Electronic and lattice properties of high-T_c superconductors due to the two-well potential for apex oxygen

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The formulation of a model for describing the interaction of current carriers in copper oxide HTSC with displacements of the apex oxygen in a two-well potential is discussed in detail. The interaction is treated using the generalized anisotropic s-d exchange model in which it is shown that the interaction matrix is determined by five independent parameters. Corrections to the electronic energy spectrum in the weak coupling regime are calculated. The corresponding contribution to the density of states changes dramatically near the Fermi energy E_F on small energy scales on the order of the characteristic collective mode frequency $\bar{\omega}$ and, what is unusual, is asymmetric about E_F, which can add substantially to the thermopower. The reaction of the conduction electrons on the lattice subsystem, in particular the suppression of the two-well feature by the pseudo-Kondo effect, is investigated. The renormalization group equations for the single-center problem are developed, and the "Kondo temperature" for the case of an anisotropic *xyz* model is found.

1. INTRODUCTION

At present it may be considered established that the apex oxygen atoms located at the apices of the elongated CuO_6 octahedra in the crystal lattices of copper oxide HTSC are in a two-well potential. Apart from direct EXAFS experiments[1], this view is supported by x-ray,[2] Mössbauer,[3] and Raman[4] data (the system $YBa_2Cu_3O_{7-\delta}$ being most closely studied in this respect), as well as by first-principle total energy calculations for $La_{2-x}Sr_xCuO_4$ using the density functional method with inclusion of correlation effects.[5] A number of workers (see, e.g., Refs. 1, 2, 6–9) have presented arguments showing the important role of apex oxygen in superconductivity mechanisms, such as temperature dependence anomalies in the relevant EXAFS parameters at T_c,[6] the correlation between the amount of apex oxygen in a unit cell and the exponent of the isotopic effect,[8] the correlation between the pressure variations of T_c and the distance from the apex oxygen to the CuO_2 plane,[7] etc. Strictly speaking all these arguments are indirect in nature (except perhaps EXAFS), but they are a sufficient motivation to raise the theoretical problem of the role of apex oxygen in determining the special properties of HTSC. Indeed this problem may be of more general interest from the viewpoint of strong correlation physics, as an opportunity to consider new multiparticle models with interesting types of behavior.

There have recently been a large number of theoretical studies on the subject.[10–15] While the particular forms of the proposed models vary, all of them consider the interaction of conduction electrons with atoms in a two-well potential, treated as two-level systems. The majority of these studies are concerned mainly with the superconductivity mechanisms possible in such models; in Ref. 10 the properties of the normal phase are briefly discussed. In all cases the strong coupling regime is considered from the outset, when the electronic spectrum near E_F is completely reshaped by the interaction with the two-level system. Because reliable estimates of interaction parameters appear at present impossible and may in addition vary from one system to another, it appears necessary to perform a detailed analysis of the electronic spectra for different regimes, starting from the perturbation theory (weak coupling) approach. It is the purpose of this study to present such an analysis.

The question of the influence of an excited two-level system on the magnitude of T_c has been investigated in a number of studies following Refs. 16 and 17 and will not be discussed here.

Apart from the mere fact of existence of two-level systems associated with apex oxygen, an essential factor in the formulation of our model is the strong evidence for the "ferroelectric" behavior of HTSC.[18–21] Therefore, unlike Refs. 11–15, our primary concern will be with the effects of interaction between two-level systems, which may lead to ferroelectric ordering (at least in a short range sense) and "pseudospin" collective excitations.[22] Even prior to any evidence for the importance of apex oxygen—and hence without the necessary specifics—a simple model for these effects was considered in Ref. 23. The problem we are discussing formally resembles the problem of magnetic Kondo lattices, in which the key factor is the competition between the resonant scattering of conduction electrons by localized spins (in our case, by two-level systems treated as pseudospins) and the spin-spin exchange interaction.[24,25] The point to note is that even in the weak coupling regime,

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a small energy scale appears in the electronic spectrum near E_F over which the density of states $N(E)$ changes sharply. The role of this scale is played by the characteristic spin excitation frequency $\bar{\omega}$.[24] The corresponding anomalous contributions to $N(E)$ are incoherent (nonquasiparticle) in nature and have a number of unusual features, in particular, the electron–hole asymmetry.[23]

However, as compared with magnetics[24,25] and with the specialized model of Ref. 23, the interaction between conduction electrons and a two-level system has a much more complicated structure (because of the nonconservation of the total "spin," for example). It is a detailed theoretical discussion of the effects of this interaction which is the objective of the present work.

In Sec. 2, the form of the initial Hamiltonian is discussed, and in particular the minimal necessary set of interaction parameters is determined and the physical meaning of the parameters is indicated. For simplicity, the lattice subsystem is described by a pseudospin formalism, corresponding to an order–disorder transition model.[22] This model presumably describes the required qualitative properties of the apex oxygen subsystem (the two-well feature, "ferroelectric" aspects, etc). Sections 3 and 4 employ second-order perturbation theory in the above parameters to evaluate the electron and lattice properties of the model respectively. In Sec. 5, the Kondo temperature T_K for the case of a single two-level center is predicted using the present model. In this case it is known[2] that the condition $\bar{\omega} > T_K$ determines the range of applicability of the results obtained in Secs. 3 and 4.

2. FORMULATION OF A PSEUDO-KONDO LATTICE MODEL

We are interested in a particular vibration mode of the apex oxygen, one in the normal direction to the CuO_2 plane. Denoting the corresponding coordinate of an ion in the ith cell by q_i, and its canonically conjugate momentum by p_i, we write the part of the lattice Hamiltonian associated with these displacements as

$$H_{\text{lat}}=\sum_i H_i+\tfrac{1}{2}\sum_{i\neq j} W(q_i,q_j),\quad H_i=\frac{P_i^2}{2M}+V(q_i), \tag{1}$$

where M is the mass of the ion, $V(q)$ is the potential for the apex oxygen ion produced by all the ions of the other type, and $W(q_i,q_j)$ is the interaction potential between the above displacements in different cells. In a quantum mechanical description of vibrations in a highly anharmonic potential, it is convenient to introduce the representation in terms of the exact eigenfunctions of the Hamiltonian H_i, and to define the corresponding projection operators,[24]

$$H_i|i\nu\rangle=E_\nu|i\nu\rangle,\quad X_i^{\nu\mu}=|i\nu\rangle\langle i\mu|. \tag{2}$$

With the picture of a two-well potential $V(q)$ for an apex oxygen in mind let us assume, as customary in two-level analyses,[27] that the first excited state is close in energy to the ground state $|0\rangle$:

$$E_1-E_0\ll E_\nu-E_0,\quad \nu>1. \tag{3}$$

According to Ref. 1, the condition (3) holds well for apex oxygen displacements in $YBa_2Cu_3O_7$ ($E_1-E_0\sim 10^2$ K, and for the remaining differences $E_\mu-E_\nu\sim 10^3$ K). Since in the electronic spectrum analysis which follows we are only interested in the vicinity $|\Delta E|<10^3$ K of the Fermi level, we may limit ourselves to only two states, $|0\rangle$ and $|1\rangle$, and change from the complete set of X operators of the form (2) to the pseudospin operators:

$$X^{01}=S^+,\quad X^{10}=S^-,\quad X^{00}=\tfrac{1}{2}+S^z,$$
$$X^{11}=\tfrac{1}{2}-S^z,\quad S^\pm=S^x\pm iS^y. \tag{4}$$

