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s-d Model with Nonspherical Fermi Surface*

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A study is made of the effects of a nonspherical and multiply connected Fermi surface on the properties of the Ruderman-Kittel-Kasuya-Yosida *s-d* interaction between localized spins and the conduction electrons. At a critical value of the conduction-electron concentration $\bar{N}_e$, the Fermi surface touches a number of Brillouin-zone faces, giving rise to a number of necks as in copper and nickel. It is shown that, in this region of electron concentration, the paramagnetic Curie temperature θ exhibits a kink associated with a discontinuity in the exchange-stiffness parameter $D \propto \sum \mathbf{R}^2 J(\mathbf{R})$, where $J(\mathbf{R})$ is the indirect-exchange parameter. These effects are expected to be more pronounced in materials with a large number of necks in the multiply connected Fermi surface. We choose the simplest possible model consistent with the crystal symmetry and the Bragg condition at the Brillouin-zone faces, i.e., a tight-binding approximation for the conduction electrons; but a number of results may be shown to be model-independent. We also neglect interband transitions, but these are shown not to affect the long-range component of the conduction-electron polarization. The long-range effects are shown to be model-independent because they are related only to the level-density function $\rho(\epsilon)$ and its derivatives at the Fermi level, whereas the short-range effects are shown to be sensitive to the details of the band structure. The paramagnetic temperature θ can be separated into a model-independent term related to $\rho(\epsilon_F)$ and a model-dependent term related to short-range effects. In the region corresponding to the spherical Fermi surface, θ is nearly proportional to $\bar{N}_e^{1/3}$, and the model-dependent contribution to θ is relatively small, at least for the simple cubic structure. It is also shown that the exchange moments $\langle \mathbf{R}^2 \rangle \propto \sum_{\mathbf{R}} \mathbf{R}^2 J(\mathbf{R})$ and $\langle \mathbf{R}^4 \rangle \propto \sum_{\mathbf{R}} \mathbf{R}^4 J(\mathbf{R})$ are model-independent and related to the level-density function $\rho(\epsilon)$ and its first and second derivatives at the Fermi level. In the neighborhood of the critical concentration, relatively large positive values of $\langle \mathbf{R}^4 \rangle / (a^2 \langle \mathbf{R}^2 \rangle)$ can be obtained for the simple cubic case, in contrast to the negative values of $\langle \mathbf{R}^4 \rangle / \langle \mathbf{R}^2 \rangle$ obtained by Kasuya in the limit $k_F a \to 0$.

I. INTRODUCTION

IT is the purpose of this paper to study the effects of a nonspherical and multiply connected Fermi surface on the properties of the Kasuya-Yosida[1,2] *s-d* interaction between localized spins and the conduction electrons, or the Ruderman-Kittel[3] indirect interaction between nuclear spins. This problem is here discussed essentially with the neglect of interband transitions; we choose a model simple enough to be treated mathematically, although some properties may be shown to be model-independent.

We consider the conduction-electron concentration $\bar{N}_e$ as a variable parameter. As we increase $\bar{N}_e$, the initially spherical Fermi surface expands and becomes increasingly deformed by approaching the Brillouin-zone boundaries. At a certain critical value of $\bar{N}_e$, the Fermi surface will touch a number of Brillouin-zone faces giving rise to a number of necks as in copper and nickel. The Brillouin-zone faces which first give rise to necks seem to be those closest to the origin in $\mathbf{k}$ space; in simple cubic structure there are six of these necks; fcc (Ni) and bcc (Fe) should have eight and 12 of them, respectively. It seems reasonable to expect that this type of effect will be more pronounced in metals with a large number of necks in the Fermi surface.

Denoting the conduction-electron single-particle unperturbed energy by $\epsilon_{\mathbf{k}}$, and the lattice parameter by a, we base our choice of model on the following requirements: (a) $\epsilon_{\mathbf{k}}$ should be proportional to $\mathbf{k}^2$ for $\mathbf{k}^2 a^2 \ll 1$, so that the results for the spherical model[1–3] can be reproduced in the limit $k_F{}^2 a^2 \ll 1$. (b) $\epsilon_{\mathbf{k}}$ must reflect the crystal symmetry. (c) $\epsilon_{\mathbf{k}}$ must fulfill the Bragg condition at the Brillouin-zone faces.

It may be shown, in general, that the above-mentioned touching points of the Fermi surface at some Brillouin-zone faces are points where $\mathrm{grad}_{\mathbf{k}} \epsilon_{\mathbf{k}} = 0$. This is a consequence of the Bragg condition. From this fact, one can show that the conduction-electron unperturbed level-density function $\rho(\epsilon)$ has a singularity when $\bar{N}_e$ reaches a critical value.

The simplest possible model, consistent with the above requirements and capable of giving rise to a multiply connected Fermi surface, can be obtained by assuming a tight-binding approximation for the conduction electrons in a band mainly of *s* character.

In Sec. II we describe the tight-binding approximation. There it is shown that, for the simple cubic structure, there are two critical values for the electron concentration.

The *s-d* Hamiltonian[1,4,5] can be written as

$$\mathcal{H}_{sd} = -N^{-1} \sum_{\mathbf{k}l} \sum_{\mathbf{k}'l'} \sum_{n} j(\mathbf{k}'l',\mathbf{k}l) e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}_n} \times \left[(a_{\mathbf{k}'l'+}{}^{\dagger} a_{\mathbf{k}l+} - a_{\mathbf{k}'l'-}{}^{\dagger} a_{\mathbf{k}l-}) S_n{}^z + a_{\mathbf{k}'l'+}{}^{\dagger} a_{\mathbf{k}l-} S_n{}^- + a_{\mathbf{k}'l'-}{}^{\dagger} a_{\mathbf{k}l+} S_n{}^+ \right], \quad (1.1)$$

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where we stress the fact that l and l' are band indices, so that $\mathbf{k}$ and $\mathbf{k}'$ are restricted to the first Brillouin zone; $a_{\mathbf{k}l\pm}^\dagger$ is the creation operator for a conduction electron with momentum $\mathbf{k}$, in band l, with spin up or down, respectively. $\mathbf{S}_n$ is the localized spin at site $\mathbf{R}_n$ of the lattice; $S_n^\pm = S_n^x \pm iS_n^y$. We assume that all sites n are occupied by d spins, so that we can preserve translational invariance. This last requirement can be relaxed in some cases. The quantity $j(\mathbf{k}l,\mathbf{k}'l')$ is a constant independent of $\mathbf{k}$ and $\mathbf{k}'$ in the case of nuclear hyperfine contact interaction; for the s-d model this quantity is given by

$$j(\mathbf{k}l,\mathbf{k}'l') = N\int \frac{e^2}{|\mathbf{r}_1-\mathbf{r}_2|}\phi_{\mathbf{k}'l'}^*(\mathbf{r}_1)\phi_d^*(\mathbf{r}_2) \times \phi_{\mathbf{k}l}(\mathbf{r}_2)\phi_d(\mathbf{r}_1)d\mathbf{r}_1 d\mathbf{r}_2. \quad (1.2)$$

