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Advanced Theoretical Condensed Matter Physics — SS09

Exercise 3

(Please return your solutions before Fr. 22.5.2009, 12h)

3.1. Linear Response Theory (15 points)

In the following we will investigate the general question: "How does a physical quantity change if an external field is applied?". We consider a many-body system H_0 and a perturbation which is explicitly time dependent:

$$\mathcal{H} = H_0 - \mu N + V_t = \mathcal{H}_0 + V_t \tag{1}$$

The perturbation V_t is switched on at time $t \to -\infty$ so that $\lim_{t\to-\infty} V_t = 0$. V_t is given by an time dependent external field ϕ_t which couples to the observable B:

$$V_t = \phi_t \hat{B}$$

For example an the electric potential will couple to the charge density $n(\mathbf{r}) = \psi^\dagger(\mathbf{r})\psi(\mathbf{r})$.

$$V_t = -e_0 \int d^3r \phi_{el}(\mathbf{r}, t) n(\mathbf{r})$$

The density matrix of the full Hamiltonian (1) in the Schroedinger picture is given by

$$\rho_t^S = \frac{\exp(-\beta\mathcal{H})}{\mathrm{tr}[\exp(-\beta\mathcal{H})]}$$

It turns out to be usefull to write all operators in the interaction picture, e.g. the density matrix

$$\rho(t) = \exp\big(\mathrm{i}\mathcal{H}_0 t\big)\rho_t^S \exp\big(-\mathrm{i}\mathcal{H}_0 t\big)$$

Note that the subscript t refers to the explicit time dependence in contrast to the time dependence introduced by the interaction picture. From now on all operators which are not explicitly marked are meant to be written in the interaction picture.

a) Derive an implicit equation for the density matrix in the interaction picture by integrating the equation of motion

$$\dot{\rho}(t) = -\mathrm{i}\big[V(t), \rho(t)\big]_-$$

and using the initial condition

$$\lim_{t\to-\infty} \rho(t) = \rho_0^S$$

b) If the perturbation is assumed to be small, it is sufficient to consider only terms which are *linear* in $V(t)$. Use the result of a) to show that the density matrix in the Schroedinger picture reads

$$\rho_t^S = \rho_0^S - \mathrm{i}\int_{-\infty}^{t} dt' \exp\bigl(-\mathrm{i}\mathcal{H}_0 t\bigr)\bigl[V(t'),\rho_0^S\bigr]_- \exp\bigl(\mathrm{i}\mathcal{H}_0 t\bigr) \tag{2}$$

We are interested in the expectation value of an observable A if an external field ϕ_t is applied which couples to the observable $\hat{B}$.

c) Calculate the expectation value $\langle A\rangle_t = \mathrm{tr}(\rho_t^S A)$. to show that

$$\Delta A_t = \langle A\rangle_t - \langle A\rangle_0 = -\mathrm{i}\int_{-\infty}^{t} dt' \phi_{t'} \langle \bigl[A(t), B(t')\bigr]_-\rangle_0$$

Hint: Use cyclic permutation under the trace.

A general retarded Green's function of the operators A and B is defined as follows

$$G_{AB}^R(t,t') = -i\Theta(t-t')\bigl\langle \bigl[A(t), B(t')\bigr]_-\bigr\rangle_0$$

Note: If you plug in $\psi^\dagger(x)$ and $\psi(x)$ for A and B you obtain the retarded single particle Green's function as it was defined in the lecture. In the same way the $\mathbf{k}$-dependent Green's function is constructed by plugging in $a_{\mathbf{k}}^\dagger$ and $a_{\mathbf{k}}$.

d) Express ΔA_t in terms of the retarded Green's function $G_{AB}^R(t,t')$.

$G_{AB}^R(t,t')$ is also called *A-B-response function.*

3.2. Feynman diagrams: 1st order perturbation theory (15 points)

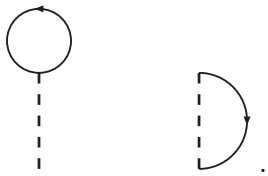
Generally, Green's function cannot be calculated exactly, but one has to use appropriate approximations. In this exercise, we want to use perturbation theory and to practice the calculation of Feynman diagrams. For that purpose, consider the Hamiltonian $\mathcal{H}$ of interacting electrons,

$$\mathcal{H} \;\equiv\; \mathcal{H}_0 + V \;=\; \sum_{\mathbf{k},\sigma} (\epsilon(\mathbf{k}) - \mu)\, c_{\mathbf{k}\sigma}^\dagger\, c_{\mathbf{k}\sigma} \;+\; \sum_{\substack{\mathbf{k},\mathbf{k}',\mathbf{q}\\ \sigma,\sigma'}} V_{\mathbf{q}}^{\sigma,\sigma'}\, c_{\mathbf{k}+\mathbf{q},\sigma}^\dagger\, c_{\mathbf{k}'-\mathbf{q},\sigma'}^\dagger\, c_{\mathbf{k}'\sigma'}\, c_{\mathbf{k}\sigma}.$$