Then the ion interaction Hamiltonian in Eq. (1) will take the form a pseudospin operator. As a result, it has been shown by the standard theory of ferroelectric order–disorder transitions[22] that, for a symmetric two-well potential and to leading order in the overlap of the ion wave functions, H_{lat} reduces to the transverse-field Ising model,

$$H_{\text{lat}}=-\Omega\sum_i S_i^z-\tfrac{1}{2}\sum_{i\neq j} J_{ij}S_i^xS_j^x, \tag{5}$$

where $\Omega=E_1-E_0$, and J_{ij} is a certain combination of the matrix elements $W(q_i,q_j)$. Here $|0\rangle$ and $|1\rangle$ are the even-parity (bonding) and odd-parity (antibonding) states, Ω is the tunneling frequency, and the dipole moment determining the difference in population numbers of the right-hand and left-hand wells is proportional to $\langle S^x\rangle$. The important point is that even in the absence of the ion–ion interaction the quantity $\langle S^z\rangle$ is nonzero due to tunneling:

$$\langle S^z\rangle=\tfrac{1}{2}\tanh\frac{\Omega}{2T}. \tag{6}$$

If the wells are asymmetric, the interaction Hamiltonian in Eq. (5) will also contain the terms $S_i^xS_j^z$ and $S_i^zS_j^z$. However, except in discussing the effect of conduction electrons on the pseudospin system (Sec. 4), this complication will not produce any qualitative effects. For simplicity in what follows we will therefore use the expression (5).

The Ising interaction J can yield a "ferroelectric" (or "antiferroelectric") transition at a certain temperature $T=T_s$. For $T<T_s$, both $\langle S^z\rangle$ and $\langle S^x\rangle$ are nonzero. In the system described by the Hamiltonian (5) there exist collective pseudospin excitations of two types, the dissipative mode and the "pseudospin waves." The frequency of these latter, in the simplest approximation, is[22]

$$\omega_{\mathbf{q}}^2=(J_0\langle S^x\rangle)^2+\Omega(\Omega-J_{\mathbf{q}}\langle S^z\rangle), \tag{7}$$

with $\langle S^z\rangle=\Omega/J_0=\text{const}$ for $T<T_s$. In the following we consider the interaction between the conduction electrons and these collective excitations while neglecting the interaction with the usual phonons.

The scattering of the conduction electrons of a metal by centers with internal degrees of freedom may give rise to special quantum-mechanical multiparticle "Kondo" resonances. In perturbation theory they are described by contributions to the scattering matrix which depend logarithmically on the electron energy measured from E_F (see Refs. 28–31). It is necessary to distinguish between two

cases, in which, as a result of the scattering event (with a change in the state of the localized center involved), the conduction electron changes only its quasimomentum, and in which it also changes either its spin or band (pseudospin) index. While Kondo type divergences exist for either situation, the formal description of the above cases differs substantially (cf. the corresponding results for electron scattering by magnetic impurities,[8] by two-level systems in metal glasses,[29,30] and by local excitons and phonons[29]). Thus, the effects of interaction between the conduction electrons and pseudospins are dependent on the presence of electron band degeneracy near E_F (because of the weak spin–orbit interaction, the spin degree of freedom is of no importance, so in what follows we will merely omit the spin index). In general, the Fermi level passes through several energy bands, so that scattering processes both with and without changing the band index occur. Restricting ourselves to the two band case, the Hamiltonian of the model is written in the form

$$H=\sum_{\mathbf{k}\tau}\varepsilon_{\mathbf{k}\tau}c^+_{\mathbf{k}\tau}c_{\mathbf{k}\tau}+H_{\rm int}+H_{\rm lat}, \tag{8}$$

where $H_{\rm lat}$ is of the form (5), $c^+_{\mathbf{k}\tau}$ is the creation operator for an electron of quasimomentum $\mathbf{k}$ and band index $\tau=\pm$, and the energy $\varepsilon_{\mathbf{k}\tau}$ is measured from E_F. For simplicity the interaction is assumed to be described by a contact Hamiltonian,

$$H_{\rm int}=\sum_{i\tau\tau'} I^\alpha_\beta \delta S^\beta_i c^+_{i\tau}\sigma^\alpha_{\tau\tau'}c_{i\tau'}, \tag{9}$$

where σ are the Pauli matrices, $\delta S^\beta_i=S^\beta_i-\langle S^\beta_i\rangle$, and I^α_β is the matrix of the interaction parameters. Here and in what follows summation over repeated cartesian indices α, β is understood. The effects of the mean field $I^\alpha_\beta\langle S^\beta_i\rangle$ may be absorbed into the definition of $\varepsilon_{\mathbf{k}\tau}$.

The model (8), (9) is an analog of the anisotropic *s-d* exchange model[21], the major difference being that the matrix I^α_β is in general nondiagonal because, unlike spin systems, there is no reason for requiring the conservation of either the total "spin" or its z projection. The only restriction is that all the I^α_β must be imaginary, as implied by the time-reversal invariance (for pseudospin systems with no spin–orbit interaction this simply reduces to complex conjugation). Since the operators σ^y and S^y contain a factor of the square root of -1, we have

$$\hat I=\begin{pmatrix} I^x_x & 0 & I^x_z\\ 0 & I^y_y & 0\\ I^z_x & 0 & I^z_z\end{pmatrix}. \tag{10}$$

Let us explain the meaning of some of the matrix elements I^α_β The $\alpha=z$ terms in Eq. (9) correspond to the change in the splitting of the degenerate electron spectrum due to the interaction with the two-level system. In particular, if $\varepsilon_{\mathbf{k}}+\equiv\mathbf{k}-$ initially, we have a static (for $\beta=x$) or dynamical (for $\beta=z$) Jahn–Teller band effect (recall that the dipole polarization is directed along the x axis). The $\alpha=x,y$ terms describe the interband scattering of the conduction electrons. The physical meaning of the parameter I^z_x will be discussed below in Sec. 4. As we shall see in the next section, the terms in I^y_y are qualitatively important because they are the only ones capable of producing an asymmetric contribution to the density of states. We note therefore that even if $I^y_y=0$ holds initially, an effective interaction of this form appears anyway in higher orders in perturbation theory (Sec. 5).

Other theoretical treatments of the interaction of current carriers with apex oxygen[11–15] are usually based on modifications of the Yu–Anderson model[32] for A15 compounds. These modified models relate to the pseudospin model in the same way as Anderson's relates to the s-d exchange model in the Kondo problem. The pseudospin operator formulation is much more convenient for a perturbative analysis because the singularities of interest to us appear in this case in lower orders.