The s-d Hamiltonian is now treated by applying perturbation theory. We assume, following Kittel and Mitchel,[6] that the conduction-electron system has a very short relaxation time so that they react very quickly to changes in the $\mathbf{S}$ coordinates. Consequently, when we calculate averages over the conduction-electron ensemble we can consider these $\mathbf{S}$ coordinates as c numbers. This is no longer true in an interval of time of the order of the localized spin relaxation time. It is also necessary to note that in the present paper we do not take into account a possible electron transfer from the d orbit to the conduction band, a mechanism proposed by Anderson and Clogston.[7]

Following Yosida,[2] the first-order perturbed wave function for the conduction electron is given by

$$\psi_{\mathbf{k}0\sigma}=\phi_{\mathbf{k}0\sigma}+\sum_{(\mathbf{k}'l'\sigma')\neq(\mathbf{k}0\sigma)} \frac{\langle \mathbf{k}'l'\sigma'|\mathcal{H}_{sd}|\mathbf{k}0\sigma\rangle}{\epsilon_{\mathbf{k}0}-\epsilon_{\mathbf{k}'l'}}\phi_{\mathbf{k}'l'\sigma'}, \quad (1.3)$$

where $\epsilon_{\mathbf{k}'l'}$ is the single-particle unperturbed energy, here assumed to be spin-independent; $\epsilon_{\mathbf{k}0}$ is the energy of an electron in the conduction band, for which we choose $l=0$, and $\sigma=\pm$ denotes the spin coordinate. Now we split the sum (1.3) in two terms: the intraband term and the interband term. The intraband contribution with $l'=0$ requires $(\mathbf{k}'\sigma')\neq(\mathbf{k}\sigma)$; the interband contribution corresponds to $l'\neq 0$, where the condition $(\mathbf{k}'\sigma')\neq(\mathbf{k}\sigma)$ is unnecessary.

Assuming that (a) the interband and intraband matrix elements of $\mathcal{H}_{sd}$ are of the same order of magnitude, and (b) the energy gap between the conduction band and the first-excited band is larger than or of the same order of the conduction-band width, then we can neglect the interband contribution. Even the assumption (b) does not seem to be essential. The reason for this is the presence of the denominator $\epsilon_{\mathbf{k}'l'}-\epsilon_{\mathbf{k}l}$. The integrals involving this denominator are mainly determined by the phase-space volume for which $\epsilon_{\mathbf{k}'l'}=\epsilon_{\mathbf{k}l}$. It is reasonable to expect the phase-space volume for $l'=l$ to be large compared with the corresponding phase volume for $l'\neq l$, where only some few special directions would allow $\epsilon_{\mathbf{k}'l'}=\epsilon_{\mathbf{k}l}$.

In Sec. III we define a momentum-dependent susceptibility function $F(\mathbf{q})$ whose Fourier transform is related to the spatial distribution of the conduction-electron spin polarization around a single magnetic ion as well as to the indirect exchange parameter $J(\mathbf{R})$. It is shown in Sec. V that the neglect of interband transitions does not effect the long-range component of the conduction-electron polarization since this is related to the behavior of the function $F(\mathbf{q})$ in the neighborhood of $\mathbf{q}=0$.

Consequently it is convenient to separate the long-range and the short-range effects. The measurable parameters related to the long-range component are shown to be model-independent since they are determined only by some features of the conduction-electron energy spectrum at the Fermi level. On the other hand, the short-range effects are model-dependent, i.e., they are sensitive to the details of band structure over the whole single-particle energy spectrum, as well as to the interband transitions here neglected.

With the neglect of interband transitions we can drop the index l, since we will be concerned only with the conduction band. The corresponding part of the s-d Hamiltonian becomes

$$\mathcal{H}_{sd} = -N^{-1}\sum_{\mathbf{k}\mathbf{k}'n} j(\mathbf{k},\mathbf{k}')e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}_n} \times[(a_{\mathbf{k}'+}^\dagger a_{\mathbf{k}+} - a_{\mathbf{k}'-}^\dagger a_{\mathbf{k}-})S_n^z + a_{\mathbf{k}'+}^\dagger a_{\mathbf{k}-}S_n^- + a_{\mathbf{k}'-}^\dagger a_{\mathbf{k}+}S_n^+]. \quad (1.4)$$

With the definitions

$$\mathbf{S}(\mathbf{k}-\mathbf{k}') = \frac{1}{N}\sum_n e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}_n}\mathbf{S}_n, \quad (1.5)$$

and

$$S_{\sigma'\sigma} = \begin{pmatrix} S^z & S^- \\ S^+ & -S^z \end{pmatrix}, \quad (1.6)$$

the s-d Hamiltonian can be separated into a diagonal part and an off-diagonal part:

$$\mathcal{H}_{sd} = \mathcal{H}_{sd}^0 + \mathcal{H}_{sd}', \quad (1.7)$$

$$\mathcal{H}_{sd}^0 = -\sum_{\mathbf{k}} j(\mathbf{k},\mathbf{k})(a_{\mathbf{k}+}^\dagger a_{\mathbf{k}+} - a_{\mathbf{k}-}^\dagger a_{\mathbf{k}-})S^z(0), \quad (1.8)$$

$$\mathcal{H}_{sd}' = -\sum_{(\mathbf{k}'\sigma')\neq(\mathbf{k}\sigma)} j(\mathbf{k},\mathbf{k}')a_{\mathbf{k}'\sigma'}^\dagger S_{\sigma'\sigma}(\mathbf{k}-\mathbf{k}')a_{\mathbf{k}\sigma}. \quad (1.9)$$

The unperturbed Hamiltonian is given by

$$\mathcal{H}_0 = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}}(a_{\mathbf{k}+}^\dagger a_{\mathbf{k}+} + a_{\mathbf{k}-}^\dagger a_{\mathbf{k}-}), \quad (1.10)$$

where $\epsilon_{\mathbf{k}}$ is the unperturbed single-particle energy, here assumed to be spin-independent.

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Using perturbation theory, in Sec. IV we determine the chemical potential and the ground-state energy of $\mathcal{H}_0'=\mathcal{H}_0+\mathcal{H}_{sd}^0$ [see (1.8) and (1.10)].

In Sec. V, the formulation given by Yosida[2] is extended by proving the model-independent result

$$\lim_{\mathbf{q}\to 0} F(\mathbf{q})=\tfrac{1}{2}\rho(\epsilon_F).$$

A study is made of the spatial distribution of the electronic polarization, with particular emphasis on parameters related to the long-range component. Some expressions are obtained for quantities that may become useful in connection with NMR, Mossbauer, and elastic neutron-scattering experiments.

