Karlsruher Institut für Technologie

Institut für Theorie der Kondensierten Materie

Theorie der Kondensierten Materie II SS 2017

PD Dr. B. Narozhny

M. Sc. M. Bard

Blatt 9

Lösungsvorschlag

---

1. Diffusion

(a) **Show that within the Matsubara technique, the density-density response function can be expressed in terms of the exact Green's function of the disordered system. Draw the corresponding diagram.**

We employ the Kubo-formula to calculate the density-density response function. Using the density fluctuation $\delta n(\mathbf{r}, t) = n(\mathbf{r}, t) - \langle n(\mathbf{r}, t)\rangle$, we find

$$K(\mathbf{r}, \mathbf{r}', t - t') = -i\theta(t - t')\langle[\delta n(\mathbf{r}, t), -\delta n(\mathbf{r}', t')]\rangle_0 \tag{1}$$

The corresponding Matsubara function has the form

$$\begin{aligned} K^M(\mathbf{r}, \mathbf{r}', \tau - \tau') = &- \langle T_\tau \bar{\Psi}(\mathbf{r}, \tau)\Psi(\mathbf{r}, \tau)\bar{\Psi}(\mathbf{r}', \tau')\Psi(\mathbf{r}', \tau')\rangle_0 \\ &+ \langle T_\tau \bar{\Psi}(\mathbf{r}, \tau)\Psi(\mathbf{r}, \tau)\rangle_0 \langle T_\tau \bar{\Psi}(\mathbf{r}', \tau'\Psi(\mathbf{r}', \tau'\rangle_0 \end{aligned} \tag{2}$$

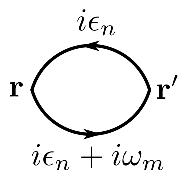
After using the Wick theorem, we end up with

$$K^M(\mathbf{r}, \mathbf{r}', \tau - \tau') = G(\mathbf{r}, \mathbf{r}', \tau - \tau')G(\mathbf{r}', \mathbf{r}, \tau' - \tau). \tag{3}$$

Transforming from the time domain to the discrete (bosonic) frequencies ω_m, we arrive at

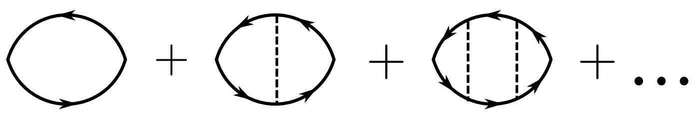
$$K^M(\mathbf{r}, \mathbf{r}', i\omega_m) = T\sum_n G(\mathbf{r}, \mathbf{r}', i\epsilon_n + i\omega_m)G(\mathbf{r}', \mathbf{r}, i\epsilon_n). \tag{4}$$

Here, ϵ_n is a fermionic frequency. The corresponding diagram is



(b) **Assuming isotropic scattering on impurities, average the above response function over disorder. Show, that the dominant contribution is given by the ladder series of diagrams, described in the lecture as the diffuson series. Sum up the series in the Matsubara technique, and expand the expression for small momenta and frequencies.**

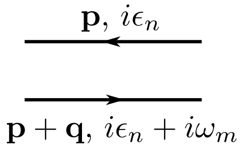
We perform now the average over the disorder realizations. We take into account all diagrams of the diffuson series (ladder diagrams):



The diagrams with crossed impurity lines are suppressed by the small parameter $1/k_{\mathrm{F}}l$ (see exercise sheet 8). The disorder-averaged Green's function is translational invariant. The corresponding function in Fourier space reads

$$G(\mathbf{p}, i\epsilon_n) = \frac{1}{i\epsilon_n - \xi_p + \frac{i}{2\tau}\mathrm{sign}(\epsilon_n)}. \tag{5}$$

Because of the assumed isotropic scattering on impurities, all diagrams consist of independent blocks that are of the form

$B =$ 

Overall we need to compute only one Matsubara summation in each diagram since we consider only elastic impurity scattering. We now perform the momentum integration in the block B:

$$B = \int \frac{\mathrm{d}^d p}{(2\pi)^d} \frac{1}{i\epsilon_n - \xi_{\mathbf{p}} + \frac{i}{2\tau}\mathrm{sign}(\epsilon_n)} \frac{1}{i(\epsilon_n + \omega_m) - \xi_{\mathbf{p}+\mathbf{q}} + \frac{i}{2\tau}\mathrm{sign}(\epsilon_n + \omega_m)} \tag{6}$$

The integral is dominated by the region close to the Fermi surface. We go over to an integration over energy and consider only small momenta $q \ll p_{\mathrm{F}}$:

$$B \approx \nu \int \mathrm{d}\xi \int \frac{\mathrm{d}\mathbf{n}}{\Omega_d} \frac{1}{i\epsilon_n - \xi + \frac{i}{2\tau}\mathrm{sign}(\epsilon_n)} \frac{1}{i(\epsilon_n + \omega_m) - \xi + v_{\mathrm{F}}\mathbf{q}\mathbf{n} + \frac{i}{2\tau}\mathrm{sign}(\epsilon_n + \omega_m)} \tag{7}$$

