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Electron Interaction in Rare-Earth Metals

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We discuss from a unified point of view various aspects of the *s-f*(*s-d*) exchange interaction in the ferromagnetically spin-ordered states of rare-earth metals, such as (1) the indirect Ruderman-Kittel-Kasuya-Yosida–type exchange interaction between localized 4*f* spins, (2) the spin-wave spectrum of the localized spins, and (3) the interaction between conduction electrons mediated by the exchange of spin waves of the localized spins. The present problem is very similar to that of the electron-phonon interaction in metals, and to obtain the electron-electron interaction we employ a similar method of using a cononical transformation. The electron interaction obtained leads to a repulsion between electrons of opposite spins at the same atomic site in the vicinity of the Fermi surface. The self-energy due to this effective electron interaction is calculated for a simplified model, and we discuss the possibility of an appreciable enhancement of the specific heat.

I. INTRODUCTION

In a previous paper[1] we discussed an effective exchange interaction between conduction electrons mediated by the flipping motion of localized spins in dilute magnetic alloys. Similar and related discussions were given also by other authors.[2–4] The rare-earth metals are another system whose main magnetic behavior may be described by the *s-f*(*s-d*) exchange interaction between conduction electrons and the localized 4*f* spins.[5] In this paper we extend our previous discussion on the dilute alloys to pure rare-earth metals. As is well known, the rare-earth metals are complicated systems in many respects. The conduction electrons consist of 5*d*, 6*s* bands and they behave quite differently from the simple free-electron band,[6,7] and as was revealed by the neutron diffraction experiment, the pattern of 4*f* spin ordering is generally screw type and this is related to the detailed nature of the anisotropy energy, crystal structure, and so on.[5] Since our primary interest is mainly to point out a new aspect of electron interaction which has been neglected so far, we drastically simplify the picture of a rare-earth metal. We approximate the conduction electrons by a single spherical electron band, and retain only the *s-f* exchange interaction as the magnetic interaction neglecting the anisotropy energy, etc., and also limit our discussion to the case of ferromagnetic ordering of the 4*f* spins. The case of Gd seems to fit most nearly to our simplified picture of the rare-earth metals.

Under the approximations mentioned above, the total Hamiltonian of our system is given by the sum of the kinetic energy of the conduction electrons, $\mathcal{H}_k$, and the *s-f* exchange interactions $\mathcal{H}_{sf}$,

$$\mathcal{H}=\mathcal{H}_k+\mathcal{H}_{sf}, \tag{1.1}$$

$$\mathcal{H}_k=\sum_{\mathbf{k}\sigma}\epsilon_{\mathbf{k}}a^\dagger{}_{\mathbf{k}\sigma}a_{\mathbf{k}\sigma}, \tag{1.2}$$

$$\begin{aligned}\mathcal{H}_{sf}=-N^{-1}\sum_i\sum_{\mathbf{k},\boldsymbol{\kappa}}&\exp(i\boldsymbol{\kappa}\cdot\mathbf{R}_i)\\ &\times J(\boldsymbol{\kappa})[S_i^z(a^\dagger{}_{\mathbf{k}\uparrow}a_{\mathbf{k}-\boldsymbol{\kappa}\uparrow}-a^\dagger{}_{\mathbf{k}\downarrow}a_{\mathbf{k}-\boldsymbol{\kappa}\downarrow})\\ &\quad+S_i^+a^\dagger{}_{\mathbf{k}\downarrow}a_{\mathbf{k}-\boldsymbol{\kappa}\uparrow}+S_i^-a^\dagger{}_{\mathbf{k}\uparrow}a_{\mathbf{k}-\boldsymbol{\kappa}\downarrow}],\end{aligned} \tag{1.3}$$

where $a^\dagger{}_{\mathbf{k}\sigma}$ is the creation operator of a conduction electron with momentum $\hbar\mathbf{k}$, energy $\epsilon_{\mathbf{k}}$, and spin $\sigma(=\uparrow$ or $\downarrow$, the quantization axis being in the direction of the z axis), $\mathbf{S}_i$ is the 4*f* localized spin at the atomic site $\mathbf{R}_i$, N is the number of atoms in the unit volume, and $J(\boldsymbol{\kappa})$ is the Fourier component of the *s-f* exchange integral. Though $J(\boldsymbol{\kappa})$ is by no means a constant independent of $\boldsymbol{\kappa}$,[8] we often approximate it by a constant J in the following.

This Hamiltonian is the same as the one treated in I except that for simplicity we have not included the Coulomb interaction between conduction electrons. Therefore, in the paramagnetic region, namely, above the Curie point T_c, where the 4*f* spins are disordered, the discussion is quite the same as in I. We present a summary of the results of I in a form which can be applied to the rare-earth metals. The main modification of the earlier argument is simply to set the number of localized spins N_0 in the dilute-alloy case equal to the number of the total atoms N for the rare-earth metal.

The usual method of discussing the spin ordering in rare-earth metals, as well as in dilute magnetic alloys, is

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[1] D. J. Kim, Phys. Rev. **149**, 434 (1966), hereafter referred to as I. In I the following correction should be made. In the energy denominator on the right side of Eq. (2.11), the sign before ϵ_l and $\epsilon_{l-\kappa}$ should be reversed. The same correction should be made in Eqs. (2.13), (2.17), (2.18), and (2.20). [In Eqs. (2.17) and (2.20), the sign before $\epsilon_{l'}$ and $\epsilon_{l'+\kappa}$ also should be reversed.]

[2] J. Kondo, Progr. Theoret. Phys. (Kyoto) **33**, 575 (1965).

[3] S. Doniach and E. P. Wohlfarth, Proc. Roy. Soc. (London) **A296**, 442 (1967).

[4] M. Bailyn, Advan. Phys. **15**, 179 (1966).

