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Quasispin model of itinerant magnetism: High-temperature theory*

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The high-temperature properties of itinerant magnetic systems are examined by using the coherent-potential approximation. We assume a local moment on each atom so that at elevated temperatures there is a number of reversed spins. The coherent potential is solved, and from that the moment on each atom is determined self-consistently. It is found that when the condition for ferromagnetic ordering is satisfied, the local moments persist even above the critical temperature. Conversely, if local moments do not exist at high temperatures, the system can at most condense into a spin-density-wave state. Furthermore, spin-flip scatterings of the conduction electrons from the local moments give rise to additional correlation not treated in the coherent-potential approximation. This correlation energy is an important part of the coupling energy of the local moments. The relations between our work and the theories of Friedel, Hubbard, and others are discussed.

I. INTRODUCTION

In an earlier paper we proposed a strong-coupling model for itinerant magnetism in transition metals.[1] The basic idea may be summarized as follows. The ground state of an itinerant magnetic system is first solved by the band-calculation method. When carried to self-consistency, there is a net spin density within every Wigner-Seitz cell, and the spin densities of different cells point in the same direction in a ferromagnetic system, but assume the alternating up and down alignment in a commensurate antiferromagnetic system. In the low-lying excited states the spin density in each cell is assumed to precess like a quasispin. We use the local-exchange approximation to formulate the interaction between the band electrons and the quasispins. The interaction Hamiltonian has the same form as the well-known s-d model except that the d spin is the total spin of each cell and the s-electron part includes all the band electrons. Then we apply standard perturbation-theory methods to calculate the magnon spectrum, the electron-magnon interaction, and the magnon-magnon interaction for the system. In every case examined, there is good agreement between theory and experiment.

The local-exchange approximation is a simple and practical way to reduce the two-body exchange interaction into a one-body effective potential.[2-4] The method is widely used in band calculations for solids, including magnetic metals. Through the use of this approximation we are able to treat the band electrons as itinerant and localized at the same time. They are itinerant because they propagate through the lattice, and they are localized because they give rise in a self-consistent manner to the quasispins.

In this paper we generalized our discussion to elevated temperatures. For simplicity we will assume a one-band model so that the local moment on each site is at most one Bohr magneton. Then the high-temperature state of the crystal may be treated as a state with a number of reversed spins. Hubbard[5] and Cyrot[6] have made analogy between this state and the ground state of a disordered binary alloy. The reversed spins give rise to two modifications to the conduction-electron propagator. On the site of a reversed spin the longitudinal part of the exchange potential has the reversed sign. This breaks the translational symmetry of the crystal and introduces the "scattering correction" of Hubbard.[5] The effect of this correction is to broaden the quasiparticle energy level in analogy with the disorder scattering in a binary alloy. Secondly, the spin on each site may flip, giving rise to the "resonance broadening" of Hubbard.[5] Since the quasispins are composed of conduction electrons, it is desirable to treat these two effects simultaneously under the same formalism because the level width of the conduction-electron state must be related to the life time of the quasispins. The coherent-potential approximation (CPA) is ideally suited for this purpose.[7-10] We show in this paper that when the calculation is carried to self-consistency, the size of the quasispin is solved from a transcendential equation in close resemblance to the Anderson model of local moments.[11] The condition for the existence of a nonzero quasispin is the same as the Stoner criterion for ferromagnetic ground state, as pointed out earlier by Friedel.[12] The quasispins persist in the paramagnetic phase as was shown by Schrieffer *et al.*[13] and Cyrot.[14] Conversely, when the Stoner criterion is not satisfied, the high-temperature susceptibility of the system is Pauli-like, and at low temperatures the system can at most order in a spin-density-wave state.

In the simple form of CPA used here, it is assumed that the reversed spins are randomly distributed in the lattice. This is not a good representation of the true state of ordering, especially near the critical temperature where short-range order exists. An improved theory taking the short-range order into consideration will be the subject of another publication.