3. ELECTRONIC SPECTRUM IN THE WEAK COUPLING REGIME

We now turn to consideration of the electronic spectrum in the model (8) using perturbation theory in $H_{\rm int}$. To this end we introduce the spinor operators $\psi^+_{\mathbf{k}}=(c^+_{\mathbf{k}+},c^-_{\mathbf{k}-})$ and the retarded matrix Green's function

$$\hat G(\mathbf{k},E)=\langle\langle\psi_{\mathbf{k}}|\psi^+_{\mathbf{k}}\rangle\rangle_E=-i\int_0^\infty dt\exp(iEt)\times\langle\{\psi_{\mathbf{k}},\psi^+_{\mathbf{k}}(t)\}\rangle,\quad \mathrm{Im}\,E>0.$$

The calculation of $\hat G(\mathbf{k},E)$ to second order in $H_{\rm int}$ and with the formally exact inclusion of $H_{\rm lat}$ (pseudospin dynamics) may be carried out either directly by the equation-of-motion method (cf. the discussion of the *s-d* exchange model in Ref. 24) or by using a diagram technique for the Matsubara Green's functions, with a subsequent analytical continuation (cf. Ref. 33). As a result we find

$$\hat G^{-1}(\mathbf{k},E)=E-\hat\varepsilon_{\mathbf{k}}-\hat\Sigma(\mathbf{k},E), \tag{11}$$

where $\hat\varepsilon_{\mathbf{k}}=\mathrm{diag}(\varepsilon_{\mathbf{k}+},\varepsilon_{\mathbf{k}-})$ is a diagonal 2×2 matrix,

$$\hat\Sigma(\mathbf{k},E)=\frac{1}{2}\sum_{\mathbf{q},\tau=\pm}\int_0^\infty d\omega\ K^{\beta\alpha}(\mathbf{q},\omega)\Big[\sigma^\beta(1+\tau\sigma^z)\times\sigma^\alpha\frac{f_{\mathbf{k}-\mathbf{q},\tau}+N_B(\omega)}{E-\varepsilon_{\mathbf{k}-\mathbf{q},\tau}+\omega}+\sigma^\alpha(1+\tau\sigma^z)\times\sigma^\beta\frac{1-f_{\mathbf{k}-\mathbf{q},\tau}+N_B(\omega)}{E-\varepsilon_{\mathbf{k}-\mathbf{q},\tau}-\omega}\Big], \tag{12}$$

where $f_{\mathbf{k}\tau}=f(\varepsilon_{\mathbf{k}\tau})$ and $N_B(\omega)$ are the Fermi and Bose distribution functions, and

$$K^{\beta\alpha}(\mathbf{q},\omega)=-\frac{1}{\pi}\mathrm{Im}\langle(h^\alpha_{\mathbf{q}}|h^\beta_{-\mathbf{q}}\rangle\rangle_\omega \tag{13}$$

is the spectral density of the components of the effective field through which acts the pseudospin system acts on the electron,

$$h^\alpha_{\mathbf{q}}=I^\alpha_\beta\delta S^\beta_q, \tag{14}$$

If the pseudospin dynamics is neglected ($H_{\rm lat} \to 0$), the Fermi function terms in (12) yield Kondo logarithmic divergences; these are substantially modified by the dynamics.

As seen from Eq. (12), the electronic density of states

$$N(E) = -\frac{1}{\pi} \mathrm{Tr} \sum_{\mathbf{k}} \mathrm{Im}\, \hat{G}(\mathbf{k},E) \tag{15}$$

contains incoherent ("nonquasiparticle") contributions due to the cuts of the Green' function

$$\delta N(E) = -\frac{1}{\pi} \mathrm{Tr} \sum_{\mathbf{k}} \mathrm{Re}\left[\frac{1}{(E-\hat{\varepsilon}_{\mathbf{k}})^2}\right] \mathrm{Im}\, \hat{\Sigma}(\mathbf{k},E). \tag{16}$$

It is these contributions which produce the sharp energy dependence of $N(E)$ (E being measured from E_F) that has been discussed in Ref. 23 for the ordered phase of an anisotropic *s-d* model.

At $T=0$, the first term in brackets in Eq. (12) has a nonzero imaginary part for $E<0$, and the second for $E>0$. Let us now separate the self-energy into contributions which are symmetric and asymmetric about E_F:

$$\hat{\Sigma}(\mathbf{k},E) = \hat{\Sigma}_s(\mathbf{k},E) + \hat{\Sigma}_a(\mathbf{k},E), \tag{17}$$

$$\begin{aligned}\hat{\Sigma}_s(\mathbf{k},E) = \frac{1}{2} \sum_{\mathbf{q}\tau} \int_0^\infty d\omega \{ &(1-\tau\sigma^z) K^{\alpha\alpha}(\mathbf{q},\omega) \\ &+ \tau\sigma^\alpha [K^{z\alpha}(\mathbf{q},\omega) + K^{\alpha z}(\mathbf{q},\omega)]\} \\ &\times \left[\frac{f_{\mathbf{k}-\mathbf{q},\tau} + N_B(\omega)}{E - \varepsilon_{\mathbf{k}-\mathbf{q},\tau} + \omega} \right. \\ &\left. + \frac{1 - f_{\mathbf{k}-\mathbf{q},\tau} + N_B(\omega)}{E - \varepsilon_{\mathbf{k}-\mathbf{q},\tau} - \omega}\right],\end{aligned} \tag{18}$$

$$\begin{aligned}\hat{\Sigma}_a(\mathbf{k},E) = \frac{i}{2} \sum_{\mathbf{q}\tau} \int_0^\infty d\omega\, K^{\beta\alpha}(\mathbf{q},\omega) (\tau\varepsilon_{\alpha\beta z} - \varepsilon_{\alpha\beta\gamma}\sigma^\gamma) \\ \times \left[\frac{f_{\mathbf{k}-\mathbf{q},\tau} + N_\beta(\omega)}{E - \varepsilon_{\mathbf{k}-\mathbf{q},\tau} + \omega} \right. \\ \left. - \frac{1 - f_{\mathbf{k}-\mathbf{q},\tau} + N_R(\omega)}{E - \varepsilon_{\mathbf{k}-\mathbf{q},\tau} - \omega}\right],\end{aligned} \tag{19}$$

where $\varepsilon_{\alpha\beta\gamma}$ is the antisymmetric unit tensor. In the symmetric part of $\delta N(E)$ due to the contribution (18), only terms in $K^{\alpha\alpha}$ survive the trace in (16). The antisymmetric part of $\delta N(E)$ arises from the terms proportional to $i(K^{xy} - K^{yx}) = K^{-+} - K^{+-}$. In view of the identity

$$\begin{aligned} i \int_{-\infty}^{\infty} d\omega [K^{xy}(\mathbf{q},\omega) - K^{yx}(\mathbf{q},\omega)] \\ = i\langle [h_0^x, h_0^y] \rangle = I_y^y (I_z^x \langle S^x \rangle - I_x^x \langle S^z \rangle)\end{aligned} \tag{20}$$

one argues that the antisymmetric part is *a priori* nonzero even in the "paraelectric" phase provided $I_y^y \neq 0, I_x^x \neq 0$.