[5] For review articles, see K. Yosida, in *Progress in Low Temperature Physics*, edited by C. J. Gorter (North-Holland Publishing Co., Amsterdam, 1964), Vol. 4, p. 265; R. J. Elliott, in *Magnetism*, edited by G. T. Rado and H. Suhl (Academic Press Inc., New York, 1965), Vol. IIA, p. 385; T. Kasuya, in *Magnetism*, edited by G. T. Rado and H. Suhl (Academic Press Inc., New York, 1967), Vol. IIB, p. 215.

[6] J. O. Dimmock and A. J. Freeman, Phys. Rev. Letters **13**, 750 (1964); A. J. Freeman, J. O. Dimmock, and R E. Watson, in *Quantum Theory of Atoms, Molecules and Solid State*, edited by P.-O. Löwdin (Academic Press Inc., New York, 1966), p. 361.

[7] A. J. Freeman, J. O. Dimmock, and R. E. Watson, Phys. Rev. Letters **16**, 94 (1966).

[8] R. E. Watson and A. J. Freeman, Phys. Rev. Letters **14**, 695 (1965).

first to derive the Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction between the localized $4f$ spins $\mathbf{S}_i$, $\mathcal{H}_f$ from a second-order perturbation calculation of the energy starting with the Hamiltonian Eq. (1.1);

$$\mathcal{H}_f=\sum_{i,j}\mathcal{J}_{ij}\mathbf{S}_i\cdot\mathbf{S}_j. \tag{1.4}$$

This procedure may be regarded as introducing an effective Hamiltonian $\mathcal{H}_{\text{eff}}$, in place of the original total Hamiltonian Eq. (1.1);

$$\mathcal{H}_{\text{eff}}=\mathcal{H}_k+\mathcal{H}_f. \tag{1.5}$$

In I we asked the question whether this $\mathcal{H}_{\text{eff}}$ is fully equivalent to the original Hamiltonian Eq. (1.1), and our answer was negative. We found a canonical transformation which transforms the original Hamiltonian Eq. (1.1) into a form similar to Eq. (1.5). Then the transformed Hamiltonian $\tilde{\mathcal{H}}$ had an extra term in addition to Eq. (1.5) which gives an effective interaction between conduction electrons:

$$\tilde{\mathcal{H}}=\mathcal{H}_k+\mathcal{H}_f+\mathcal{H}_e. \tag{1.6}$$

$\mathcal{H}_e$ is given as

$$\mathcal{H}_e=-\tfrac{2}{3}\sum_{\mathbf{l},\mathbf{l}',\kappa}C(\mathbf{l},\mathbf{l}',\boldsymbol{\kappa})\big[\tfrac{1}{4}(a^\dagger{}_{\mathbf{l}\uparrow}a_{\mathbf{l}-\kappa\uparrow}-a^\dagger{}_{\mathbf{l}\downarrow}a_{\mathbf{l}-\kappa\downarrow})\\ \times(a^\dagger{}_{\mathbf{l}'\uparrow}a_{\mathbf{l}'+\kappa\uparrow}-a^\dagger{}_{\mathbf{l}'\downarrow}a_{\mathbf{l}'+\kappa\downarrow})+\tfrac{1}{2}a^\dagger{}_{\mathbf{l}\downarrow}a_{\mathbf{l}-\kappa\uparrow}a^\dagger{}_{\mathbf{l}'\uparrow}a_{\mathbf{l}'+\kappa\downarrow}\\ +\tfrac{1}{2}a^\dagger{}_{\mathbf{l}\uparrow}a_{\mathbf{l}-\kappa\downarrow}a^\dagger{}_{\mathbf{l}'\downarrow}a_{\mathbf{l}'+\kappa\uparrow}\big], \tag{1.7}$$

with

$$C(\mathbf{l},\mathbf{l}',\boldsymbol{\kappa})=-N^{-1}\,|\,J(\boldsymbol{\kappa})\,|^2\\ \times\langle S_i{}^z[(\epsilon_{\mathbf{l}'+\kappa}-\epsilon_{\mathbf{l}'}-g\mu_BH_i{}^z)^{-1}-(\epsilon_{\mathbf{l}-\kappa}-\epsilon_{\mathbf{l}}+g\mu_BH_i{}^z)^{-1}]\rangle, \tag{1.8}$$

where g is the g factor of the localized spin, μ_B is the Bohr magneton, $H_i{}^z$ is the local field at the ith spin site from surrounding localized spins due to the interaction $\mathcal{H}_f$ and the direction of $\mathbf{H}_i$ is taken as the quantization axis of $\mathbf{S}_i$ and $\langle\cdots\rangle$ means a thermal average. $C(\mathbf{l},\mathbf{l}',\boldsymbol{\kappa})$ depends on the lattice site i, as discussed in I; however, since we are considering the paramagnetic situation, we have assumed that it becomes independent of i if the thermal average is taken appropriately for the completely random distribution of the orientation of the localized spins.

