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Advanced Theoretical Condensed Matter Physics — SS11

Exercise 1

(Please return your solutions before Tue. 26.04.2011)

1.1. Green's functions for noninteracting electrons

In the lecture the position dependent Green's function was defined. In the same way one can define a momentum dependent retarded Green's function:

$$G^R_{\mathbf{k}\sigma}(t,t') = -\mathrm{i}\Theta(t-t')\frac{1}{Z_G}\mathrm{tr}\left\{\mathrm{e}^{-\beta(\hat{H}-\mu\hat{N})}\left[c_{\mathbf{k}\sigma}(t), c^\dagger_{\mathbf{k}\sigma}(t')\right]_+\right\} \tag{1}$$

(The advanced and time-ordered momentum dependent Green's functions are defined in complete analogy to the lecture). We will consider a system of noninteracting electrons here

$$\mathcal{H}_0 = H_0 - \mu N = \sum_{\mathbf{k}\sigma}(\epsilon(\mathbf{k})-\mu)c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}$$

a) Determine the time-dependence of $c_{\mathbf{k}\sigma}(t)$ and $c^\dagger_{\mathbf{k}\sigma}(t')$ for the noninteracting system $\mathcal{H}_0$ by using the equation of motion for a Heisenberg operator.

b) Compute the retarded Green's function (1) for the noninteracting system using the results of a).

$$G^{R,0}_{\mathbf{k}\sigma}(t,t') = -\mathrm{i}\Theta(t-t')\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}(\epsilon(\mathbf{k})-\mu)(t-t')} = G^{R,0}_{\mathbf{k}\sigma}(t-t') \tag{2}$$

c) Derive the Fourier transform

$$G^{R,0}_{\mathbf{k}\sigma}(E) = \int_{-\infty}^{\infty} d(t-t')\, G^{R,0}_{\mathbf{k}\sigma}(t-t')\,\mathrm{e}^{\mathrm{i}E(t-t')} = \frac{1}{E-(\epsilon(\mathbf{k})-\mu)+\mathrm{i}0^+} \tag{3}$$

Hint: Use the residue theorem to show first that

$$\Theta(t-t') \quad = \quad \mathrm{i}\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\,\frac{\mathrm{e}^{-\mathrm{i}\omega(t-t')}}{\omega+\mathrm{i}0^+}.$$

The Green's function can also be defined as the resolvent of a wave operator. In our case this is the Schrödinger operator:

$$(\mathrm{i}\partial_t - \mathcal{H}_0)G^{R,0}(t-t') = \delta(t-t')$$

d) Show that this equation is fullfilled by (2) by writing it in momentum space representation. What is the corresponding equation in energy space? Show that (3) is the resolvent of the Schröedinger operator in energy space.

In general, the retarded Green's function contains a non-infinitesimal imaginary part in the denominator

$$G^R_{\mathbf{k}\sigma}(\omega) = \frac{1}{\omega - (\epsilon(\mathbf{k}) - \mu) + \mathrm{i}\tau^{-1}}$$

e) Use the residue theorem to calculate the time-dependent Green's function by Fourier transform. How does the Green's function behave for large $(t - t')$? How can one interprete τ? Try to explain why a finite $\tau > 0$ might occur.

1.2. Green's functions: general properties

In the previous exercise, you calculated explicitely the retarded Green's function G for the special case of a diagonal Hamiltonian. However, in most cases the system is much more complex, e.g., in the presence of interactions. Nevertheless some analytical properties of G will always hold. We will discuss some of them in this exercise.

a) Normalization:
Use the explicit definition of the spectral function $A_{\mathbf{k}\sigma}(\omega)$ (see lecture),

$$A_{\mathbf{k}\sigma}(\omega) = \frac{1}{Z_G}\sum_{n,m} |\langle n|c_{\mathbf{k}\sigma}|m\rangle|^2 \left(e^{-\beta E_n} + e^{-\beta E_m}\right) \delta(\omega + E_n - E_m), \quad (4)$$

to show that $A_{\mathbf{k}\sigma}(\omega)$ is normalized,

$$\int_{-\infty}^{\infty} d\omega\, A_{\mathbf{k}\sigma}(\omega) = 1.$$

Use the spectral representation of $G^{\mathrm{R}}_{\mathbf{k}\sigma}(\omega)$ (see lecture),

$$G^{\mathrm{R}}_{\mathbf{k}\sigma}(\omega) = \int_{-\infty}^{\infty} d\omega' \frac{A_{\mathbf{k}\sigma}(\omega')}{\omega - \omega' + \mathrm{i}0^+}, \quad (5)$$

to find the relation between $\mathrm{Im}G^{\mathrm{R}}_{\mathbf{k}\sigma}(\omega)$ and $A_{\mathbf{k}\sigma}(\omega)$. Calculate

$$\int_{-\infty}^{\infty} d\omega\, \mathrm{Im}G^{\mathrm{R}}_{\mathbf{k}\sigma}(\omega).$$

b) Analytic properties:
We will now investigate some additional analytic properties of the zero-temperature Green's functions. We can write the definition of the Green's function as given in (5) in the following way

$$G_{\mathbf{k}\sigma}(z) = \int_{-\infty}^{\infty} d\omega' \frac{A_{\mathbf{k}\sigma}(\omega')}{z - \omega'}, \quad (6)$$

where z is now an arbitrary complex number, and notice that the "Green's function" has for the moment arbitrary analytic properties (it does not have a R-superscript).

