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Effective Temperature Scattering Matrix and Kinematic Mechanism of Cooper Instability in Antiferromagnetic Rare-Earth Intermetallides

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Abstract—An effective temperature-dependent scattering matrix for a localized subsystem is obtained in the periodic Anderson model by summing itinerant variables in the diagrammatic series of perturbation theory. The effective interaction that occurs in this case can lead to an antiferromagnetic phase, a superconducting phase, and the phase of coexisting superconductivity and antiferromagnetism observed in heavy-fermion intermetallic compounds.

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INTRODUCTION

Extensive studies of the phase of coexisting superconductivity and antiferromagnetism (SC + AFM) began after the discovery of a number of rare-earth heavy-fermion intermetallic compounds in which such states were observed [1]. The SC + AFM phase induced by externally applied pressure occurs in such cerium intermetallic compounds as $CeIn_3$, $CeRhIn_5$, and $CePt_2In_7$ (of the group $Ce_nT_mIn_{3n+2m}$ [2]).

Recent experimental investigations of $CeRhIn_5$ raised problems relating to fundamentals of the structure of heavy-fermion systems.

Under atmospheric pressure, $CeRhIn_5$ is an antiferromagnet with a Neél temperature of 3.8 K [3]. Applying external pressure to a sample lowers its Neél temperature, evidence of the suppression of long-range antiferromagnetic (AFM) order. In the region of pressures where the AFM order is greatly suppressed, a reduction in temperature is accompanied by the onset of the superconducting (SC) state [4]. In a number of NQR and neutron diffraction experiments, it was shown that a microscopically homogeneous SC+AFM phase exists in $CeRhIn_5$ up to critical pressures at which the AFM state is destroyed [5, 6].

The most probable nonphonon SC mechanism in heavy-fermion systems is one involving interaction of a magnetic nature and spin fluctuations [7, 8]. Other nonphonon mechanisms are directly related to fluctuations of nonmagnetic nature in the vicinity of a quantum critical point. In [9], it was suggested that the onset of Cooper instability is related to valence fluctuations. The possibility of Cooper pairing in the vicinity of local quantum critical point, where the Kondo regime is violated, was demonstrated in [10].

A model of Kondo lattice [11] is often used in microscopic descriptions of the magnetism of heavy-fermion systems. This adequately describes the situation when a localized *f*-level is far from the Fermi level. With mixed valence (which is common in cerium compounds), the *f*-level and the Fermi level are close. In this regime, the minimum microscopic model is the periodic Anderson model (PAM).

It is known that the Shrieffer–Wolf transformation often used to obtain effective exchange interaction cannot be applied to the PAM Hamiltonian if the system is in the mixed valence regime [12]. At the same time, exchange interaction between localized electrons can be induced via high-energy hybridization processes [13]. The resulting exchange interaction is actually the Cooper pairing mechanism that produces the SC + AFM phase in heavy-fermion systems [14, 15]. This approach allows a qualitative description of the phase transitions observed in $CeRhIn_5$ at low temperatures as pressure grows.

In this work, a more general approach is presented that uses an effective temperature-dependent scattering matrix for a quasi-localized subsystem and allows us to consider the kinematic mechanism behind the formation of AFM, SC, and SC + AFM phases in cerium intermetallic compounds.

It should be noted that the temperature of the onset of AFM ordering in the above compounds does not exceed several degrees Kelvin. The temperature of SC formation is on the same order of magnitude. We therefore assume that both orderings are induced by the same interaction. When hybridization is taken into account, the exchange mean-field theory yields rather high values of the critical temperature for the AFM phase [16]. The method proposed in this work allows

us to develop a spin-wave theory of antiferromagnetism in the low temperature region with allowance for hybridization between itinerant and localized electron subsystems. Calculations for the temperature-dependent scattering matrix are based on using the diagram technique in atomic representation with Hubbard operators [17, 18].