In the region near the Fermi surface when the energy differences are such as $|\,\epsilon_{\mathbf{l}-\kappa}-\epsilon_{\mathbf{l}}\,|$, $|\,\epsilon_{\mathbf{l}'}-\epsilon_{\mathbf{l}'+\kappa}\,|<|\,g\mu_BH_i\,|$, the expression for $C(\mathbf{l},\mathbf{l}',\boldsymbol{\kappa})$ is simplified to

$$C(\mathbf{l},\mathbf{l}',\boldsymbol{\kappa})\cong2(J^2/N)\langle S_i{}^z/g\mu_BH_i{}^z\rangle\equiv C, \tag{1.9}$$

and accordingly $\mathcal{H}_e$ reduces to

$$\mathcal{H}_e=-\tfrac{2}{3}C\sum_{\kappa}\boldsymbol{\sigma}(\boldsymbol{\kappa})\cdot\boldsymbol{\sigma}(-\boldsymbol{\kappa}), \tag{1.10}$$

where $\boldsymbol{\sigma}(\boldsymbol{\kappa})$ is the Fourier component of the spin density of the conduction electrons

$$\sigma^z(\boldsymbol{\kappa})=\tfrac{1}{2}\sum_{\mathbf{k}}(a^\dagger{}_{\mathbf{k}\uparrow}a_{\mathbf{k}-\kappa\uparrow}-a^\dagger{}_{\mathbf{k}\downarrow}a_{\mathbf{k}-\kappa\downarrow}),\ \text{etc.} \tag{1.11}$$

C can be reduced further if we notice that the bracketed quantity in Eq. (1.9) is simply the magnetic susceptibility of the individual localized spin which in the paramagnetic region is just the Curie law

$$C=\tfrac{2}{3}(J^2/N)(k_BT)^{-1}S(S+1), \tag{1.12}$$

where S is the magnitude of $\mathbf{S}_i$.

If we calculate the Curie point of the conduction electrons by a random-phase approximation (RPA) as in I using Eqs. (1.10) and (1.12), we obtain

$$k_BT_c=\tfrac{2}{3}N^{-1}J^2\rho(\epsilon_F)\,S(S+1), \tag{1.13}$$

where $\rho(\epsilon_F)$ is the density of states of conduction electrons at the Fermi surface. What is interesting about Eq. (1.13) is that it coincides with the Curie temperature of the localized spins which would be obtained from $\mathcal{H}_f$ using a molecular-field approximation.[5] This means that both the conduction electrons and the localized spins order at $T=T_c$.

In Sec. II we extend the previous theory given in I to rare-earth metals and generalize the results of the present section to the spin-ordered state. The extension can be done very naturally and it seems very instructive in the sense that it teaches us what the spin-wave analog in the paramagnetic region is. Already in I we pointed out the similarity between our problem and the electron-phonon-interaction problem.[9,10] We pictured our electron interaction as mediated by the exchange of Zeeman energy of the flipping motion of the localized spins under the local field. In the spin-ordered state the spin wave of the $4f$ localized spins is a well-defined excitation and now a pair of conduction electrons interact through the exchange of this spin wave. Thus the analogy between our case and the electron-phonon case becomes more direct in the spin-ordered state. In the vicinity of the Fermi surface, the electron interaction obtained takes the form of repulsion between electrons of opposite spin on the same atomic site (in the case of simple s band) and thus, as is well known, one obtains a ferromagnetic interaction.[11]

In Sec. III we discuss the change in the electronic specific heat of rare-earth metals resulting from the electron spin-wave interaction. This problem has been discussed by others.[12–14] [*Note added in proof.* Since this paper was submitted, a few papers, other than that mentioned in Ref. 14, dealing with the same subject have appeared.[14a]] A recent paper by Nakajima[14] formulated this problem by following Migdal's treatment of the electron-phonon interaction,[15] and corre-

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[9] H. Frohlich, Phys. Rev. **79**, 845 (1950).

[10] J. Bardeen and D. Pines, Phys. Rev. **99**, 1140 (1955).

[11] See, for instance, J. Hubbard, Proc. Roy. Soc. (London) **A276**, 238 (1963).

[12] J. Kondo (private communication).

[13] W. F. Brinkman (private communication).

[14] S. Nakajima, Progr. Theoret. Phys. (Kyoto) **38**, 23 (1967).

[14a] L. C. Davis and S. H. Liu, Phys. Rev. **163**, 503 (1967); H. S. D. Cole and R. E. Turner, Phys. Rev. Letters **19**, 501 (1967).

[15] A. Migdal, Zh. Eksperim. i Teor. Fiz. **34**, 1438 (1958) [English transl.: Soviet Phys.—JETP **7**, 996 (1958)].

sponds to our result in Sec. III concerning self-energy of conduction electrons. Our treatment, however, follows closely the Bardeen and Pines's treatment of electron-phonon interaction[10] and it seems much simpler. Also, our method can equally treat the problem in the temperature region both above and below T_c.

II. ELECTRON INTERACTION BELOW T_c

We consider in the temperature region sufficiently below T_c, $T \ll T_c$, where the localized 4f spins are aligned ferromagnetically (assume in the z direction) and the conduction electron spins are polarized. In this region the spin wave of the 4f localized spin (or of the coupled system of 4f localized spin and conduction electrons) is a well-defined excitation mode. In this section we derive an effective electron interaction between conduction electrons mediated by this spin wave. In obtaining the effective electron interaction we also determine the spin-wave spectrum of the 4f spins which includes the dynamic effect.[16]

We rewrite the total Hamiltonian Eq. (1.1) in the following way:

$$\mathcal{H}=\mathcal{H}_0+\mathcal{H}'_{sf}-\mathcal{H}_e-\mathcal{H}_f, \tag{2.1}$$

$$\mathcal{H}_0=\mathcal{H}_k+\mathcal{H}_e+\mathcal{H}_f+\mathcal{H}_{sf}{}^z(0), \tag{2.2}$$

where $\mathcal{H}_e$ is the electron-electron interaction, $\mathcal{H}_f$ is of the form of Eq. (1.4), and both of them will be determined self-consistently later. $\mathcal{H}_{sf}{}^z(0)$ is the diagonal part of $\mathcal{H}_{sd}$, which corresponds to the terms proportional to S_i^z and with $\kappa=0$ in Eq. (1.3) and gives rise to a uniform polarization of conduction electrons and $\mathcal{H}'_{sf}=\mathcal{H}_{sf}-\mathcal{H}_{sf}{}^z(0)$. As in I we find a canonical transformation in such a way as would eliminate $\mathcal{H}'_{sf}$ to first order with respect to J. The transformed Hamiltonian $\tilde{\mathcal{H}}$ is expanded in the following way:

$$\begin{aligned}\tilde{\mathcal{H}}&=e^{-U}\mathcal{H}e^{U}\\&=\mathcal{H}+[\mathcal{H},U]+\tfrac{1}{2}[[\mathcal{H},U],U]+\cdots.\end{aligned} \tag{2.3}$$