II. FERROMAGNETIC SYSTEMS AT ELEVATED TEMPERATURES

In Ref. 1, we proposed the band Hamiltonian for the quasispin problem to be

$$H=\frac{p^2}{2m}+V(\vec{r})+\sum_i W_0(\vec{r}-\vec{R}_i)\hat{\eta}_i\cdot\vec{\sigma}\,, \tag{2.1}$$

where $V(\vec{r})$ is the spin-independent part of the crystal potential, and $W_0(\vec{r}-\vec{R}_i)$ is the spin-dependent potential which is defined in the unit cell around the site $\vec{R}_i$. The unit vector $\hat{\eta}_i$ is the direction of the quasispin at $\vec{R}_i$. In a single-band and constant-matrix-element approximation the Hamiltonian has the form

$$\begin{aligned}H=&\sum_{\vec{k}\sigma}\epsilon_{\vec{k}}C^{\dagger}_{\vec{k}\sigma}C_{\vec{k}\sigma}\\&-\Delta\sum_{\vec{k}\vec{k}'}\sum_i\big[\hat{\eta}^z_i(C^{\dagger}_{\vec{k}\uparrow}C_{\vec{k}'\uparrow}-C^{\dagger}_{\vec{k}\downarrow}C_{\vec{k}'\downarrow})\\&\qquad+\hat{\eta}^+_iC^{\dagger}_{\vec{k}\downarrow}C_{\vec{k}'\uparrow}+\hat{\eta}^-_iC^{\dagger}_{\vec{k}\uparrow}C_{\vec{k}'\downarrow}\big]e^{i(\vec{k}'-\vec{k})\cdot\vec{R}_i}\,,\end{aligned} \tag{2.2}$$

where $\hat{\eta}^{\pm}_i=\hat{\eta}^x_i\pm i\hat{\eta}^y_i$.

For the ferromagnetic system the ground-state electron levels are

$$\epsilon_{\vec{k}s}=\epsilon_{\vec{k}}\mp\Delta\,,$$

and the spin per atom is given by

$$S=\frac{1}{2N}\sum_{\vec{k}}\left[f(\epsilon_{\vec{k}\uparrow})-f(\epsilon_{\vec{k}\downarrow})\right],$$

where $f(\epsilon)$ is the Fermi distribution function, and N is the total number of atoms. The sum on $\vec{k}$ can be transformed into an integral on energy by defining a density of states per spin per atom

$$N(\epsilon)=\frac{1}{N}\sum_{\vec{k}}\delta(\epsilon_{\vec{k}}-\epsilon)\,.$$

Then

$$S=\frac{1}{2}\int N(\epsilon)\left[f(\epsilon-\Delta)-f(\epsilon+\Delta)\right]d\epsilon\,. \tag{2.3}$$

To make contact with the more familiar results we further assume that the interaction matrix element Δ is proportional to the spin, i.e., $\Delta=US$, where U is the proportionality constant. Note that U is not the bare Coulomb repulsion between two electrons on the same site, which is of the order of 10 eV. Instead, it is related to the average Slater exchange in the ferromagnetic state. The size of U has been determined from self-consistent band calculations to be about 2 eV.[15] Under this assumption Eq. (2.3) becomes a self-consistent equation for S, and the condition for nonzero solution for S is the Stoner criterion $UN(\mu)>1$, where μ is the Fermi energy.

Now we consider the system at an elevated temperature so that there is a number of reversed spins at random sites. At any time the probability of a site to be in spin-up state is p_+, and in spin-down state p_-, with $p_++p_-=1$. The magnetization per spin is $S(T)=S(p_+-p_-)$. In the lowest order we treat the z component of the scattering potential by the coherent-potential approximation. A spin-up electron sees a potential $-\Delta$ at a spin-up site and a potential Δ at a spin-down site. The numbers of spin-up and spin-down sites are given by Np_+ and Np_-. In the coherent-potential method this fluctuating potential is approximately represented by a complex energy-dependent potential $V_+(E)$ such that the Green's function for the electron is

$$G_+(\vec{k},E)=\left[E-\epsilon_{\vec{k}}+\mu-V_+(E)\right]^{-1}, \tag{2.4}$$

where E is measured from the Fermi level. The t matrix for repeated scattering of a spin-up electron from a site i is solved from

$$t_{i+}=V_{i+}+V_{i+}G_{ii+}t_{i+}\,, \tag{2.5}$$

where

$$\begin{aligned}G_{ii+}(E)&=\frac{1}{N}\sum_{\vec{k}}G_+(\vec{k},E)\\&=\int\frac{N(\epsilon)\,d\epsilon}{E-\epsilon+\mu-V_+(E)}\,.\end{aligned} \tag{2.6}$$

