QMB - HW 10 WS2022/2023

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1 Green's function and density of states

First of all, let us establish a connection between the retarded Green's function $G^{\mathrm{ret}}(\mathbf{k},\omega)$ and the density of states of the system `$\rho(\omega)$`. Show that for **free particles**,

$$\rho(\omega) = -\frac{1}{\pi}\mathrm{Im}\sum_{\mathbf{k}}\left[G^{\mathrm{ret}}(\mathbf{k},\omega)\right]$$

How can we express $\rho(\omega)$ in terms of the spectral function $A(\mathbf{k},\omega)$?

The free fermion Hamiltonian:

$$\hat{H} = \sum_{k}\frac{\hbar^2 k^2}{2m}\hat{c}_k^{\dagger}\hat{c}_k$$

The retarded greens function is the retarded (two-point) correlation for the creation and annihilation operators of the same state:

$$G^{\mathrm{ret}} = C^r\left(t_1 - t_2\right) = -i\Theta\left(t_1 - t_2\right)\left\langle\left\{c_k\left(t_2\right), c_k^{\dagger}\left(t_1\right)\right\}\right\rangle$$

or

$$G^{\mathrm{ret}} = C^r\left(t\right) = -i\Theta\left(t\right)\left\langle\left\{c_k\left(t\right), c_k^{\dagger}\left(0\right)\right\}\right\rangle$$

We have seen the imaginary-time cousin of this function before - see the lecture notes sec 2.4.4 for review.

The required Green's function has a very simple form:

$$C^r\left(\omega\right) = \frac{1}{\omega - E_{\boldsymbol{k}}}$$

To derive this, we need the the Lehman representation the Green's function assumes the form:

1. Fourier transform the real-time retarded Green's function:

$$C^r\left(\omega\right) = -i\int\limits_{-\infty}^{\infty} dt\, e^{i\omega t - \mu|t|}C^r\left(t\right) = -i\int\limits_{0}^{\infty} dt\, e^{i\omega t - \mu|t|}\left\langle\left\{c_k\left(t\right), c_k^{\dagger}\left(0\right)\right\}\right\rangle$$

μ is introduced to ensure convergence, and later we will take $\lim_{\mu\to 0}$.

2. Then we substitute for the expectation value

$$\left\langle \left\{ c_k(t), c_k^\dagger(0) \right\} \right\rangle = \frac{1}{Z} Tr\left[\rho_H \left\{ c_k(t), c_k^\dagger(0) \right\} \right] = \frac{1}{Z} \sum_n e^{-\beta E_n} \left\langle n \left| \left\{ c_k(t), c_k^\dagger(0) \right\} \right| n \right\rangle$$

where ρ_H is the free-fermion equilibrium density function and $|n\rangle$ are the system's eigenstates. So far all of this was completely general. In our case $\rho_H(\beta) = e^{-\beta \hat{H}}$ and we emphasize $n = \{n_i\} \in \{0,1\}^N$ to denote the multi-particle state $|n\rangle = \prod_{n_i} \hat{c}_i^{\dagger n_i} |0\rangle$.

3. Time evolution of operators is given by

$$c_k^\dagger(t) = e^{i\hat{H}t} c_k^\dagger e^{-i\hat{H}t}$$

Therefore each element in the sum is actually

$$\begin{aligned}
\sum_n e^{-\beta E_n} \left\langle n \left| \left\{ c_k^\dagger(t), c_k(0) \right\} \right| n \right\rangle &= \sum_n e^{-\beta E_n} \left(\left\langle n \left| c_k(t) c_k^\dagger(0) \right| n \right\rangle + \zeta \left\langle n \left| c_k^\dagger(0) c_k(t) \right| n \right\rangle \right) = \\
&= \sum_n e^{-\beta E_n} \left(\left\langle n \left| e^{i\hat{H}t} c_k e^{-i\hat{H}t} c_k^\dagger(0) \right| n \right\rangle + \zeta \left\langle n \left| c_k^\dagger(0) e^{i\hat{H}t} c_k e^{-i\hat{H}t} \right| n \right\rangle \right) = \\
&= \sum_n e^{-\beta E_n} \left(e^{iE_n t} \left\langle n \left| c_k e^{-i\hat{H}t} c_k^\dagger(0) \right| n \right\rangle + \zeta e^{-iE_n t} \left\langle n \left| c_k^\dagger(0) e^{i\hat{H}t} c_k \right| n \right\rangle \right) =
\end{aligned}$$