In Sec. VI we study the indirect effective exchange interaction, and it is shown in Sec. VII that, as a consequence of the fluctuations in the localized spin coordinates $\mathbf{S}_n$ and the almost instantaneous response of the conduction electrons to these fluctuations, the conduction-electron spin polarization $\rho(\mathbf{r}=0)$ at the nuclear site also fluctuates around a certain average. These fluctuations in $\rho(\mathbf{r}=0)$ are expected to produce a broadening of the NMR linewidth as well as a broadening of the Mossbauer lines. At low temperatures, in the ferromagnetic state, the average squared fluctuation is shown to follow a T^3 law; in the paramagnetic region, the same quantity should be nearly proportional to $T\chi \propto T/(T-\theta)$, where χ is the magnetic susceptibility.

In Sec. VIII A it is shown that the paramagnetic temperature θ is the sum of a model-independent term proportional to the level-density function at the Fermi level and a term related to short-range effects which is model-dependent. In the limit corresponding to the spherical model, i.e., for $k_Fa\ll 1$, one can show that the model-dependent term is relatively small, at least in the simple cubic case; in this limit, the paramagnetic temperature may be shown to depend on the electron concentration through a term nearly proportional to $\bar{N}_e^{1/3}\propto \rho(\epsilon_F)$.

In Sec. VIII B we study some effects related to the thermal excitation of the conduction electrons in the neighborhood of the Fermi surface. This is shown to give rise to a temperature dependence of the indirect exchange parameter $J(\mathbf{R})$. Now, the critical temperature T_c is related to $\sum_{\mathbf{R}\neq 0} J(\mathbf{R})$, in the molecular-field approximation, so that T_c itself is temperature-dependent. Solving the self-consistency equation $T_c=\text{function}(T)=\text{function}(T_c)$ we obtain a correction for the critical temperature.

In Sec. VIII C it is obtained that in ferromagnetic dilute disordered alloys (as Fe:Au) the critical temperature T_c is a function of c, the concentration of magnetic impurity, and that T_c/c may decrease with concentration, as a consequence of the effect considered in Sec. VIII B.

The pressure dependence of T_c is shown in Sec. VIII D to contain a term which is not very sensitive to the details of band structure.

In Sec. IX we obtain the result that the exchange moments $\langle \mathbf{R}^2\rangle=\text{const}\sum_{\mathbf{R}} \mathbf{R}^2 J(\mathbf{R})$ and $\langle \mathbf{R}^4\rangle=\text{const}\times\sum_{\mathbf{R}} \mathbf{R}^4 J(\mathbf{R})$ related to the long-range component of $J(\mathbf{R})$ are determined by the level-density function $\rho(\epsilon)$ and its first and second derivatives at the Fermi level. Explicit expressions in terms of tabulated functions are obtained for $\langle \mathbf{R}^2\rangle$, $\langle \mathbf{R}^4\rangle$, $\langle R_x^4+R_y^4+R_z^4\rangle$, as well as for the paramagnetic temperature θ, and the quantity $(\partial/\partial\epsilon_F)J(\mathbf{R}=0)$, in the case of the simple cubic structure.

In the region of electron concentration corresponding to the spherical model, i.e., for $k_Fa\ll 1$, the results obtained by Kasuya for $\langle \mathbf{R}^2\rangle$ and $\langle \mathbf{R}^4\rangle$ are reproduced; in this region of electron concentration (for $k_Fa\ll 1$), we obtain

$$\langle R_x^4+R_y^4+R_z^4\rangle/\langle \mathbf{R}^4\rangle\approx \tfrac{3}{5}.$$

In the neighborhood of the first critical electron concentration, just before the formation of necks in a multiply connected Fermi surface (for $\omega\lesssim -1$, see text), we obtain a positive value for $\langle \mathbf{R}^2\rangle$ (as in the spherical model) and relatively large positive values for the ratio $\langle \mathbf{R}^4\rangle/(a^2\langle \mathbf{R}^2\rangle)$ in contrast with a negative ratio obtained by Kasuya[1] in the spherical model; for $\omega=-1-\eta$, with $0<\eta\ll 1$, we obtain for the simple cubic case the result

$$\langle R_x^4+R_y^4+R_z^4\rangle/\langle \mathbf{R}^4\rangle\approx 9/7,$$

that is, a value about twice as large as the one obtained in the region $k_Fa\ll 1$, where the Fermi surface is nearly spherical.

In the final section, some applications are made to rare-earth metallic compounds and alloys.

II. TIGHT-BINDING APPROXIMATION

The unperturbed Schrödinger equation is given by[8]

$$\mathcal{H}_0\phi_{\mathbf{k}}(\mathbf{r})=[-(h^2/2m)\nabla^2+V(\mathbf{r})]\phi_{\mathbf{k}}(\mathbf{r})=\epsilon_{\mathbf{k}}\phi_{\mathbf{k}}(\mathbf{r}), \quad (2.1)$$

where

$$V(\mathbf{r})=\sum_n U(\mathbf{r}-\mathbf{R}_n) \quad (2.2)$$

is the periodic potential and $U(\mathbf{r}-\mathbf{R}_n)$ is the local potential in the neighborhood of ion $\mathbf{R}_n$. In the tight-binding approximation, the wave function $\phi_{\mathbf{k}}(\mathbf{r})$ is constructed from the localized s-wave functions $\phi_s(\mathbf{r}-\mathbf{R}_n)$,

$$\phi_{\mathbf{k}}(\mathbf{r})=e^{i\mathbf{k}\cdot\mathbf{r}}u_{\mathbf{k}}(\mathbf{r}), \quad (2.3)$$

where

$$u_{\mathbf{k}}(\mathbf{r})=\sum_n e^{i\mathbf{k}\cdot(\mathbf{R}_n-\mathbf{r})}\phi_s(\mathbf{r}-\mathbf{R}_n) \quad (2.4)$$

is periodic from cell to cell in the crystal, and $\phi_s(\mathbf{r})$ is the solution of the local Schrödinger equation

$$[-(h^2/2m)\nabla^2+U(\mathbf{r})]\phi_s(\mathbf{r})=E_s\phi_s(\mathbf{r}). \quad (2.5)$$

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[8] See, for example, A. H. Wilson, *The Theory of Metals* (Cambridge University Press, Cambridge, England, 1958), 2nd ed., Sec. 2.7.

The single-particle energy $\epsilon_{\mathbf{k}}$ in (2.1) is obtained as

$$\epsilon_{\mathbf{k}}=\int_V \phi_{\mathbf{k}}^*(\mathbf{r})\mathcal{H}_0\phi_{\mathbf{k}}(\mathbf{r})d\mathbf{r}\Big/\int_V \phi_{\mathbf{k}}^*(\mathbf{r})\phi_{\mathbf{k}}(\mathbf{r})d\mathbf{r}\,, \tag{2.6}$$

where V is the volume of the sample.