The potential V_{i+} on site i is $V_{i+}=-\Delta-V_+(E)$ if the spin state of that site is up, and $V_{i+}=\Delta-V_+(E)$ if the site has spin down. Thus for a spin-up site

$$t_{++}=\frac{-\Delta-V_+(E)}{1-\left[-\Delta-V_+(E)\right]G_{ii+}(E)}\,,$$

and for a spin-down site

$$t_{+-}=\frac{\Delta-V_+(E)}{1-\left[\Delta-V_+(E)\right]G_{ii+}(E)}\,. \tag{2.7}$$

The coherent potential is determined self-consistently by the requirement that the average t matrix vanishes, i.e.,

$$p_+t_{++}+p_-t_{+-}=0\,. \tag{2.8}$$

Similarly, for spin-down electrons we obtain a set of equation with all Δ replaced by $-\Delta$. The equations are solved self-consistently to find the local electron propagators and the local densities of states

$$\rho_{i\sigma}(E) = (1/\pi)\,\mathrm{Im}G_{ii\sigma}(E). \tag{2.9}$$

Then the average spin per site is

$$\bar{S} = \frac{1}{2}\int_{-\infty}^{\infty} [\rho_{i+}(E) - \rho_{i-}(E)] f(E)\, dE, \tag{2.10}$$

where $f(E)$ is the Fermi distribution function.

The meaning of these results becomes clear when we examine the atomic limit, $N(\epsilon) = \delta(\epsilon - \epsilon_d)$, where ϵ_d is the energy of the one-electron orbital. In this limit the CPA is trivially exact. Equations (2.5)–(2.8) and their spin-down counterparts are easy to solve. The results for $\rho_{i\sigma}(E)$ and S are

$$\rho_{i\sigma}(E) = p_+\delta(E - \epsilon_d + \mu \pm \Delta) + p_-\delta(E - \epsilon_d + \mu \mp \Delta),$$

and

$$\bar{S} = \tfrac{1}{2}(p_+ - p_-)\int_{-\infty}^{\infty} [\delta(E - \epsilon_d + \mu + \Delta) - \delta(E - \epsilon_d + \mu - \Delta)] f(E)\, dE.$$

The integral in the expression for S is just the number of unpaired electrons per site, so

$$\bar{S} = S(p_+ - p_-), \tag{2.11}$$

where S is the spin per site. Therefore, in the following discussion we will use Eq. (2.11) to relate the size of the local moment to the average local spin in Eq. (2.10).

We now show that when the spins are not completely ordered the criterion for the existence of local moments is identical to the Stoner criterion. For this purpose we substitute the expressions for the t matrices in Eq. (2.7) into the self-consistent condition Eq. (2.8) to obtain a relation between the Green's function and the coherent potential

$$(V_\pm^2 - \Delta^2)G_{ii\pm}(E) + V_\pm \pm \Delta(p_+ - p_-) = 0. \tag{2.12}$$

At the threshold of local moment formation the local level splitting Δ is infinitesimal, so we may solve for V_σ to obtain

$$V_\pm \cong \mp\Delta(p_+ - p_-).$$

This may be recognized as the same result as predicted by the random-phase approximation. It follows that

$$\rho_{i\sigma}(E) \cong N[E + \mu \pm \Delta(p_+ - p_-)],$$

and

$$\bar{S} \cong (p_+ - p_-)\Delta\int_{-\infty}^{\infty} \frac{dN(E+\mu)}{dE} f(E)\, dE.$$

The last result, together with Eq. (2.11), give the threshold value of U for the formation of local moments

$$1 = U\int_{-\infty}^{\infty} \frac{dN(E+\mu)}{dE} f(E)\, dE. \tag{2.13}$$

For transition metals $\mu \cong 1$ eV measured from the bottom of the d bands. So even up to the typical Curie temperature of 1000 K the temperature effect of the Fermi distribution function is entirely negligible. Then Eq. (2.13) reduces to the Stoner criterion $1 = UN(\mu)$. Thus, if the material is ferromagnetic at low temperatures, the local moments persist up to the Curie temperature.

