# Zener Theory

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In the narrow-band limit, the correlation between two localized magnetic moments with spin  $S = \frac{1}{2}$  is calculated exactly in the case where both moments are subjected to a direct antiferromagnetic Heisenberg interaction of strength G as well as a ferromagnetic  $s-d$  interaction of strength J with the conduction electrons. It appears that the correlation exhibits <sup>a</sup> discontinuity as a function of  $J/G$  in the case where the spin clouds, which are built up by the electron gas around the moments, overlap. Another interesting feature is the fact that the two types of interaction are unable to cancel out each other, i. e. , a correlation which equals zero does not appear. It also appears that the two moments can never be coupled in a purely antiferromagnetic way unless in the trivial case  $J=0$ .

#### I. INTRODUCTION

In the Zener theory' the ferromagnetism in the transition metals is attributed to the ferromagnetic s-d interaction of the conduction electrons with the magnetic moments. Although the direct interaction between the localized magnetic moments is antiferromagnetic, the indirect coupling via the s-d interaction with the conduction electrons dominates in a sufficient way in order to obtain ferromagnetism in these materials. In order to treat the Zener theory in a purely quantum-mechanical way, it is important first to concentrate on the more simple problem of two magnetic moments  $\bar{S}_1$  and  $\bar{S}_2$  with spin  $S = \frac{1}{2}$ , which directly interact via an antiferromagnetic Heisenberg interaction of strength  $G$  ( $G$  < 0) and have an indirect coupling via a ferromagnetic s-d interaction of strength  $J(J>0)$ with the conduction electrons. The exact solution of this problem would result in a definite answer to the interesting question of whether the correlation between the two magnetic moments as a function of  $|G/J|$  gradually changes from a ferromagnetic to an antiferromagnetic character, or in a discontinuous way jumps from a purely ferromagnetic correlation to a purely antiferromagnetic one with increasing  $|G/J|$ . Although a number of approximation schemes have been developed for this problem, the most prominent being the concept of the Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction,  $2-4$  the exact nature of the solution of this problem is still unknown. This is largely due to the breakdown of the RKKY interaction in the case where higher-order terms in the perturbation expansion are taken into account.

In this paper the exact solution is given for the case of a narrow conduction band which is half-

filled. The solution of the present model is quite analogous to the one of the corresponding model without a direct interaction between the two localized magnetic moments.  $6$  The assumption of a narrow conduction band is equivalent to making the kinetic energy of all one-particle levels the same. This feature is essential for the solvability of the model. Taking into account one-particle levels with different kinetic energies complicates the problem tremendously. Undoubtedly this narrowband assumption limits the physical applicability of the present model. The fact, however, that this model can be solved exactly more than makes up for this deficiency, because the exact solvability makes it possible to analyze the competition between an indirect and a direct interaction in every detail. As such, this model joins the small class of nontrivial model Hamiltonians in solid-state physics which can be analyzed exactly and in complete detail. Moreover, the model presents a very useful testing ground for approximations made in order to solve the original Hamiltonian.

This paper is organized in the following way: In Sec. II the model is defined, in Sec. III the results are given as far as the ground state is concerned, and in Sec. IV the results are discussed.

#### II. MODEL

Because in the case of a narrow conduction band the kinetic energy of all one-particle levels can be assumed to be the same, i. e., to equal the constant  $\epsilon$ , the Hamiltonian of the system is given by

 $H = \epsilon \sum_{n=1}^{N} c_{\vec{k}_n \sigma}^{\dagger} c_{\vec{k}_n \sigma} - \frac{J}{2\Omega} \sum_{n,m=1}^{N} \sum_{\rho=1}^{2} e^{i(\vec{k}_m - \vec{k}_n) \cdot \vec{R}_{\rho}}$ 

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 $\overline{4}$ 

$$
\times \left[ (c_{\vec{k}_{n^*}}^{\dagger} c_{\vec{k}_{m^*}} - c_{\vec{k}_{n^-}}^{\dagger} c_{\vec{k}_{m^-}}) S_{\rho}^2 + c_{\vec{k}_{n^*}}^{\dagger} c_{\vec{k}_{m^-}} S_{\rho}^{\dagger} + c_{\vec{k}_{n^-}}^{\dagger} c_{\vec{k}_{m^*}} S_{\rho}^{\dagger} \right] - G \, \vec{S}_1 \cdot \vec{S}_2 \,, \tag{1}
$$

where  $\Omega$  is the volume of the system,  $\vec{R}_{p}$  denotes the position of magnetic moment p with spin  $\bar{S}_{\rho}$  of magnitude  $S = \frac{1}{2}$ , and the total number of states is given by  $2N$ , N spin-up and N spin-down states.