Defining the overlap integrals

$$\mathcal{H}(\mathbf{R}_n)=\int_V \phi_s^*(\mathbf{r}+\mathbf{R}_n)\mathcal{H}_0\phi_s(\mathbf{r})d\mathbf{r}\,, \tag{2.7}$$

$$S(\mathbf{R}_n)=\int_V \phi_s^*(\mathbf{r}+\mathbf{R}_n)\phi_s(\mathbf{r})d\mathbf{r}\,, \tag{2.8}$$

we obtain

$$\epsilon_{\mathbf{k}}=\sum_n e^{i\mathbf{k}\cdot\mathbf{R}_n}\mathcal{H}(\mathbf{R}_n)/\sum_n e^{i\mathbf{k}\cdot\mathbf{R}_n}S(\mathbf{R}_n)\,,$$

or

$$\epsilon_{\mathbf{k}}\approx[\mathcal{H}(0)+\sum_{\langle n\rangle} e^{i\mathbf{k}\cdot\mathbf{R}_n}\mathcal{H}(\mathbf{R}_n)]/[S(0)+\sum_{\langle n\rangle} e^{i\mathbf{k}\cdot\mathbf{R}_n}S(\mathbf{R}_n)]\,, \tag{2.9}$$

where $\sum_{\langle n\rangle}$ is the sum over the nearest neighbors, and more distant integrals are neglected. Furthermore, $\mathcal{H}(0)=E_s$ and $S(0)=1$ may be assumed relatively large, so that the single-particle energy becomes

$$\epsilon_{\mathbf{k}}\approx E_s+B\gamma_{\mathbf{k}}\,. \tag{2.10}$$

Here B is a negative constant (the local potential is attractive) related to the overlapping integrals $\mathcal{H}(nn)$ and $S(nn)$, and $\gamma_{\mathbf{k}}$ is the nearest-neighbor structure factor

$$\gamma_{\mathbf{k}}=\frac{1}{z}\sum_{\langle n\rangle} e^{i\mathbf{k}\cdot\mathbf{R}_n}\,, \tag{2.11}$$

where z is the number of nearest neighbors. We also note that in (2.9) we have used the equivalence of all nearest neighbors.

In the particular case of the simple cube lattice we can write

$$\epsilon_{\mathbf{k}}\approx\tfrac{1}{3}B\sum_j \cos(ak_j)\,, \tag{2.12}$$

where we have dropped the constant E_s, since we are concerned only with differences of energies. Here we note that $-|B|<\epsilon_{\mathbf{k}}<|B|$, so that

$$-|B|<\epsilon_F<|B|\,. \tag{2.13}$$

Defining the dimensionless parameter

$$\omega=3\epsilon_F/|B|\,, \tag{2.14}$$

we obtain

$$-3<\omega<+3\,. \tag{2.15}$$

It is easy to see that expression (2.12) gives rise to the necks mentioned in the Introduction. The Bragg condition tells us that the vector $\mathrm{grad}_{\mathbf{k}}\epsilon_{\mathbf{k}}$ is parallel to the Brillouin-zone face at the intersection of the Fermi surface with the Brillouin-zone boundary. If one considers, for example, the plane square net, from geometrical considerations one can show that $\mathrm{grad}_{\mathbf{k}}\epsilon_{\mathbf{k}}=0$ at the touching (critical) points mentioned in the Introduction.

For the simple cubic structure, the condition

$$\mathrm{grad}_{\mathbf{k}}\epsilon_{\mathbf{k}}=0 \tag{2.16}$$

gives rise to a set of three equations

$$\sin(ak_j)=0 \quad (j=x,y,z)\,,$$

so that $ak_j=0,\pm\pi$. Then we obtain the following set of points, for which the Eq. (2.16) is satisfied:

(a) $a\mathbf{k}=(0,0,0)$;

(b) $a\mathbf{k}=(0,0,\pm\pi)$, $(0,\pm\pi,0)$, and $(\pm\pi,0,0)$;

(c) $a\mathbf{k}=(0,\pm\pi,\pm\pi)$, $(\pm\pi,0,\pm\pi)$, and $(\pm\pi,\pm\pi,0)$;

(d) $a\mathbf{k}=(\pm\pi,\pm\pi,\pm\pi)$.

The parameter ω defined in (2.14) assumes the values $\omega_a=-3$, $\omega_b=-1$, $\omega_c=+1$, and $\omega_d=+3$, respectively, at the above points.

We also note that, from symmetry considerations, the exchange parameter $j(\mathbf{k},\mathbf{k})$ defined in (1.2), with $\mathbf{k}'=\mathbf{k}$, has the same value at the different points belonging to the same set.

In this way one can see that the region $\omega\gtrsim-3$ corresponds to a spherical Fermi surface, as well as the region $\omega\lesssim+3$. The former is of particle character and the latter of hole character.

As we increase ω from the bottom of the band, where $\omega=-3$, when ω reaches the critical value $\omega_b=-1$, the Fermi surface will just touch the Brillouin-zone cubic faces at the points of type (b), i.e., at the center of the Brillouin-zone cubic faces.

For $-1<\omega<1$, the Fermi surface becomes multiply connected and with six necks. As we increase ω from -1 to $+1$ it seems difficult to ascertain the shape of the Fermi surface for $\omega=+1$. But if we start from $\omega\leqslant+3$, first recomposing the eight pieces of the Fermi surface to obtain a continuous sphere, then, as we decrease the value of ω, we again obtain, for $\omega\leqslant+1$, a multiply connected Fermi surface with six necks and whose interior is empty.

III. *q*-DEPENDENT SUSCEPTIBILITY FUNCTION

The spin-dependent perturbed wave function is given by

$$\psi_{\mathbf{k}\pm}(\mathbf{r})=\phi_{\mathbf{k}\pm}-\sum_{\mathbf{k}'\neq\mathbf{k}}{}'\frac{j(\mathbf{k},\mathbf{k}')}{\epsilon_{\mathbf{k}}-\epsilon_{\mathbf{k}'}}\times[\pm S^z(\mathbf{k}-\mathbf{k}')\phi_{\mathbf{k}'\pm}+S^{\pm}(\mathbf{k}-\mathbf{k}')\phi_{\mathbf{k}'\mp}]\,, \tag{3.1}$$

where the prime in the summation is to indicate that $\mathbf{k}'$ is restricted to the first Brillouin zone. For the simple cubic system this condition is given by $-\pi<ak_j'\leqslant\pi$.

The polarization of the conduction-electron band can be obtained by calculating the density of electrons with spin up and down:

$$\rho_{\pm}(\mathbf{r})=\sum_{\text{occ. states}}\psi_{\mathbf{k}\pm}{}^{*}(\mathbf{r})\psi_{\mathbf{k}\pm}(\mathbf{r})\,. \tag{3.2}$$

Using (3.1) and the representation (2.3) for $\phi_{\mathbf{k}}(\mathbf{r})$, we obtain

$$\rho_{\pm}(\mathbf{r})=\sum_{\mathbf{k}} n_{\mathbf{k}}{}^{\pm}u_{\mathbf{k}}{}^{*}(\mathbf{r})u_{\mathbf{k}}(\mathbf{r}) \mp\Bigg[\sum_{\mathbf{k}'\neq\mathbf{k}}{}' n_{\mathbf{k}'}\frac{j(\mathbf{k},\mathbf{k}')}{\epsilon_{\mathbf{k}}-\epsilon_{\mathbf{k}'}}S^{z}(\mathbf{k}-\mathbf{k}')e^{i(\mathbf{k}'-\mathbf{k})\mathbf{r}} \times u_{\mathbf{k}}{}^{*}(\mathbf{r})u_{\mathbf{k}'}(\mathbf{r})+\text{c.c.}\Bigg], \tag{3.3}$$

where $n_{\mathbf{k}}{}^{\pm}$ is the Fermi distribution function for the two sets of spins up and down, respectively. The second term in (3.3) involves a sum over the indices $\mathbf{k}$ and $\mathbf{k}'$. In the second term we do not have to distinguish $n_{\mathbf{k}}{}^{-}$ from $n_{\mathbf{k}}{}^{+}$ since this produces only a second-order correction in j^2, whereas in the first term this distinction is necessary because it corresponds to a correction in first order of j.

