Theorie der Kondensierten Materie II   SS 2017

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1. Ruderman-Kittel effect at $T > 0$:

We consider the Ruderman-Kittel effect at $T > 0$ similarly to what was done in Exercise 5 at $T = 0$. In particular, we use the Green's function in the coordinate representation. The calculation involves the Fourier transform of the now Matsubara Green's function from the momentum to coordinate representation. We will only consider here the approximate calculation valid at large distances, which technically amounts to linearizing the excitation spectrum and using the trick of "ξ-integration". In full analogy with the previous calculation we find:

$$G_0(i\omega_n, \boldsymbol{r}) = \int \frac{d^3p}{(2\pi)^3} \frac{e^{i\boldsymbol{pr}}}{i\omega_n - \xi_p} \approx \frac{\nu_0}{pr} \int d\xi \frac{\sin(p_F + \xi/v_F)r}{i\omega_n - \xi} = -\frac{m}{2\pi r} e^{ir(p_F + i\omega_n/v_F)\operatorname{sign}\omega_n}.$$

The magnetization or spin density can be expressed in terms of the Green's function similarly to the case at $T = 0$. Formally, the only difference is that one has to replace factors of $-i$ by -1 in the definitions of the Green's functions and the perturbation operator. This way we find

$$\sigma^i(r) = 2JS^i T \sum_{\omega_n} G_0^2(i\omega_n, \boldsymbol{r}),$$

which leads to

$$\sigma^i(r) = 2JS^i \frac{m^2}{4\pi^2 r^2} T \left[\sum_{\omega_n > 0} e^{2ip_F r - 2\omega_n r/v_F} + \sum_{\omega_n < 0} e^{-2ip_F r + 2\omega_n r/v_F} \right].$$

The sums can be directly evaluated without any further approximations. The result is

$$\sigma^i(r) = JS^i \frac{m^2 T}{2\pi^2 r^2} \frac{\cos(2p_F r)}{\sinh(2\pi T r/v_F)}.$$

At $T = 0$ this results reproduces the leading term in the zero-temperature result found in the Exercise 5. Also here one could perform the exact integration for parabolic spectrum and find the generalization of the full result of the Exercise 5 to nonzero temperatures.

One can see from the above result that the oscillatory behavior persists at length scales smaller than the thermal length $v_F/(2\pi T)$. Given the approximate nature of the calculation, the result is relevant for length scales

$$p_F^{-1} \ll r \ll v_F/(2\pi T).$$

Assuming low enough temperatures $T \ll E_F$ this is still a rather wide interval. For longer length scales the oscillatory behavior is exponentially suppressed.

2. Matsubara susceptibility:

(a) Here we prove that the analytic continuation of the Matsubara susceptibility yields the Kubo formula.

Consider the Matsubara correlation function

$$\chi_{AB}^{M}(i\omega_n) = \frac{1}{2} \int_{-1/T}^{1/T} d\tau\, e^{i\omega_n\tau} \left\langle \mathrm{T}_\tau \hat{A}^M(\tau)\hat{B}^M(0) \right\rangle_T.$$

Here the subscript M denotes the Matsubara operator, i.e.

$$\hat{A}^M(\tau) = e^{-\tau\hat{H}}\hat{A}e^{\tau\hat{H}}.$$

The brackets indicate thermal averaging

$$\langle\ldots\rangle_T = \frac{1}{Z}\mathrm{Tr}\left(\ldots e^{-\hat{H}/T}\right), \qquad Z = \mathrm{Tr}\, e^{-\hat{H}/T}.$$

Consider now the basis of te exact eigenstates of the system

$$\hat{H}|n\rangle = E_n|n\rangle.$$

Note, that these are the exact many-body states of the system rather than single-particle states.

In terms of the eigenstates $|n\rangle$, the above expression for the Matsubara susceptibility can be made explicit as follows

$$\chi_{AB}^{M}(i\omega_n) = \frac{1}{2Z} \int_0^{1/T} d\tau\, e^{i\omega_n\tau} \sum_{n_1,n_2} e^{-E_{n_1}/T} e^{-(E_{n_1}-E_{n_2})\tau} \langle n_1|\hat{A}|n_2\rangle\langle n_2|\hat{B}|n_1\rangle$$

$$+ \frac{1}{2Z} \int_{-1/T}^{0} d\tau\, e^{i\omega_n\tau} \sum_{n_1,n_2} e^{-E_{n_1}/T} e^{(E_{n_1}-E_{n_2})\tau} \langle n_1|\hat{B}|n_2\rangle\langle n_2|\hat{A}|n_1\rangle$$

In the second sum we can now exchange the indices. After that we can evaluate the τ integral (recall that $\omega_n/T = 2\pi n$). As a result, we find

$$\chi_{AB}^{M}(i\omega_n) = \sum_{n_1,n_2} \frac{e^{-E_{n_1}/T} - e^{-E_{n_2}/T}}{i\omega_n - (E_{n_1} - E_{n_2})} \langle n_1|\hat{A}|n_2\rangle\langle n_2|\hat{B}|n_1\rangle.$$

Let us now compare this result with the Kubo formula:

$$\chi_{AB}(\omega) = i \int_0^\infty dt\, e^{i\omega t} \left\langle \left[\hat{A}(t), \hat{B}(0)\right] \right\rangle_T.$$