nest we insert resolutions of the identity $\sum_m |m\rangle \langle m|$ to get read from the other time evolution operators

$$\begin{aligned}
C^r(t) &= \sum_n e^{-\beta E_n} \left\langle n \left| \left\{ c_k^\dagger(t), c_k(0) \right\} \right| n \right\rangle = \\
&= \sum_n e^{-\beta E_n} \sum_m \left(e^{iE_n t} \left\langle n \left| c_k e^{-i\hat{H}t} \right| m \right\rangle \left\langle m \left| c_k^\dagger \right| n \right\rangle + \zeta e^{-iE_n t} \left\langle n \left| c_k^\dagger \right| m \right\rangle \left\langle m \left| e^{i\hat{H}t} c_k \right| n \right\rangle \right) = \\
&= \sum_n e^{-\beta E_n} \sum_m \left(e^{i(E_n - E_m)t} \langle n | c_k | m \rangle \left\langle m \left| c_k^\dagger \right| n \right\rangle + \zeta e^{-i(E_n - E_m)t} \left\langle n \left| c_k^\dagger \right| m \right\rangle \langle m | c_k | n \rangle \right) = \\
&= \sum_n e^{-\beta E_n} \sum_m e^{i(E_n - E_m)t} \langle n | c_k | m \rangle \left\langle m \left| c_k^\dagger \right| n \right\rangle + \zeta \sum_n \sum_m e^{-\beta E_m} e^{-i(E_m - E_n)t} \left\langle m \left| c_k^\dagger \right| n \right\rangle \langle n | c_k | m \rangle = \\
&= \sum_n \sum_m \left(e^{-\beta E_n} e^{i(E_n - E_m)t} \left\langle m \left| c_k^\dagger \right| n \right\rangle \langle n | c_k | m \rangle + \zeta e^{-\beta E_m} e^{-i(E_m - E_n)t} \left\langle m \left| c_k^\dagger \right| n \right\rangle \langle n | c_k | m \rangle \right) = \\
&= \sum_n \sum_m \left(e^{-\beta E_n} e^{i(E_n - E_m)t} + \zeta e^{-\beta E_m} e^{-i(E_m - E_n)t} \right) \langle n | c_k | m \rangle \left\langle m \left| c_k^\dagger \right| n \right\rangle
\end{aligned}$$

$$C^r(t) = \frac{1}{Z} \sum_n \sum_m \left(e^{-\beta E_n} + \zeta e^{-\beta E_m} \right) \langle n | c_k | m \rangle \left\langle m \left| c_k^\dagger \right| n \right\rangle e^{i(E_n - E_m)t}$$

Now perform the time integration:

$$\begin{aligned}
C^r(\omega) &= -i \frac{1}{Z} \sum_n \sum_m \langle n | c_k | m \rangle \left\langle m \left| c_k^\dagger \right| n \right\rangle \int_0^\infty dt\, e^{i\omega t - \mu|t|} \left(e^{-\beta E_n} e^{i(E_n - E_m)t} - \zeta e^{-\beta E_m} e^{-i(E_m - E_n)t} \right) = \\
&= i \frac{1}{Z} \sum_n \sum_m \langle n | c_k | m \rangle \left\langle m \left| c_k^\dagger \right| n \right\rangle \left[\frac{e^{-\beta E_n}}{i\omega - \mu + i(E_n - E_m)} - \frac{\zeta e^{-\beta E_m}}{i\omega - \mu + i(E_n - E_m)} \right] = \\
&= \frac{1}{Z} \sum_n \sum_m \left[\frac{e^{-\beta E_n}}{\omega + i\mu + (E_n - E_m)} - \frac{\zeta e^{-\beta E_m}}{\omega + i\mu + (E_n - E_m)} \right] \left| \left\langle m \left| c_k^\dagger \right| n \right\rangle \right|^2
\end{aligned}$$

Note $\langle n \left| c_k \right| m \rangle = \left(\left\langle m \left| c_k^\dagger \right| n \right\rangle \right)^*$ and $\left\langle m \left| c_k^\dagger \right| n \right\rangle = \left(\langle n \left| c_k \right| m \rangle \right)^*$.