If U is determined so as to satisfy

$$[\mathcal{H}_0,U]+\mathcal{H}'_{sf}=0, \tag{2.4}$$

then the transformed Hamiltonian becomes

$$\begin{aligned}\mathcal{H}=\mathcal{H}_k+\mathcal{H}_{sf}{}^z(0)+\tfrac{1}{2}[\mathcal{H}'_{sf},U]\\-[\mathcal{H}_e,U]-[\mathcal{H}_f,U]+\cdots.\end{aligned} \tag{2.5}$$

As will be shown below, in order to satisfy Eq. (2.4), U must be proportional to J, and $\mathcal{H}_e$ and $\mathcal{H}_f$ are proportional to J^2. In this paper assuming $J/\epsilon_F \ll 1$, we retain only the first three terms on the right side of Eq. (2.5) by keeping terms to order J^2. Our task in the following part of this section is to find U so as to satisfy Eq. (2.4) and then to calculate the commutator of $[\mathcal{H}'_{sf},U]$ with that U to obtain $\mathcal{H}_f$ and $\mathcal{H}_e$. The operator U needed to satisfy Eq. (2.4) is obtained as

$$\begin{aligned}U=-\sum_{\mathbf{l},\kappa}J(\boldsymbol{\kappa})\left[\frac{S^{+}(-\boldsymbol{\kappa})}{\tilde{\epsilon}_{\mathbf{l}-\kappa\uparrow}-\tilde{\epsilon}_{\mathbf{l}\downarrow}-2J\langle S^z(0)\rangle+\omega(\boldsymbol{\kappa})}\,a^{\dagger}{}_{\mathbf{l}\downarrow}a_{\mathbf{l}-\kappa\uparrow}+\frac{S^{-}(-\boldsymbol{\kappa})}{\tilde{\epsilon}_{\mathbf{l}-\kappa\downarrow}-\tilde{\epsilon}_{\mathbf{l}\uparrow}+2J\langle S^z(0)\rangle-\omega(-\boldsymbol{\kappa})}\,a^{\dagger}{}_{\mathbf{l}\uparrow}a_{\mathbf{l}-\kappa\downarrow}\right]\\-\sum_{\mathbf{l}}\sum_{\kappa}{}'J(\boldsymbol{\kappa})S^z(-\boldsymbol{\kappa})\left[\frac{a^{\dagger}{}_{\mathbf{l}\uparrow}a_{\mathbf{l}-\kappa\uparrow}}{\tilde{\epsilon}_{\mathbf{l}-\kappa\uparrow}-\tilde{\epsilon}_{\mathbf{l}\uparrow}}-\frac{a^{\dagger}{}_{\mathbf{l}\downarrow}a_{\mathbf{l}-\mathbf{k}\downarrow}}{\tilde{\epsilon}_{\mathbf{l}-\kappa\downarrow}-\tilde{\epsilon}_{\mathbf{l}\downarrow}}\right],\end{aligned} \tag{2.6}$$

where

$$S^z(\boldsymbol{\kappa})=N^{-1}\sum_i\exp(-i\boldsymbol{\kappa}\cdot\mathbf{R}_i)\,S_i{}^z\ \text{etc.}, \tag{2.7}$$

and the prime on the summation excludes $\boldsymbol{\kappa}=0$. It should be noticed, as in the case of the electron-phonon interaction, U given by Eq. (2.6) satisfies Eq. (2.4) only under certain approximations: (1) $S^z(0)$ is often replaced by the thermal average $\langle S^z(0)\rangle$. (2) $\mathcal{H}_e$, which is an electron-electron interaction as will be discussed below in this section, is diagonalized by a Hartree approximation to give a self-energy of the conduction electron, and $\tilde{\epsilon}_{\mathbf{l}\sigma}$ is the one-particle energy which includes this self-energy. This procedure of obtaining the self-energy is the theme of Sec. III. (3) The spin-wave energy of the localized spin $\omega(\kappa)$ is introduced by a molecular-field approximation as follows:

$$[\mathcal{H}_{sf}{}^z(0)+\mathcal{H}_f,S^{-}(\boldsymbol{\kappa})]=\omega(\boldsymbol{\kappa})S^{-}(\boldsymbol{\kappa}). \tag{2.8}$$

Or, more explicitly,

$$\begin{aligned}\omega(\boldsymbol{\kappa})=-N^{-1}[-J(0)\sum_{\mathbf{k}}(f_{\mathbf{k}\uparrow}-f_{\mathbf{k}\downarrow})\\-2(\mathcal{J}^{+-}(\boldsymbol{\kappa})+\mathcal{J}^{-+}(\boldsymbol{\kappa}))\langle S^z(0)\rangle],\end{aligned} \tag{2.9}$$

where the number operator of conduction electrons $a^{\dagger}{}_{\mathbf{k}\sigma}a_{\mathbf{k}\sigma}$ is replaced by a Fermi distribution $f_{\mathbf{k}\sigma}$, and the tensor $\mathcal{J}(\boldsymbol{\kappa})$ is the Fourier transform of the RKKY interaction $\mathcal{H}_f$, and is given explicitly by Eq. (2.11) below. The spin-wave frequency determined from Eq. (2.9) should contain an imaginary part. However, for simplicity in this paper we will not consider the imaginary part and assume $\omega(\boldsymbol{\kappa})$ to be a real quantity.

