Karlsruher Institut für Technologie
Institut für Theorie der Kondensierten Materie

Theorie der Kondensierten Materie II SS 2015

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Blatt 6
Lösung

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1. Ruderman-Kittel effect:

Consider a localized spin immersed into a free Fermi-gas. The spin interacts with the local electronic spin density by means of the Hamiltonian

$$\hat{H}_{int} = J\hat{S}^i\hat{\sigma}^i(\vec{r}=0),$$

where the local spin density is given by

$$\hat{\sigma}^i(\vec{r}) = \psi^\dagger_\alpha(\vec{r})\sigma^i_{\alpha\beta}\psi_\beta(\vec{r}),$$

and $\sigma^{x,y,z}_{\alpha\beta}$ are the Pauli matrices.

Find the average spin polarization in the electronic system

$$\sigma^i(\vec{r}) = \langle\hat{\sigma}^i(\vec{r})\rangle,$$

at large distances awayt from the impurity spin (i.e., for $k_F r \gg 1$).

Show that the polarization oscillates as a function of r and find the oscillation period. J can be assumed to be small.

The spin polarization of the electron gas can be found using the exact Green's function as follows

$$\sigma^j(\vec{r}) = -i\mathrm{Tr}\left(\hat{\sigma}^j\hat{G}\right) = -i\lim_{t'\to t+0}\left(\sigma^j_{\alpha\beta}G_{\beta\alpha}(\vec{r},t;\vec{r},t')\right).$$

The exact Green's function G can be found as a perturbation series in the external potential describing the impurity spin

$$\hat{V} = J\int d^3r S^j\delta^{(3)}(\vec{r})\psi^\dagger_\alpha(\vec{r})\hat{\sigma}^j_{\alpha\beta}\psi_\beta(\vec{r}).$$

Consider the first-order correction

$$G^{(1)}_{\alpha\beta}(\epsilon,\vec{r},\vec{r}\,') = JS^j\sigma^j_{\alpha\beta}G_0(\epsilon,\vec{r})G_0(\epsilon,-\vec{r}\,').$$

Here $G_0(\epsilon,\vec{r})$ is the free electronic Green's function in the coordinate representation. This function can be found as

$$G_0(\epsilon,\vec{r}) = \int\frac{p^2dp\sin\theta d\theta}{(2\pi)^2}\frac{e^{ipr\cos\theta}}{\epsilon-\xi(p)+i\delta\mathrm{sign}\epsilon} = \frac{1}{2\pi^2 r}\int\limits_0^\infty\frac{dp\ p\sin pr}{\epsilon-\xi(p)+i\delta\mathrm{sign}\epsilon}.$$

As usual, here $\xi(p) = p^2/(2m) - E_F$.

It is instructive to perform the ramining integration in two ways:

(i) first, one can evaluate the integral exactly and find

$$G_0(\epsilon,\vec{r}) = -\frac{m}{2\pi r} e^{i\mathrm{sign}\epsilon\, \varkappa r}, \qquad \varkappa = \sqrt{2m(E_F+\epsilon+i\delta\mathrm{sign}\epsilon)}.$$

(ii) one can evaluate the integral also approximately, replacing the integral over p by an integral over ξ

$$G_0(\epsilon,\vec{r}) \approx \frac{1}{2\pi^2 r}\int\limits_{-\infty}^{\infty} \frac{p_F d\xi}{v_F}\frac{\sin(p_F+\xi/v_F)r}{\epsilon-\xi+i\delta\mathrm{sign}\epsilon} = -\frac{m}{2\pi r} e^{ir(p_F\mathrm{sign}\epsilon+|\epsilon|/v_F}.$$

The approximate solution works well at large distances $rp_F \gg 1$.

Now we can evaluate the spin polarization in the leading order. Using the above first-order correction to the Green's function we find

$$\sigma^j(\vec{r}) = -2iJS^j \int \frac{d\epsilon}{2\pi} G_0^2(\epsilon,\vec{r}).$$

The frequency integral can be evaluated with both the exact and approximate expressions for G_0.

At large distances, $rp_F \gg 1$, we can use the approximate form and find

$$\sigma^j(r) = JS^i \frac{mp_F}{4\pi^3}\frac{\cos 2p_F r}{r^3}.$$

This solution oscillates with the pariod π/p_F and decays as r^{-3}.

