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MICROSCOPIC FERMI-LIQUID APPROACH TO THE RESONANT EFFECTS OF SPIN-ORBIT INTERACTION IN SOLIDS

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Kondo effect, saturation magnetization and heat capacity of ferromagnetic are calculated from the first principles in the spirit of Landau's Fermi-liquid theory. Temperature dependence of resistivity of metal with magnetic impurity is obtained in a good agreement with existing experimental data. Resistance curves demonstrate a minimum due to the resonance character of the interaction between spins of the localized and conduction electrons. It has been demonstrated that both temperature dependence of magnetic momentum and internal energy of ferromagnetic are in a good agreement with those predicted by the Heisenberg's model.

Keywords: *Kondo effect, saturation magnetization, magnon, heat capacity, ferromagnetic.*

METODA FERMI-LICHID MICROSCOPICĂ PENTRU EFECTELE DE REZONANȚĂ A INTERACȚIUNII SPIN-ORBITE ÎN SUBSTANȚELE SOLIDE

Efectul Kondo, magnetizarea de saturație și căldura specifică a unui feromagnet sunt calculate folosind principiile fundamentale în spiritul teoriei Fermi-lichid Landau. Dependența de temperatură a rezistenței metalului cu impurități magnetice este în concordanță cu experimentul. Rezistența minimă este legată de natura rezonantă a interacțiunii unui electron de conducție cu un electron localizat. Se arată că dependența de temperatură a momentului magnetic și energia interioară este în bună concordanță cu modelul Heisenberg.

Cuvinte-cheie: *Efect Kondo, magnetizare de saturație, magnon, capacitate termică, ferromagnetic.*

Introduction

Heisenberg model [1,2] play an important role in quantum theory of magnetism. Heisenberg effective spin-Hamiltonian in which the non-relativistic exchange interaction is expressed as a spin-spin interaction allowed explaining many experimental results. The temperature dependence of the heat capacity and the saturation magnetization of the ferromagnetic cannot be understood without involvement of the concept of spin waves into the consideration. In our previous work [3] it was found from the first principles that the spin-orbit interaction is important for understanding the temperature dependence of the magnetic moment and the internal energy of a ferromagnet. In this paper, we calculate the temperature corrections to the model results using the developed approach [3]. The constant of the spin-Hamiltonian is the sum of contributions of the exchange and the spin-orbit interaction, which is usually neglected. But the spin-orbit interaction in resonant cases [3] can provide a compatible with exchange contribution.

This work is devoted to study of the Kondo effect, saturation magnetization and heat capacity of the ferromagnetic at low temperature from the first principles in the spirit of Landau theory of Fermi-liquid. Comparison of obtained results and known results of model theory [1, 2] are performed.

1. General consideration

Investigation of electron and phonon properties of solids is based on various theoretical models [3-8]. In the paper [3], we have obtained a Hartree-Fock equation for the energy spectrum of electrons with account of the correlations of the charge density [5,8] and with account the spin-orbit interaction in the framework of the calculation of the average value $P_{mm} = \langle a_m^+ a_n \rangle$, where a_m^+ , a_n creation and annihilation operators of electrons. Electrical resistance, magnetization and internal energy of ferromagnetic is dependent on the value of the $P_{mm} = \langle a_m^+ a_n \rangle$, which in thermal equilibrium is represented as a series in powers of fluctuations $\Delta V(\sigma)$ about the average value $\langle V(\sigma) \rangle_0$ given in the interaction picture. All designations in this paper are the same as introduced in the work [3]. To avoid Coulomb divergence one may sum up diverging terms or use the fluctuation-dissipation theorem and find the next result for P_{mm} [3].

$$P_{mm} = n_m \delta_{nm} + \frac{n_n - n_m}{\hbar \omega_{nm}} (\hbar c - \varepsilon_n \delta_{nm}) - \sum_q V_q \int_{-\infty}^{\infty} \frac{d\omega}{\pi \hbar} (n(\omega) + 1) \text{Im}\{-G(q, \omega)\} \sum_l e_{nl}(q) e_{lm}(-q) \left\{ \frac{n_m(1-n_l)}{(\omega + \omega_m)(\omega + \omega_{ln})} - \frac{n_l(1-n_m)}{(\omega - \omega_m)(\omega - \omega_{ln})} \right\} \quad (1)$$