The integral over ξ is non-vanishing only if both poles lie on different sides. We obtain

$$B = 2\pi\nu\tau f(\epsilon_n, \omega_m) \int \frac{\mathrm{d}\mathbf{n}}{\Omega_d} \frac{1}{1 + |\omega_m|\tau - i v_{\mathrm{F}}\, \mathbf{q}\mathbf{n}\, \mathrm{sign}(\omega_m)}, \tag{8}$$

where the function

$$f(\epsilon_n, \omega_m) = \theta(-\omega_m)\theta(\epsilon_n)\theta(-\omega_m - \epsilon_n) + \theta(\omega_m)\theta(-\epsilon_n)\theta(\epsilon_n + \omega_m) \tag{9}$$

handles the different cases related to the location of the two poles in Eq. (7). We expand now for small frequencies $|\omega_m|\tau \ll 1$ and small momenta $v_{\mathrm{F}}\tau q = ql \ll 1$. The term linear in q vanishes after the integration over the directions $\mathbf{n}$. We find

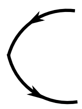
$$B \approx 2\pi\nu\tau f(\epsilon_n, \omega_m) \left(1 - |\omega_m|\tau - \frac{v_{\mathrm{F}}^2 \tau^2 q^2}{d}\right) = 2\pi\nu\tau f(\epsilon_n, \omega_m) \left[1 - \tau(|\omega_m| + Dq^2)\right], \tag{10}$$

where we introduced the diffusion constant, $D = v_{\mathrm{F}}^2\tau/d$. In order to perform the Matsubara sum in each diagram (that might contain many blocks), we note that

$f^2 = f$ (both terms in Eq. (9) exclude each other). Hence, in each diagram we need to perform the same summation

$$T \sum_n f(\epsilon_n, \omega_m) = T|m| = \frac{|\omega_m|}{2\pi}. \tag{11}$$

Let us for a moment ignore the first diagram and sum all diagrams with at least one impurity line. The diagram with $l \geq 1$ impurity lines contains $k = l - 1$ blocks B. We see that if we want to sum all diagrams, we need to calculate the block at finite frequency or momentum (convergence of geometric progression). Each diagram contains additionally two ends of the form



that give the same result as Eq. (10). We can set ω_m and q to zero for the ends since each diagrams has two ends such that they do not produce a divergence. From each end we get a factor $2\pi\nu\tau$. Furthermore, each impurity line contributes a factor $\Gamma = (2\pi\nu\tau)^{-1}$. We thus get for the sum of all diagrams with at least one impurity line

$$K^{(1)} = \frac{|\omega_m|}{2\pi}(2\pi\nu\tau)^2 \sum_{k=0}^{\infty} \frac{1}{(2\pi\nu\tau)^{k+1}} \left[2\pi\nu\tau(1 - \tau(|\omega_m| + Dq^2))\right]^k \tag{12}$$

$$= \frac{\nu|\omega_m|}{|\omega_m| + Dq^2}. \tag{13}$$

The diagram without impurity line can be calculated at zero frequency and momentum (proper limit: $\omega_m = 0$ and then $q \to 0$). The diagram is closely related to the polarization operator (here: disordered Green's functions). We take a shortcut and do not explicitly calculate the diagram in the Matsubara technique:

$$K^{(0)} = T \sum_n \int \frac{\mathrm{d}^3 p}{(2\pi)^d} G^2(i\epsilon_n, \mathbf{p}) = -\frac{\partial}{\partial\mu} T \sum_n \int \frac{\mathrm{d}^3 p}{(2\pi)^d} G(i\epsilon_n, \mathbf{p}) = -\frac{\partial n}{\partial \mu} = -\nu. \tag{14}$$

Adding both parts together, we finally obtain

$$K(i\omega_m, \mathbf{q}) = K^{(0)} + K^{(1)} = -\frac{\nu D q^2}{|\omega_m| + Dq^2}. \tag{15}$$

(c) **Compare your results to the classical diffusion equation. Write down the diffusion equation in the presence of an external force and find the classical response function. Show that the result corresponds to the above result of the diagrammatic calculation (after analytic continuation). Consider the diffuson diagrams in real space and explain why do they correspond to diffusion.**

The classical diffusion equation with an external force $\mathbf{F} = -\nabla V$ (drift-diffusion equation or Smoluchowski equation) reads

$$\partial_t n = D\nabla^2 n - \eta \nabla \cdot (\mathbf{F} n), \tag{16}$$

where η is the mobility that can be related to the diffusion constant by

$$\eta = \frac{\nu D}{n_0}. \tag{17}$$

Here n_0 is the average density in the system. If we assume now that the density varies slowly on the length scale of the variations of $\mathbf{F}$, we can replace the n in the term that contains the external force by n_0. We thus find

$$\partial_t n - D\nabla^2 n = \nu D \nabla^2 V \tag{18}$$

In Fourier space we obtain the same result as in part b) after the analytic continuation ($\omega_m > 0, i\omega_m \to \omega + i\delta$):

$$n(\mathbf{q}, \omega) = -\frac{\nu D q^2}{-i\omega + Dq^2} V(\mathbf{q}, \omega) \tag{19}$$