Earlier, expansion of the Green functions by semi-invariants [19] and the method of Kubo invariants [20] were used to construct a theory of perturbations within the PAM. Using the diagram technique in the atomic representation and the generalized random phase approximation [22], the dynamic magnetic susceptibility of the paramagnetic PAM phase was calculated in [21].

MODEL

In a two-sublattice representation, the PAM Hamiltonian can be written in the form

$$H = H_0 + H_{\text{mix}}, \tag{1}$$

where H_0 operator allows for the noninteracting subsystems of localized and itinerant electrons

$$\begin{aligned} H_0 = &\sum_{p\sigma}\left[\left(\varepsilon_{\alpha p\sigma}-\mu\right)\alpha^{\dagger}_{p\sigma}\alpha_{p\sigma}+\left(\varepsilon_{\beta p\sigma}-\mu\right)\beta^{\dagger}_{p\sigma}\beta_{p\sigma}\right] \\ &+\sum_{f\sigma}\left(E_0-\mu\right)d^{\dagger}_{f\sigma}d_{f\sigma}+\sum_{f}Un_{f\uparrow}n_{f\downarrow} \\ &+\sum_{g\sigma}\left(E_0-\mu\right)d^{\dagger}_{g\sigma}d_{g\sigma}+\sum_{g}Un_{g\uparrow}n_{g\downarrow}, \end{aligned} \tag{2}$$

and the H_{mix} operator considers hybridization processes involving the two groups of electrons:

$$\begin{aligned} H_{\text{mix}} = &\frac{1}{\sqrt{N/2}}\sum_{pf\sigma}e^{-ipf}\frac{1}{\sqrt{2}}\left[\left(V_p+W_p\right)\alpha^{+}_{p\sigma}d_{f\sigma}\right. \\ &\left.+\left(W_p-V_p\right)\beta^{+}_{p\sigma}d_{f\sigma}\right]+\frac{1}{\sqrt{N/2}}\sum_{pg\sigma}e^{-ipg}\frac{1}{\sqrt{2}}\left[\left(V_p+W_p\right)\right. \\ &\left.\times\alpha^{+}_{p\sigma}d_{g\sigma}+\left(V_p-W_p\right)\beta^{+}_{p\sigma}d_{g\sigma}\right]+h.c. \end{aligned} \tag{3}$$

Here $\alpha_{p\sigma}$ and $\beta_{p\sigma}$ are the operators for annihilation of itinerant electrons with quasi-momentum p and spin projection σ in the first and second AFM zones with energies $\varepsilon_{\alpha p\sigma}$ and $\varepsilon_{\beta p\sigma}$, respectively; μ is the system chemical potential; $d_{f\sigma}\left(d_{g\sigma}\right)$ is the operator of electron annihilation on localized site $f(g)$ belonging to $F(G)$ sublattice; E_0 is the localized level energy; $n_{f\sigma}=d^{\dagger}_{f\sigma}d_{f\sigma}$ is the operator of the number localized electrons on site f with spin projection σ; U is the parameter of on-site Coulomb interaction between localized electrons. In the H_{mix} summand, quantities V_p and W_p represent Fourier transforms of hybridization matrix elements belonging to the same sublattice and to different sublattices, respectively; and N is the total number of sites in the two sublattices.

TEMPERATURE-DEPENDENT SCATTERING MATRIX OF A QUASI-LOCALIZED SUBSYSTEM

To calculate the properties of the normal and SC phases with AFM ordering, we employ Matsubara Green functions constructed using Hubbard operators

$$D_{\lambda\nu}\left(l\tau;l'\tau'\right)=-\left\langle T_{\tau}X^{\lambda}_{l}\left(\tau\right)X^{-\nu}_{l'}\left(\tau'\right)S\left(1/T\right)\right\rangle_{0,c}, \tag{4}$$

where

$$S\left(1/T\right)=T_{\tau}\exp\left(-\int_{0}^{1/T}H_{\text{mix}}(\tau)\,d\tau\right). \tag{5}$$

In these expressions, the operator time dependence is contained in their interaction representation. The related averaging is performed using a zero-order Hamiltonian. Symbols λ and ν determine the root vectors for the Hubbard operator and T is the temperature. The dimension of the root vector coincides with that of the atomic states basis and the root vector n-component is represented in the simple universal form $\lambda_n(r,t)=\delta_{nr}-\delta_{nt}$ [18].

