TKM2 Übungsblatt 8: Lösungen

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1 Magnetic / Non-Magnetic Impurities

Hamiltonian

$$H_0 = \int d^3r \left[\sum_{\alpha=\pm} \psi^\dagger_\alpha(\boldsymbol{r})\epsilon(-i\boldsymbol{\nabla})\psi_\alpha(\boldsymbol{r}) - \Delta\left(\psi_\uparrow(\boldsymbol{r})\psi_\downarrow(\boldsymbol{r}) + \text{h.c.}\right)\right] \tag{1}$$

$$H_1 = \int d^3r \left[\sum_{\alpha=\pm} V_1(\boldsymbol{r})\psi^\dagger_\alpha(\boldsymbol{r})\psi_\alpha(\boldsymbol{r}) + \sum_{\alpha\beta=\pm} V_{2,i}(\boldsymbol{r})\psi^\dagger_\alpha\sigma_{i,\alpha\beta}\psi_\beta(\boldsymbol{r})\right] \tag{2}$$

which we can rewrite as

$$H_0 = \int d^3r \left[\sum_{\alpha=\pm} \psi^\dagger_\alpha(\boldsymbol{r})\epsilon(-i\boldsymbol{\nabla})\psi_\alpha(\boldsymbol{r}) - \sum_{\alpha\beta} i\sigma_{y,\alpha\beta}\Delta\left(\psi_\alpha(\boldsymbol{r})\psi_\beta(\boldsymbol{r}) + \text{h.c.}\right)\right] \tag{3}$$

$$H_1 = \int d^3r \left[\sum_{\alpha=\pm} V_1(\boldsymbol{r})\psi^\dagger_\alpha(\boldsymbol{r})\psi_\alpha(\boldsymbol{r}) + \sum_{\alpha\beta=\pm} V_{2,i}(\boldsymbol{r})\psi^\dagger_\alpha\sigma_{i,\alpha\beta}\psi_\beta(\boldsymbol{r})\right] \tag{4}$$

a) Equation of motion

$$\begin{aligned}
\partial_\tau\psi_\alpha &= -\epsilon(-i\boldsymbol{\nabla})\psi_\alpha - i\Delta\sum_\beta \sigma_{2,\alpha\beta}\psi^\dagger_\beta - V_1(\boldsymbol{r})\psi_\alpha - \sum_\beta V_{2,i}(\boldsymbol{r})\sigma_{i,\alpha\beta}\psi_\beta \\
\partial_\tau\psi^\dagger_\alpha &= \epsilon(-i\boldsymbol{\nabla})\psi^\dagger_\alpha + i\Delta\sum_\beta \sigma_{2,\alpha\beta}\psi^\dagger_\beta V_1(\boldsymbol{r})\psi_\alpha + \sum_\beta V_{2,i}(\boldsymbol{r})\tilde{\sigma}_{i,\alpha\beta}\psi^\dagger_\beta
\end{aligned} \tag{5}$$

where $\tilde{\sigma}_i = \sigma^*_i = -\sigma_y\sigma_i\sigma_y$. If we further introduce the notation

$$\Phi_{\alpha,+} = \psi_\alpha, \qquad \text{and} \qquad \Phi_{\alpha,-} = \psi^\dagger_\alpha \tag{6}$$

Then we can write the equation of motion as

$$\begin{aligned}
\partial_\tau\Phi_{\alpha,\mu} = -\epsilon(-i\boldsymbol{\nabla})\sum_\nu(\tau_3)_{\mu\nu}\Phi_{\alpha,\nu} + \Delta\sum_{\beta,\nu}(\tau_2)_{\mu\nu}(\sigma_2)_{\alpha\beta}\Phi_{\alpha,\nu} - V_1(\boldsymbol{r})\sum_\nu(\tau_3)_{\mu\nu}\Phi_{\alpha,\nu} \\
- V_{2,i}(\boldsymbol{r})\sum_{\beta\nu}\frac{1}{2}\left[(1+\tau_z)_{\mu\nu}\sigma_{i,\alpha\beta} + (1-\tau_z)_{\mu\nu}\tilde{\sigma}_{i,\alpha\beta}\right]\Phi_{\beta,\nu}
\end{aligned} \tag{7}$$