As far as the electron system is concerned, the only relevant operators are

$$
\alpha_{\rho\sigma}^{\dagger} = \frac{1}{\sqrt{N}} \sum_{n=1}^{N} e^{-i\vec{k}_{n}\cdot\vec{R}} c_{\vec{k}_{n}\sigma}^{\dagger} \quad (p=1, 2) . \tag{2}
$$

The physical meaning of the operator  $\alpha_{\rho\sigma}^{\dagger}$  is that it creates a spin cloud (in other words a wave packet with spin  $\sigma$ )  $g_{\rho\sigma}(\vec{x})$  of the following form:

$$
g_{\rho\sigma} = \frac{1}{\sqrt{N}} \sum_{n=1}^{N} \phi_{\vec{\mathbf{k}}_n, t}(\vec{\mathbf{x}}) e^{i\vec{\mathbf{k}}_n \cdot (\vec{\mathbf{x}} - \vec{\mathbf{R}}_p)}, \qquad (3)
$$

where  $e^{i\vec{\bf k}\cdot \vec{\bf x}}\phi_{\vec{\bf k}_n,t}(\vec{x})$  are the Bloch functions and the index  $t$  denotes the conduction band considered. In general the two spin clouds  $g_{1g}(\vec{x})$  and  $g_{2g}(\vec{x})$  are not independent but overlap. This overlap  $f(R)$  is given by

$$
f(R) = \frac{1}{N} \sum_{n=1}^{N} e^{-i\vec{\mathbf{k}}_n \cdot (\vec{\mathbf{R}}_1 - \vec{\mathbf{R}}_2)},
$$
 (4)

where  $R = |\vec{R}_1 - \vec{R}_2|$  and  $|f(R)| < 1$ . Because of this overlap, it is advantageous to introduce a new set of fermion operators which are linear combinations of the old ones. This new set is defined by

$$
d_{1\sigma}^{\dagger} = \frac{1}{\left[1 - f^2(R)\right]^{1/2}} \left(A_{+} \alpha_{1\sigma}^{\dagger} - A_{-} \alpha_{2\sigma}^{\dagger}\right),
$$
  
\n
$$
d_{2\sigma}^{\dagger} = \frac{1}{\left[1 - f^2(R)\right]^{1/2}} \left(A_{+} \alpha_{2\sigma}^{\dagger} - A_{-} \alpha_{1\sigma}^{\dagger}\right),
$$
\n
$$
(5)
$$

where

$$
A_{\pm} = \frac{1}{2} [1 + f(R)]^{1/2} \pm \frac{1}{2} [1 - f(R)]^{1/2} , \qquad (6)
$$

while the remaining operators  $d_{i\sigma}^{\dagger}(l=3, 4, \ldots, N)$ can be obtained by the well-known Schmidt process of orthogonalization. The Hamiltonian in this new representation is

$$
H = \epsilon \sum_{i=1, \sigma}^{N} d_{1\sigma}^{\dagger} d_{1\sigma} - \sum_{i=1}^{3} O_i - G \vec{S}_1 \cdot \vec{S}_2 , \qquad (7)
$$

where the operators  $O_i$  (*i*=1, 2, 3) are defined by

$$
O_1 = \frac{JN}{4\Omega} \left\{ 1 + \left[ 1 - f^2(R) \right]^{1/2} \right\} \sum_{p=1}^{2} \left[ \left( d_{p+}^{\dagger} d_{p+} - d_{p-}^{\dagger} d_{p-} \right) S_p^{\sharp} + d_{p+}^{\dagger} d_{p-} S_p^{\dagger} + d_{p-}^{\dagger} d_{p+} S_p^{\dagger} \right], \qquad (8a)
$$