The value $\sum_{m,n} P_{mn} = \sum_n n_n$ is in accordance with Landau Fermi liquid theory. Landau theory of Fermi-

liquid is founded on the representation about the quasiparticles and equation $n = n_0 + \delta n$. Second term in Eq.(1) is equal to zero due to the Hartree-Fock equation for the energy spectrum of quasiparticles [3]. Correction δn to the Fermi-Dirac distribution n_0 is in terms of $G(q, \omega)$ Eq.(1). We calculate function $G(q, \omega)$ by taking into account two components of the Coulomb interaction $\mathcal{V} = (V_q^T + V_{-q}^T)/2$, $\mathcal{H} = H - \mathcal{V}$ as the perturbation. These terms lead to the Coulomb divergences, and should be taken into the consideration for example by using the random phase approximation. Carrying out the simple decoupling the retarded Green's function $G(q, \omega)$ can be evaluated

$$G(q, \omega) = \tilde{G}(q, \omega) / \{1 - \tilde{G}(q, \omega) - \tilde{G}_C^{SO}(q, \omega) - \tilde{G}_{SO}^C(q, \omega) + \tilde{G}_C^C(q, \omega) \tilde{G}_C^{SO}(q, \omega) - \tilde{G}_{SO}^{SO}(q, \omega) \tilde{G}(q, \omega)\} \quad (2)$$

by taking the spin-orbit interaction into the consideration. Averaging with using the equilibrium density matrix of the quasiparticles with Hamiltonian $H_0 = \sum_l \varepsilon_l a_l^\dagger a_l + \sum_{qj} \hbar \omega_{qj} b_{qj}^\dagger b_{qj}$, we find

$$G(q, \omega) = \left(\frac{\varepsilon(q, 0)}{\varepsilon(q, 0) - 1} + \tilde{G}_{SO}^{SO}(q, \omega) \right)^{-1}, \quad \tilde{G}_{SO}^{SO}(q, \omega) = 2 \frac{V_q}{\hbar} \sum_{nl} |e_{nl}^{SO}(q)|^2 \frac{n_n - n_l}{(\omega + i\delta)^2 - \omega_{ln}^2} \omega_{ln}, \quad \tilde{G}(q, \omega) \cong 1 - \varepsilon(q, 0) \quad (3)$$

Electrons interact with quasiparticles, which spectrum is determined by the poles of the $G(q, \omega)$.

$$2 \frac{(\varepsilon(q, 0) - 1) V_q}{\hbar \varepsilon(q, 0)} \sum_{nl} |e_{nl}^{SO}(q)|^2 \frac{n_n - n_l}{\omega_{ln}^2 - \omega^2} \omega_{ln} = 1 \quad (4)$$

Two-band approximation leads to the formula $\omega_{ln} = \Delta_{ln} + \hbar(k_l^2 - k_n^2)/2m^*$. In accordance with the Hubbard model [9], we assume that initial state $n \uparrow$ is discrete energy level state, and $l \downarrow$ state is the band state. Magnons frequencies are lower than the electron transition frequency ω_{ln} . It was established [3] that magnon dispersion law is determined by the electron state $l \downarrow$ energy band structure. Thus for magnon frequency one finds the next expression

$$\omega_q = \omega(q) \{1 - f(q)\}^{1/2}, \quad f(q) = 2 \frac{(\varepsilon(q, 0) - 1) V_q}{\hbar \omega^2(q) \varepsilon(q, 0)} \sum_{nl} |e_{nl}^{SO}(q)|^2 (n_n - n_l) \omega_{ln}, \quad \omega(q) = \Delta + \hbar q^2 / 2m^* \quad (5)$$

An energy band of bulk semiconductors dispersion law at low momentum is quadratic Eq.(5). However, in low-dimensional semiconductors magnons may have a different dispersion law. So magnons in the doped graphene lattice Kondo must have a linear dispersion law.