Using the tight-binding approximation we obtain

$$u_{\mathbf{k}}{}^{*}(\mathbf{r})u_{\mathbf{k}'}(\mathbf{r})\approx U_{\mathbf{k}'-\mathbf{k}}(\mathbf{r})\,, \tag{3.4}$$

where

$$U_{\mathbf{q}}(\mathbf{r})=\sum_{n} e^{i\mathbf{q}\cdot(\mathbf{R}_n-\mathbf{r})}|\phi_s(\mathbf{r}-\mathbf{R}_n)|^2 \tag{3.5}$$

is a periodic function of $\mathbf{r}$ from cell to cell. The next term in (3.4) involves nearest-neighbor overlap products $\phi_s(\mathbf{r}-\mathbf{R}_n)\phi_s(\mathbf{r}-\mathbf{R}_n+\mathbf{R}_m)$. Some properties of the function $U_{\mathbf{q}}(\mathbf{r})$ are

$$U_{-\mathbf{q}}(\mathbf{r})=U_{\mathbf{q}}(-\mathbf{r}) \tag{3.6}$$

and

$$U_{\mathbf{q}}{}^{*}(\mathbf{r})=U_{-\mathbf{q}}(\mathbf{r})\,. \tag{3.7}$$

We now assume that $j(\mathbf{k},\mathbf{k}')$ depends only on the vector $\mathbf{k}'-\mathbf{k}$. We will see that sometimes it is possible to lift this restriction. Then we obtain

$$\rho_{\pm}(\mathbf{r})=U_0(\mathbf{r})\sum_{\mathbf{k}} n_{\mathbf{k}}{}^{\pm} \pm\Big[\sum_{\mathbf{q}\neq 0}{}' j(\mathbf{q})S^{z}(-\mathbf{q})e^{i\mathbf{q}\cdot\mathbf{r}}U_{\mathbf{q}}(\mathbf{r})F(\mathbf{q})+\text{c.c.}\Big], \tag{3.8}$$

where

$$F(\mathbf{q})=\sum_{k}{}'\frac{n_{\mathbf{k}}}{\epsilon_{\mathbf{k}+\mathbf{q}}-\epsilon_{\mathbf{k}}}, \tag{3.9}$$

and the prime in summation (3.9) is to indicate that $\mathbf{q}$ is to be restricted in such a way that $\mathbf{k}$ and $\mathbf{k}'=\mathbf{k}+\mathbf{q}$ belong to the first Brillouin zone. To avoid this complication we can write

$$\sum_{\mathbf{k}}{}'\frac{n_{\mathbf{k}}}{\epsilon_{\mathbf{k}+\mathbf{q}}-\epsilon_{\mathbf{k}}}=\frac{V}{8\pi^3}\int_{\text{BZ}}' d\mathbf{k}\frac{n_{\mathbf{k}}}{\epsilon_{\mathbf{k}+\mathbf{q}}-\epsilon_{\mathbf{k}}},$$

or

$$F(\mathbf{q})=\frac{V}{8\pi^3}\int_{\text{BZ}} d\mathbf{k}\,n_{\mathbf{k}}\int_{\text{BZ}} d\mathbf{k}'\frac{1}{\epsilon_{\mathbf{k}'}-\epsilon_{\mathbf{k}}}\delta(\mathbf{k}'-\mathbf{k}-\mathbf{q})\,, \tag{3.10}$$

so that the restriction for $\mathbf{k}$ and $\mathbf{k}'$ in the first Brillouin zone is explicitly taken into account. It is important to realize the necessity of this restriction, in connection with the fact that l and l' are band indices and that we are not using the extended zone scheme.

The function $F(\mathbf{q})$, here called the momentum-dependent susceptibility function, will be the center of our discussion. For the simple cubic case, the vectors $\mathbf{k}$ and $\mathbf{k}'$ are restricted by $-\pi<ak_j\leqslant\pi$ and $-\pi<ak_j'\leqslant\pi$, and consequently $\mathbf{q}$ is limited to the interior of the cube $-2\pi<aq_j<2\pi$, where the equal sign is not allowed. Outside this volume $F(\mathbf{q})$ is zero as we can see from (3.10). For other lattice structures, as long as we use (3.10) we can extend the sum over $\mathbf{q}$ in (3.8) to infinity. To determine this function $F(\mathbf{q})$ we need the explicit k dependence of $\epsilon_{\mathbf{k}}$, not only near the Fermi surface but throughout the Brillouin zone.

The fact that $F(\mathbf{q})$ is zero outside the region $-2\pi<aq_j<2\pi$ results from the neglect of the interband terms in (1.3). This corresponds to cutting Yosida's function $f(|\mathbf{q}|)$ at a point where $f(|\mathbf{q}|)$ is already small. This becomes more evident if we take in the Yosida spherical model a value $ak_F\sim\frac{1}{2}\pi$, for example. We note that $k_F\sim\pi/a$ corresponds roughly to a completely filled Brillouin zone. Then, for $|\mathbf{q}|>2\pi/a$, we obtain $q/2k_F\sim qa/\pi>2$. In other words, the region $|q_j|>2\pi/a$ corresponds to $q/2k_F\gtrsim 2$, where the Yosida function $f(|\mathbf{q}|)$ is already small compared to unity.

It is shown in Sec. V that the conduction-electron spin polarization $P(\mathbf{r})$ [see (5.19)] produced by a single localized magnetic ion has a spatial distribution related to the Fourier transform of the susceptibility function $F(\mathbf{q})$. This becomes clearer in Sec. IX, where the indirect exchange parameter $J(\mathbf{R})$ [see (9.11)] is shown to be also related to the Fourier transform of $F(\mathbf{q})$.

Now, from the Fourier theorem, we know that the behavior of the Fourier transform of $F(\mathbf{q})$ at large distances is determined by the properties of the function $F(\mathbf{q})$ in the neighborhood of $\mathbf{q}=0$. Being more explicit, if we know the function $F(\mathbf{q})$ in the finite region $|\mathbf{q}|<q_0$, then we can determine the behavior of its Fourier transform in the region $|\mathbf{r}|>10/q_0$, say.