Using the exact form of the Green's function one can find the expression that is valid for any r:

$$\sigma^j(r) = JS^i \frac{mp_F}{4\pi^3}\left(\frac{\cos 2p_F r}{r^3} - \frac{\sin 2p_F r}{2p_F r^4}\right).$$

Again, at large distances, the two results coinside. However, the total spin polarization given by the integral over the volume should be evaluated with the help of the exact expression: the approximate solution yields a divergence at $r=0$ which is the artifact of the approximation; the approximate solution is invalid in that region.

2. Dynamical spin susceptibility:

Find the paramagnetic contribution to the electronic spin susceptibility $\chi(\omega,k)$ at $T=0$. The spin susceptibility describes the response of the electronic system to an external magnetic field. Consider the limit $\omega \ll E_F$, $k \ll k_F$.

Verify that in the limit $\omega/k \to 0$, $k \to 0$ you recover the Pauli susceptibility. Discuss the importance of the proper limiting procedure and the order of limits.

Solve the problem in two ways - first, by a direct evaluation of the corresponding diagram, and second, by finding the imaginary part of $\chi(\omega,k)$ first, and then restoring the real part using the Kramres-Kronig relations.

The diagram for the spin susceptibility looks very similar to the diagram for the polarization operator. The obvious difference is the two spin vertices, which however, do not yields any significant difference since

$$\mathrm{Tr}\sigma^i\sigma^j = \delta_{ij}.$$

However, the analytic properties of the susceptibility and polarization operator are different

$$\Pi(-\omega) = \Pi(\omega), \qquad \chi(-\omega^*) = \chi^*(\omega).$$

The technical reason is that the polarization operator is given by the loop diagram with the causal Green's functions, while the susceptibility should be calculated with the help of retarded and advanced functions.

This can be derived from the Kubo formula

$$\chi(\omega) = i\int\limits_0^\infty dt e^{i\omega t}\langle[\hat{A}(t), \hat{B}(0)]\rangle.$$

as follows.

Consider the operator

$$\hat{s}_z(\vec{r}, t) = \mu_B\left[\hat{\psi}^\dagger_\uparrow(\vec{r}, t)\hat{\psi}_\uparrow(\vec{r}, t) - \hat{\psi}^\dagger_\downarrow(\vec{r}, t)\hat{\psi}_\downarrow(\vec{r}, t)\right],$$

and use it in the Kubo formula as both $\hat{A}$ and $\hat{B}$. Then using Wick's theorem (note, that the averaging in the Kubo formula does not involve time ordering) one finds

$$\chi(\omega, \vec{q}) = 2i\mu_F^2\int dt d^3r e^{i\omega t + i\vec{q}\vec{r}}\left[\langle\hat{\psi}^\dagger_\uparrow(\vec{r}, t)\hat{\psi}_\uparrow(0, 0)\rangle\langle\hat{\psi}_\uparrow(\vec{r}, t)\hat{\psi}^\dagger_\uparrow(0, 0)\rangle - \langle\hat{\psi}^\dagger_\uparrow(0, 0)\hat{\psi}_\uparrow(\vec{r}, t)\rangle\langle\hat{\psi}_\uparrow(0, 0)\hat{\psi}^\dagger_\uparrow(\vec{r}, t)\rangle\right].$$

The averages can be calculated by the usual rules of second quantization

$$\langle\hat{\psi}^\dagger_\uparrow(\vec{r}, t)\hat{\psi}_\uparrow(\vec{r}\,', t')\rangle = \sum_{\vec{p}} e^{i\xi(\vec{p})(t-t') - i\vec{p}(\vec{r}-\vec{r}\,')}n[\xi(\vec{p})],$$

$$\langle\hat{\psi}_\uparrow(\vec{r}, t)\hat{\psi}^\dagger_\uparrow(\vec{r}\,', t')\rangle = \sum_{\vec{p}} e^{i\xi(\vec{p})(t-t') - i\vec{p}(\vec{r}-\vec{r}\,')}\{1 - n[\xi(\vec{p})]\}.$$