2. Resonant effects of spin-orbit interaction in solids

Using equation (1) it can be obtained that a non-zero contribution of the temperature correction to the saturation magnetization $\Delta M(T) = M(0) - M(T)$ is determined by the transitions with spin flip due to the spin-orbit coupling

$$\Delta M(T) = 2 \frac{\mu_B}{V} \sum_q V_q \frac{(\varepsilon(q, 0) - 1)}{\varepsilon(q, 0)} \frac{(\omega^2(q) - \omega_q^2)}{\hbar \omega_q} \sum_{nl} \frac{|e_{nl}^{SO}(q)|^2}{(\omega_q - \omega_{ln})^2} (n(\omega_q) n_n (1 - n_l) - [n(\omega_q) + 1] n_l (1 - n_n)), \quad (6)$$

The factor $(\omega_q - \omega_{ln})^{-2}$ in the resonance conditions gives rise to contribution enhance of the processes of inelastic scattering of electrons with spin flip in the absorption of magnons. As a result of the calculation performed, the temperature correction for the saturation magnetization is expressed by the next equation

$$\Delta M(T) = 2 \mu_B \sum_q n(\omega_q) (n(\omega_q) + 1) (1 - \exp[\beta(\omega_q - \omega(q))]) / V \cong 2 \mu_B \sum_q n(\omega_q) / V, \quad n_n (1 - n_l) (n(\omega_q) + 1)^{-1} = (n_n - n_l) \quad (7)$$

Equation (7) is identical to that in the model theory of magnons [1,2] at low temperature $T \rightarrow 0$, when $n(\omega_q) + 1 \cong 1$ and $\exp[\beta(\omega_q - \omega(q))] \ll 1$, $\beta = \hbar / k_B T$. Similarly we calculate the magnon contribution to

the electronic internal energy of a ferromagnetic $U_e = \sum_l \varepsilon_l \langle a_l^\dagger a_l \rangle$. Using the formula (1), one gets

the next ab-initio result

$$\Delta U(T) = \sum_q \hbar \omega_q n(\omega_q) (n(\omega_q) + 1) (1 - \exp[\beta(\omega_q - \omega(q))]) \cong \sum_q \hbar \omega_q n(\omega_q) \quad (8)$$

At low temperature and at $\omega(q) = \hbar q^2 / 2m^*$, $\Delta \cong 0$ we obtain that $\Delta M \approx T^{3/2}$, $\Delta U \approx T^{5/2}$, $\Delta C_V \approx T^{3/2}$ in accordance with Holstein-Primakov theory [1,2]. Factor $(n(\omega_q) + 1)(1 - \exp[\beta(\omega_q - \omega(q))])$ in equations (7,8) changes the magnitudes of ΔM , ΔU . Finally, the calculated temperature correction ΔM (Bloch $T^{3/2}$ law (7)) together with results for the magnon dispersion law (5) and the heat capacity of ferromagnetic are in agreement with the Heisenberg model [1,2].

Resistance minimum of metals with magnetic impurities is connected with the interaction between spins of the localized and conduction electrons in the exchange model [10]. We consider Kondo effect with account of spin-orbit coupling from the first principles. According to the standard theory, conductivity is determined by the equation

$$\sigma = -\frac{1}{3V} \left(\frac{\hbar e}{m} \right)^2 \sum_k k^2 \tau(k) \frac{dP_{kk}}{d\varepsilon_k} = 1/\rho, \quad (9)$$

Here $\tau(k)$ -is transport relaxation time. According to the Eq.(9), conductivity is dependent on the $dP_{kk}/d\varepsilon_k$. But P_{kk} (1) deviates from the standard Fermi-Dirac distribution. With account of correlation in thermal equilibrium, distribution function $P_{kk} = \langle a_k^\dagger a_k \rangle$ has the next form

$$P_{kk} = n_k - \sum_q V_q \int_{-\infty}^{\infty} \frac{d\omega}{\pi \hbar} n(\omega) \text{Im}\{-G(q, \omega)\} \sum_l |e_{kl}^{SO}(q)|^2 \left\{ \frac{n_k(1-n_l)}{(\omega + \omega_{kl})^2} - \frac{n_l(1-n_k)}{(\omega - \omega_{kl})^2} \right\}, \quad (10)$$

Sum over l includes impurity states; k subscript denotes the quantum numbers sets of conduction electrons. Let us first consider the case when impurity level with energy ε_l is below the Fermi level and inequality $\varepsilon_l < \varepsilon_k$ is satisfied. Hence $\omega_{kl} = \hbar k^2 / 2m + \Delta = \omega(k)$ In this case dispersion law of the lattice Kondo magnon is determined by the equation (5). Integrating over ω with account of magnon absorption and emission processes at low temperature one gets

$$P_{kk} = n_k + n(\omega_k) (n(\omega_k) + 1) (1 - \exp[\beta(\omega_k - \omega(q))]) \quad (11)$$