We now turn to the calculation of the commutator $\frac{1}{2}[\mathcal{H}'_{sf},U]$ which is the third term on the right side of Eq. (2.5) and from which we expect to obtain $\mathcal{H}_f$ and $\mathcal{H}_e$. This commutator consists of two qualitatively different parts which may be written symbolically as

$$\begin{aligned}\tfrac{1}{2}[\mathcal{H}'_{sf},U]&=[\sum\mathbf{S}(\boldsymbol{\kappa})a^{\dagger}a,\sum\mathbf{S}(\boldsymbol{\kappa}')a^{\dagger}a]\\&=\sum\mathbf{S}(\boldsymbol{\kappa})\mathbf{S}(\boldsymbol{\kappa})[a^{\dagger}a,a^{\dagger}a]\\&\qquad+\sum[\mathbf{S}(\boldsymbol{\kappa}),\mathbf{S}(\boldsymbol{\kappa}')]a^{\dagger}aa^{\dagger}a\\&\equiv\tfrac{1}{2}[\mathcal{H}'_{sf},U]_{\mathrm{I}}+\tfrac{1}{2}[\mathcal{H}'_{sf},U]_{\mathrm{II}}.\end{aligned} \tag{2.10}$$

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[16] Y. Nagaoka, Progr. Theoret. Phys. (Kyoto) **28**, 1033 (1962).

From a simple calculation,

$$\tfrac{1}{2}[\mathcal{H}'_{sf}, U]_{\mathrm{I}}=\tfrac{1}{2}\sum_{\mathrm{l}}\sum_{\kappa}{}'\,|J(\boldsymbol{\kappa})|^2\left[\frac{f_{\mathrm{l}-\kappa\uparrow}-f_{\mathrm{l}\uparrow}}{\tilde{\epsilon}_{\mathrm{l}-\kappa\uparrow}-\tilde{\epsilon}_{\mathrm{l}\uparrow}}+\frac{f_{\mathrm{l}-\kappa\downarrow}-f_{\mathrm{l}\downarrow}}{\tilde{\epsilon}_{\mathrm{l}-\kappa\downarrow}-\tilde{\epsilon}_{\mathrm{l}\downarrow}}\right]S^z(\boldsymbol{\kappa})S^z(-\boldsymbol{\kappa})$$

$$+\tfrac{1}{2}\sum_{\mathrm{l}}\sum_{\kappa}|J(\boldsymbol{\kappa})|^2\left[\frac{f_{\mathrm{l}-\kappa\uparrow}-f_{\mathrm{l}\downarrow}}{\tilde{\epsilon}_{\mathrm{l}-\kappa\uparrow}-\tilde{\epsilon}_{\mathrm{l}\downarrow}-2J\langle S^z(0)\rangle+\omega(\boldsymbol{\kappa})}S^-(\boldsymbol{\kappa})S^+(-\boldsymbol{\kappa})\right.$$

$$\left.+\frac{f_{\mathrm{l}-\kappa\downarrow}-f_{\mathrm{l}\uparrow}}{\tilde{\epsilon}_{\mathrm{l}-\kappa\downarrow}-\tilde{\epsilon}_{\mathrm{l}\uparrow}+2J\langle S^z(0)\rangle-\omega(-\boldsymbol{\kappa})}S^+(\boldsymbol{\kappa})S^-(-\boldsymbol{\kappa})\right]\equiv\sum_{\kappa}{}'\mathcal{J}^{zz}(\boldsymbol{\kappa})S^z(\boldsymbol{\kappa})S^z(-\boldsymbol{\kappa})$$

$$+\sum_{\kappa}[\mathcal{J}^{-+}(\boldsymbol{\kappa})S^-(\boldsymbol{\kappa})S^+(-\boldsymbol{\kappa})+\mathcal{J}^{+-}(\boldsymbol{\kappa})S^+(\boldsymbol{\kappa})S^-(-\boldsymbol{\kappa})]\equiv\mathcal{H}_f. \quad (2.11)$$

In Eq. (2.11) we retained only the diagonal part of the conduction electron number operator and replaced it by the Fermi distribution function. This is a dynamic RKKY interaction between localized spins. [To be exact, to obtain an ordinary RKKY interaction we have to incorporate $\mathcal{H}_{sd}{}^z(0)$ to the above $\mathcal{H}_f$; the $\mathcal{H}_f$ appearing in Sec. I, therefore, should be understood to include $\mathcal{H}_{sf}{}^z(0)$.]

Similarly, the second part of the commutator, Eq. (2.10), is calculated as

$$\tfrac{1}{2}[\mathcal{H}'_{sf}, U]_{\mathrm{II}}=N^{-1}\sum_{\mathrm{k},\kappa,\mathrm{l}}|J(\boldsymbol{\kappa})|^2\left[\frac{\langle S^z(0)\rangle}{\tilde{\epsilon}_{\mathrm{l}-\kappa\downarrow}-\tilde{\epsilon}_{\mathrm{l}\uparrow}+2J\langle S^z(0)\rangle-\omega(-\boldsymbol{\kappa})}a^\dagger{}_{\mathrm{k}\downarrow}a_{\mathrm{k}+\kappa\uparrow}a^\dagger{}_{\mathrm{l}\uparrow}a_{\mathrm{l}-\kappa\downarrow}\right.$$

$$\left.-\frac{\langle S^z(0)\rangle}{\tilde{\epsilon}_{\mathrm{k}+\kappa\uparrow}-\tilde{\epsilon}_{\mathrm{k}\downarrow}-2J\langle S^z(0)\rangle+\omega(-\boldsymbol{\kappa})}a^\dagger{}_{\mathrm{l}\uparrow}a_{\mathrm{l}-\kappa\downarrow}a^\dagger{}_{\mathrm{k}\downarrow}a_{\mathrm{k}+\kappa\uparrow}\right]\equiv\mathcal{H}_e. \quad (2.12)$$

This is an effective electron-electron interaction which is mediated by the exchange of spin-wave excitation and it originates from the fact that the localized spin $\mathbf{S}_i$ is a dynamic entity.