For the introduced Green functions, summing over the degrees of freedom that correspond to the itinerant subsystem can be performed explicitly, and the effective temperature-dependent scattering matrix can be obtained:

$$\begin{aligned} \tilde{S}\left(1/T\right)=T_{\tau}\exp\left\{-\int_{0}^{1/T}d\tau_1\int_{0}^{1/T}d\tau_2\sum_{p\sigma}\sum_{ijr=1}^{2}\left[Z^{+}_{p\sigma}\left(\tau_1\right)\right]_i\right. \\ \left.\times\left(\hat{V}^{+}_{p}\right)_{ij}G_{j\sigma}\left(p,\tau_1-\tau_2\right)\left(\hat{V}_p\right)_{jr}\left[Z_{p\sigma}\left(\tau_2\right)\right]_r\right\}, \end{aligned}$$

where the $\left[Z_{p\sigma}\left(\tau\right)\right]_i$ operators are given by expressions

$$\left[Z_{p\sigma}\left(\tau\right)\right]_1=\frac{1}{\sqrt{N/2}}\sum_{f}e^{-ipf}d_{f\sigma}\left(\tau\right),$$

$$\left[Z_{p\sigma}\left(\tau\right)\right]_2=\frac{1}{\sqrt{N/\ 2}}\sum_{g}e^{-ipg}d_{g\sigma}\left(\tau\right),$$

matrix $\hat{V}_p$ has the form

$$\hat{V}_p=\frac{1}{\sqrt{2}}\begin{pmatrix}V_p+W_p, & V_p+W_p\\ W_p-V_p, & V_p-W_p\end{pmatrix},$$

and $G_{j\sigma}\left(p,\tau_1-\tau_2\right)$ are bare Green functions for itinerant electrons.

Construction of the effective scattering matrix simplifies calculations of localized Green functions due to the equality

$$\begin{aligned} D_{\lambda\nu}\left(l\tau;l'\tau'\right)&=-\left\langle T_{\tau}X^{\lambda}_{l}\left(\tau\right)X^{-\nu}_{l'}\left(\tau'\right)S\left(1/T\right)\right\rangle_{0} \\ &=-\left\langle T_{\tau}X^{\lambda}_{l}\left(\tau\right)X^{-\nu}_{l'}\left(\tau'\right)\tilde{S}\left(1/T\right)\right\rangle_{0,\text{loc}}. \end{aligned}$$

As a result, the averaging operation is accomplished with allowance for the zero-order Hamiltonian of the localized subsystem only, and the effective Hamiltonian acquires the structure of the Hubbard Hamilto-

nian. The kinematic mechanism arising from the non-Fermi character of commutation relations of the Hubbard operators in this case leads to both AFM ordering and Cooper pairing in the presence of long-range AFM order. The ensuing dependence of the effective parameters on Matsubara variables describes the retardation effects and brings about renormalization of the energy parameters.

CONCLUSIONS

Exact regrouping of the diagram series was accomplished in the periodic Anderson model after summation under the sign of average in every order of perturbation theory by dynamic variables relating to an itinerant subsystem. Calculating the Green functions for a quasi-localized subsystem was thus reduced to calculating these functions for an effective Hubbard Hamiltonian. This allowed us to determine the kinematic mechanism behind the formation of antiferromagnetism, superconductivity, and the coexistence phase of superconductivity and antiferromagnetism in cerium heavy-fermion intermetallic compounds.

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