We want to calculate the single-particle Matsubara Green's function $G_{\mathbf{k}\sigma}(\mathrm{i}\omega)$ by treating the potential V as a perturbation. According to Dyson's equation,

$$G_{\mathbf{k}\sigma}(\mathrm{i}\omega) = G_{\mathbf{k}\sigma}^0(\mathrm{i}\omega) + G_{\mathbf{k}\sigma}^0(\mathrm{i}\omega)\Sigma_{\mathbf{k}\sigma}(\mathrm{i}\omega)G_{\mathbf{k}\sigma}(\mathrm{i}\omega),$$

we have to calculate the self energy $\Sigma_{\mathbf{k}\sigma}(\mathrm{i}\omega)$. Restricting to 1st order in V this corresponds to the evaluation of the two Feynman diagrams



a) General case:
Use the Feynman rules to show that the first diagram  (Hartree term) yields

$$\Sigma^{(\mathrm{H})}_{k\sigma}(\mathrm{i}\omega) \;=\; \left(V^{\sigma,\sigma}_{\mathbf{q}=0} + V^{\sigma,-\sigma}_{\mathbf{q}=0}\right) \sum_{\mathbf{k}'} f(\epsilon(\mathbf{k}') - \mu)$$

and the second one  (Fock term) yields

$$\Sigma^{(\mathrm{F})}_{k\sigma}(\mathrm{i}\omega) \;=\; -\sum_{\mathbf{q}} V^{\sigma,\sigma}_{\mathbf{q}} f(\epsilon(\mathbf{k}-\mathbf{q}) - \mu).$$

Hint: Recall that for a holomorphic function $F(z)$

$$\frac{1}{\beta}\sum_{\omega} F(\mathrm{i}\omega) \;=\; -\oint_{C_1} \frac{dz}{2\pi\mathrm{i}}\, f(z)\, F(z) \;=\; \oint_{C_2} \frac{dz}{2\pi\mathrm{i}}\, f(z)\, F(z),$$

where C_1 encloses only the poles of $f(z)$ and C_2 only those of $F(z)$.

b) Coulomb interaction:
Consider the concrete example of a Coulomb interaction of a gas of free electrons in three dimensions. The Fourier transform of the Coulomb potential is

$$V^{\sigma,\sigma'}_{\mathbf{q}} \;=\; \begin{cases} 0 & , \quad \mathbf{q} = 0 \\ \frac{1}{V}\frac{4\pi e_0^2}{q^2} & , \quad \mathbf{q} \neq 0 \end{cases} \qquad (e_0\text{: elementary electric charge}).$$

Use the result from a) to obtain

$$\Sigma_{k\sigma}(\mathrm{i}\omega) \;=\; -\sum_{\mathbf{q}} V^{\sigma\sigma}_{\mathbf{k}-\mathbf{q}}\, f(\epsilon(\mathbf{q}) - \mu) \;\overset{T\to 0}{=}\; \frac{e_0^2}{2\pi} k_{\mathrm{F}} \left(2 + \frac{k_{\mathrm{F}}^2 - k^2}{k k_{\mathrm{F}}} \ln\left|\frac{k_{\mathrm{F}} + k}{k_{\mathrm{F}} - k}\right|\right).$$

Hint:

$$\int_0^x dy\, y\, \ln\left|\frac{y-1}{y+1}\right| \;=\; -x - \frac{1}{2}\left(1 - x^2\right) \ln\left|\frac{x-1}{x+1}\right|$$

c) Hubbard interaction:
In metals the bare Coulomb interaction gets screened by the conduction band electrons. Therefore, the effective two-particle potential becomes short-ranged, $V(x) \approx e^{-x/\xi}\, \frac{e_0^2}{x}$ (Thomas-Fermi approximation). Assuming the screening length ξ to be on the order of one lattice spacing one can approximate the potential as point-like and arrives at the important Hubbard model

$$\mathcal{H}_{\mathrm{Hub}} \;\equiv\; \mathcal{H}_0 + V \;=\; \sum_{\mathbf{k},\sigma} (\epsilon(\mathbf{k}) - \mu)\, c^\dagger_{\mathbf{k}\sigma}\, c_{\mathbf{k}\sigma} \;+\; \frac{U}{2} \sum_{i,\sigma} c^\dagger_{i,\sigma}\, c^\dagger_{i,-\sigma}\, c_{i,-\sigma}\, c_{i,\sigma},$$

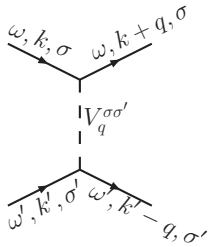
where the index i labels the lattice sites.

Show that the Fourier transform of the Hubbard potential is $V^{\sigma,\sigma'}_{\mathbf{q}} \;=\; \frac{U}{2V}\, \delta_{\sigma,-\sigma'}$ and obtain from a)

$$\Sigma_{k\sigma}(\mathrm{i}\omega) \;=\; \frac{1}{2} U n, \qquad n \;=\; \frac{\langle N \rangle}{V}.$$

Feynman rules: (Matsubara representation)

1) Draw all connected, topologically distinct diagrams of order n.

2) Each vertex corresponds to 

$= \quad -\frac{1}{\beta} V_{\mathbf{q}}^{\sigma,\sigma'}.$

3) Each line $\xrightarrow{\omega, k, \sigma}$ corresponds to $-G^0_{\mathbf{k}\sigma}(\mathrm{i}\omega) = \dfrac{-1}{\mathrm{i}\omega - \epsilon(\mathbf{k}) + \mu}$.

4) Each non-propagating line,  and  , gets a factor $e^{\mathrm{i}\omega 0^+}$.

5) Each closed fermion loop gets an additional factor (-1).

6) All internal indices (momenta, spins, energies, ...) have to be summed.