The coupling constant appearing in our electron interaction contains a complicated wave-number dependence. To see a qualitative feature of $\mathcal{H}_e$ in Eq. (2.12) we neglect this wave-number dependence in the narrow region near the Fermi surface of the spin-polarized conduction electrons such that

$$|\tilde{\epsilon}_{\mathrm{l}-\kappa\downarrow}-\tilde{\epsilon}_{\mathrm{l}\uparrow}+2J\langle S^z(0)\rangle|,$$

$$|\tilde{\epsilon}_{\mathrm{l}+\kappa\uparrow}-\tilde{\epsilon}_{\mathrm{l}\downarrow}-2J\langle S^z(0)\rangle|<\omega(\boldsymbol{\kappa}) \quad (2.13)$$

and approximate the coupling constant by a positive constant C;

$$C\equiv(2/N)J^2\langle S^z(0)\rangle(1/\omega_0), \quad (2.14)$$

where ω_0 is a representative spin-wave energy. With this approximation $\mathcal{H}_e$, Eq. (2.12), is written as

$$\mathcal{H}_e=-C\sum_{\kappa}\sigma^+(\boldsymbol{\kappa})\sigma^-(-\boldsymbol{\kappa}), \quad (2.15)$$

apart from a constant term. For an s band, Eq. (2.15) is transformed to the more familiar form,[11] aside from a constant term

$$\mathcal{H}_e=NC\sum_i n_{i\uparrow}n_{i\downarrow}, \quad (2.16)$$

where $n_{i\sigma}$ is the number operator for the conduction electron at the ith atomic site. In the case of degenerate bands, as in real rare-earth metals, we would obtain intra- and interband repulsive interaction between electrons with opposite spins on the same atomic site. The strength of this interaction near the Fermi surface is not small. The order of magnitude of ω_0 can be estimated from Eqs. (2.9) and (2.11) as follows:

$$\omega_0=\lambda(J^2/N)\rho(\epsilon_F)\langle S^z(0)\rangle \quad (2.17)$$

by assuming $\mathcal{H}_{sf}{}^z(0)$ is the dominant factor leading to the conduction-electron spin polarization and neglecting the possible effect of $\mathcal{H}_e$. λ is a positive constant of order 1. Then from Eqs. (2.14) and (2.17),

$$C=2\lambda\rho(\epsilon_F)^{-1}, \quad (2.18)$$

and therefore NC appearing as the repulsive energy in Eq. (2.16) is on the order of the Fermi energy. It should be noticed, however, as we have stressed, that this interaction is effective only in a small energy interval near the Fermi surface as defined by Eq. (2.13).

Our spin-wave dispersion relation, Eq. (2.9), with Eq. (2.11) would reduce to the ordinary one[16] if we neglect the effect of the self-energy due to $\mathcal{H}_e$ by replacing $\tilde{\epsilon}_{\mathrm{k}\sigma}$ simply by ϵ_{k}.

Since the model that Doniach and Wohlfarth[3] used in discussing the dilute alloys below the spin-ordering temperature and our model are similar, we may compare the two results. In the static limit their effective electron interaction [the second term on the right side side of Eq. (3.20) of Ref. 3 with $\omega=0$] is of the form of our Eq. (2.16), with ω_0 in Eq. (2.14) taking only the first term on the right side of Eq. (2.9), but they do not need to impose the restriction Eq. (2.13) for the validity of Eq. (2.16). We plan to discuss further the relation between the two results.

III. ELECTRON SELF-ENERGY AND SPECIFIC HEAT

By applying the Hartree approximation to our effective electron-electron interaction $\mathcal{H}_e$, Eq. (2.12), quite similarly to the case of dilute alloys,[2] we obtain the self-energy $\Sigma_\sigma(\mathbf{l}, \bar\epsilon_{l\sigma})$ associated to the electron with momentum $\hbar\mathbf{l}$, energy $\bar\epsilon_{l\sigma}$, and spin σ[17]:

$$\Sigma_\uparrow(\mathbf{l}, \bar\epsilon_{l\uparrow}) = -(J^2/N)\langle S^z(0)\rangle \sum_{\mathbf{k}} \frac{2f_{\mathbf{k}\downarrow}-1}{\bar\epsilon_{\mathbf{k}\downarrow}-\bar\epsilon_{l\uparrow}+2J\langle S^z(0)\rangle-\omega(\mathbf{k}-\mathbf{l})}, \tag{3.1a}$$

$$\Sigma_\downarrow(\mathbf{l}, \bar\epsilon_{l\downarrow}) = -(J^2/N)\langle S^z(0)\rangle \sum_{\mathbf{k}} \frac{2f_{\mathbf{k}\uparrow}-1}{\bar\epsilon_{l\downarrow}-\bar\epsilon_{\mathbf{k}\uparrow}+2J\langle S^z(0)\rangle-\omega(\mathbf{l}-\mathbf{k})}. \tag{3.1b}$$

The renormalized one particle energy $\bar\epsilon_{\mathbf{k}\sigma}$, aside from the spin splitting due to the molecular field of localized spin $\pm J\langle S^z(0)\rangle$, is determined from

$$\bar\epsilon_{\mathbf{k}\sigma}=\epsilon_{\mathbf{k}}+\Sigma_\sigma(\mathbf{k}, \bar\epsilon_{\mathbf{k}\sigma}). \tag{3.2}$$

