Universität Bonn 04 November, 2016
Physikalisches Institut
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Special Topics in Condensed Matter Theory
Winter term 2016/17

Exercise 3

(Solutions due on 25 November, 2016)

1 Green's functions: general properties (10 points)

1 Solution

a)

$$A_{\mathbf{k}\sigma}(\omega) = \frac{1}{Z_G}\sum_{n,m}|\langle n|c_{\mathbf{k}\sigma}|m\rangle|^2(e^{-\beta E_n}+e^{-\beta E_m})\delta(\omega+E_n-E_m)$$

Integrate over ω,

$$\begin{aligned}
\int_{-\infty}^{\infty} d\omega\, A_{\mathbf{k}\sigma}(\omega) &= \int_{-\infty}^{\infty} d\omega\,\frac{1}{Z_G}\sum_{n,m}|\langle n|c_{\mathbf{k}\sigma}|m\rangle|^2(e^{-\beta E_n}+e^{-\beta E_m})\delta(\omega+E_n-E_m)\\
&=\sum_{nm}\underbrace{\int_{-\infty}^{\infty} d\omega\,\delta(\omega-E_n-E_m)}_{1}\frac{1}{Z_G}|\langle n|c_{\mathbf{k}\sigma}|m\rangle|^2(e^{-\beta E_n}+e^{-\beta E_m})\\
&=\frac{1}{Z_G}\sum_{nm}\langle n|c_{\mathbf{k}\sigma}|m\rangle\langle m|c^\dagger_{\mathbf{k}\sigma}|n\rangle(e^{-\beta E_n}+e^{-\beta E_m})\\
&=\frac{1}{Z_G}(\sum_m\langle m|c^\dagger_{\mathbf{k}\sigma}\sum_n|n\rangle\langle n|c_{\mathbf{k}\sigma}|m\rangle e^{-\beta E_m}+(m\leftrightarrow n, c\leftrightarrow c^\dagger))\\
&=\frac{1}{Z_G}(\sum_m\langle m|c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}|m\rangle e^{-\beta E_m}+\sum_n\langle n|c_{\mathbf{k}\sigma}c^\dagger_{\mathbf{k}\sigma}|n\rangle e^{-\beta E_n})\\
&=\frac{1}{Z_G}(\sum_n\langle n|c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}|n\rangle e^{-\beta E_n}+\sum_n\langle n|c_{\mathbf{k}\sigma}c^\dagger_{\mathbf{k}\sigma}|n\rangle e^{-\beta E_n})\\
&=\frac{1}{Z_G}\sum_n\langle n|\underbrace{c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}+c_{\mathbf{k}\sigma}c^\dagger_{\mathbf{k}\sigma}}_{1}|n\rangle e^{-\beta E_n}\\
&=\frac{\sum_n e^{-\beta E_n}}{Z_G}=1
\end{aligned}$$

b)Here simply apply the identity (say Kramers-Kronig relation),

$$\frac{1}{x+i\epsilon}=\mathcal{P}\frac{1}{x}-i\pi\delta(x). \tag{1}$$

Where the $\mathcal{P}$ denotes principal value. Then

$$\begin{aligned} G^R_{\mathbf{k}\sigma}(\omega) &= \int_{-\infty}^{\infty} d\omega' \, \frac{A_{\mathbf{k}\sigma}(\omega')}{\omega - \omega' + i0^+} \\ &= \int_{-\infty}^{\infty} d\omega' \left(\frac{A_{\mathbf{k}\sigma}(\omega')}{\omega - \omega'} - i\pi\delta(\omega - \omega') A_{\mathbf{k}\sigma}(\omega') \right) \\ &= \int_{-\infty}^{\infty} d\omega' \frac{A_{\mathbf{k}\sigma}(\omega')}{\omega - \omega'} - i\pi A_{\mathbf{k}\sigma}(\omega) \end{aligned}$$

Then we integrate the imaginary part of retarded Green's function over ω,

$$\int_{-\infty}^{\infty} d\omega \, \mathrm{Im} G^R_{\mathbf{k}\sigma}(\omega) = \int_{-\infty}^{\infty} d\omega \, [-\pi A_{\mathbf{k}\sigma}(\omega)] = -\pi \tag{2}$$

b)In this problem we consider a finite band width for lattice systems, i.e. $A_{\mathbf{k}\sigma}(\omega) = 0$ if $|\omega| \geq \omega_{max}$ or $A_{\mathbf{k}\sigma}(\omega) = A_{\mathbf{k}\sigma}(\omega)$.