The cutoff introduced in $F(\mathbf{q})$ by the neglect of interband transitions occurs only outside a region sufficiently large (a cube of side $4\pi/a$ in the simple cubic case). In the simple cubic case,

$$q_0\approx 2\pi/a\,,$$

so that we can determine the conduction-electron polarization in the region $|\mathbf{r}|>r_0$, where

$$r_0\approx 10a/2\pi\approx 2a\,,$$

and in this way we obtain the result that the interband transitions of the type considered in this paper (see the Introduction) do not affect the long-range component of the conduction-electron spin polarization $P(\mathbf{r})$ or of the indirect-exchange parameter $J(\mathbf{R})$.

It is demonstrated in Sec. V that in the first term of (3.8), the difference between $n_\mathbf{k}^+$ and $n_\mathbf{k}^-$ gives rise to a term which is just that required to complete the sum over $\mathbf{q}$ in the second term of (3.8). The first term in (3.8) can be shown to be related to the diagonal part of $\mathcal{H}_{sd}$, whereas the second term in $\mathbf{q}\neq 0$ is related to the off-diagonal part.

IV. PERTURBED ENERGY

A. Chemical Potential

Using (1.7) and (1.10), the total Hamiltonian can be written as

$$\mathcal{H}=\mathcal{H}_0'+\mathcal{H}_{sd}', \tag{4.1}$$

where $\mathcal{H}_{sd}'$ is given by (1.9) and

$$\mathcal{H}_0'=\mathcal{H}_0+\mathcal{H}_{sd}^0=\sum_\mathbf{k}\left(\epsilon_\mathbf{k}^+a_{\mathbf{k}+}^\dagger a_{\mathbf{k}+}+\epsilon_\mathbf{k}^-a_{\mathbf{k}-}^\dagger a_{\mathbf{k}-}\right), \tag{4.2}$$

$$\epsilon_\mathbf{k}^\pm=\epsilon_\mathbf{k}\mp A\,, \tag{4.3}$$

and

$$A=j(0)S^z(0)\,, \tag{4.4}$$

as one obtains from (1.8) and (1.10).

Denoting by $|0\rangle$ the ground state of $\mathcal{H}_0'$ and by $|\Psi_0\rangle$ the ground state of $\mathcal{H}$, the perturbation expansion for $\langle\Psi_0|\mathcal{H}|\Psi_0\rangle$ is given by[9]

$$\langle\Psi_0|\mathcal{H}|\Psi_0\rangle=\langle 0|\mathcal{H}_0'|0\rangle+\langle 0|\mathcal{H}_{sd}'|0\rangle+\sum_{n\neq 0}\frac{\langle 0|\mathcal{H}_{sd}'|n\rangle\langle n|\mathcal{H}_{sd}'|0\rangle}{E_0-E_n}, \tag{4.5}$$

where E_0 and E_n are the eigenvalues of $\mathcal{H}_0'$ in the ground state $|0\rangle$ and in the excited state $|n\rangle$, respectively; $\langle 0|\mathcal{H}_{sd}'|0\rangle$ is equal to zero since $\mathcal{H}_{sd}'$ contains only off-diagonal terms.

The state $|0\rangle$ is characterized by the fact that all single-particle states $\epsilon_\mathbf{k}^\pm$ below a certain energy μ are occupied and all others are unoccupied. Later, when necessary, we will replace this square distribution by the Fermi distribution appropriate to a temperature T. We also note that the chemical potential μ for $\mathcal{H}_0'$ is different from ϵ_F, the corresponding quantity for $\mathcal{H}_0$. Denoting by N_e the total number of conduction electrons, the perturbed chemical potential μ is determined by the condition

$$\begin{aligned}N_e&=\sum_{\mathbf{k}\ (\epsilon_\mathbf{k}^+<\mu)}1+\sum_{\mathbf{k}\ (\epsilon_\mathbf{k}^-<\mu)}1\\&=\frac{V}{8\pi^3}\left[\int_{\epsilon_\mathbf{k}<\mu+A}d\mathbf{k}+\int_{\epsilon_\mathbf{k}<\mu-A}d\mathbf{k}\right]\\&=\int_{E_b}^{\mu+A}\rho(\epsilon)d\epsilon+\int_{E_b}^{\mu-A}\rho(\epsilon)d\epsilon,\end{aligned} \tag{4.6}$$

where E_b is the single-particle energy corresponding to the bottom of the unperturbed band and $\rho(\epsilon)$, the unperturbed energy-level density of the conduction electron for each spin state, is given by

$$\rho(\epsilon)=\frac{V}{8\pi^3}\int_{\mathrm{BZ}}\delta(\epsilon-\epsilon_\mathbf{k})d\mathbf{k}. \tag{4.7}$$

The *s-d* Hamiltonian conserves the total number of conduction electrons. Consequently, in absence of the interaction we can write

$$N_e=2\int_{E_b}^{\epsilon_F}\rho(\epsilon)d\epsilon. \tag{4.8}$$

Using the Taylor-series expansion of $\rho(\epsilon)$ in the region $\mu-A<\epsilon<\mu+A$, and equating (4.8) and (4.6), we obtain

$$2\int_{E_b}^{\epsilon_F}\rho(\epsilon)d\epsilon=2\int_{E_b}^{\mu}\rho(\epsilon)d\epsilon+A^2\rho'(\mu)\,, \tag{4.9}$$

where we have kept only terms up to second order in A. From (4.9) we derive

$$2\int_{\epsilon_F}^{\mu}\rho(\epsilon)d\epsilon=-A^2\rho'(\mu) \tag{4.10}$$

or

$$\mu\approx\epsilon_F-\tfrac{1}{2}A^2\frac{\rho'(\epsilon_F)}{\rho(\epsilon_F)}\,, \tag{4.11}$$

where we can see that μ differs from ϵ_F only by a term in second order of the *s-d* interaction. From (4.11) we can derive a necessary condition for the validity of perturbation theory, which is

$$\tfrac{1}{2}A^2\left|\frac{\rho'(\epsilon_F)}{\epsilon_F\rho(\epsilon_F)}\right|\ll 1. \tag{4.12}$$

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[9] See, for example, C. Kittel, *Quantum Theory of Solids* (John Wiley & Sons, Inc., New York, 1963).

B. Ground-State Energy of $\mathcal{H}_0'$

The ground-state energy of $\mathcal{H}_0'$ defined in (4.1) and (4.2) can now be obtained as

$$\begin{aligned}\langle 0|\mathcal{H}_0'|0\rangle &= \sum_{\mathbf{k}\ (\epsilon_{\mathbf{k}}^+<\mu)} \epsilon_{\mathbf{k}}^+ + \sum_{\mathbf{k}\ (\epsilon_{\mathbf{k}}^-<\mu)} \epsilon_{\mathbf{k}}^- \\ &= \int_{E_b}^{\mu+A} (\epsilon-A)\rho(\epsilon)d\epsilon \\ &\qquad + \int_{E_b}^{\mu-A} (\epsilon+A)\rho(\epsilon)d\epsilon. \end{aligned} \tag{4.13}$$

Using the expansion

$$\rho(\epsilon)=\rho(\mu)+(\epsilon-\mu)\rho'(\mu)+\tfrac{1}{2}(\epsilon-\mu)^2\rho''(\mu)+\cdots, \tag{4.14}$$

the expression (4.13) becomes

$$\langle 0|\mathcal{H}_0'|0\rangle = 2\int_{E_b}^{\mu} \epsilon\rho(\epsilon)d\epsilon + A^2[-\rho(\mu)+\mu\rho'(\mu)], \tag{4.15}$$

where, in the second term, we can replace $-\rho(\mu)+\mu\rho'(\mu)$ by $-\rho(\epsilon_F)+\epsilon_F\rho'(\epsilon_F)$ with an error of order A^4. Taking into account the result (4.11) the final expression becomes

$$\langle 0|\mathcal{H}_0'|0\rangle = 2\int_{E_b}^{\epsilon_F} \epsilon\rho(\epsilon)d\epsilon - A^2\rho(\epsilon_F), \tag{4.16}$$

where the first term is the total energy of the conduction electrons in absence of the s-d interaction.