For simplicity we will not consider the imaginary part of the self-energy as in the spin-wave frequency. We may define more appropriately one-particle energy $\tilde{E}_{\mathbf{k}\sigma}$ of a conduction electron by incorporating the part of the exchange splitting due to $\mathcal{H}_{sf}{}^z(0)$ into $\bar\epsilon_{\mathbf{k}\sigma}$;

$$\tilde{E}_{\mathbf{k}\sigma}=\bar\epsilon_{\mathbf{k}\sigma}-J\langle S^z(0)\rangle\theta_\sigma, \tag{3.3}$$

where

$$\begin{aligned}\theta_\sigma &= 1 \quad \text{for} \quad \sigma=\uparrow\\ &=-1 \quad \text{for} \quad \sigma=\downarrow.\end{aligned} \tag{3.4}$$

The effective mass of the σ-spin conduction electron, m^*_σ, which gives the electronic specific heat, is obtained from the following relation:

$$(m^*_\sigma)^{-1}=(\hbar k_{F\sigma})^{-1}[d\tilde{E}_{l\sigma}/d(\hbar l)]\,|_{l=k_{F\sigma}}, \tag{3.5}$$

where $k_{F\sigma}$ is the Fermi wave number of the spin-polarized conduction electron with spin σ. From Eqs. (3.5), (3.2), and (3.3),

$$(m^*_\sigma)^{-1}=m^{-1}+(m^*_\sigma)^{-1}(\partial/\partial\tilde{E}_{l\sigma})\Sigma_\sigma(\mathbf{l}, \tilde{E}_{l\sigma})\,|_{l=k_{F\sigma}}, \tag{3.6}$$

where m is the electron mass without the effect of $\mathcal{H}_e$.

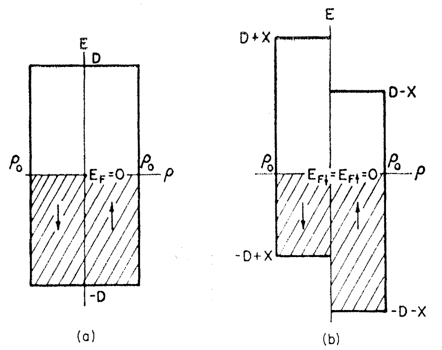

FIG. 1. (a) The density of states for the paramagnetic state for a square band. The Fermi level is assumed to be at the center of the band and the energy is measured from there. ρ_0 is the density of states of electrons and is assumed to be constant within the bandwidth $2D$. (b) The density of states for the ferromagnetic state. The bands given in (a) are split in energy by $2X=2J\langle S^z(0)\rangle$.

In this paper we will not attempt to carry out any exact calculation of Eqs. (3.1a), (3.1b), and (3.6). Since our purpose is only to obtain qualitative features, we will estimate the effective mass by adopting as simple a model as possible. (1) On the right side of Eqs. (3.1a) and (3.1b) we replace $\tilde{E}_{\mathbf{k}\sigma}$ by $E_{\mathbf{k}\sigma}$, which neglects the contribution from the self-energy due to $\mathcal{H}_e$. (2) For the energy band $E_{\mathbf{k}\sigma}[=\epsilon_{\mathbf{k}}-J\langle S^z(0)\rangle\theta_\sigma]$ we assume a square band with a constant density of states ρ_0 and width $2D$, such as shown in Fig. 1. (3) We represent the spin-wave spectrum by a constant frequency ω_0 (Einstein approximation) as given by Eq. (2.17) and neglect the effects of the finite maximum wave number in the spin-wave spectrum. The latter approximation may be justified from the fact that the maximum wave number which is on the order of inverse atomic distance or k_F is much larger than $k_{F\uparrow}-k_{F\downarrow}$, say, for Gd, as will be seen from the discussion below. Under these approximations and for zero temperature the self-energy, Eqs. (3.1a) and (3.1b), is calculated as

$$\begin{aligned}\Sigma_\uparrow(\mathbf{l}, \tilde{E}_{l\uparrow}) = -2(J^2/N)\langle S^z(0)\rangle\rho_0[&\ln|-\tilde{E}_{l\uparrow}-\omega_0|\\ &-\tfrac{1}{2}\ln|D+X-\tilde{E}_{l\uparrow}-\omega_0| -\tfrac{1}{2}\ln|-D+X-\tilde{E}_{l\uparrow}-\omega_0|],\end{aligned} \tag{3.7a}$$

$$\begin{aligned}\Sigma_\downarrow(\mathbf{l}, \tilde{E}_{l\downarrow}) = -2(J^2/N)\langle S^z(0)\rangle\rho_0[&-\ln|\tilde{E}_{l\downarrow}-\omega_0|\\ &+\tfrac{1}{2}\ln|\tilde{E}_{l\downarrow}-D+X-\omega_0| +\tfrac{1}{2}\ln|\tilde{E}_{l\downarrow}+D+X-\omega_0|],\end{aligned} \tag{3.7b}$$

and accordingly the effective mass is obtained as

$$\begin{aligned}m^*_\uparrow/m&=m^*_\downarrow/m\\ &=1+2(J^2/N)\langle S^z(0)\rangle\rho_0\{\tfrac{1}{2}[(D+X-\omega_0)^{-1}\\ &\qquad-(D-X+\omega_0)^{-1}]+(\omega_0)^{-1}\},\end{aligned} \tag{3.8}$$

where $2X$ is the exchange splitting of conduction electrons (see Fig. 1) which, neglecting the effect of $\mathcal{H}_e$, is given as $2X=2J\langle S^z(0)\rangle$, where in Fig. 1, J is assumed to be positive. If

$$D+X,\ D-X\gg\omega_0, \tag{3.9}$$

then

$$\begin{aligned}m^*_\sigma/m&\approx1+2(J^2/N)\langle S^z(0)\rangle\rho_0(1/\omega_0)\\ &=1+2/\lambda,\end{aligned} \tag{3.10}$$

where λ is a positive constant of order 1 defined in Eq. (2.17).