$$\begin{aligned} \lim_{\omega \to \pm\infty} \omega \cdot G^R_{\mathbf{k}\sigma}(\omega) &= \lim_{\omega \to \pm\infty} \omega \int_{-\infty}^{\infty} d\omega' \, \frac{A_{\mathbf{k}\sigma}(\omega')}{\omega(1 - \frac{\omega'}{\omega} + \frac{i0^+}{\omega})} \\ &= \lim_{\omega \to \pm\infty} \int_{-\infty}^{\infty} d\omega' \, A_{\mathbf{k}\sigma}(\omega')(1 + (\frac{\omega'}{\omega} - \frac{i0^+}{\omega}) + (\frac{\omega'}{\omega} - \frac{i0^+}{\omega})^2) \\ &= 1 + \lim_{\omega \to \pm\infty} \int_{-\infty}^{\infty} d\omega' \, A_{\mathbf{k}\sigma}(\omega')(\frac{\omega'}{\omega} - \frac{i0^+}{\omega}) \\ &= 1 + \lim_{\omega \to \pm\infty} \frac{1}{\omega} \int_{-\omega_{max}}^{\omega_{max}} d\omega' \, A_{\mathbf{k}\sigma}(\omega')(\omega' - i0^+) \\ &= 1 \end{aligned}$$

Which means $G^R_{\mathbf{k}\sigma}(\omega) \sim 1/\omega$ for large energies.

2 Density of states (10 points)

Spectral function can be defined by,

$$A_{\mathbf{k}\sigma}(\omega) = -2\mathrm{Im} G^R_{\mathbf{k}\sigma}(\omega) \tag{3}$$

Then (Kramers-Kronig),

$$N^{(d)}(\omega) = \int d^d k A_{\mathbf{k}\sigma}(\omega) = \int d^d k - 2\mathrm{Im} G^R_{\mathbf{k}\sigma}(\omega) = 2\pi\delta(\omega - \epsilon_{\mathbf{k}}) \tag{4}$$

Use the identity for delta function

$$\int_{-\infty}^{\infty} f(x)\delta(g(x))dx = \sum_i \frac{f(x_i)}{g'(x_i)} \tag{5}$$

which I checked from Wikipeida then,

$$\begin{aligned}A_{\mathbf{k}\sigma}(\omega) =&\delta(\omega - (\epsilon_{\mathbf{k}} - \mu)) \\ =&\delta(\omega - \frac{\hbar^2}{2m}k^2 + \mu) \\ =&\frac{1}{\left|-\frac{\hbar^2}{m}k\right|}\delta(|\mathbf{k}| - k_\omega)\end{aligned}$$

where $k_\omega = \sqrt{\frac{2m}{\hbar^2}(\omega + \mu)}$, and $k = |\mathbf{k}|$, so that,

$$\begin{aligned}N^{(d)}(\omega) &= \int d\Omega \int dk k^{d-1}\frac{m}{\hbar k}\delta(k - k_\omega) \\ &= \int d\Omega \frac{m}{\hbar^2}(\frac{2m}{\hbar^2}(\omega + \mu))^{d-2/2}\end{aligned}$$

and the volume $\int d\Omega 1$ equal to 2, 2π, 4π for dimensions $d = 1, 2, 3$ respectively.

$$\begin{aligned}N^{(1)}(\omega) =&\sqrt{\frac{m}{2\hbar^2}}\frac{2}{\sqrt{\omega + \mu}} \\ N^{(2)}(\omega) =&2\pi\frac{m}{\hbar^2} \\ N^{(3)}(\omega) =&\sqrt{32}(\frac{m}{\hbar^2})^{3/2}\sqrt{\omega + \mu}\end{aligned}$$

To sketch, simply capture the properties $N^{(1)} \sim \omega^{-1/2}$, $N^{(2)} \sim 1$ and $N^{(3)} \sim \omega^{1/2}$.