Making the Fourier transform we finally obtain

$$\chi(\omega, \vec{q}) = 2i\mu_F^2\int\frac{d\epsilon d^3p}{(2\pi)^4}\left[G^R(\epsilon+\omega, \vec{p}+\vec{q})G^A(\epsilon, \vec{p}) - G^A(\epsilon+\omega, \vec{p}+\vec{q})G^R(\epsilon, \vec{p})\right]n(\vec{p})[1-n(\vec{p}+\vec{q})].$$

For small $q \ll p_F$

$$\int d\epsilon G^R(\epsilon+\omega, \vec{p}+\vec{q})G^A(\epsilon, \vec{p}) = \frac{2\pi i}{\omega - v_F q cos\theta + i\delta},$$

and

$$\int d\xi n(\xi)[1 - n(\xi + v_F q\cos\theta)] = \begin{cases} v_F q\cos\theta & \cos\theta > 0, \\ 0 & \cos\theta < 0. \end{cases}$$

As a result

$$\chi(\omega,q)=\mu_B^2\nu_0\int\limits_0^\pi \sin\theta d\theta\frac{v_Fq\cos\theta}{\omega-v_Fq\cos\theta+i\delta}.$$

This differs from the Lindhardt function found in the previous exercise by the sign of the imaginary part:

$$\chi(\omega,q)=2\mu_B^2\nu_0\left[1+\frac{\omega}{2v_Fq}\ln\left|\frac{\omega-v_Fq}{\omega+v_Fq}\right|+\frac{i\pi}{2}\frac{\omega}{v_Fq}\theta(v_Fq-|\omega|)\right].$$

In the limit $\omega/k\to 0$, $k\to 0$ we find the usual Pauli susceptibility

$$\chi_{para}=2\mu_B\nu_0.$$

Second solution

Consider first the imaginary part of the susceptibility using the imaginary part of the Green's function

$$\mathrm{Im}G^R(\epsilon,\vec{p})=-i\pi\delta(\epsilon-\xi_{\vec{p}}).$$

Physically, the imaginary part of the susceptibility describes dissipation in the system, that corresponds to excitation of electron-hole pairs by time-dependent field. This can be described by the same diagram as in the above solution, but now with "on-shell" (real) states. Then, the imaginary part of the susceptibility is given by

$$\mathrm{Im}\chi(\omega,q)=2\mu_B^2\pi^2\int\frac{d^3p}{(2\pi)^3}\frac{d\epsilon}{2\pi}\delta(\epsilon-\xi_{\vec{p}})\delta(\epsilon+\omega-\xi_{\vec{p}+\vec{q}})n(\vec{p})[1-n(\vec{p}+\vec{q})].$$

This expression describes the process where as a result of absorbtion of the energy "quant" (ω) of the external field, an electron in a state under the Fermi surface (with the energy $\xi_{\vec{p}}$) is excited to a state above the Fermi surface (with the energy $\xi_{\vec{p}+\vec{q}}$). This yields $\mathrm{Im}\chi$ only for $\omega>0$. The values at negative frequencies can be restored by using the relation $\chi(-\omega)=\chi^*(\omega)$.

Integrating over the frequency ϵ yields

$$\mathrm{Im}\chi(\omega,q)=\mu_B^2\int\frac{d^3p}{(2\pi)^2}\delta(\omega-\xi_{\vec{p}+\vec{q}}+\xi_{\vec{p}})n(\vec{p})[1-n(\vec{p}+\vec{q})].$$

Focusing on the long wavelength limit $q\ll p_F$, we can use the ξ integration trick that yields $qv_F\cos\theta$ for $\cos\theta>0$ and zero otherwise. The remaining angular integration can be performed as follows

$$\int\limits_0^{\pi/2}d\theta\sin\theta v_Fq\cos\theta\delta(\omega-v_Fq\cos\theta)=\begin{cases}\omega, & 0<\omega<v_Fq,\\ 0, & \omega>v_Fq.\end{cases}.$$

Since the imaginary part of the susceptibility is an odd function of ω, we find

$$\mathrm{Im}\chi(\omega,q)=\mu_B^2\nu_0\begin{cases}\omega, & |\omega|<v_Fq,\\ 0, & |\omega|>v_Fq.\end{cases}.$$

The real part can now be restored from the analiticity, i.e. the Kramers-Kronig relation. This results in the same integration as in the above solution with the same result.