Using results obtained, inserting the equation (11) into (9) we can calculate the temperature dependence of resistivity $\rho(T)$ in units of $\rho(0)$ with account of absorptions and emissions of magnons at the Fermi surface in the lattice of Kondo. Introducing the next designations

$$a = \hbar \omega_{k_F} / k_B, bC = \hbar(\omega(k_F) - \omega_{k_F}) / k_B \cong \hbar \omega(k_F) f(k_F) / 2k_B, bC \ll a \text{ we obtain}$$

$$\rho(T) / \rho(0) = (1 + AT^5 / C) \left\{ 1 + 2 \text{Sh} \left(\frac{a}{T} \right) \left[\text{Ch} \left(\frac{a}{T} \right) - 1 \right]^{-2} \left(1 - \exp \left[-\frac{bC}{T} \right] \right) \right\}^{-1} \quad (12)$$

Where C is the concentration of impurities in arbitrary units. Term AT^5 shows the contribution from the acoustic vibrations. Equation (12) do not changes and in the case when impurity level with energy ε_l is above the Fermi level. But in that case $\omega_{lk} = \Delta - \hbar k^2 / 2m = \omega(k)$, and $P_{kk} = n_k - n(\omega_k) (n(\omega_k) + 1) (1 - \exp[\beta(\omega_k - \omega(q))])$. Contribution into the transport relaxation time $\tau(k)$ due to the electron scattering by collisions with magnons is negligible $1/\tau_{SO}(k_F) \approx \omega(k_F) f(k_F)$. Really, making use of equation (1) with account of damping γ_{kl} we obtain $\gamma_{kl}(k) = (\omega(k) - \omega_k) \{ 2[1 + 2n(\omega_k) - (n_l - n_k)] / (n_l - n_k) \}^{1/2}$. Here function $f(k_F)$ is determined in Eq. (5).

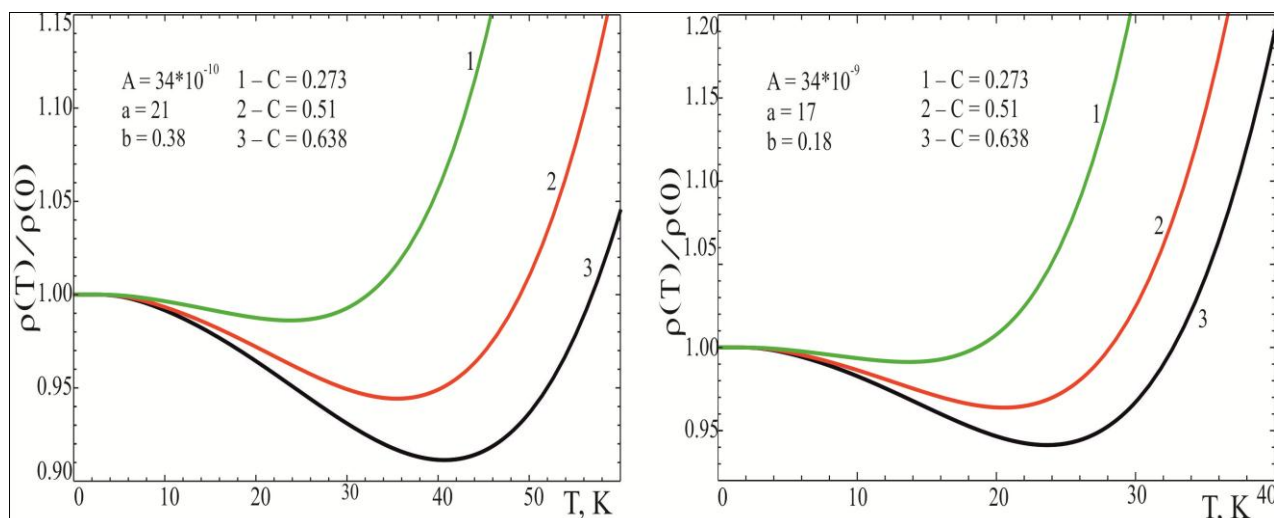


Fig.1. Temperature dependence of resistivity $\rho(T)/\rho(0)$ (12) for different values of concentration C .

In Figure 1 there are represented results of resistivity calculation generated by equation (12) for different values of concentrations and magnon frequencies. Temperature dependence of resistivity of metal with magnetic impurity is in accordance with experiment. Resistance minimum is related to the resonance character of the interaction between spins of the localized and conduction electrons. The results obtained reflect the Abrikosov-Shul aka Kondo resonance character of the spin-flip scattering transitions due to the spin-orbit coupling.

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