The incoherent contribution $\delta N(E)$ changes near the Fermi level dramatically in the energy interval $|E| \sim \bar{\omega}$, where $\bar{\omega}$ is the characteristic pseudospin excitation frequency. From Eqs. (16), (17)–(19) it follows that $\delta N(E \to 0) \to 0$ for $T=0$ (Ref. 23), in a manner determined by the specific form of $K^{\alpha\beta}(\omega)$ (pseudospin dynamics). Thus, the total density of states can be represented in the form

$$\frac{N(E)}{\rho(E)} = 1 + \Phi(E/\bar{\omega}) \approx \begin{cases} 1+\Phi_+, & E \gg \bar{\omega}, \\ 1, & |E| \ll \bar{\omega}, \\ 1+\Phi_-, & E<0, \quad |E| \gg \bar{\omega}, \end{cases} \tag{21}$$

where $\rho(E)$ is the bare density of states and $\Phi_\pm \sim I^2 \rho^2(0)$ ($\Phi_+ \neq \Phi_-$ if $I_y^y \neq 0$).

The asymmetry in $N(E)$ yields a substantial contribution to the thermopower $S(T)$. According to the Mott–Jones formula,[23] for elastic scattering we have

$$S(T) = \frac{1}{eT\sigma(T)} \int_{-\infty}^{\infty} dE \left(-\frac{\partial f(E)}{\partial E}\right) E\sigma(E), \tag{22}$$

$$\sigma(T) = \int_{-\infty}^{\infty} dE \left(-\frac{\partial f(E)}{\partial (E)}\right) \sigma(E), \tag{23}$$

where e is the electron charge, $\sigma(T)$ is the conductivity, and $\sigma(E)$ is the contribution to this latter from the layer with the given energy. Setting $\delta\sigma(E) \sim \delta N(E)$, we find that for $T > \bar{\omega}$

$$eS(T) \propto \Phi_+ - \Phi_- \sim \rho^2(0) I_y^y I_x^x \langle S^z \rangle \tag{24}$$

(the last estimate applies to the para phase). We see that the thermopower does not contain the usual small factor T/E_F. An alternative means for detecting the antisymmetric part of $\delta N(E)$ may be provided by tunneling experiments.

In order to find the temperature dependence of the nonquasiparticle contributions to $\sigma(T)$ and $S(T)$ for $T < \bar{\omega}$, it is necessary to specify the form of the spectral density (13). At low temperatures short-wavevector pseudospin excitations dominate, so for the frequency of the pseudospin waves (7) we have

$$\omega_{\mathbf{q}}^2 = \omega_0^2 + v^2 q^2, \tag{25}$$

where $\omega_0 \to 0$ for $T \to T_s$. After we average over $\mathbf{q}$ the corresponding contribution to K takes the form

$$\bar{K}_1(\omega) \propto (\omega - \omega_0)^{(d/2-1)} \theta(\omega - \omega_0), \tag{26}$$

where $\theta(x)$ is the Heaviside function, and $d=2$, 3 is the space dimensionality. Then, if the function $\rho(E)$ is smooth near E_F, we find

$$\delta\sigma_1(T), \delta S_1(T) \propto T^{d/2} \exp(-\omega_0/T). \tag{27}$$

In the presence of a two-dimensional van Hove singularity at the Fermi level, when $\rho(E) \propto -\ln|E|$, the expression (27) is multiplied by $\ln(W/T)$, where W is on the order of the conduction bandwidth.

In the ferroelectric phase the spectral density exhibits a "central peak"[22]

$$\bar{K}_2(\omega) \propto \frac{1}{\pi} \langle S^x \rangle^2 \frac{\Gamma}{\Gamma^2 + \omega^2}, \tag{28}$$

where $\Gamma=1/T_1$ is the inverse time for the longitudinal relaxation of the dipole moment. Substitution of (28) yields

$$\delta N_2(E) \propto \text{const}+\arctan(E/\Gamma). \tag{29}$$

A nonzero contribution to (23) from the odd-parity term in (29) arises from including the energy dependence of the smooth factors in $\sigma(e)$:

$$\delta\sigma(T) \propto T\int_{-\infty}^{\infty} dE(-\partial f(E)/\partial E)$$
$$\times(\sigma_0+\sigma_1 E+\ldots)\arctan(E/\Gamma). \tag{30}$$

Then

$$\delta\sigma_2(T), \quad T\delta S_2(T) \propto \langle S^x\rangle^2 \frac{T}{\max\{T,\ \Gamma(T)\}}. \tag{31}$$

If $\Gamma(T) \gg T$ for all T, a linear temperature contribution to the conductivity and a large constant contribution to the thermopower arise (cf. Ref. 24).

4. EFFECT OF CURRENT CARRIERS ON THE PSEUDOSPIN SUBSYSTEM

The perturbation theory framework also makes it possible to consider the reaction of the conduction electrons on the lattice pseudospin subsystem. At present, experimental information about this latter is rather limited (to EXAFS data,[1,6] in fact). Nevertheless, the pseudospin dynamics can in principle be separated in inelastic neutron scattering superposed on the usual phonon contributions. Therefore its theoretical study may be of use in designing an appropriate experimental research problem.

Here it is necessary, however, to remember the simplifications we employ in the model (pseudospin formalism, or the assumption of a ferroelectric order–disorder transition; and the use of the Hamiltonian (5), which implies the symmetry of the two-well potential). Consequently the results obtained in this section should be regarded as only qualitative when applied to real HTSC materials.

The effect of conduction electrons on the pseudospin dynamics is conveniently analyzed by the method of retarded-commutator Green's functions for pseudospin operators,

$$\Gamma^{\lambda\mu}(\mathbf{q},\omega)=\langle\langle S^2_{\mathbf{q}}|S^{\mu}_{-\mathbf{q}}\rangle\rangle_{\omega} \tag{32}$$

in an analogous fashion to the RKKY interaction in the *s-d* exchange model. By decoupling to second order in I we find

$$\omega\Gamma^{\lambda\mu}(\mathbf{q},\omega)-\langle\langle[S^{\lambda}_{\mathbf{q}},H_{\text{lat}}]|S^{\mu}_{-\mathbf{q}}\rangle\rangle_{\omega}=i\varepsilon_{\lambda\mu\nu}\langle S^{\nu}\rangle$$
$$-iI^{\alpha}_{\beta}\varepsilon_{\lambda\beta\nu}\sum_{\mathbf{k}\tau\tau'}\sigma^{\alpha}_{\tau\tau'}\Big[f_{\mathbf{k}\tau}\delta_{\tau\tau'}\Gamma^{\nu\mu}(\mathbf{q},\omega)$$
$$-\langle S^{\nu}\rangle I^{\gamma}_{\delta}\sigma^{\gamma}_{\tau'\tau}\frac{f_{\mathbf{k}\tau}-f_{\mathbf{k}+\mathbf{q},\tau'}}{\omega-\varepsilon_{\mathbf{k}+\mathbf{q},\tau'}+\varepsilon_{\mathbf{k}\tau}}+\Gamma^{\delta\mu}(\mathbf{q},\omega)\Big]. \tag{33}$$