Above the Curie temperature we have the condition $p_+ = p_- = \frac{1}{2}$, so the equation for the local moment becomes ambiguous. However, if an infinitesimal magnetic field is applied to polarize the system ever so slightly, we again find local moments on the sites if the Stoner criterion is satisfied. We therefore conclude that in a ferromagnetic metal the disordered state is a state of persistent but randomly oriented quasispins. Neutron scattering experiments in the paramagnetic state of Fe support this view.[16] Conversely, if the Stoner criterion is not satisfied there can be no local moments in the paramagnetic phase. Furthermore, if the system orders, it cannot order ferromagnetically. Examples of systems which order at low temperatures but have no local moments at high temperatures are chromium and its alloys.[17]

The CPA equations are also easy to solve near the Curie temperature where $p_+ - p_- = \xi \ll 1$. The solutions are of the form

$$G_{ii\pm}(E) = G(E) \pm \xi g(E),$$
$$V_\pm(E) = V(E) \pm \xi\nu(E),$$

where

$$G(E) = \int \frac{N(\epsilon)\, d\epsilon}{E - \epsilon + \mu - V(E)},$$
$$G(E) = V(E)/[\Delta^2 - V^2(E)],$$
$$g(E) = -\Delta/\{V^2(E) - \Delta^2 + [2G(E)V(E) + 1]/\phi(E)\},$$
$$\nu(E) = g(E)/\phi(E),$$
$$\phi(E) = \int \frac{N(\epsilon)\, d\epsilon}{[E - \epsilon + \mu - V(E)]^2}. \tag{2.14}$$

The size of the local moment is given by

$$S = \frac{1}{\pi}\int_{-\infty}^{0} \mathrm{Im}g(E)\, dE. \tag{2.15}$$

Given a density of states function $N(\epsilon)$ one can solve the above set of equations to find S. The result also applies to the paramagnetic phase as discussed earlier. In general we expect the size of S in the paramagnetic state to differ from that in the ordered state.

III. RESULTS OF MODEL CALCULATIONS

In this section we report the results of a few model calculations to further illustrate the nature

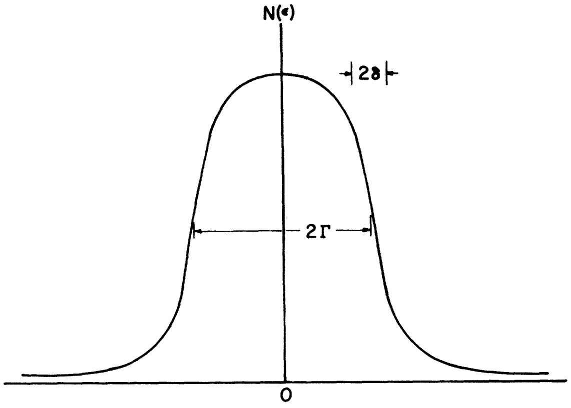

FIG. 1. Nearly square density of states model.

of the CPA. A particularly simple model density of states is the Lorentzian model

$$N(\epsilon)=(1/\pi)\Gamma/[(\epsilon-\mu)^2+\Gamma^2],$$

where $\epsilon>0$. The local moment in the ordered phase is given by

$$S=(1/\pi)\tan^{-1}(\Delta/\Gamma).$$

At elevated temperatures the solution of the CPA equations are

$$G_{ii\sigma}(E)=[E-V_\sigma(E)+i\Gamma(E)]^{-1} \tag{3.1}$$

and

$$V_\sigma(E)=\frac{\Delta^2\mp[E+i\Gamma(E)]\Delta(p_+-p_-)}{E+i\Gamma(E)\mp\Delta(p_+-p_-)}, \tag{3.2}$$

where $\Gamma(E)=\pm\Gamma$ according to whether $E>0$ or $E<0$, and E is measured from the Fermi level. The expressions for the Green's functions may be reduced to

$$G_{ii\sigma}(E)=\frac{p_+}{E\pm\Delta+i\Gamma(E)}+\frac{p_-}{E\mp\Delta+i\Gamma(E)}. \tag{3.3}$$

The local electron densities are

$$\rho_{i\sigma}(E)=\frac{\Gamma}{\pi}\left(\frac{p_+}{(E\pm\Delta)^2+\Gamma^2}+\frac{p_-}{(E\mp\Delta)^2+\Gamma^2}\right),$$

and the size of the local moment is identical to that in the ordered phase.

