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Advanced Theoretical Condensed Matter Physics — SS09

Exercise 2

(Please return your solutions before Fr. 8.5.2009, 12h)

2.1. Green's functions for noninteracting electrons (10 points)

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:

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

(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 b).

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

c) Derive the Fourier transform

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

Hint: Use the residue theorem to show first that

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

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.

2.2. Green's functions: general properties (10 points)

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),

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

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

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

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

2.3. Stability of Fermi Surface (10 points)

As you know from statistical mechanics, (free) Fermi systems possess a Fermi surface, i.e., at zero temperature the occupation number, $\langle n_{\vec{k}\sigma}\rangle$, jumps discontinuously at $\epsilon_{\mathbf{k}} = \mu$. This discontinuity is the origin of many physical properties of solids.

a) Show that $\langle n_{\vec{k}\sigma} \rangle$ can be expressed via

$$\langle n_{\mathbf{k}\sigma} \rangle \;=\; \int_{-\infty}^{\infty} d\omega\, f(\omega)\, A_{\mathbf{k}\sigma}(\omega) \stackrel{T\to 0}{=} \int_{-\infty}^{0} d\omega\, A_{\mathbf{k}\sigma}(\omega), \quad \text{with } f(\omega) \;=\; \frac{1}{e^{\beta\omega}+1}. \quad (5)$$

Hint: To derive Eq. (5) rewrite the expectation value $\langle n_{\mathbf{k}\sigma} \rangle = \langle c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} \rangle$ in its spectral representation and compare the result with (4).

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

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

(For simplicity, in exercise 2.1 e) we approximated $\Sigma_{\mathbf{k}\sigma}(\omega) \approx const.$)

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. One can show that $G^{\mathrm{incoh}}_{\mathbf{k}\sigma}(\omega)$ is a smooth function and you can neglect it in the following.

c) Consider now the limits $\tilde{\epsilon}^{*}(\mathbf{k}) \nearrow 0$ and $\tilde{\epsilon}^{*}(\mathbf{k}) \searrow 0$ to show that $\langle n_{\mathbf{k}\sigma} \rangle$ remains discontinuous. Compare the result with the noninteracting case from exercise 2.1. Why can one deduce $z \in [0, 1]$ from exercise 2.2 a)?