$$
O_2 = \frac{JN}{4\Omega} \left\{ 1 - \left[ 1 - f^2(R) \right]^{1/2} \right\} \left[ (d_{1*}^{\dagger} d_{1*} - d_{1*}^{\dagger} d_{1*}) S_2^* + | 1 - 2 - \rangle (\left| \beta \right| + \left| \gamma \right|) \right] + d_{1*}^{\dagger} d_{1*} S_2^* + d_{1*}^{\dagger} d_{1*} S_2^* + (d_{2*}^{\dagger} d_{2*} - d_{2*}^{\dagger} d_{2*}) S_1^* \right\}
$$

$$
+ d_{2+}^{\dagger} d_{2-} S_{1}^{-} + d_{2-}^{\dagger} d_{2+} S_{1}^{\dagger} \, , \qquad \text{(8b)}
$$

$$
O_3 = \frac{JN}{4\Omega} f(R) \left[ (d_{1*}^{\dagger} d_{2*} + d_{2*}^{\dagger} d_{1*} - d_{1*}^{\dagger} d_{2*} - d_{2*}^{\dagger} d_{1*}) \right]
$$
  
×  $(S_1^{\epsilon} + S_2^{\epsilon}) + (d_{1*}^{\dagger} d_{2*} + d_{2*}^{\dagger} d_{1*}) (S_1^{\epsilon} + S_2^{\epsilon})$   
+  $(d_{1*}^{\dagger} d_{2*} + d_{2*}^{\dagger} d_{1*}) (S_1^{\epsilon} + S_2^{\epsilon}) \right].$  (8c)

Obviously it is sufficient to study the Hamiltonian

$$
H' = \epsilon \sum_{l=1,\sigma}^{2} d_{l\sigma}^{\dagger} d_{l\sigma} - \sum_{i=1}^{3} O_i - G \tilde{S}_1 \cdot \tilde{S}_2
$$
 (9)

in order to obtain the exact nature of the competition between the indirect and direct interaction. The relevant information is contained in the behavior of the correlation function  $\langle 0|\bar{S}_1\cdot\bar{S}_2|0\rangle$ , where  $|0\rangle$  denotes the ground state of Hamiltonian  $H'$ .

## III. RESULTS

By putting

$$
\left|\alpha\right\rangle = \left|m_1 = \frac{1}{2}\right\rangle \left|m_2 = \frac{1}{2}\right\rangle,
$$
  
\n
$$
\left|\beta\right\rangle = \left|m_1 = \frac{1}{2}\right\rangle \left|m_2 = -\frac{1}{2}\right\rangle,
$$
  
\n
$$
\left|\gamma\right\rangle = \left|m_1 = -\frac{1}{2}\right\rangle \left|m_2 = \frac{1}{2}\right\rangle,
$$
  
\n
$$
\left|\delta\right\rangle = \left|m_1 = -\frac{1}{2}\right\rangle \left|m_2 = -\frac{1}{2}\right\rangle,
$$
  
\n(10)

where

$$
S_{p}^{\boldsymbol{\ell}} \mid m_{p} = \pm \frac{1}{2} \rangle = \pm \frac{1}{2} \mid m_{p} = \pm \frac{1}{2} \rangle \quad (p = 1, 2)
$$
 (11)

and

$$
d_{k_1\sigma_1}^{\dagger} d_{k_2\sigma_2}^{\dagger} \Phi_{\text{vac}} = |k_1\sigma_1, k_2\sigma_2\rangle| , \qquad (12)
$$

the following results are obtained as far as the ground state of Hamiltonian  $H'$  is concerned:

(i) In the case where  $-2\Omega G/JN < f^2(R) < 1$ , the ground -state energy reads

$$
E_1 = 2\epsilon - (JN/2\Omega) - \frac{1}{4}G \t\t(13)
$$

It appears that this state is fivefold degenerate. The eigenvectors are

$$
|E_1,1\rangle = |1+,2+\rangle \,|\alpha\rangle \;, \tag{14a}
$$

$$
|E_1, 2\rangle = |1-, 2-\rangle |0\rangle , \qquad (14b)
$$

$$
|E_1, 3\rangle = \frac{1}{2} [ (|1+, 2-\rangle + |1-, 2+\rangle) | \alpha \rangle
$$

$$
+\left|1+2+\rangle\left(\left|\beta\right\rangle+\left|\gamma\right\rangle\right)\right],\qquad(14c)
$$

$$
|E_1, 4\rangle = \frac{1}{2} \left[ (|1+, 2-\rangle + |1-, 2+\rangle) | \delta \rangle \right. \\
\left. + |1-, 2-\rangle (|\beta\rangle + |\gamma\rangle) \right], \qquad (14d)
$$

$$
|E_1, 5\rangle = (1/\sqrt{6}) [(|1+, 2-\rangle + |1-, 2+\rangle)
$$

$$
(|\beta\rangle+|\gamma\rangle)+|1+,2+\rangle|\delta\rangle+|1-,2-\rangle|\alpha\rangle]. \tag{14e}
$$