We can consider the block B, that we used in part b) in real space. We need to calculate it now for arbitrary momenta and frequencies since we need to perform a Fourier transform. In three spatial dimensions, this block reads

$$B = 2\pi\nu\tau \int \frac{\mathrm{d}\Omega}{4\pi} \frac{1}{1 + |\omega_m|\tau + i\mathbf{qn}\tau v_\mathrm{F}\,\mathrm{sign}(\omega_m)} \tag{20}$$

$$= \frac{\pi\nu \mathrm{sign}(\omega_m)}{iqv_\mathrm{F}} \ln \frac{1 + |\omega_m|\tau + iql\,\mathrm{sign}(\omega_m)}{1 + |\omega_m|\tau - iql\,\mathrm{sign}(\omega_m)} \tag{21}$$

Analytically continuing to the real frequencies gives

$$B(\mathbf{q}, \omega) = \frac{\pi\nu}{iqv_\mathrm{F}} \ln \frac{1 - i\omega\tau + iql}{1 - i\omega\tau - iql} \tag{22}$$

Transforming back to real space yields

$$B(\mathbf{r}, t) = \frac{\nu}{2r^2}\delta(r - v_\mathrm{F}t)\mathrm{e}^{-r/l}. \tag{23}$$

Hint: The opposite Fourier transform of this result to momentum and frequency space might be easier. We observe that the propagation is ballistic for length scales smaller than the mean free-path and exponentially damped for longer length scales.

(d) **Consider the classical diffusion equation and find its Greens function (as the Greens function of the linear differential equation). Use the Greens function of the diffusion equation to find the probability of the particle to return to a given point in space. Explain, how your results can be used to justify the qualitative arguments used in the lecture to describe the weak localization correction.**

The Green's function of the diffusion equation can be found from

$$(\partial_t - D\nabla^2)G(\mathbf{r}, t) = \delta(r)\delta(t). \tag{24}$$

In Fourier space the solution reads

$$G(\mathbf{q}, \omega) = \frac{1}{Dq^2 - i\omega}. \tag{25}$$

We now transform this result back to real space (3D):

$$G(\mathbf{r},t) = \int \frac{\mathrm{d}^3 q}{(2\pi)^3} \int \frac{\mathrm{d}\omega}{2\pi} \mathrm{e}^{i(\mathbf{qr}-\omega t)} \frac{1}{Dq^2 - i\omega} \tag{26}$$

$$= \theta(t) \frac{1}{4\pi^2} \int_{-1}^{1} \mathrm{d}\cos\theta \int_0^\infty \mathrm{d}q\, q^2\, \mathrm{e}^{iqr\cos\theta} \mathrm{e}^{-Dtq^2} \tag{27}$$

$$= \theta(t) \frac{1}{4\pi^2 r} \int_{-\infty}^{\infty} \mathrm{d}q\, q\, \sin(qr) \mathrm{e}^{-Dtq^2} \tag{28}$$

$$= -\theta(t) \frac{1}{8\pi^2 r} \frac{\partial}{\partial r} \int_{-\infty}^{\infty} \mathrm{d}q\, (\mathrm{e}^{iqr} + \mathrm{e}^{-iqr}) \mathrm{e}^{-Dtq^2} \tag{29}$$

$$= -\theta(t) \frac{1}{4\pi^2 r} \frac{\partial}{\partial r} \mathrm{e}^{-r^2/4Dt} \sqrt{\frac{\pi}{Dt}} \tag{30}$$

$$= \theta(t) \left(\frac{1}{4\pi Dt}\right)^{3/2} \mathrm{e}^{-r^2/(4Dt)} \tag{31}$$

This function describes the probability distribution of a particle, that is placed at the origin at $t = 0$. The probability of the particle to come back close to origin at the time t is given by

$$\left(\frac{1}{4\pi Dt}\right)^{3/2} \Delta V, \tag{32}$$

where ΔV is a "small" volume element.

The weak localization correction is produced by the interference of time reversed paths. In classical physics the probabilities of two paths add up. Hence, the total return probability due to the "direct" and time reversed path is given by $p_{\mathrm{cl}} = 2p_1$, where p_1 is the probability for the "direct" path. In quantum mechanics, the total probability is given by adding the amplitudes and then taking the modulus squared. If we denote both amplitudes by $A_1 = \sqrt{p_1}\mathrm{e}^{i\phi_1}$ and $A_2 = \sqrt{p_2}\mathrm{e}^{i\phi_2}$, the total return probability is given by $p_{\mathrm{qm}} = p_1^2 + p_2^2 + 2\sqrt{p_1 p_2}\cos(\phi_1 - \phi_2)$. This expression contains an interference therm that averages to zero after the disorder average if both path are unrelated. However, since both paths are related by time reversal, we have $p_1 = p_2$ and $\phi_1 = \phi_2$. Consequently, the interference term survives the disorder average and we obtain $p_{\mathrm{qm}} = 4p_1 = 2p_{\mathrm{cl}}$. This phenomenon is also known under the name "enhanced backscattering".