More conveniently, we can define the four-component vector:

$$\Phi = \begin{pmatrix} \Phi_{+,+} \\ \Phi_{-,+} \\ \Phi_{+,-} \\ \Phi_{-,-} \end{pmatrix} = \begin{pmatrix} \psi_\uparrow \\ \psi_\downarrow \\ \psi_\uparrow^\dagger \\ \psi_\downarrow^\dagger \end{pmatrix} \tag{8}$$

For which the equation of motion is given by

$$\partial_\tau \Phi = [-\epsilon(-i\boldsymbol{\nabla})\tau_3 + \Delta\tau_2\sigma_2 - V_1(\boldsymbol{r})\tau_3 - V_{2,i}(\boldsymbol{r})\alpha_i]\,\Phi \tag{9}$$

where the matrices τ_3, $\tau_2\sigma_2$ and α_i have the block-structures

$$\tau_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \qquad \tau_2\sigma_2 = \begin{pmatrix} 0 & -i\sigma_2 \\ i\sigma_2 & 0 \end{pmatrix} \tag{10}$$

and

$$\alpha_i = \frac{1}{2}\,[(1+\tau_z)\sigma_i + (1-\tau_z)\tilde{\sigma}_i] = \begin{pmatrix} \sigma_i & 0 \\ 0 & -\tilde{\sigma}_i \end{pmatrix} \tag{11}$$

b) It then follows that the Green's function

$$\hat{G}(\boldsymbol{r},\boldsymbol{r}',\tau) = -\langle T_\tau \Phi(\boldsymbol{r},\tau)\Phi^\dagger(\boldsymbol{r}',0)\rangle \tag{12}$$

satisfies the equation of motion

$$[-\partial_\tau - \epsilon(-i\boldsymbol{\nabla})\tau_3 + \Delta\tau_2\sigma_2 - V_1(\boldsymbol{r})\tau_3 - V_{2,i}(\boldsymbol{r})\alpha_i]\,\hat{G}(\boldsymbol{r},\boldsymbol{r}',\tau) = \delta(\tau)\hat{1}\delta(\boldsymbol{r}-\boldsymbol{r}') \tag{13}$$

To verify, consider the equation of motion of each component

$$\begin{aligned} G_{\alpha\mu,\beta\nu}(\boldsymbol{r},\boldsymbol{r}',\tau) &= -\langle T_\tau \Phi_{\alpha,\mu}(\boldsymbol{r},\tau)\Phi^\dagger_{\beta,\nu}(\boldsymbol{r},0)\rangle \\ &= -\Theta(\tau)\langle \Phi_{\alpha,\mu}(\boldsymbol{r},\tau)\Phi^\dagger_{\beta,\nu}(\boldsymbol{r}',0)\rangle + \Theta(-\tau)\langle \Phi^\dagger_{\beta,\nu}(\boldsymbol{r}',0)\Phi_{\alpha,\mu}(\boldsymbol{r},\tau)\rangle \end{aligned} \tag{14}$$

Using Equation (7), together with the anti-commutation relations $\{\Phi_{\alpha,\mu}, \Phi^\dagger_{\beta,\nu}\} = \delta_{\alpha\beta}\delta_{\mu\nu}$ to evaluate the discontinuity from the Theta-functions, the equation of motion of the GF follows immediately.[1]

c) In frequency space we have

$$[i\omega_n - \epsilon(-i\boldsymbol{\nabla})\tau_3 + \Delta\tau_2\sigma_2 - V_1(\boldsymbol{r})\tau_3 - V_{2,i}(\boldsymbol{r})\alpha_i]\,\hat{G}(\boldsymbol{r},\boldsymbol{r}',i\omega_n) = \hat{1}\delta(\boldsymbol{r}-\boldsymbol{r}') \tag{15}$$