The correlation function  $\langle E_1, i | \overline{\hat{S}}_1 \cdot \overline{\hat{S}}_2 | E_1, i \rangle$  (*i*=1, 2, 3, 4, 5) simply reads

$$
\langle E_1 | \mathbf{\bar{S}}_1 \cdot \mathbf{\bar{S}}_2 | E_1 \rangle = \frac{1}{4} \,, \tag{15}
$$

i.e., the two magnetic moments are coupled in a ferromagnetic way.

(ii) In the case where  $f^2(R) < -2\Omega G/JN$ , the ground-state energy is given by

$$
E_2 = 2\epsilon + \frac{JN}{2\Omega} + \frac{1}{4}G - \frac{1}{2}\left\{\frac{J^2 N^2}{\Omega^2} \left[4 - 3f^2(R)\right] - 2G\frac{JN}{\Omega} + G^2\right\}^{1/2}.
$$
 (16)

This state is nondegenerate. The eigenvector has the following form:

$$
|E_2\rangle = a |E_2\rangle_+ + b |E_2\rangle_-,
$$
 (17)

where

 $\overline{\mathscr{L}}$ 

$$
|E_2\rangle_{\pm} = A_{\pm}(|1+,2-\rangle|\beta\rangle + |1-,2+\rangle|\gamma\rangle) + B_{\pm}(|1+,2-\rangle|\gamma\rangle + |1-,2+\rangle|\beta\rangle) + C_{\pm}(|1+,2+\rangle|\delta\rangle + |1-,2-\rangle|\alpha\rangle),
$$
\n(18a)

$$
A_4 = -\frac{2 - f^2(R) - 2[1 - f^2(R)]^{1/2} + [4 - 3f^2(R)]^{1/2} + [4 - 7f^2(R) + 3f^4(R)]^{1/2}}{2[32 - 32f^2(R) + 6f^4(R) + [16 - 10f^2(R)][4 - 3f^2(R)]^{1/2}]^{1/2}},
$$
\n(18b)

$$
B_4 = -\frac{2 - 2f^2(R) + 2[1 - f^2(R)]^{1/2} \pm [4 - 3f^2(R)]^{1/2} \pm [4 - 7f^2(R) + 3f^4(R)]^{1/2}}{2[32 - 32f^2(R) + 6f^4(R) \pm [16 - 10f^2(R)][4 - 3f^2(R)]^{1/2}]^{1/2}},
$$
\n(18c)

$$
C_{\pm} = \frac{2 - f^2(R) \pm [4 - 3f^2(R)]^{1/2}}{\left[32 - 32f^2(R) + 6f^4(R) \pm [16 - 10f^2(R)] \left[4 - 3f^2(R)\right]^{1/2}\right]^{1/2}},
$$
\n(18d)

$$
a = \frac{1}{2}\sqrt{2} G[3 - 3f^{2}(R)]^{1/2} [4 - 3f^{2}(R)]^{-1/2} \left[ \frac{J^{2}N^{2}}{\Omega^{2}} [4 - 3f^{2}(R)] - 2G \frac{JN}{\Omega} + G^{2} \right]
$$
  
+ 
$$
\left( \frac{JN}{\Omega} - G[4 - 3f^{2}(R)]^{-1} \right) [4 - 3f^{2}(R)]^{1/2} \left( \frac{J^{2}N^{2}}{\Omega^{2}} [4 - 3f^{2}(R)] - 2G \frac{JN}{\Omega} + G^{2} \right)^{1/2} \Big]^{-1/2}, \quad (18e)
$$
  

$$
b = -\frac{1}{2}\sqrt{2} \left[ \left( \frac{JN}{\Omega} - G[4 - 3f^{2}(R)]^{-1} \right) [4 - 3f^{2}(R)]^{1/2} + \left( \frac{J^{2}N^{2}}{\Omega^{2}} [4 - 3f^{2}(R)] - 2G \frac{JN}{\Omega} + G^{2} \right)^{1/2} \right]^{1/2}
$$

$$
\times \left(\frac{J^2 N^2}{\Omega^2} \left[4 - 3f^2(R)\right] - 2G \frac{JN}{\Omega} + G^2\right)^{-1/4}.
$$
 (18f)