The expressions (4.11) and (4.16) are generalizations of previous results obtained by Yosida[2] using the spherical model with $\epsilon_{\mathbf{k}}=\hbar^2\mathbf{k}^2/2m$. The above results are general; in other words, they do not depend on any specific assumption on the $\mathbf{k}$ dependence of the single-particle energies $\epsilon_{\mathbf{k}}$. The only condition for their validity is that $j(\mathbf{k},\mathbf{k}')u_{\mathbf{k}}^*(\mathbf{r})u_{\mathbf{k}'}(\mathbf{r})$ must depend only on the vectors $\mathbf{k}'-\mathbf{k}$, and $\mathbf{r}$, obviously.

V. SPIN POLARIZATION

Now we are prepared to discuss the first term in (3.8). If we define $n^\pm=\sum_{\mathbf{k}} n_{\mathbf{k}}^\pm$, we obtain

$$n^\pm = \int_{E_b}^{\mu\pm A} \rho(\epsilon)d\epsilon \approx \int_{E_b}^{\epsilon_F\pm A} \rho(\epsilon)d\epsilon, \tag{5.1}$$

up to terms linear in A, since from (4.11), μ differs from ϵ_F only by a term in A^2. The result is that

$$n^\pm = n\pm A\rho(\epsilon_F), \tag{5.2}$$

where $n=\tfrac{1}{2}N_e$ and $A=j(0)S^z(0)$.

Replacing (5.2) in (3.8), we obtain

$$\begin{aligned}\rho_\pm(\mathbf{r}) &= U_0(\mathbf{r})n \pm j(0)S^z(0)U_0(\mathbf{r})\rho(\epsilon_F) \\ &\quad \pm \sum_{\mathbf{q}\neq 0} [j(\mathbf{q})S^z(-\mathbf{q})e^{i\mathbf{q}\cdot\mathbf{r}}U_{\mathbf{q}}(\mathbf{r})F(\mathbf{q})+\text{c.c.}], \end{aligned} \tag{5.3}$$

where the second term is the Zener-Fröhlich-Nabarro[10,11] (ZFN) polarization.

It is possible to prove that the correct form for the ZFN polarization, in the general case, should read

$$\langle j(\mathbf{k},\mathbf{k})|u_{\mathbf{k}}(\mathbf{r})|^2\rangle_F S^z(0)\rho(\epsilon_F), \tag{5.4}$$

where the average of a function $\Phi(\mathbf{k})$ over the Fermi surface is defined by

$$\langle\Phi(\mathbf{k})\rangle_F = \int_{\mathrm{BZ}} \Phi(\mathbf{k})\delta(\epsilon-\epsilon_{\mathbf{k}})d\mathbf{k} \Big/ \int_{\mathrm{BZ}} \delta(\epsilon-\epsilon_{\mathbf{k}})d\mathbf{k}, \tag{5.5}$$

or

$$\langle\Phi(\mathbf{k})\rangle_F = \int_{\mathrm{FS}} \Phi(\mathbf{k})\frac{dS_{\mathbf{k}}}{|\mathbf{v}_k|} \Big/ \int_{\mathrm{FS}} \frac{dS_{\mathbf{k}}}{|\mathbf{v}_k|}, \tag{5.6}$$

where $\mathbf{v}_{\mathbf{k}}=(1/\hbar)\mathrm{grad}_{\mathbf{k}}\epsilon_{\mathbf{k}}$ is the conduction-electron group velocity. In (5.6) the integrals are to be extended over the Fermi surface, where $\epsilon_{\mathbf{k}}=\epsilon_F$.

In the right-hand side of (5.3) we note that the second term involving $\mathbf{q}=0$ is related to a factor $\rho(\epsilon_F)$, whereas the term $\mathbf{q}=0$ absent in the third term involves a factor $2F(0)$.

Now we prove the following important theorem, valid at $T=0$°K:

$$\lim_{\mathbf{q}\to 0} F(\mathbf{q}) = +\tfrac{1}{2}\rho(\epsilon_F). \tag{5.7}$$

The result (5.7) can be proved by calculating separately $\rho(\epsilon_F)$ and the limit in the simple cubic case; this proof is given in Appendix A. We prefer the demonstration given here which has the advantage of being model-independent.

At $T=0$°K, Eq. (3.10) becomes

$$F(\mathbf{q}) = \frac{V}{8\pi^3}\int_{\mathrm{BZ}} d\mathbf{k}\,\theta(\epsilon_F-\epsilon_{\mathbf{k}}) \int_{\mathrm{BZ}} \frac{d\mathbf{k}'}{\epsilon_{\mathbf{k}'}-\epsilon_{\mathbf{k}}}\delta(\mathbf{k}'-\mathbf{k}-\mathbf{q}), \tag{5.8}$$

where $\theta(x)$ is the step function, with value 1 for $x>0$, and zero for $x<0$.

The above expression, as it stands, is not defined at $\mathbf{q}=0$. If we follow Van Vleck[12] and replace $1/(\epsilon_{\mathbf{k}'}-\epsilon_{\mathbf{k}})$ by its principal part we can see that the limit of $F(\mathbf{q})$, for $\mathbf{q}\to 0$, is a well-defined quantity.

Differentiating $F(\mathbf{q})$ with respect to ϵ_F we obtain

$$\begin{aligned} G(\mathbf{q}) &= \frac{\partial F(\mathbf{q})}{\partial\epsilon_F} \\ &= \frac{V}{8\pi^3}\int_{\mathrm{BZ}} d\mathbf{k}\,\delta(\epsilon_F-\epsilon_{\mathbf{k}}) \int_{\mathrm{BZ}} P\frac{d\mathbf{k}'}{\epsilon_{\mathbf{k}'}-\epsilon_{\mathbf{k}}}\delta(\mathbf{k}'-\mathbf{k}-\mathbf{q}) \\ &= \frac{V}{8\pi^3}\int_{\mathrm{BZ}} d\mathbf{k}\,\delta(\epsilon_F-\epsilon_{\mathbf{k}}) \int_{\mathrm{BZ}} P\frac{d\mathbf{k}'}{\epsilon_{\mathbf{k}'}-\epsilon_F}\delta(\mathbf{k}'-\mathbf{k}-\mathbf{q}), \end{aligned} \tag{5.9}$$

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[10] C. Zener, Phys. Rev. **81**, 440 (1951).