The fact that the size of local moment is independent of the ordering is easy to understand. The assumption of Lorentzian density of states reduces the band to a set of local resonances. This has the effect of decoupling the atoms and making the coherent-potential method exact. Nevertheless, the results are useful in demonstrating the following point. The propagator in Eq. (3.1) is clearly in the form written down by Hubbard after making the scattering correction. On the other hand, the equivalent form in Eq. (3.3) indicates that the site i switches back and forth between spin up and spin down with relative probabilities p_+ and p_-. This is just the resonance broadening effect discussed by Hubbard. Thus, our theory, though different in mathematical approach from Hubbard's work, actually treats the scattering and resonance effects under the same formalism.

For a nontrivial model we choose the nearly square density of states

$$N(\epsilon)=\frac{1}{2\pi\Gamma}\left[\tan^{-1}\left(\frac{\epsilon+\Gamma}{\delta}\right)-\tan^{-1}\left(\frac{\epsilon-\Gamma}{\delta}\right)\right],$$

where 2Γ is a measure of the bandwidth and 2δ a measure of the squareness as shown in Fig. 1. In the limit $\delta\to 0$ the shape of $N(\epsilon)$ becomes square. The CPA equations must be solved numerically. We find that for energies near the maximum of $N(\epsilon)$ the numerical solutions for the potential $V_\sigma(E)$ converge very slowly. To avoid this difficulty we assume 0.8 electron per site so that the Fermi level is slightly to the left of the maximum. The size of the local moment S is computed as a function of U for $\delta=0.2\Gamma$ in both the ferromagnetic phase and the paramagnetic phase, and the results are plotted in Fig. 2. Both curves approach the limit $S=0.4$ in the large U limit, but the spin value in the paramagnetic phase falls consistently below that in the ferromagnetic phase. The explanation of this effect can be traced to the line broadening in the paramagnetic phase due to random spin scattering of the electrons. The added broadening in the paramagnetic phase gives an effectively broader band and smaller density of states at the Fermi level. For intermediate ordering the spin value is bounded by the two curves.

The decrease in spin value with increasing disorder gives rise to an increase in internal energy

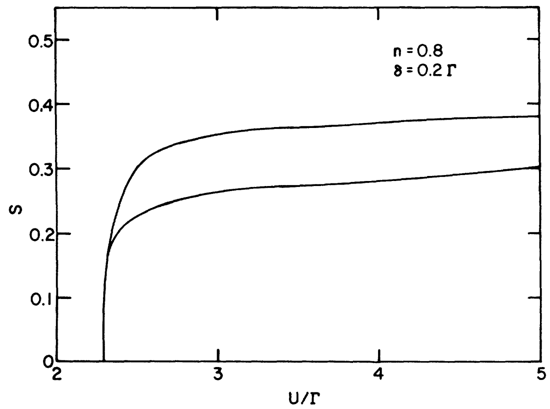

FIG. 2. S-vs-U curves for the nearly square density of states model. The upper curve is for the ferromagnetic state and the lower curve for the paramagnetic state.

of the system. This energy is in part the coupling energy between the local moments. In Sec. IV we discuss another important contribution of the coupling energy which comes from spin-flip scattering effects not treated in the CPA.

IV. CORRELATION ENERGY DUE TO SPIN-FLIP SCATTERING

The spin-flip scattering terms in Eq. (2.2) are not effective in the ground state. With a number of reversed spins a spin-up electron may undergo a spin flip when it encounters a spin-down site and then flips again at a spin-up site. Similarly, a spin-down electron may go through two spin flips when it interacts with a spin-up and a spin-down site in succession. Both processes contribute to the self-energy of the electrons. For a spin-up electron the self-energy is found to be

$$\Sigma^{(1)}_{lm+}(E) = V_l^{(+-)} G_{lm-}(E) V_m^{(-+)},$$

where $V_l^{(+-)}$ and $V_m^{(-+)}$ are spin-flip matrix elements at site l and m, respectively. The self-energy for a spin-down electron has a similar expression.