The correlation function  $\langle E_2 | \overline{\mathcal{S}}_1 \cdot \overline{\mathcal{S}}_2 | E_2 \rangle$  is given by

$$
\langle E_2 | \vec{S}_1 \cdot \vec{S}_2 | E_2 \rangle = \frac{1}{4} - \left( a \frac{2[1 - f^2(R)]^{1/2} + [4 - 7f^2(R) + 3f^4(R)]^{1/2}}{32 - 32f^2(R) + 6f^4(R) + [16 - 10f^2(R)][4 - 3f^2(R)]^{1/2}]^{1/2}} + b \frac{2[1 - f^2(R)]^{1/2} - [4 - 7f^2(R) + 3f^4(R)]^{1/2}}{32 - 32f^2(R) + 6f^4(R) - [16 - 10f^2(R)][4 - 3f^2(R)]^{1/2}]^{1/2}} \right)^2.
$$
 (19)

(iii) In the case where  $f^2(R) = -2\Omega G/JN$ , a peculiar thing happens—the two energy levels  $E_1$  and  $E_2$  coincide. The degeneracy of this level is further enlarged because, for this particular value of  $f^2(R)$ , this level coincides with the energy level

$$
E_3 = 2\epsilon + \frac{1}{4}G - \frac{1}{2}\left\{J^2N^2/(\Omega^2)\left[1 - f^2(R)\right] + G^2\right\}^{1/2} \tag{20}
$$

The degeneracy of the energy level  $E_3$  equals 3. The eigenvectors are given by

$$
|E_3,1\rangle = \frac{1}{2}c\left[\left(\left|1+,2-\right\rangle-\left|1-,2+\right\rangle\right)\right]\alpha\right\rangle + \left|1+,2+\right\rangle\left(\left|\beta\right\rangle-\left|\gamma\right\rangle\right)\right] + \frac{1}{2}d\left[\left(\left|1+,2-\right\rangle-\left|1-,2+\right\rangle\right)\right]\alpha\right\rangle - \left|1+,2+\right\rangle\left(\left|\beta\right\rangle-\left|\gamma\right\rangle\right)\right],
$$
\n
$$
|E_3,2\rangle = \frac{1}{2}c\left[\left(\left|1+,2-\right\rangle-\left|1-,2+\right\rangle\right)\right]\delta\right\rangle + \left|1-,2-\right\rangle\left(\left|\beta\right\rangle-\left|\gamma\right\rangle\right)\right]
$$
\n(21a)

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$$
+\frac{1}{2}d\left[\left(\left|1_{+},2_{-}\right\rangle-\left|1_{-},2_{+}\right\rangle\right)\left|\delta\right\rangle-\left|1_{-},2_{-}\right\rangle\left(\left|\beta\right\rangle-\left|\gamma\right\rangle\right)\right],\tag{21b}
$$

$$
|E_3, 3\rangle = (c/\sqrt{2}) (|1_+, 2_- \rangle |\beta\rangle - |1_-, 2_+ \rangle |\gamma\rangle) + (d/\sqrt{2}) (|1_+, 2_- \rangle |\gamma\rangle - |1_-, 2_+ \rangle |\beta\rangle), \qquad (21c)
$$

where

$$
c = \frac{G}{(2(J^2N^2/\Omega^2)[1 - f^2(R)] + 2G^2 - (2JN/\Omega)[1 - f^2(R)]^{1/2}\{(J^2N^2/\Omega^2)[1 - f^2(R)] + G^2\}^{1/2}} \,,
$$
 (22a)

$$
d = \frac{-(JN/\Omega)\left[1 - f^2(R)\right] + \left\{(J^2N^2/\Omega^2)\left[1 - f^2(R)\right] + G^2\right\}^{1/2}}{(2(J^2N^2/\Omega^2)\left[1 - f^2(R)\right] + 2G^2 - (2JN/\Omega)\left[1 - f^2(R)\right]^{1/2}\left\{(J^2N^2/\Omega^2)\left[1 - f^2(R)\right] + G^2\right\}^{1/2}\right\}^{1/2}} \tag{22b}
$$