The system of linear equations for the Green's functions, Eq. (33), determines the spectrum of pseudospin excitations. In contrast to the usual *s-d* model, the population difference between electronic energy subbands

$$\Delta n=\sum_{\mathbf{k}}(f_{\mathbf{k}+}-f_{\mathbf{k}-}) \tag{34}$$

is not small in I (except for the case of a degenerate bare band to be discussed below). It is therefore possible to limit ourselves to first-order terms by retaining only the first term in the brackets in (33) [note that $\alpha=z$ and, by (10), $\beta=x,z$]. Then we obtain for the spectrum

$$\omega^2=\tilde{\Omega}(\tilde{\Omega}-J_q\langle S^z\rangle)+g^2, \tag{35}$$

where

$$\tilde{\Omega}=\Omega+I^z_z\Delta n, \quad g=I^z_x\Delta n+J_0\langle S^x\rangle. \tag{36}$$

Expression (35) differs from (7) by the renormalizations (36). While the replacement $\Omega\to\tilde{\Omega}$ does not lead to any radical consequences, the appearance of the Δn term in g is very important. Its implication is that the conduction electrons cause a spontaneous distortion of the lattice at any temperatures (the left-hand and right-hand wells become inequivalent). If there is no physical reason to expect this inequivalence, then it is necessary to set $I^z_x=0$ in Eq. (10); generally speaking, it is only in this case that a ferroelectric phase transition may occur.

In the case of the band Jahn–Teller effect, when in the absence of electrons $\varepsilon_{\mathbf{k}+}=\varepsilon_{\mathbf{k}-}$ holds and Δn is small in I, the "mixing" of $\langle S^z\rangle$ and $\langle S^x\rangle$ due to the I^z_x and I^x_z interactions arises only in higher orders of perturbation theory. For this case, the dependence on the pseudospin indices may be neglected in the second-order terms on the right-hand side of Eq. (33). Then Eqs. (33) become

$$\omega\Gamma^{x\beta}(\mathbf{q},\omega)-i[\tilde{\Omega}+\langle S^z\rangle(I^y_y)^2\Pi_{\mathbf{q}\omega}]\Gamma^{y\beta}(\mathbf{q},\omega)=i\varepsilon_{x\beta\gamma}\langle S^{\gamma}\rangle;$$

$$i\{\tilde{\Omega}-J_{\mathbf{q}}\langle S^z\rangle+\langle S^z\rangle[(I^x_x)^2+(I^z_x)^2]\Pi_{\mathbf{q}\omega}$$
$$-\langle S^x\rangle(I^x_zI^x_x+I^z_zI^z_x)\Pi_{q\omega}\}\Gamma^{x\beta}(\mathbf{q},\omega)+\omega\Gamma^{y\beta}(\mathbf{q},\omega)$$
$$-i\{g-\langle S^z\rangle(I^x_xI^x_z+I^z_xI^z_z)\Pi_{\mathbf{q}\omega}$$
$$+\langle S^x\rangle[(I^z_z)^2+(I^x_z)^2]\Pi_{\mathbf{q}\omega}\}\Gamma^{z\beta}(\mathbf{q},\omega)=i\varepsilon_{y\beta\gamma}\langle S^{\gamma}\rangle;i[g$$
$$+\langle S^x\rangle(I^y_y)^2\Pi_{\mathbf{q}\omega}]\Gamma^{y\beta}(\mathbf{q},\omega)+\omega\Gamma^{z\beta}(\mathbf{q},\omega)=i\varepsilon_{z\beta\gamma}\langle S^{\gamma}\rangle, \tag{37}$$

where

$$\Pi_{\mathbf{q}\omega}=\sum_{\mathbf{k}}\frac{f_{\mathbf{k}}-f_{\mathbf{k}+\mathbf{q}}}{\omega+\varepsilon_{\mathbf{k}}-\varepsilon_{\mathbf{k}+\mathbf{q}}} \tag{38}$$

is the polarization operator in the random phase approximation. Restricting ourselves for simplicity to the case of a paraelectric phase ($\langle S^x\rangle=0$), we find that to within second-order terms,

$$\Gamma^{xx}(\mathbf{q},\omega)=\frac{\tilde{\Omega}+\langle S^z\rangle (I_y^y)^2\Pi_{\mathbf{q}\omega}}{\omega^2-\Lambda_{\mathbf{q}\omega}^2}\langle S^z\rangle,$$

$$\Gamma^{xy}(\mathbf{q},\omega)=-\Gamma^{yx}(\mathbf{q},\omega)=\frac{i\omega\langle S^z\rangle}{\omega^2-\Lambda_{\mathbf{q}\omega}^2}, \tag{39}$$

$$\Gamma^{yy}(\mathbf{q},\omega)=\frac{\tilde{\Omega}-J_{\mathbf{q}}\langle S^z\rangle+\langle S^z\rangle[(I_x^x)^2+(I_x^z)^2]\Pi_{\mathbf{q}\omega}}{\omega^2-\Lambda_{\mathbf{q}\omega}^2}\langle S^z\rangle,$$

where the square of the renormalized frequency has the form

$$\Lambda_{\mathbf{q}\omega}^2=\tilde{\Omega}(\tilde{\Omega}-J_{\mathbf{q}}\langle S^z\rangle)+\langle S^z\rangle\Pi_{\mathbf{q}\omega}\{\tilde{\Omega}-J_{\mathbf{q}}\langle S^z\rangle)(I_y^y)^2 +\tilde{\Omega}[(I_x^x)^2+(I_x^z)^2]\}. \tag{40}$$

The imaginary part of the quantity Λ describes the damping of the pseudospin waves due to their interaction with electrons. Since

$$\mathrm{Im}\,\Pi_{\mathbf{q}\omega}\simeq-\pi\omega\sum_{\mathbf{k}}\delta(\varepsilon_{\mathbf{k}})\delta(\varepsilon_{\mathbf{k}+\mathbf{q}})\quad(|\omega|\ll W), \tag{41}$$

the damping is linear in frequency. Analogous to the case of Kondo magnetics,[24,25] this damping gives rise to logarithmic contributions to the pseudospin correlation functions $\langle S_{\mathbf{q}}^{\alpha}S_{-\mathbf{q}}^{\beta}\rangle$ and the means $\langle S^{\beta}\rangle$. Using the spectral representation we obtain

$$\langle S^z\rangle=\tfrac{1}{2}-\langle S_i^+S_i^-\rangle=\tfrac{1}{2}+\frac{1}{\pi}\mathrm{Im}\sum_{\mathbf{q}}\int_{-\infty}^{\infty}d\omega\,N_B(\omega) \times\langle\langle S_{\mathbf{q}}^x+iS_{\mathbf{q}}^y|S_{-\mathbf{q}}^x-iS_{-\mathbf{q}}^y\rangle\rangle_{\omega}. \tag{42}$$