To calculate the spin-flip matrix elements we need to know the quantum-mechanical nature of the quasispins. In Ref. 1 we gave an intuitive way of handling this problem base on the interconfiguration fluctuation model of Hirst.[18] In this model the quasispin is a mixture of spin-zero and spin-$\frac{1}{2}$ states so that the state of an atom is represented by

$$\Psi = b_1 |\tfrac{1}{2}, \tfrac{1}{2}\rangle + b_0 |0, 0\rangle$$

for a spin-up site and

$$\Psi' = b_1 |\tfrac{1}{2}, -\tfrac{1}{2}\rangle + b_0 |0, 0\rangle$$

for a spin-down site. The coefficients b_0 and b_1 are determined by the normalization, $|b_0|^2 + |b_1|^2 = 1$, and the size of the quasispin,

$$S = \langle \Psi | S^z | \Psi \rangle = \tfrac{1}{2} |b_1|^2 .$$

In a spin-flip transition we can easily establish that

$$\langle \Psi' | S^- | \Psi \rangle = \langle \Psi | S^+ | \Psi' \rangle = |b_1|^2 = 2S .$$

Using the definition $\eta^{\pm} = S^{\pm}/S$, we obtain the spin-flip matrix elements

$$V^{(+-)} = V^{(-+)} = 2\Delta .$$

When averaged over an ensemble of crystals with all possible distributions of reversed spins, we get

$$\Sigma^{(1)}_{lm\sigma}(E) = 4p_+ p_- \Delta^2 G_{lm,-\sigma}(E).$$

Upon Fourier analysis we obtain

$$\Sigma^{(1)}_{\sigma}(\vec{k}, E) = 4p_+ p_- \Delta^2 G_{-\sigma}(\vec{k}, E) . \tag{4.1}$$

The contribution of spin-flip scatterings to the internal energy is

$$E_f^{(1)}(T) = -\frac{1}{2} \sum_{\vec{k}\sigma} \int \frac{dE}{2\pi i} \Sigma^{(1)}_{\sigma}(\vec{k}, E) G_\sigma(\vec{k}, E)$$
$$= N[S^2 - S^2(T)] \mathcal{J}(T) , \tag{4.2}$$

where

$$\mathcal{J}(T) = -\frac{4U^2}{N} \sum_{\vec{k}} \int \frac{dE}{2\pi i} G_+(\vec{k}, E) G_-(\vec{k}, E) . \tag{4.3}$$

The physical meaning of the quantity $\mathcal{J}(T)$ is easy to understand if we write Eq. (4.3) as

$$\mathcal{J}(T) = \sum_l J(\vec{R}_l) , \tag{4.4}$$

where

$$J(\vec{R}_l) = -\frac{4U^2}{N^2} \sum_{\vec{k}\vec{k}'} \int \frac{dE}{2\pi i} G_+(\vec{k}, E)$$
$$\times G_-(\vec{k}', E) e^{i(\vec{k}-\vec{k}')\cdot \vec{R}_l} . \tag{4.5}$$

The quantity $J(\vec{R}_l)$ is the Ruderman-Kittel interaction between two spins separated by a distance $\vec{R}_l$.[19] In the ground state the interaction $J(\vec{R}_l)$ can be put into the more familiar form

$$J(\vec{R}_l) = \frac{4U^2}{N^2} \sum_{\vec{k}\vec{k}'} \frac{f_{\vec{k}\uparrow} - f_{\vec{k}'\downarrow}}{E_{\vec{k}'\downarrow} - E_{\vec{k}\uparrow}} e^{i(\vec{k}-\vec{k}')\cdot \vec{R}_l} , \tag{4.6}$$

and it follows that $\mathcal{J}(0) = 4U$. In the excited state the presence of the complex self-energy in the Green's functions gives rise to a complicated temperature dependence to the interaction.

