon(\vec{k})}}$$

(c) Spectral function from retarded G:

$$G^R(\vec{k}, t, t') \equiv \Theta(t-t')\left[G^>(t,t') - G^<(t,t')\right]$$

$$G^>(\vec{k}, t, t') = i\left(f(\varepsilon(\vec{k})) - 1\right) e^{i\varepsilon(\vec{k})(t'-t)}$$

$$G^<(\vec{k}, t, t') = i\, f(\varepsilon(\vec{k}))\, e^{i\varepsilon(\vec{k})(t'-t)}$$

$$\Rightarrow G^R(\vec{k}, t, t') = -i\,\Theta(t-t')\, e^{i\varepsilon(\vec{k})(t'-t)}$$

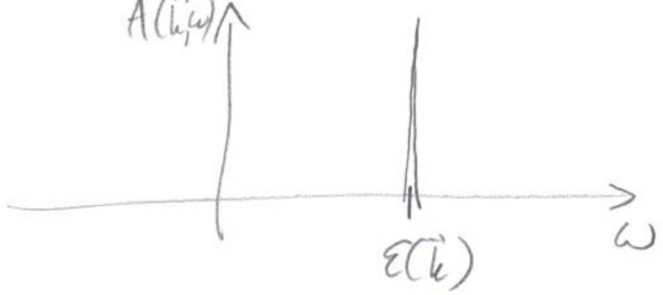
independent of distribution !!!

$$\Rightarrow G^R(\vec{k}, \omega+i0^+) = -i\int_0^\infty dt\, e^{-i\varepsilon(\vec{k})t}\, e^{i(\omega+i0^+)t} = \frac{1}{\omega+i0^+ - \varepsilon(\vec{k})}$$

Dirac identity: $\frac{1}{x + i0^+} = \mathcal{P}\frac{1}{x} - i\pi\,\delta(x)$

$$\Rightarrow \; -\frac{1}{\pi}\,\mathrm{Im}\, G^R(\vec{k},\omega+i0^+) \equiv A(\vec{k},\omega) \quad \text{Spectral function}$$

$$= \delta(\omega - \varepsilon(\vec{k}))$$



δ-peak at excitation energy $\varepsilon(\vec{k})$

(d) $e^{i\varepsilon(\vec{k})(t'-t)} \rightarrow e^{i\int_t^{t'} d\bar{t}\; \varepsilon(\vec{k} - A(\bar{t}))}$

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