We can evaluate the elements $\left| \left\langle m \left| c_k^\dagger \right| n \right\rangle \right|^2$. The state $|n\rangle$ must have no $\boldsymbol{k}$ particles, Therefore adding such a particle changes the energy $E_m = E_n + E_{\boldsymbol{k}}$. If $|n\rangle$ contained a $\boldsymbol{k}$ particle, that $c_{\boldsymbol{k}}^\dagger$ annihilates it.

$$C^r(\omega) = \frac{1}{Z} \sum_{n,n_k=0} \left[\frac{e^{-\beta E_n} - \zeta e^{-\beta(E_n + E_k)}}{\omega + i\mu - E_k} \right] = \frac{1}{Z} \sum_{n,n_k=0} \frac{e^{-\beta E_n}\left(1 - \zeta e^{-\beta E_k}\right)}{\omega + i\mu - E_k} =$$

$$= \frac{1}{Z} \frac{1}{\omega + i\mu - E_k} \left(1 + e^{-\beta E_k}\right) \sum_{n,n_k=0} e^{-\beta E_n}$$

The sum over m we can replace by $\sum_{m,m_k=0} e^{-\beta E_m} = \prod_{\vec{\boldsymbol{m}},m_k=0} \left(1 + e^{-\beta E_{\boldsymbol{m}}}\right)$. Hence we notice that we found the partition function Z:

$$Z = \sum_{\vec{\boldsymbol{m}}} e^{-\beta E_{\boldsymbol{m}}} = \prod_{\boldsymbol{m}} \left(1 + e^{-\beta E_{\boldsymbol{m}}}\right) = \left(1 + e^{-\beta E_{\boldsymbol{k}}}\right) \prod_{\vec{\boldsymbol{m}},m_k=0} \left(1 + e^{-\beta E_{\boldsymbol{m}}}\right)$$

Now we arrived at the result we initially claimed:

$$C^r(t) = \frac{1}{Z} \frac{1}{\omega + i\mu - E_{\boldsymbol{k}}} \left(1 + e^{-\beta E_{\boldsymbol{k}}}\right) \sum_{n,n_k=0} e^{-\beta E_n} = \frac{1}{Z} \frac{1}{\omega + i\mu - E_{\boldsymbol{k}}} Z = \frac{1}{\omega - E_{\boldsymbol{k}} + i\mu} = G^{ret}(\boldsymbol{k}, \omega)$$

Now using Dirac's identity

$$\lim_{\mu \to 0^+} \frac{1}{\omega - E_k + i\mu} = -i\pi\delta(\omega - E_k) + P\frac{1}{x}$$

(Note this identity is meaningful strictly only under integration - it is valid for distributions).

We find the spectral function

$$A(\boldsymbol{k}, \omega) = -\frac{1}{\pi} Im C^r(\omega) = \delta(\omega - E_k)$$

To conclude the question, we remember that the density of states is defined as

$$\rho(\omega) = \sum_n \delta(\omega - \omega_n)$$

where ω_n are the eigenenergies of the system, so we found what we were looking for:

$$\rho(\omega) = -\frac{1}{\pi} Im \sum_k C^r(\omega) = \sum_k A(\boldsymbol{k}, \omega)$$

2 Properties of the spectral function

We want to show that the spectral function $A(\boldsymbol{k},\omega)$ can be interpreted as a probability distribution over ω. For this, A must satisfy two conditions:

1. Normalization: $\int d\omega A(\boldsymbol{k},\omega)=1$.
2. Positivity: $A(\boldsymbol{k},\omega)\geq 0$.

Postivity is guaranteed by $A(\boldsymbol{k},\omega)=\delta(\omega-E_k)$ having a positive coefficient. for the case without interactions the normalization follows immediately:

$$\int d\omega A(\boldsymbol{k},\omega)=\int d\omega\delta(\omega-E_k)=1$$

With interaction the result still holds. The spectral function is then

$$A(\boldsymbol{k},\epsilon)=\frac{1}{Z}\sum_{n,m}\langle n|c_k|m\rangle\left\langle m\left|c_k^\dagger\right|n\right\rangle\left(e^{-\beta E_m}-\zeta e^{-\beta E_n}\right)\delta(\omega+E_n-E_m)$$