The idea that the local moments in ferromagnetic transition metals are coupled together by the long-range Ruderman-Kittel interaction was first suggested by Friedel[12] and formulated by Cyrot[6] and Capellmann.[20] The experimental evidence for this view has been reported recently by Stearns.[21] However, there is an important distinction between our result in Eq. (4.5) and the results in Refs. 6 and 20. In our work the quasiparticle damping is explicitly contained in the expression for $J(\vec{R})$, whereas the earlier works all take the quasiparticles as free from damping even in the disordered spin state. Physically the damping effect shortens the range of $J(\vec{R})$ such that with increasing temperature the distant spin pairs are progressively out of touch with each other. Consequently we expect a weakening of the total coupling strength at high temperatures. The experimental evidence of this effect can be found in the neutron scattering data on Ni for which the spin-wave stiffness constant is found to be 555 meV Å² at helium temperature but 280 meV Å² near the Curie temperature.[22] Therefore, unlike magnetic insulators, the spin coupling in ferromagnetic transition metals depends on temperature through the spin disorder scattering of the band electrons.

The effect of spin disorder on the energy bands may be appreciated by studying the imaginary part of the electron self-energy, which is the inverse scattering time. Taking only the CPA part of the self-energy and using the explicit result of the Lorentzian model, we find

$$\tau_\sigma^{-1}(T) = \mathrm{Im}\,V_\sigma(E) = \left(1 - \frac{S^2(T)}{S^2}\right)\frac{\Gamma\Delta^2}{U^2S^2(T)+\Gamma^2}, \qquad (4.7)$$

for electrons near the Fermi level $E \cong 0$. As the temperature increases the scattering time decreases steadily until the Curie temperature is reached. Beyond that point the scattering time levels off to a constant value. The asymptotic value for the scattering time is

$$\tau_\sigma^{-1}(\infty) = \Delta^2/\Gamma > \pi U S^2 . \qquad (4.8)$$

For Ni with $U \cong 2$ eV,[23] and $S = 0.3$, we estimate $\tau_\sigma^{-1}(\infty) > 0.6$ eV, which is a substantial fraction of the total bandwidth of about 3 eV for the d states. The corresponding mean free path of the electron is of the order of the nearest-neighbor distance. Therefore, near T_c only nearest-neighbor interactions are important.

The quasiparticle scattering gives rise to a large, temperature-dependent spin disorder electrical resistivity. The temperature dependence of the resistivity for the Lorentzian model has the form

$$\rho(T) = \rho(\infty)\left(1 - \frac{S^2(T)}{S^2}\right)\frac{\Gamma^2}{U^2S^2(T)+\Gamma^2}, \qquad (4.9)$$

where $\rho(\infty)$ is the spin disorder resistivity of the paramagnetic phase. This result is very similar to those of Kasuya[24] and deGennes and Friedel[25] which are derived from the s-d model by using perturbation theory.

The contribution of the spin-flip scattering to the quasiparticle level width is also of interest. This is because the total level width determines the size of the quasispins, so it may be necessary to include the spin-flip scattering effect self-consistently in the calculation of S. As discussed previously the spin-flip scattering is unimportant at low temperatures when there are few reversed spins. So we will limit our study to the paramagnetic state for which $p_+ = p_- = \frac{1}{2}$. Then the relative importance of the spin-slip scattering versus the CPA contribution to the level width may be assessed by looking at the imaginary parts of $\Sigma_\sigma^{(1)}(\vec{k}, E)$ in Eq. (4.1) and $V_\sigma(E)$ in Eq. (3.2) for electrons on the Fermi level, $\epsilon_{\vec{k}}^{\sigma} = \mu$, $E = 0$. We find

$$\mathrm{Im}\,\Sigma_\sigma^{(1)}(k_F, 0) = \Gamma$$

and

$$\mathrm{Im}\,V_\sigma(0) = \Delta^2/\Gamma .$$

The ratio of the two terms is $(\Gamma/\Delta)^2$. Thus the spin-flip scattering is unimportant when the bandwidth is small compared with the band splitting, i.e., the condition under which local moments are stable. We conclude that the concept of quasispins coupled by spatially damped Ruderman-Kittel interaction is valid under this condition.

