Universität Bonn 10.11.2005
Physikalisches Institut
Prof. Dr. H. Kroha, P. Henseler
http://www.th.physik.uni-bonn.de/th/Groups/kroha

Condensed Matter Theory I — WS05/06

Exercise 3

(Please return your solutions before 22.11., 13:00 h)

3.1 Density of states (DOS) (4 points)

a) Derive the DOS $N(E)$ for a general dispersion relation ϵ_k in d dimensions, starting with the definition:

$$N(E) := \sum_k \delta(E - \epsilon_k) \tag{1}$$

(*hint:* Use the equation for the group velocity, given in the lecture.)

b) Calculate $N(E)$ for the $1d$ chain ($\epsilon_k = -2tcos(ka)$).

3.2 Green's functions - equation of motion (8 points)

a) Derive an equation of motion for an operator A, which does not depend explicitely on time, in the Heisenberg picture.

b) Determine the time-dependence of $c_{k\sigma}(t)$ and $c^\dagger_{k\sigma}(t)$ for the free electron gas with $H = \sum_{k\sigma} \epsilon_k c^\dagger_{k\sigma} c_{k\sigma}$.

c) Compute the free retarded Green's function $G^{0,R}_{k\sigma}(t - t')$, using the result of b).

d) Derive the Fourier transform $G^{0,R}_{k\sigma}(\omega) = \int d\tau G^{0,R}_{k\sigma}(\tau) e^{i(\omega + i\eta)\tau}$ with $|\eta| \to 0$. What is the sign of η? Why?

3.3 Equation of motion for the Green's function with local pair interaction (10 points)

If one considers an electron gas with a local pair interaction between two electrons, the Hamiltonian in position representation in 2nd quantization looks like this:

$$
\begin{aligned}
H_0 &= \frac{\hbar^2}{2m}\sum_\sigma \int d^3x \nabla\Psi^\dagger_\sigma(x)\nabla\Psi_\sigma(x) \\
V &= \frac{1}{2}\sum_{\sigma\sigma'}\int d^3x d^3x' v(x,x')\Psi^\dagger_\sigma(x)\Psi^\dagger_{\sigma'}(x')\Psi_{\sigma'}(x')\Psi_\sigma(x)
\end{aligned}
\tag{2}
$$

where the pair interaction is given by: $v(x,x') = (2\pi)^3 V_0 \delta(x-x') \cdot \delta_{\sigma'-\sigma}$.

In a real system, the local pair interaction can be explained be a strongly screended Coulomb interaction.

a) Transform the Hamiltonian (Eqn.2) to momentum space and show, using $\epsilon_k = -\frac{\hbar^2 k^2}{2m}$, that:

$$
H = H_0 + V = \sum_{k\sigma} \epsilon_k c^\dagger_{k\sigma} c_{k\sigma} + \frac{1}{2} V_0 \sum_{\substack{kpq \\ \sigma\sigma'}} \delta_{\sigma'-\sigma} c^\dagger_{k+q\sigma} c^\dagger_{p-q\sigma'} c_{p\sigma'} c_{k\sigma} \tag{3}
$$

b) The equation of motion of the retarded Green's function for the Hamiltonian H was shown in the lecture to be:

$$
\begin{aligned}
i\hbar\partial_t G^{\mathrm{R}}_{\kappa\tau}(t,t') &= \hbar\delta(t-t')\langle[c_{\kappa\tau}, c^\dagger_{\kappa\tau}]_+\rangle - i\theta(t-t')\langle[[c_{\kappa\tau}, H_0]_-(t), c^\dagger_{\kappa\tau}(t')]_+\rangle \\
&- i\theta(t-t')\langle[[c_{\kappa\tau}, V]_-(t), c^\dagger_{\kappa\tau}(t')]_+\rangle
\end{aligned}
$$

Write down the equation of motion for the Hamiltonian of part a) and show that the interaction term depends on the higher Green's function

$$
\Gamma^{-\tau\tau}_{pq\kappa} = -i\theta(t-t')\langle[(c^\dagger_{p+q-\tau} c_{p-\tau} c_{\kappa+q\tau})(t), c^\dagger_{\kappa\tau}(t')]_+\rangle \tag{4}
$$

c) For the following approximation, fluctuations of the operators A and B around their expectation values are neglected, i.e. one considers $A - \langle A\rangle = B - \langle B\rangle = 0$. Thus show that in general the following relation holds: $AB = \langle A\rangle B + \langle B\rangle A - \langle A\rangle\langle B\rangle$.

d) Use the approximation of part c) with $A = c^\dagger_{p+q\sigma} c_{p\sigma}$, $B = c_{\kappa+q\tau}$ and show that the retarded Green's function for the Hamiltonian of Eqn. (2) in momentum space becomes:

$$
G^{\mathrm{R}}_{\kappa\tau}(\omega) = \frac{1}{\omega - \epsilon_\kappa - V_0 \sum_p \langle n_{p-\tau}\rangle + i\eta}
$$

In this case the approximation of part c) is called *mean field approximation.*

e) Derive an expression for the magnetization $m := \langle n_\uparrow\rangle - \langle n_\downarrow\rangle$ and the particle number $n := \langle n_\uparrow\rangle + \langle n_\downarrow\rangle$ and show, that $m = 0$ is always a solution. One can show, that for $1 \leq V_0 N(\epsilon_F)$ there exist (numerical) solutions (Fig. 1) with finite magnetization.

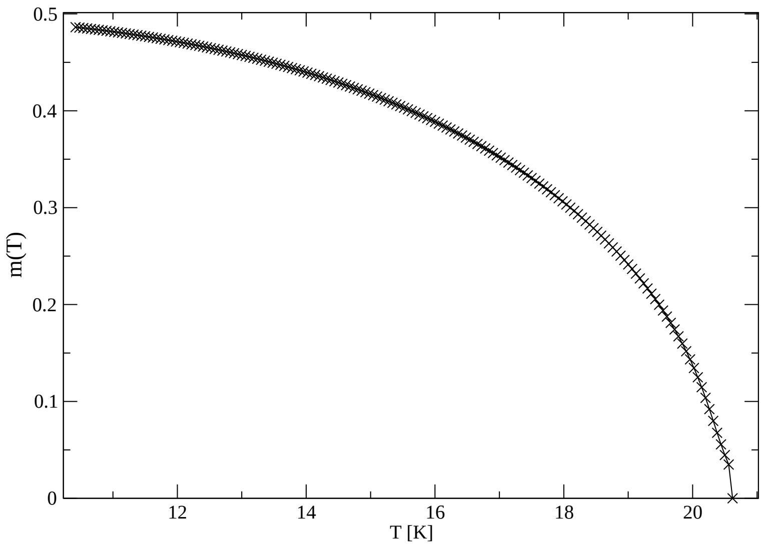

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Figure 1: Example for the numerical solution of the magnetization in the mean-field approximation