Where the states $|n\rangle,|m\rangle$ and energies E_n,E_m
are the eigenstates and eigenenergies of the total (interacting) Hamiltonian.

$$\begin{aligned}\int d\epsilon A(\boldsymbol{k},\epsilon)&=\int d\epsilon\frac{1}{Z}\sum_{n,m}\langle n|c_k|m\rangle\left\langle m\left|c_k^\dagger\right|n\right\rangle\left(e^{-\beta E_m}-\zeta e^{-\beta E_n}\right)\delta(\omega+E_n-E_m)=\\&=\frac{1}{Z}\sum_{n,m}\langle n|c_k|m\rangle\left\langle m\left|c_k^\dagger\right|n\right\rangle\left(e^{-\beta E_m}-\zeta e^{-\beta E_n}\right)\delta(\omega+E_n-E_m)=\\&=\frac{1}{\pi}\sum_{n,m}e^{-\beta E_n}\left\langle n\left|c_k^\dagger\right|m\right\rangle\langle m|c_k|n\rangle-\zeta\frac{1}{\pi}\frac{1}{Z}\sum_{n,m}e^{-\beta E_m}\left\langle n\left|c_k^\dagger\right|m\right\rangle\langle m|c_k|n\rangle=\\&=\frac{1}{Z}Tr\left[\rho_H\left[c_k^\dagger,c_k\right]_\zeta\right]\end{aligned}$$

For fermionic operators $\left\{c_k^\dagger,c_k\right\}=\mathbb{I}$ so $\int d\epsilon A(\boldsymbol{k},\epsilon)=\frac{1}{Z}Tr[\rho_H\mathbb{I}]=\frac{1}{Z}Tr[\rho_H]=1$. The result can be shown for any density matrix, not only those of thermal equilibrium. Postivity still holds for the interacting case because all of the terms in the sum are positive (The matrix elements contribute their squared absolute value, the exponents are positive and are summed for fermionc operators).

The spectral function can be used to calculate the expected occupancy $n_{B/f}(\boldsymbol{k})=\frac{1}{e^{\beta E_{\boldsymbol{k}}}-\zeta}$ of the eigenstates:

$$\int d\omega n_{B/F}(\hbar\omega)A(\boldsymbol{k},\omega)=\int d\omega n_{B/F}(\hbar\omega)\delta(\omega+E_{\boldsymbol{k}})=n_{B/F}(E_{\boldsymbol{k}})=\left\langle n_{B/F}(E_{\boldsymbol{k}})\right\rangle$$

And also in the interacting case:

$$\int d\omega n_{B/F}(\omega) A(\boldsymbol{k},\omega) = \int d\omega \frac{1}{Z}\sum_{n,m} \langle n |c_k| m\rangle \left\langle m \left|c_k^\dagger\right| n\right\rangle \left(e^{-\beta E_n} - \zeta e^{-\beta E_m}\right)\delta(\omega + E_n - E_m) n_{B/F}(\omega) =$$

$$= \frac{1}{Z}\sum_{n,m} \langle n |c_k| m\rangle \left\langle m \left|c_k^\dagger\right| n\right\rangle \left(e^{-\beta E_n} - \zeta e^{-\beta E_m}\right) n_{B/F}(E_m - E_n) =$$

$$= \frac{1}{Z}\sum_{n,m} \langle n |c_k| m\rangle \left\langle m \left|c_k^\dagger\right| n\right\rangle e^{-\beta E_m}\left(e^{-\beta(E_n - E_m)} - \zeta\right) n_{B/F}(E_m - E_n) =$$

$$= \frac{1}{Z}\sum_{n,m} \langle n |c_k| m\rangle \left\langle m \left|c_k^\dagger\right| n\right\rangle e^{-\beta E_m}\left(e^{\beta(E_m - E_n)} - \zeta\right) \frac{1}{e^{\beta(E_m - E_n)} - \zeta} =$$