When the condition (3.9) is satisfied, we may simplify the expression of the self-energy, Eqs. (3.7a)

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[17] Our expression, Eqs. (3.1a) and (3.1b), for the self-energy is slightly different from that of Nakajima [Eqs. (5.5) and (5.6) of Ref. 14]. If we replace $2f_{k\downarrow}-1$ and $2f_{k\uparrow}-1$, respectively, by $2f_{k\downarrow}$ and $2(f_{k\uparrow}-1)$ in Eqs. (3.1a) and 3.1b), our results reduce to that that of Nakajima. The possible origin of this difference might be traced in the procedure of reducing Eq. (2.12) to Eqs. (3.1a) and (3.1b). We have followed Ref. 2 by putting $a^\dagger_{k\sigma}a_{k\sigma}=f_{k\sigma}+(a^\dagger_{k\sigma}a_{k\sigma}-f_{k\sigma})$ and neglecting $(a^\dagger_{k\sigma}a_{k\sigma}-f_{k\sigma})(a^\dagger_{k'\sigma'}a_{k'\sigma'}-f_{k'\sigma'})$. As can be easily checked, this difference, however, does not affect our conclusion, for instance, Eq. (3.10).

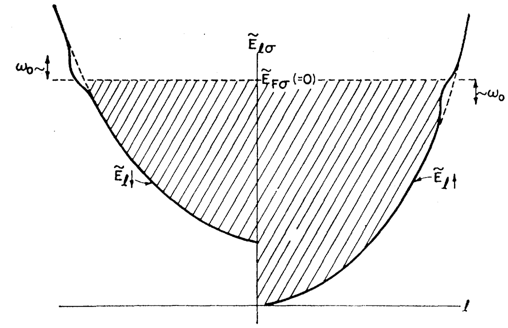

FIG. 2. A schematic graph of the energy-dispersion curve for conduction electrons including the self-energy modifications. Note that the self-energy contributions for up- and down-spin electrons are of opposite sign; however, since they also appear on opposite sides of the Fermi surface, their contributions to the enhancement of the density of states at the Fermi surface do not cancel.

and (3.7b), near the Fermi surface as

$$\Sigma_{\uparrow}(1, \tilde{E}_{1\uparrow}) \approx -2(J^2/N)\langle S^z(0)\rangle \rho_0 \ln|(\tilde{E}_{1\uparrow}+\omega_0)/D|, \tag{3.7a$'$}$$

$$\Sigma_{\downarrow}(1, \tilde{E}_{1\downarrow}) \approx 2(J^2/N)\langle S^z(0)\rangle \rho_0 \ln|(\tilde{E}_{1\downarrow}-\omega_0)/D|, \tag{3.7b$'$}$$

where $\tilde{E}_{l\sigma}$ is measured from the Fermi surface. The self-energy of an up-spin electron near the Fermi surface is positive and therefore its *maximum* lies approximately ω_0 below the Fermi surface, whereas the self-energy of a down-spin electron is negative and its *minimum* lies approximately ω_0 above the Fermi surface. We illustrate the situation schematically in Fig. 2.

It was suggested that the exchange splitting of the conduction band would drastically suppress the mass enhancement due to the spin-wave mechanism,[12,13] but in our calculation we do not see such a tendency. We believe that this was a result of the fact that the self-energies for up- and down-spin electrons are of opposite sign. What may not have been realized is that they contribute to opposite sides of the Fermi surface. Though we will not make any further effort to evaluate the more exact expressions for the self-energies by abandoning the Einstein model for the spin-wave spectrum, we believe that the assumption of the constant spin-wave frequency is not a vital assumption needed to obtain the result presented in this section.

In real rare-earth metals, for instance in Gd, however, the condition (3.9) is very likely to be realized from the fact that $(J/N)\rho(\epsilon_F)\,(\approx J/D)\ll 1$.[6] Actually a large electronic specific heat is observed in most rare-earth metals. For instance, in Gd, the specific heat is eight times that given by the free-electron model.[18] From a band calculation on Gd, Dimmock and Freeman[6] gave the density of states three times that of the free-electron value and attributed the remaining part to the electron-phonon interaction effect. It seems fairly possible that our spin-wave mechanism also would contribute here.

IV. DISCUSSION

Though we have said that we eliminated $\mathcal{H}'_{sf}$ to first order in Sec. II, to be exact, this statement is incorrect. As in the case of the electron-phonon interaction,[8,9] the part of $\mathcal{H}'_{sf}$ which corresponds to the energy-conserving processes such as $\tilde{E}_{1-\kappa\uparrow}-\tilde{E}_{1\downarrow}+\omega(\kappa)=0$ and $\tilde{E}_{1-\kappa\sigma}-\tilde{E}_{1\sigma}=0$ cannot be eliminated, as is seen from the structures of the canonical transformation we used [see Eq. (2.6)], and this part of $\mathcal{H}'_{sf}$ not eliminated gives rise to the ordinary electrical resistance. This part of $\mathcal{H}'_{sf}(0)$ not eliminated, as well as $\mathcal{H}_{sf}{}^z(0)$, should be incorporated to $\mathcal{H}_f$ of Sec. II, to give the ordinary RKKY-type interaction.[19]

As to the effect of our effective electron interaction $\mathcal{H}_e$, we discussed only the problem of the electronic specific heat. Its effect in many other problems, especially magnetic ones, will be considered in a future publication.

As has been stressed repeatedly, our model may be too crude; however, we believe that our results are qualitatively correct for rare-earth metals.

ACKNOWLEDGMENTS

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