In the absence of impurities $V_1 = V_{2,i} = 0$ we have

$$[i\omega_n - \epsilon(-i\boldsymbol{\nabla})\tau_3 + \Delta\tau_2\sigma_2]\,\hat{G}(\boldsymbol{r},\boldsymbol{r}',i\omega_n) = \hat{1}\delta(\boldsymbol{r}-\boldsymbol{r}') \tag{16}$$

and it is easy to make the transition to momentum space

$$[i\omega_n - \epsilon_{\boldsymbol{k}}\tau_3 + \Delta\tau_2\sigma_2]\,\hat{G}_0(\boldsymbol{k},i\omega_n) = \hat{1} \tag{17}$$

and the Green's function is given by

$$\hat{G}(\boldsymbol{k},i\omega_n) = [i\omega_n - \epsilon_{\boldsymbol{k}}\tau_3 + \Delta\tau_2\sigma_2] \tag{18}$$

[1] By writing the Eqm. for each component we avoid complications with the matrix structure, i.e. $\Phi\Phi^\dagger$ is a (operator-valued) matrix while $\Phi^\dagger\Phi$ is a (operator valued) scalar.

d) We treat the impurities as a perturbation and define the unperturbed propagator $\hat{G}_0(\boldsymbol{r}-\boldsymbol{r'}, i\omega_n) = \frac{1}{\mathcal{V}}\sum_{\boldsymbol{k}} \hat{G}_0(\boldsymbol{k}, i\omega_n)e^{i\boldsymbol{k}\cdot\boldsymbol{r}}$ with

$$\hat{G}_0(\boldsymbol{k}, i\omega_n) = (i\omega_n - \epsilon_{\boldsymbol{k}}\tau_3 + \Delta\tau_2\sigma_2)^{-1} \tag{19}$$

as well as the vertices

$$V_1(\boldsymbol{r})\tau_3, \qquad \text{and} \qquad \sum_i V_{2,i}(\boldsymbol{r})\alpha_i \tag{20}$$

We assume s-wave scattering of the impurities and thus write

$$\begin{aligned} V_1(\boldsymbol{r}) &= \sum_n U_1\delta(\boldsymbol{r}-\boldsymbol{R}_n^1) = U_1\sum_{\boldsymbol{k}}\sum_n e^{i\boldsymbol{k}\cdot(\boldsymbol{r}-\boldsymbol{R}_n^1)}, \\ V_{2,i}(\boldsymbol{r}) &= \sum_n S_{n,i}U_2\delta(\boldsymbol{r}-\boldsymbol{R}_n^2) = U_2\sum_{\boldsymbol{k}}\sum_n S_{n,i}e^{i\boldsymbol{k}\cdot(\boldsymbol{r}-\boldsymbol{R}_n^2)} \end{aligned} \tag{21}$$

We assume that the positions of the magnetic and non-magnetic impurities are uncorrelated and that the direction of the spins are also uncorrelated. The average over magnetic spins is given by $\langle S_{n,i}S_{n,j}\rangle = \frac{1}{3}S(S+1)\delta_{ij}$. We get two contributions to the self-energy

$$\hat{\Sigma}(\boldsymbol{k}, i\omega_n) = N_i|U_1|^2\sum_{\boldsymbol{k'}}\tau_3\hat{G}(\boldsymbol{k'}, i\omega_n)\tau_3 + \frac{1}{3}S(S+1)N_\beta|U_2|^2\sum_{\boldsymbol{k'}}\sum_i \alpha_i\hat{G}(\boldsymbol{k'}, i\omega_n)\alpha_i \tag{22}$$

We make the ansatz

$$\hat{G}(\boldsymbol{k}, i\omega_n) = (i\tilde{\omega}_n - \epsilon_{\boldsymbol{k}}\tau_3 - \tilde{\Delta}\tau_2\sigma_2)^{-1} = \frac{i\tilde{\omega}_n + \epsilon_{\boldsymbol{k}}\tau_3 + \tilde{\Delta}\tau_2\sigma_2}{(i\omega_n)^2 - \epsilon_{\boldsymbol{k}}^2 - \tilde{\Delta}^2} \tag{23}$$

where $\tilde{\omega}_n$ and $\tilde{\Delta}$ are renormalized frequency and superconducting gap, respectively. From the Dyson equation $\hat{G}^{-1} = \hat{G}_0^{-1} - \hat{\Sigma}$ we have

$$\hat{G}^{-1} - \hat{G}_0^{-1} = -\hat{\Sigma} \Rightarrow (i\tilde{\omega}_n - i\omega_n) - \left(\tilde{\Delta} - \Delta\right)\tau_2\sigma_2 = -\hat{\Sigma} \tag{24}$$