i) Write down the definition of the spectral function $A(\omega)$ in terms of the difference of retarded and advanced Green's functions.

ii) We now assume a certain analyticity property for z. Let $\mathrm{Im}z > 0$. Remind yourself also of the analyticity properties of the retarded $G^{\mathrm{R}}_{\mathbf{k}\sigma}(\omega)$ and advanced $G^{\mathrm{A}}_{\mathbf{k}\sigma}(\omega)$ Green's function. Therefore, show, using Cauchy's theorem, that

$$G_{\mathbf{k}\sigma}(z) \quad = \quad -\frac{1}{2\pi i}\int_{-\infty}^{\infty} d\omega' \, \frac{G^{R}_{\mathbf{k}\sigma}(\omega')}{z-\omega'}, \tag{7}$$

iii) At this point set $z = \omega + \mathrm{i}0^+$ in (7). Show that our Green's functions obey the *Kramers - Kronig* relations:

$$\mathrm{Im}G^{\mathrm{R}}_{\mathbf{k}\sigma}(\omega) = -\frac{1}{\pi}P\int_{-\infty}^{\infty} d\omega' \, \frac{\mathrm{Re}G^{\mathrm{R}}_{\mathbf{k}\sigma}(\omega')}{\omega'-\omega} \tag{8}$$

$$\mathrm{Re}G^{\mathrm{R}}_{\mathbf{k}\sigma}(\omega) = \frac{1}{\pi}P\int_{-\infty}^{\infty} d\omega' \, \frac{\mathrm{Im}G^{\mathrm{R}}_{\mathbf{k}\sigma}(\omega')}{\omega'-\omega} \tag{9}$$

where the symbol P in front of the integral sign denotes the principal part of the integral.
Hint: Use the relation $\frac{1}{\omega'-\omega\pm i\delta} = P\left(\frac{1}{\omega'-\omega}\right) \mp i\pi\delta(\omega'-\omega)$
This means that the real and imaginary parts of the Green's function are not to be found independently, but rather can be calculated from one another. This is an important feature of the Green's function in that from it one sees that the Green's functions obey *causality*, and therefore corresponds to physical correlation functions.

iv) As an exercise on the application of the *Kramers - Kronig* relations, show, using (9) that the real part of the function $G^{\mathrm{R}}_{\mathbf{k}\sigma}(\omega)$ with the imaginary part

$$\mathrm{Im}G^{\mathrm{R}}_{\mathbf{k}\sigma}(\omega) = -\frac{1}{1+\omega^2}$$

is given by

$$\mathrm{Re}G^{\mathrm{R}}_{\mathbf{k}\sigma}(\omega) = \frac{\omega}{1+\omega^2}$$

c) Asymptotic behavior:
You can assume that $A_{\mathbf{k}\sigma}(\omega) \equiv 0$ if $|\omega| > \omega_{max}$ for some $0 < \omega_{max} < \infty$. Show

$$\lim_{\omega\to\pm\infty} \omega \cdot G^{\mathrm{R}}_{\mathbf{k}\sigma}(\omega) \quad = \quad 1,$$

i.e., $G^{\mathrm{R}}_{\mathbf{k}\sigma}(\omega) \approx 1/\omega$ for large energies.

d) In general, the retarded Green's function is of the form

$$G_{\mathbf{k}\sigma}(\omega) \quad = \quad \frac{1}{\omega - \tilde{\epsilon}(\mathbf{k}) - \Sigma_{\mathbf{k}\sigma}(\omega)}, \qquad \text{with } \tilde{\epsilon}(\mathbf{k}) \;=\; \epsilon(\mathbf{k}) - \mu.$$

(For simplicity, in exercise 1.1 e) we approximated $\Sigma_{\mathbf{k}\sigma}(\omega) \approx \mathit{const.}$)

Assume $\mathrm{Im}\Sigma_{\mathbf{k}\sigma}(\omega) = -\mathrm{i}0^+ + \mathcal{O}(\omega^2)$ and expand the Green's function around $(\tilde{\epsilon}(\mathbf{k}) = 0, \omega = 0)$ up to first order and show that it takes the form

$$G_{\mathbf{k}\sigma}(\omega) = \frac{z}{\omega - \tilde{\epsilon}^*(\mathbf{k}) + \mathrm{i}0^+} + G^{\mathrm{incoh}}_{\mathbf{k}\sigma}(\omega),$$

where $G^{\mathrm{incoh}}_{\mathbf{k}\sigma}(\omega)$ contains all higher order contributions. What are the explicit forms of the expression z and $\tilde{\epsilon}^*(\mathbf{k})$? We have seen, in exercise 1.1e), that the imaginary part of the Green's function represents a "decay parameter" for the Green's function. What role, which you can conclude from this exercise, does the real part play?