Singular contributions arise from the imaginary part of the numerators in (39) (note that we can set $\Lambda_{\mathbf{q}\omega}=\omega_{\mathbf{q}}$ in the denominators). Then we have

$$\delta\langle S^z\rangle=-[(I_x^x)^2+(I_y^y)^2+(I_x^z)^2] \times\langle S^z\rangle^2\sum_{\mathbf{k}\mathbf{k}'}\frac{f_{\mathbf{k}}(1-f_{\mathbf{k}'})}{(\varepsilon_{\mathbf{k}}-\varepsilon_{\mathbf{k}'})^2-\omega_{\mathbf{k}-\mathbf{k}'}^2}. \tag{43}$$

To logarithmic accuracy we find

$$\frac{\delta\langle S^z\rangle}{\langle S^z\rangle}\approx-\langle S^z\rangle\rho^2(0)[(I_x^x)^2 +(I_y^y)^2(I_x^z)^2]\ln\frac{W}{\max(\bar{\omega},T)}. \tag{44}$$

Thus, Kondo singularities reduce $\langle S^z\rangle$ in proportion to the tunnel splitting and hence suppress the two-well nature of the potential; this effect is similar to the suppression of local moments in Kondo systems. According to Ref. 1, the effective separation between the apex oxygen potential wells is a minimum at the superconducting transition point $T=T_c$. The explanation is that the reduction in $\langle S^z\rangle$ with decreasing temperature follows Eq. (44) only in the normal phase. For $T<T_c$, the logarithm is cut off at the value of the superconducting gap $\Delta(T)$, where $\Delta(T\ll T_c)$ is much greater than T and $\bar{\omega}$, so that the decrease in $\langle S^z\rangle$ becomes growth. A similar conclusion was reached in Ref. 10 based on a calculation of the static "susceptibility" (S^z,S^z).

5. THE RENORMALIZATION GROUP AND THE KONDO TEMPERATURE

The appearance of logarithmical singularities in the self-energy and in the "local moment" correction raises the problem of summing them in order to examine the low-temperature (low-energy) behavior. This problem has been repeatedly considered for a single-impurity *s-d* model with $I_{\alpha}^{\beta}=I\delta_{\alpha\beta}$ (isotropic case) and $I=\mathrm{diag}(I_{\perp},I_{\perp},I_{\parallel})$ (see Ref. 35 for a review). We will examine a single-center model with an arbitrary $\hat{I}$ matrix and $H_{\mathrm{lat}}\to 0$.

The simplest, and easiest to grasp, approach to the summation of singularities at low temperatures is the renormalization method in Anderson's "poor man's scaling."[34] In order to derive the equations for the effective interaction parameters, let us evaluate the electron Green's function averaged over the states of the electronic subsystem (but not over the pseudospin states). The result may be written

$$\hat{G}_{\mathbf{k}\mathbf{k}'}(E)=\langle\langle\psi_{\mathbf{k}}|\psi_{\mathbf{k}'}^{+}\rangle\rangle_E =\hat{G}_{\mathbf{k}}^{(0)}(E)\delta_{\mathbf{k}\mathbf{k}'}+\hat{G}_{\mathbf{k}}^{(0)}(E)\hat{T}(E)\hat{G}_{\mathbf{k}'}^{(0)}(E), \tag{45}$$

where

$$\hat{G}_{\mathbf{k}}^{(0)}(E)=\mathrm{diag}\left(\frac{1}{E-\varepsilon_{\mathbf{k}+}},\frac{1}{E-\varepsilon_{\mathbf{k}-}}\right) \tag{46}$$

is the free-electron spinor Green's function and the T matrix is (for the contact interaction) independent of $\mathbf{k}$ and $\mathbf{k}'$, and has the spinor structure of

$$\hat{T}(E)=-(I_{\mathrm{eff}})_{\beta}^{\alpha}(E)S^{\beta}\hat{\sigma}^{\alpha}, \tag{47}$$

with $I_{\mathrm{eff}}=I$ to within first-order perturbation terms [see Eq. (9)]. When we evaluate the Green's function (45) by the equation-of-motion method, corrections to I_{eff} appear in second order which contain $\xi=\ln|W/E|$ (W is the cutoff parameter of the order of the bandwidth). The corresponding renormalization group equations are obtained by the replacement $I\to I_{\mathrm{eff}}$ in $\partial I_{\mathrm{eff}}/\partial\xi$ (cf. Refs. 36, 35, 31, 25). After calculations which are in principle analogous to those for the usual Kondo problem[36] we find

$$\frac{\partial g_{\nu}^{\mu}}{\partial\xi}=-\varepsilon_{\nu\alpha\gamma}\varepsilon_{\mu\beta\lambda}g_{\alpha}^{\beta}g_{\gamma}^{\lambda}, \tag{48}$$

where, for simplicity, we have set $\rho_+(0)=\rho_-(0)=\rho$ and introduced the dimensionless interaction constants $g_{\nu}^{\mu}=\rho(I_{\mathrm{eff}})_{\nu}^{\mu}$ It is convenient to introduce the vectors

$$\mathbf{g}^{\mu}=(g_x^{\mu},g_y^{\mu},g_z^{\mu}).$$

Then Eq. (48) becomes

$$\frac{\partial\mathbf{g}^{\mu}}{\partial\xi}=2\varepsilon_{\mu\beta\gamma}[\mathbf{g}^{\beta}\mathbf{g}^{\gamma}]. \tag{49}$$

From Eq. (49) it follows that if the bare interaction matrix is of the form (10), i.e., $\mathbf{g}^y \perp \mathbf{g}^x, \mathbf{g}^z$ for $\xi=0$, the same will be true after renormalization. In this case Eqs. (49) take the form

$$\frac{\partial g_x^x}{\partial \xi}=-2g_x^z g_y^y, \quad \frac{\partial g_z^z}{\partial \xi}=-2g_z^x g_y^y,$$

$$\frac{\partial g_y^y}{\partial \xi}=2(g_z^x g_x^z-g_x^x g_z^z), \quad \frac{\partial g_x^z}{\partial \xi}=2g_x^z g_y^y, \quad \frac{\partial g_z^x}{\partial \xi}=2g_x^z g_y^y. \quad (50)$$

We see that setting $I_y^y=0$ in the Hamiltonian would in general be dangerous because from Eq. (50) it follows that in higher orders in perturbation theory the corresponding interaction processes are induced anyway. Thus, the main physical result of the interaction I_y^y—the appearance of an electron–hole asymmetry in the density of states (Sec. 3)—is true even for $I_y^y=0$. At the same time, if the matrix I is diagonal (i.e., $I_x^z=I_z^x=0$), this structure will remain in all orders in perturbation theory. The discussion which follows is restricted to this latter case, in which Eqs. (50) can be integrated in full. Then we have

$$g_\nu^\mu=g_\mu \delta_{\mu\nu}, \quad \frac{\partial g_\mu}{\partial \xi}=-2\varepsilon_{\mu\beta\lambda} g_\beta g_\lambda. \quad (51)$$

From (51),

$$g_x^2-g_y^2=C_1, \quad g_x^2-g_z^2=C_2, \quad (52)$$

where the constants are defined in terms of the bare parameters as

$$C_1=\rho^2[(I_x^x)^2-(I_y^y)^2], \quad C_2=\rho^2[(I_x^x)^2-(I_z^z)^2]. \quad (53)$$

Specifically, let us assume that

$$|I_x^x| \geqslant |I_y^y|, \quad |I_z^z|, \quad (54)$$

so that we have $C_1 \geqslant 0, C_2 \geqslant 0$ (otherwise permute the indices x,y,z). Two cases then arise.