The correlation function  $\langle E_3, i | \mathbf{\bar{\hat{S}}_1 \cdot \bar{\hat{S}_2}} | E_3, i \rangle$   $(i=1,$ 2, 2) reads

$$
\langle E_3 | \bar{S}_1 \cdot \bar{S}_2 | E_3 \rangle
$$
  
=  $-\frac{1}{4} + \frac{G}{2\{(J^2N^2/\Omega^2) [1 - f^2(R)] + G^2\}^{1/2}}$ . (23)

Therefore the total degeneracy equals 9 in the ease where  $f^2(R) = -2\Omega G/JN$ . The relevant correlation function is given by

$$
\frac{1}{9}(5\langle E_1|\overline{S}_1\cdot\overline{S}_2|E_1\rangle+\langle E_2|\overline{S}_1\cdot\overline{S}_2|E_2\rangle
$$
  
+3 $\langle E_3|\overline{S}_1\cdot\overline{S}_2|E_3\rangle)$   
= 
$$
-\frac{f^2(R)[10-3f^2(R)]}{12[2-f^2(R)]\ 4-f^2(R)}
$$
(24)

#### IV. DISCUSSION

As follows from the above, the correlation function  $\langle 0|\bar{S}_1 \cdot \bar{S}_2|0\rangle$ , which gives the information concerning the mutual direction of the magnetic moments in the ground state  $|0\rangle$ , is a quite intricate

function of  $|J/G|$  and  $f(R)$ . For this reason the correlation function has been plotted as a function of  $|J N/4\Omega G|$  for three values of  $|f(R)|$ , namely  $|f(R)| = 0$ , 0.4, and 0.9 (see Fig. 1). The behavior of the correlation function for other values of  $|f(R)|$ can easily be guessed from Fig. 1. The correlation function behaves in a peculiar way. With increasing direct interaction, it discontinuously jumps from a purely ferromagnetic to an antiferromagnetie character.

It is certainly noteworthy that the two types of interaction are unable to cancel out each other, i.e., a correlation which equals zero does not appear. It follows that the two moments are always coupled either in a purely ferromagnetic way,  $\langle 0|\bar{S}_1\cdot\bar{S}_2|0\rangle$  $=\frac{1}{4}$ , or in an antiferromagnetic way, where  $\langle 0|\bar{S}_1\cdot\bar{S}_2|0\rangle = -\frac{3}{4}$  holds only in the case that  $|JN/$  $4G\Omega$  = 0, i.e., the coupling is never antiferromaged netic unless  $J=0$ . The peculiar point which lies in the gap is due to the fact that in the case that  $f^2(R)$  $=-2\Omega G/JN$ , the energy levels  $E_1$  and  $E_2$  cross each other, while the degeneracy is enlarged by a third energy level  $E_3$ . Nothing further can be said about the nature of this point; its existence just follows from a purely quantum-mechanical calculation. It



FIG. 1. Correlation function  $\langle 0 | \bar{S}_1 \cdot \bar{S}_2 | 0 \rangle$  as a function of  $|JN/4\Omega G|$ plotted on a logarithmic scale. Curve a denotes the case  $f(R) = 0$ , curve b  $|f(R)|$ = 0. 4, and curve  $c |f(R)| = 0.9$ .

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is, however, noteworthy that the correlation between the two magnetic moments, as given by this point, tends to zero in the case that  $|2\Omega G/JN| \ll 1$ . In other words, when the  $s-d$  interaction strongly dominates the direct antiferromagnetic interaction, and because of the oscillating character of  $f(R)$ , there may exist a finite number of distances  $R_n$  between the two magnetic moments such that the correlation between these moments approximately equals zero in the case that  $f^2(R_n) = -2\Omega G/JN$  and  $f^2(R_n) \ll 1$ , while the correlation changes its character as soon as such a distance  $R_n$  has been passed by.