Using the approximation $\sum_{\boldsymbol{k'}} = \frac{N(0)}{2}\int_{-\infty}^{\infty} d\epsilon$ we can write

$$\begin{aligned} \sum_{\boldsymbol{k'}}\hat{G}(\boldsymbol{k'}, i\omega_n) &= \frac{N(0)}{2}\int_{-\infty}^{\infty} d\epsilon \frac{i\tilde{\omega}_n + \epsilon\tau_3 + \tilde{\Delta}\tau_2\sigma_2}{-\tilde{\omega}_n^2 - \epsilon^2 - \tilde{\Delta}^2} = -\frac{N(0)}{2}\int_{-\infty}^{\infty} d\epsilon \frac{i\tilde{\omega}_n + \tilde{\Delta}\tau_2\sigma_2}{\epsilon^2 + \tilde{\omega}_n^2 + \tilde{\Delta}^2} \\ &= -\frac{N(0)}{2}\frac{i\tilde{\omega}_n + \tilde{\Delta}\tau_2\sigma_2}{\sqrt{\tilde{\omega_n}^2 + \tilde{\Delta}^2}} \end{aligned} \tag{25}$$

and the self-energy is given by

$$\begin{aligned} \hat{\Sigma} &= -\frac{1}{2\tau_i}\frac{\tau_3(i\tilde{\omega}_n + \tilde{\Delta}\tau_2\sigma_2)\tau_3}{\sqrt{\tilde{\omega_n}^2 + \tilde{\Delta}^2}} - \frac{1}{6\tau_\beta}\sum_i \frac{\alpha_i(i\tilde{\omega}_n + \tilde{\Delta}\tau_2\sigma_2)\alpha_i}{\sqrt{\tilde{\omega_n}^2 + \tilde{\Delta}^2}} \\ &= -\frac{1}{2\tau_i}\frac{i\tilde{\omega}_n - \tilde{\Delta}\tau_2\sigma_2}{\sqrt{\tilde{\omega_n}^2 + \tilde{\Delta}^2}} - \frac{1}{2\tau_\beta}\frac{i\tilde{\omega}_n + \tilde{\Delta}\tau_2\sigma_2}{\sqrt{\tilde{\omega_n}^2 + \tilde{\Delta}^2}} \end{aligned} \tag{26}$$

where we used $\tau_3\tau_3 = 1$ and $\tau_3\tau_2\tau_3 = -\tau_2$ as well as

$$\alpha_i\alpha_i = \begin{pmatrix} \sigma_i\sigma_i & 0 \\ 0 & \tilde{\sigma}_i\tilde{\sigma}_i \end{pmatrix} = \hat{1} \tag{27}$$

and

$$\alpha_i\tau_2\sigma_2\alpha_i = \begin{pmatrix}\sigma_i & 0\\ 0 & -\tilde{\sigma}_i\end{pmatrix}\begin{pmatrix}0 & -i\sigma_2\\ i\sigma_2 & 0\end{pmatrix}\begin{pmatrix}\sigma_i & 0\\ 0 & -\tilde{\sigma}_i\end{pmatrix} = \begin{pmatrix}0 & i\sigma_i\sigma_2\tilde{\sigma}_i\\ -i\tilde{\sigma}_i\sigma_2\sigma_i & 0\end{pmatrix} = \tau_2\sigma_2 \quad (28)$$

where we used $\tilde{\sigma}_i = -\sigma_2\sigma_i\sigma_2$ such that $\sigma_i\sigma_2\tilde{\sigma}_i = -\sigma_i\sigma_2\sigma_2\sigma_i\sigma_2 = -\sigma_2$ and $\tilde{\sigma}_i\sigma_2\sigma_i = -\sigma_2\sigma_i\sigma_2\sigma_2\sigma_i = -\sigma_2$. We thus have

$$\tilde{\omega}_n = \omega_n + \frac{1}{2}\left(\frac{1}{\tau_i} + \frac{1}{\tau_\beta}\right)\frac{\tilde{\omega}_n}{\sqrt{\tilde{\omega_n}^2 + \tilde{\Delta}^2}} \quad (29)$$

and

$$\tilde{\Delta} = \Delta + \frac{1}{2}\left(\frac{1}{\tau_i} - \frac{1}{\tau_\beta}\right)\frac{\tilde{\Delta}}{\sqrt{\tilde{\omega_n}^2 + \tilde{\Delta}^2}} \quad (30)$$