Here $\hat{A}(t)$ is the Heisenberg operator

$$\hat{A}(t) = e^{-it\hat{H}}\hat{A}e^{it\hat{H}}.$$

In the basis of the eigen functions of the Hamiltonian, we find

$$\chi_{AB}(\omega) = \frac{i}{Z}\int_0^\infty dt e^{i\omega t}\sum_{n_1,n_2} e^{-E_{n_1}/T}e^{-i(E_{n_1}-E_{n_2})t}\langle n_1|\hat{A}|n_2\rangle\langle n_2|\hat{B}|n_1\rangle$$

$$-\frac{i}{Z}\int_0^\infty dt e^{i\omega_n t}\sum_{n_1,n_2} e^{-E_{n_1}/T}e^{i(E_{n_1}-E_{n_2})t}\langle n_1|\hat{B}|n_2\rangle\langle n_2|\hat{A}|n_1\rangle$$

Again, interchanging the indices in the second line and integrating over t we find

$$\chi_{AB}(\omega) = \sum_{n_1,n_2}\frac{e^{-E_{n_1}/T}-e^{-E_{n_2}/T}}{\omega-(E_{n_1}-E_{n_2})+i0}\langle n_1|\hat{A}|n_2\rangle\langle n_2|\hat{B}|n_1\rangle.$$

The imaginary part in the denominator appears due to the formal divergence of the time integral. In order to make the integral formally convergent one typically adds a factor $e^{-\delta t}$ to the integrand, which results in the infinitesimal imaginary part $(\delta \to 0)$.

The proof of the equivalence of the two approaches follows from comparison between the obtained results for $\chi_{AB}^M(i\omega_n)$ and $\chi_{AB}(\omega)$. Since the susceptibility $\chi_{AB}(\omega)$ is an analytic function in the upper half-plane of complex ω, it can be analytically continued from the real axis onto the imaginary half axis with $\text{Im}\,\omega > 0$. There it coinsides with $\chi_{AB}^M(i\omega_n)$ for points $i\omega_n = 2\pi i nT$, $n > 0$. Assuming now that the Matsubara susceptibility can be continued from the imaginary half axis onto the uper half-plane, we find that this continuation'must coinside with $\chi_{AB}(\omega)$ (as guaranteed by the general theorems of the complex analysis).

(b) Consider now the dynamical spin susceptibility. In the Exercise 6 this quantity was found at $T = 0$ with the help of the Kubo formula. Now we would like to find it with the help of the Matsubara susceptibility. The latter is given by the loop diagram corresponding to the expression

$$\chi_{\alpha\beta}^M(i\omega_n, k) = -2\mu_B^2\delta_{\alpha\beta}T\sum_{\omega_m}\int\frac{d^3p}{(2\pi)^3}G(i\omega_m, \boldsymbol{p})G(i\omega_m+i\omega_n, \boldsymbol{p}+\boldsymbol{k}).$$

The Matsubara sum can be calculated explicitly

$$T\sum_{\omega_m}\frac{1}{(i\omega_m+i\omega_n-\xi_{\boldsymbol{p}+\boldsymbol{k}})(i\omega_m-\xi_{\boldsymbol{p}})} = \frac{n_F(\xi_{\boldsymbol{p}+\boldsymbol{k}})-n_F(\xi_{\boldsymbol{p}})}{i\omega_n-\xi_{\boldsymbol{p}+\boldsymbol{k}}+\xi_{\boldsymbol{p}}}.$$

Here we have used the identity

$$\sum_{n=-\infty}^\infty\frac{1}{(2n+1)^2+a^2} = \frac{\pi}{2a}\tanh\frac{\pi a}{2}.$$

As a result, the Matsubara susceptibility has the form

$$\chi_{\alpha\beta}^M(i\omega_n, k) = -2\mu_B^2\delta_{\alpha\beta}\int\frac{d^3p}{(2\pi)^3}\frac{n_F(\xi_{\boldsymbol{p}+\boldsymbol{k}})-n_F(\xi_{\boldsymbol{p}})}{i\omega_n-\xi_{\boldsymbol{p}+\boldsymbol{k}}+\xi_{\boldsymbol{p}}}.$$

This integral cannot be evaluated analytically for arbitrary values of the parameters. Consider however the case of low temperatures $T \ll E_F$ and long wavelengthes $k \ll p_F$. In this case, we can use the trick of the "ξ-integration". Using the identity

$$\int d\xi \left[n_F(\xi) - n_F(\xi + \boldsymbol{v}\boldsymbol{k}) \right] = \boldsymbol{v}\boldsymbol{k},$$

we find

$$\chi^M_{\alpha\beta}(i\omega_n, k) = 2\mu_B^2 \nu_0 \delta_{\alpha\beta} \int \frac{d\Omega}{4\pi} \frac{v_F \boldsymbol{n}\boldsymbol{k}}{i\omega_n - v_F \boldsymbol{n}\boldsymbol{k}}.$$

The angular integration is identical to that discussed in the Exercise 6. The result is given by

$$\chi^M_{\alpha\beta}(i\omega_n, k) = 2\mu_B^2 \nu_0 \delta_{\alpha\beta} \left[1 + \frac{i\omega_n}{2v_F k} \ln \frac{i\omega_n - v_F k}{i\omega_n + v_F k} \right].$$

The analytic continuation amounts to the replacement $i\omega_n \to \omega + i0$. The result coinsides with the $T = 0$ result of the Exercise 6:

$$\chi(\omega, k) = 2\mu_B^2 \nu_0 \left[1 + \frac{\omega}{2v_F k} \ln \left| \frac{\omega - v_F k}{\omega + v_F k} \right| \right].$$