When  $|JN/2\Omega G| \leq 1$ , the relative influence of the direct antiferromagnetic interaction increases with increasing  $f^2(R)$ . When  $|JN/2\Omega G| > 1$ , the relative influence of the direct interaction increases with increasing  $f^2(R)$  until  $f^2(R)$  reaches the value  $-2\Omega G /$ <br>JN; for larger values of  $f^2(R)$ , the correlation will then switch to a purely ferromagnetic one. The fact that the antiferromagnetic correlation increases with increasing  $|f(R)|$  seems to be surprising for the following reason: As has been shown, the electron gas builds up a quasiparticle around each magnetic moment. The two quasiparticles are in general not independent-their wave functions overlap. This overlap  $f(R)$  is an oscillatory function of the distance  $R$  between the two magnetic moments; its amplitude decreases with increasing  $R$ , and it holds that  $|f(R)| < 1$ . The fact that the two quasiparticles are not independent induces the correlation between the magnetic moments via the  $s-d$  interaction. It is, therefore, remarkable that when  $f(R) = 0$ , i.e., the two quasiparticles are not interacting at all with each other, the ferromagnetic  $s-d$  interaction still influences the correlation between both magnetic moments, even in the maximal way, except of course when  $G = 0$ . This effect is caused by the fact that the Heisenberg interaction mixes the states  $|E_2\rangle$ , and  $|E_2\rangle$ , which are both eigenvectors of the Hamiltonian without this direct interaction. The resulting state is no longer an eigenstate of the  $G = 0$  Hamiltonian, and therefore the ferromagnetic s-d interaction will even influence the correlation between the two magnetic moments when  $f(R) = 0$ . This also follows directly from the fact that when  $f(R) = 0$ , the ground state is equivalent to the ground state of the following Hamiltonian:

 $H = -(JN/\Omega) (\bar{S}_1 \cdot \bar{S}_1 + \bar{S}_2 \cdot \bar{S}_2) - G \bar{S}_1 \cdot \bar{S}_2,$  (25)

where  $\bar{s}_1$  and  $\bar{s}_2$  are the spin operators of the two

spin clouds which are built up by the electron gas around the magnetic moments. It is obvious that the correlation between  $\bar{S}_1$  and  $\bar{S}_2$  will be influenced by  $\bar{s}_1$  and  $\bar{s}_2$ , i.e., by the ferromagnetic s-d coupling. Apparently the effect of an increasing overlap between the spin clouds is to strengthen the antiferromagnetic character of the coupling between the magnetic moments. Increasing the overlap, however, also means enlarging the energy of the system. Therefore, when the energy of the accompanying eigenstate becomes too large, the correlation switches to one of an entirely different character, namely, a purely ferromagnetic one. As follows from the calculations, the  $f(R) = 0$  situation has the lowest energy.

In conclusion it can be said that when the direct interaction strongly dominates the ferromagnetic s-d interaction, the correlation between the two magnetic moments will always be of an antiferromagnetic character. In the opposite ease it depends strongly on the distance between the two moments. Because of the fact that  $f(R)$  depends on the solid in which the two magnetic moments are imbedded, the situation might occur that for the same distance between the moments and for the same values of the coupling constants  $J$  and  $G$ , the correlation is ferromagnetic for one solid but antiferromagnetic for another. If, for instance, the assumption is made that the  $s-d$  interaction mainly operates within a small region around the Fermi surface of a freeelectron system, then  $f(R)$  can be approximated by  $f(R) = (\sin k_F R)/k_F R$ , where  $k_F$  clearly depends on the type of solid.

In the case of a dilute magnetic alloy, which has a narrow conduction band and mell-defined impurity spins, it has to be expected that  $|JN/4G\Omega| > 1$  up to  $|JN/4G\Omega| \gg 1$ . This means that the alloy is in the region of the discontinuity of  $\langle 0 | \bar{S}_1 \cdot \bar{S}_2 | 0 \rangle$  as a function of  $|JN/4G\Omega|$  and  $f(R)$ .

Finally, it should be remarked that most of the results mentioned above cannot be obtained by theories of the HKKY type.

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<sup>&</sup>lt;sup>1</sup>C. Zener, Phys. Rev.  $81, 440$  (1951).

 ${}^{2}$ M. A. Ruderman and C. Kittel, Phys. Rev. 96, 99 (1954).

 $3$ T. Kasuya, Progr. Theoret. Phys. (Kyoto)  $16, 45$ (1956).

 ${}^{4}$ K. Yosida, Phys. Rev. 106, 893 (1957).

<sup>&</sup>lt;sup>5</sup>G. Vertogen and W. J. Caspers, Phys. Status Solidi 25 721 (1968).

 $6G.$  Vertogen, Physica  $48, 509$  (1970).