When Δ and Γ are comparable in size, the CPA may result in stable local moments but the spin-flip scattering may severely modify the size of the moments in the disordered phase. It becomes questionable whether the concept of quasispin is meaningful. However, one must bear in mind that the CPA ignores completely the short-range order of the spins near the ordering temperature. It therefore leaves out the cooperative effects of many sites in the formation of a cluster of partially ordered spins. At the same time the spin-flip scattering effect is overestimated because such scattering events between nearby sites are inhibited by short-range order. What is needed is an alloy theory which includes the short-range order effects as the starting approximation. Such a theory has been formulated recently by Kittler and Falicov,[26] and the application of their method to the itinerant magnetic system is now under investigation.

V. SUMMARY AND CONCLUSION

The results of this work may be summarized as follows: (i) the disordered phase of an itinerant ferromagnetic material is better described by a collection of randomly oriented local moments; (ii) the effective coupling energy between pairs of local moments progressively weakens with increasing disorder; and (iii) the disruption of electron bands gives rise naturally to the magnetic contribution to the electrical resistivity.

These conclusions are only of qualitative validity because (a) the one-band model is an oversimplification of real transition metals; (b) the CPA is a mean-field theory, and is therefore quantitatively unreliable in dealing with long-range, oscillatory spin pair interactions; and (c) the separate treatment of the longitudinal and transverse electron-spin scattering is not valid at high temperatures. Although the third point may be studied within the framework of CPA by including higher-order effects, e.g., vertex corrections, we feel that the additional insight that may be gained from such a calculation will be minimal.

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[1] S. H. Liu, Phys. Rev. B 13, 3962 (1976).

[2] J. C. Slater, Phys. Rev. 81, 385 (1951).

[3] W. Kohn and L. J. Sham, Phys. Rev. 140, A1133 (1965).

[4] R. Gaspar, Acta Phys. (Hung.) 3, 163 (1954).

[5] J. Hubbard, Proc. R. Soc. A 276, 401 (1964).

[6] M. Cyrot, J. Phys. (Paris) 33, 125 (1972).

[7] J. L. Beeby, Phys. Rev. 135, A130 (1964).

[8] P. Soven, Phys. Rev. 156, 809 (1967); 178, 1136 (1969).

[9] S. Kirkpatrick, B. Velicky, and H. Ehrenreich, Phys. Rev. B 1, 3250 (1970).

[10] K. Levin, R. Bass, and K. H. Bennemann, Phys. Rev. B 6, 1865 (1972).

[11] P. W. Anderson, Phys. Rev. 124, 41 (1961).

[12] J. Friedel, G. Leman, and S. Olszewski, J. Appl. Phys. 32, 325S (1961).

[13] S. W. Wang, W. E. Evenson, and J. R. Schrieffer, Phys. Rev. Lett. 23, 92 (1969); J. Appl. Phys. 41, 1199 (1970).

[14] M. Cyrot, Phys. Rev. Lett. 25, 871 (1970).

[15] See the list of references in Ref. 1.

[16] M. K. Wilkinson and C. G. Shull, Phys. Rev. 103, 516 (1956).

[17] M. K. Wilkinson, E. O. Wollan, W. C. Koehler, and J. W. Cable, Phys. Rev. 127, 2080 (1962).

[18] L. L. Hirst, J. Phys. Chem. Solids 35, 1285 (1974).

[19] M. A. Ruderman and C. Kittel, Phys. Rev. 96, 99 (1954).

[20] H. Capellmann, J. Phys. F 4, 1112 (1974); 4, 1466 (1974).

[21] M. B. Stearns, Phys. Rev. B 8, 4383 (1973).

[22] H. A. Mook, J. Lynn, and R. M. Nicklow, Phys. Rev. Lett. 30, 556 (1973).

[23] L. Hodges, H. Ehrenreich, and N. D. Lang, Phys. Rev. 152, 505 (1973).

[24] T. Kasuya, Prog. Theor. Phys. 16, 58 (1956).

[25] P.-G. deGennes and J. Friedel, J. Phys. Chem. Solids 4, 71 (1958).

[26] R. C. Kittler and L. M. Falicov, J. Phys. C 9, 4259 (1976).