$$= \frac{1}{Z}\sum_{n,m} \langle n |c_k| m\rangle \left\langle m \left|c_k^\dagger\right| n\right\rangle e^{-\beta E_m} = \frac{1}{Z}\sum_{m} \left\langle n \left|c_k^\dagger c_k\right| n\right\rangle e^{-\beta E_m} = \left\langle c_k^\dagger c_k\right\rangle = n_{B/F}(E_{\boldsymbol{k}}) = \langle n_{B/F}(E_{\boldsymbol{k}})\rangle$$

This results is applies both for fermions and bosons. Generically the pole will be non-negative, so for the bosonic spectral function will also be a probability amplitudes, but this needs to be verified. Then the frequencies can be thought of as the energy, or the Bohr frequencies associated with the energies of the system's allowed transitions.

The spectral function describes how the systems reacts to the addition of a single particles $\hat{c}_k^\dagger$. The Hamiltonian couples (or not, depends on its interactions) the particle to the systems eigenstates. So initially the state is $\hat{c}_k^\dagger |\psi(t=0)\rangle$ which is a pure state, and after a certain time of evolution by the full Hamiltonian, the system will be in a super position of eigenstates that is dictated by the spectral function.

3 Just add interactions

The addition of interactions introduces the self energy operator $\Sigma(\omega) = \Sigma' + i\Sigma''$ (note Σ'' is negative). As a result, the simple spectral function with a single pole at E_k will be replaced by a distribution of poles, whose center now shifted to $E_k + \Sigma'$, with a width characterized by Σ''. The intensity of the singularities decays with the distance from the center. A Fourier transform of the Green\s function allows to estimate the excitation's life time:

$$G^{ret}(\boldsymbol{k},\omega) = \frac{1}{\omega - E_k - \Sigma} = \frac{1}{\omega - E_k - \Sigma' - i\Sigma''}$$

To do the Fourier transform $G^{ret}(t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega e^{-i\omega t} G^{ret}(\boldsymbol{k},\omega)$, compute the integral by considering a complex frequency z and a suitable contour integral for $f(z) = \frac{e^{-izt}}{\omega - z}$.

1. First shift $\omega \to \omega' = \omega - E_k - \Sigma'$. This will brings out a phase factor $e^{-i\left(E_k + \Sigma'\right)t}$.

2. For $t < 0$, notice the pole is below the real line. Close the contour by parameterizing $z(\theta) = Re^{i\theta}$, $\theta \in [0,\pi]$ on a semi-circular path, and on the real line $z \in [-R, R]$. On the circular path $e^{-izt} = e^{-iR\cos\theta} e^{R\sin\theta t}$

which decays strongly because of the positive $\sin\theta$ and negative time. Therefore the integral on this part is 0, and since the contour closes over no poles the integral on the other part vanishes as well.

3. For $t > 0$, do a similar parametrization, however below the real line. The signs of t and $\sin\theta$ will be exchanged. Now there is a single simple pole with residue $Res\left[e^{-izt}\frac{1}{z-i\Sigma''}\right] = \lim_{z\to i\Sigma''}(z - i\Sigma'')\, f(z) = e^{-i\left(i\Sigma''\right)t}$, and $\oint dz e^{-izt}\frac{e^{-izt}}{\omega-z} = 2\pi i \mathrm{Res}\left[e^{-izt}\frac{1}{z-i\Sigma''}\right]$.

To conclude:

$$G^{ret}(t) \propto \Theta(t)\, i e^{-i\left(E_k+\Sigma'\right)t} e^{\Sigma''|t|}$$

Since $G(t)$ measures the particles probability to still exist at time t (the amplitude of the single particle state) , the exponential decay ($\Sigma'' < 0!$) in G indicates the particle will not survive.

To which order in the Coulomb interaction do need to go to actually see this?Second order is sufficient because there we have a diagram that contains a virtual particle with the same mass as the initial additional particle. In the diagram there will be three propagators, each contributing a factor of i which will not vanish thank to the virtual particle.