2 | Renormalized gap

We define $u = \tilde{\omega}_n/\tilde{\Delta}$ and write

$$\tilde{\omega}_n = \omega_n + \frac{1}{2}\left(\frac{1}{\tau_i} + \frac{1}{\tau_\beta}\right)\frac{u}{\sqrt{u^2+1}} \quad (31)$$

and

$$\tilde{\Delta} = \Delta + \frac{1}{2}\left(\frac{1}{\tau_i} - \frac{1}{\tau_\beta}\right)\frac{1}{\sqrt{u^2+1}} \quad (32)$$

Dividing the top line with the second one gives

$$u = \frac{\omega_n + \frac{1}{2}\left(\frac{1}{\tau_i} + \frac{1}{\tau_\beta}\right)\frac{u}{\sqrt{u^2+1}}}{\Delta + \frac{1}{2}\left(\frac{1}{\tau_i} - \frac{1}{\tau_\beta}\right)\frac{1}{\sqrt{u^2+1}}} = \frac{\frac{\omega_n}{\Delta} + \frac{1}{2}\left(\frac{1}{\tau_i} + \frac{1}{\tau_\beta}\right)\frac{u}{\Delta\sqrt{u^2+1}}}{1 + \frac{1}{2}\left(\frac{1}{\tau_i} - \frac{1}{\tau_\beta}\right)\frac{1}{\Delta\sqrt{u^2+1}}} \quad (33)$$

Solving for ω_n/Δ we get

$$\begin{aligned}\frac{\omega_n}{\Delta} &= u\left(1 + \frac{1}{2}\left(\frac{1}{\tau_i} - \frac{1}{\tau_\beta}\right)\frac{1}{\Delta\sqrt{u^2+1}}\right) - \frac{1}{2}\left(\frac{1}{\tau_i} + \frac{1}{\tau_\beta}\right)\frac{u}{\Delta\sqrt{u^2+1}}\\ &= u\left(1 - \frac{1}{\tau_\beta}\frac{1}{\Delta\sqrt{u^2+1}}\right)\end{aligned} \quad (34)$$

we see that the scattering rate of the non-magnetic impurities gets cancelled in this expression, and only the magnetic impurity scattering rate influences the ratio ω_n/Δ, and for $\tau_\beta \to \infty$ we have $u = \tilde{\omega}_n/\tilde{\Delta} = \omega_n/\Delta$.

We consider now the gap equation

$$\Delta = V\sum_{\boldsymbol{k}}\langle c_{-\boldsymbol{k}\downarrow}c_{\boldsymbol{k}\uparrow}\rangle = \frac{V}{4}\frac{1}{\beta}\sum_{\omega_n}\sum_{\boldsymbol{k}}\mathrm{Tr}\left(\tau_2\sigma_2\hat{G}(\boldsymbol{k}, i\omega_n)\right) = -\frac{VN(0)}{2}\frac{1}{\beta}\sum_{\omega_n}\frac{\tilde{\Delta}}{\sqrt{\tilde{\omega}_n^2 + \tilde{\Delta}^2}} \quad (35)$$

Switching summation variables to $\omega_n \to \tilde{\omega}_n \to u$ we have then

$$\Delta = -\frac{VN(0)}{2\beta}\sum_u \frac{1}{\sqrt{u^2+1}} \quad (36)$$

Now we recall that for $\tau_\beta \to \infty$ we have $u = \omega_n/\Delta$ which is independent of the impurity scattering rate. Thus the gap equation is not changed when we introduce non-magnetic scattering, and thus the solution is also insensitive to non-magnetic scattering. This result is known as Anderson's theorem.