For $g_x g_y g_z > 0$, the sign of g_x is the same as that of the product $g_y g_z$ and, according to Eq. (51), renormalization reduces the absolute value of g_x. This case, similar to the "ferromagnetic" *s-d* exchange Kondo problem, does not lead to the strong coupling regime and is not overly revealing physically. We will not discuss this case below.

Let $g_x g_y g_{zx} < 0$, that is, either one or three interaction constants are negative. Then we have from (51), using (52), that

$$\frac{\partial |g_x|}{\partial \xi}=2[(g_x^2-C_1)(g_x^2-C_2)]^{1/2}. \quad (55)$$

Equation (55) can be represented in the form

$$2\rho |I_x^x| \xi=\int_{1/\psi}^1 \frac{dt}{[(1-\eta_1 t^2)(1-\eta_2 t^2)]^{1/2}}, \quad (56)$$

in which

$$\eta_1=1-\frac{(I_y^y)^2}{(I_x^x)^2}, \quad \eta_2=1-\frac{(I_z^z)^2}{(I_x^x)^2}, \quad \psi=(I_{\text{eff}})_x^x/I_x^x, \quad (57)$$

whence it is possible to express ψ in terms of ξ with the aid of Jacobi elliptical functions. We will not give this expression because of its length, but restrict ourselves to a discussion of the "Kondo temperature" T_K. This is defined as the boundary of the strong coupling region, at which the quantity g_x goes to infinity when evaluated perturbatively. From (57) with $\psi=\infty, \xi=\ln(W/T_K)$ we find

$$T_K=W \exp\left[-\frac{1}{2\rho |I_x^x| \sqrt{\eta_+}} F\left(\arcsin \sqrt{\eta_+}, \sqrt{\frac{\eta_-}{\eta_+}}\right)\right], \quad (58)$$

$$\eta_+=\max(\eta_1,\eta_2), \quad \eta_-=\min(\eta_1,\eta_2),$$

where

$$F(\varphi,\kappa)=\int_0^\varphi \frac{dt}{(1-\kappa^2 \sin^2 t)^{1/2}}$$

is the elliptic integral of the first kind. Of special interest is the case in which

$$|I_x^x| > |I_y^y|=|I_z^z|. \quad (59)$$

Then from Eq. (58) we obtain

$$T_K=W \exp\left[-\frac{1}{4\rho |I_x^x| \sqrt{\eta}} \ln\left|\frac{1+\sqrt{\eta}}{1-\sqrt{\eta}}\right|\right], \quad (59')$$

which agrees with the corresponding result for anisotropic *s-d* model[35] in the weak interaction case.

From (52) it is seen that as $E \to T_K$, all three effective constants diverge, their signs coinciding with those of the bare constants. If one of the latter is equal to zero (apart from the already assumed condition $I_z^x=I_x^z=0$), we are dealing with a peculiar—"marginal"—case in which the usual strong coupling regime is not realized. For example, for $I_y^y=0$ we have $g_x=\text{const}$, $g_z=\text{const}$, and g_y grows linearly with ξ.

The above results are valid for $T_K > \bar{\omega}$ (for a one-center case this condition implies $T_K > \Omega$). For the simultaneous inclusion of the Kondo effect and pseudospin dynamics, the Kondo divergences are cut off at $\bar{\omega}$, this latter in turn being renormalized by the conduction electrons [to lowest perturbation order, via the renormalization in $\langle S^z \rangle$, Eq. (44)]. Thus, there is a need for a self-consistent treatment of the problem. An analogous Kondo lattice problem (isotropic, periodic *s-d* model with Heisenberg type dynamics) has been solved in Ref. 25. In the present case the situation is much more complicated because both the effective interaction and dynamics are characterized by several relevant variables. The construction of a scaling theory for the "pseudo-Kondo lattice" seems to be an interesting problem for future investigation.

In concluding this section, we emphasize that the usual perturbation theory considered in Secs. 3 and 4 is valid for all temperatures and energies (including the case $T, |E| < T_K$) provided $T_K \ll \bar{\omega}$. This follows from the fact that, because of the "cutoff" of the Kondo logarithm at $|E| \sim \bar{\omega}$ [see Eq. (44)], the quantity ξ is bounded by the inequality $\xi \ll \ln(W/\bar{\omega})$ and its entire variation is within the weak coupling region (small renormalization of $\hat{g}$) for $\bar{\omega} > T_K$. According to Eq. (40), the conduction electron contribution to $\bar{\omega}$ is of order g^2, while T_K depends expo-

nentially on $|g|$. Consequently, for a weak electron–pseudospin interaction and high density of two-level systems perturbation theory is always applicable except in the case of a "spurious" smallness of $\bar{\omega}$ due to the cancellation of the direct, J_{ij}, and indirect, $\propto g^2$, interactions. At the same time, for dilute systems $\bar{\omega}$ may be small (for small Ω) because of the large separation between the two-level systems involved.

6. DISCUSSION AND CONCLUSIONS

Let us emphasize the most essential points of our discussion.

1. We have relied on the pseudospin description of the anharmonic vibrations of apex oxygen, which is obtained by considering atomic displacements after first projecting onto a space of states, each center of which contains the ground and first excited states of a two-well potential. Such an approach relates to the usual phonon picture in the same way as the description of electronic states in the language of atomic terms relates to the band description. In other words, if the phonon–phonon interaction at a single center exceeds the characteristic phonon frequency, we go over to the "Hubbard subband" description of atomic displacement dynamics, the pseudomagnetic mode (7) corresponding to excitations from the lower to upper subband.

In fact, if the interaction between d-electrons in a narrow energy band is large enough to lead to the formation of localized magnetic moments, then the interaction of the wide-s-band with the d-electrons reduces to an s-d exchange and leads to the Kondo effect. This case is in sharp contrast to the situation in which both subsystems retain their band (or, more precisely Fermi-liquid) character. Consequently, the interaction of the conduction electrons with highly anharmonic local atomic displacements has different properties than the usual electron–phonon interaction.

In the problem of localized magnetic moments one can interpolate between the cases of a weak and strong d-electron correlation within the framework of the Anderson model. For the electron–lattice problem the role of such a model is played by that of Yu and Anderson,[32] in which the two-well nature of the potential is due to a strong electron–phonon interaction and its appearance is described by formal analogy with the appearance of the localized moment. Unlike Ref. 32, we do not specify the nature of the two-well potential (it may arise for purely lattice reasons) and instead describe the electron–ion interaction phenomenologically with the use of the interaction matrix (10). This approach appears to be more suitable for constructing a perturbation theory as well as for including the effects of center–center interactions.

2. For the weak coupling regime, the major result of our discussion is that corrections to the density of states change dramatically near the Fermi level on the scale of the characteristic dynamics frequency $\bar{\omega}$ and, in contrast to the usual electron–phonon interaction, do not have an electron–hole symmetry and so may lead to large values of thermopower even in a perturbative regime.

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[1] J. Mustre de Leon, S. D. Conradson, I. Baltistić, and A. R. Bishop, Phys. Rev. Lett. **65**, 1675 (1990); Phys. Rev. **B 44**, 2422 (1991).
[2] S. D. Conradson and D. Raistrick, Science **243**, 1340 (1989).
[3] T. Nishida, M. Katada, and Y. Matsumoto, Japan. J. Appl. Phys. **29**, 259 (1990).
[4] L. V. Gasparov, V. D. Kulakovskiĭ, V. B. Timofeev, and E. Ya. Sherman, Zh. Eksp. Teor. Fiz. **100**, 1981 (1991) [Sov. Phys. JETP **73**, 929 (1991)].
[5] V. I. Anisimov, M. A. Korotin, J. Zaanen, and O. K. Andersen, Phys. Rev. Lett. **68**, 345 (1992).
[6] H. Maruyama, T. Ishii, N. Bamba *et al.*, Physica **C 160**, 524 (1989).
[7] E. Kaldis, P. Fisher, and A. W. Hewat, Physica **C 159**, 668 (1989).
[8] K. A. Müller, Z. Phys. **B 80**, 193 (1990).
[9] H. Yamazaki, H. Kimura, H. Maeda *et al.*, Physica **C 185–189**, 879 (1991).
[10] V. Yu. Irkhin, M. I. Katsnelson, and A. V. Trefilov, Europhys. Lett. **15**, 649, (1991); Pis'ma Zh. Eksp. Teor. Fiz. **53**, 242 (1991) [JETP Lett. **53**, 255 (1991)].
[11] A. Heinz and R. Tscheuschner, Phys. Rev. **B 43** , 5601 (1991).
[12] Y. Ohta, T. Tohyama, and S. Maekawa, Phys. Rev. **B 43**, 2968 (1991).
[13] M. Zoli, Phys. Rev. **B 44**, 7163 (1991); Physica **C 178**, 390 (1991).
[14] M. Frick, I. Morgenstern, and W. von der Linden, Z. Phys. **B 82**, 339 (1991).
[15] A. Zawadowsky, K. Penc, and G. T. Zimanyi, Progr. Theor. Phys. Suppl. N108, 11 (1991).
[16] G. M. Vujičić, V. L. Aksenov, N. M. Plakida, and S. Stamenkovic, Phys. Lett. **A 73**, 439 (1979); J. Phys. **C 14**, 2377 (1981).
[17] N. M. Plakida, V. L. Aksenov, and S. L. Drechsler, Europhys. Lett. **4**, 1309 (1987).
[18] A. S. Shcherbakov, M. I. Katsnelson, A. V. Trefilov *et al.*, Pis'ma Zh. Eksp. Teor. Fiz. **46**, 111 (1987); **49**, 102 (1989) [JETP Lett. **46**, 136 (1987); **49**, 121 (1987)].
[19] S. K. Kurtz, J. R. Hardy, and J. W. Flocken, Ferroelectrics **87**, 29, (1988).
[20] V. V. Lemanov, A. B. Sherman, G. O. Andrianov, and I. Érgashev, Fiz. Tverd. Tela **32**, 2161 (1990) [Sov. Phys. Solid State **32**, 1258 (1990)].
[21] D. Mihailovic and A. J. Heeger, Solid St. Commun., **75**, 319 (1990).
[22] R. Blinc and B. Žekš, *Ferroelectrics and Antiferroelectrics. Lattice Dynamics*, North-Holland, Amsterdam (1984).
[23] V. Yu. Irkhin, M. I. Katsnelson, and A. V. Trefilov, Physica **C 160**, 397 (1989).
[24] V. Yu. Irkhin and M. I. Katsnelson, Z. Phys. **B 75** , 67 (1989); **B 82**, 77 (1991).
[25] V. Yu. Irkhin and M. I. Katsnelson, J. Phys.: Cond. Mat. **4**, 9661 (1992).
[26] J. Hubbard, Proc. Roy. Soc. **285**, 542 (1965).
[27] W. A. Fillips, Rep. Prog. Phys. **50**, 1657 (1987).
[28] J. Kondo, in *Solid State Physics*, Vol. 23, Academic Press, New York (1969).
[29] J. Kondo, Physica **B 84**, 40, 207 (1976).
[30] A. Zawadowsky, Phys. Rev. Lett. **45**, 211 (1980).
[31] V. Yu. Irkhin and M. I. Katsnelson, Z. Phys. **B 70** , 371 (1988).
[32] C. Yu and P. W. Anderson, Phys. Rev. **B 29**, 6165 (1984).
[33] W. F. Brinkman and S. Engelsberg, Phys. Rev. **169** , 417 (1968).
[34] J. M. Ziman, *Electrons and Phonons: The Theory of Transport Phenomena in Solids*, Oxford Univ. Press (1960).
[35] A. M. Tsvelick and P. B. Wiegmann, Adv. Phys. **32** , 453 (1983).
[36] P. W. Anderson, J. Phys. **C 3**, 2346 (1970).
[37] G. Zwicknagl, Adv. Phys. **41**, 203 (1992).
[38] C. L. Kane, P. A. Lee, and N. Read, Phys. Rev. **B 39**, 6880 (1989); K. J. von Szczepanski, P. Horsch, W. Stephan, and M. Ziegler, Phys. Rev. **B 41**, 2017 (1990).
[39] Y. Chen, D. Foerster, and A. I. Larkin, Phys. Rev. **B 46**, 5370 (1992).
[40] X. Li, T. Kawai, and S. Kawai, Japan J. Appl. Phys. **31**, L934 (1992).
[41] S. V. Vonsovskiĭ, Yu. A. Izyumov, and É. Z. Kurmaev, *Superconductivity of the Transition Metals and of their Alloys and Compounds* [in Russian], Nauka, Moscow (1972).
[42] *Superconductivity in Ternary Compounds I. Structural, Electronic and Lattice Properties*, edited by Ø. Fischer and M. B. Maple, Springer, Berlin–Heidelberg–New York (1982).

[43] A. I. Liechtenstein, I. I. Mazin, C. O. Rodriguez *et al.*, Phys. Rev. **B 44**, 5388 (1991).
[44] K. Miyake, T. Matsuura, and C. M. Varma, Solid St. Commun., **71**, 1149 (1989).

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