[11] H. Fröhlich and F. R. N. Nabarro, Proc. Roy. Soc. (London) **A175**, 382 (1940).

[12] J. H. Van Vleck, Rev. Mod. Phys. **34**, 681 (1962).

or

$$G(\mathbf{q}\to 0)=\frac{V}{8\pi^3}\int_{\mathrm{BZ}} d\mathbf{k}\,\delta(\epsilon_F-\epsilon_{\mathbf{k}})P\frac{1}{\epsilon_{\mathbf{k}}-\epsilon_F}\,. \qquad (5.10)$$

Now, using the representations

$$\pi\delta(\epsilon_F-\epsilon_{\mathbf{k}})=\frac{1}{2i}\left(\frac{1}{\epsilon_F-\epsilon_{\mathbf{k}}-i\lambda}-\frac{1}{\epsilon_F-\epsilon_{\mathbf{k}}+i\lambda}\right), \qquad (5.11)$$

$$P\frac{1}{\epsilon_F-\epsilon_{\mathbf{k}}}=\frac{1}{2}\left(\frac{1}{\epsilon_F-\epsilon_{\mathbf{k}}-i\lambda}+\frac{1}{\epsilon_F-\epsilon_{\mathbf{k}}+i\lambda}\right), \qquad (5.12)$$

where $\lambda=+0$, we obtain

$$\begin{aligned}G(\mathbf{q}\to 0)&\\ &=-\frac{V}{8\pi^3}\int_{\mathrm{BZ}} d\mathbf{k}\frac{1}{4\pi i}\left[\frac{1}{(\epsilon_F-\epsilon_{\mathbf{k}}-i\lambda)^2}-\frac{1}{(\epsilon_F-\epsilon_{\mathbf{k}}+i\lambda)^2}\right]\\ &=\frac{V}{8\pi^3}\frac{\partial}{\partial\epsilon_F}\int_{\mathrm{BZ}} d\mathbf{k}\left[\frac{1}{\epsilon_F-\epsilon_{\mathbf{k}}-i\lambda}-\frac{1}{\epsilon_F-\epsilon_{\mathbf{k}}-i\lambda}\right]\frac{1}{4\pi i}\\ &=\frac{1}{2}\frac{V}{8\pi^3}\frac{\partial}{\partial\epsilon_F}\int_{\mathrm{BZ}} d\mathbf{k}\,\delta(\epsilon_F-\epsilon_{\mathbf{k}})=\tfrac{1}{2}\rho'(\epsilon_F)\,. \qquad (5.13)\end{aligned}$$

If we make use of the property

$$\theta(\epsilon_F-\epsilon_{\mathbf{k}})=\int_{-\infty}^{\epsilon_F}\delta(\epsilon-\epsilon_{\mathbf{k}})d\epsilon, \qquad (5.14)$$

and the fact that $\rho(\epsilon)=0$ for ϵ below the bottom of the band, we obtain

$$F(\mathbf{q}\to 0)=\frac{1}{2}\int_{-\infty}^{\epsilon_F}\rho'(\epsilon)d\epsilon=\tfrac{1}{2}\rho(\epsilon_F)\,. \qquad (5.15)$$

This is a model-independent result valid for arbitrary lattice structure; it is also independent of the assumption of a tight-binding approximation. The physical reason for this fact is related to the nature of the *s-d* Hamiltonian which allows only excitations of particle-hole pairs with energy $\epsilon_{\mathbf{k}+\mathbf{q}}-\epsilon_{\mathbf{k}}$, where $\epsilon_{\mathbf{k}+\mathbf{q}}$ is above the Fermi level, say, and $\epsilon_{\mathbf{k}}$ is below the Fermi level. Consequently, for $\mathbf{q}\to 0$,

$$\epsilon_{\mathbf{k}+\mathbf{q}}\approx\epsilon_{\mathbf{k}}\approx\epsilon_F\,, \qquad (5.16)$$

so that, in this limit, the excitations are possible only in the neighborhood of the Fermi surface, at sufficiently low temperatures, when the conduction-electron mean free path is sufficiently large.

In the above demonstration we also note that the quantity λ appearing in (5.12) should be the same as the corresponding quantity at (5.11), so that, if we want to include phenomenologically the effect of a finite mean free path, we should include a finite relaxation rate λ not only in $P[1/(\epsilon_{\mathbf{k}'}-\epsilon_{\mathbf{k}})]$ but also in the δ function (5.11).

As we see from (5.15) and (5.3), the second term in (5.3) is exactly the term necessary to complete the sum in the third term of (5.3), so that we can now write

$$\rho_\pm(\mathbf{r})=U_0(\mathbf{r})n\pm\sum_{\mathbf{q}}\,[j(\mathbf{q})S^z(-\mathbf{q})e^{i\mathbf{q}\cdot\mathbf{r}}U_{\mathbf{q}}(\mathbf{r})\times F(\mathbf{q})+\text{c.c.}], \qquad (5.17)$$

where we have adopted the definition

$$F(\mathbf{0})\equiv\lim_{\mathbf{q}\to 0}F(\mathbf{q});$$

in (5.17), the first term is the periodic charge distribution in absence of the *s-d* interaction. We note that $U_0(\mathbf{r})=u_{\mathbf{k}}^*(\mathbf{r})u_{\mathbf{k}}(\mathbf{r})$ is normalized by $\int_V U_0(\mathbf{r})d\mathbf{r}=1$, and therefore, $U_0(\mathbf{r})\approx 1/V$ in the plane-wave approximation, so that $\rho_\pm(\mathbf{r})$ has the dimension of number of electrons per unit volume.

Using the expressions (1.5) and (5.17), the spin polarization defined as $\rho(\mathbf{r})=\rho_+(\mathbf{r})-\rho_-(\mathbf{r})$ has a spatial distribution given by

$$\rho(\mathbf{r})=\sum_n S_n^zP(\mathbf{r}-\mathbf{R}_n)\,, \qquad (5.18)$$

with

$$P(\mathbf{r}-\mathbf{R}_n)=\frac{2}{N}\sum_{\mathbf{q}} j(\mathbf{q})e^{i\mathbf{q}\cdot(\mathbf{r}-\mathbf{R}_n)}U_{\mathbf{q}}(\mathbf{r}-\mathbf{R}_n)\times F(\mathbf{q})+\text{c.c.}, \qquad (5.19)$$

where we have used the periodicity of $U_{\mathbf{q}}(\mathbf{r})$. We note that $P(\mathbf{r}-\mathbf{R}_n)$ is not periodic in $\mathbf{r}$.

As we see in (5.18), each localized spin $\mathbf{S}_n$ gives rise to a linearly independent contribution to the conduction-electron polarization at point $\mathbf{r}$. This fact is a consequence of the first-order perturbation theory.

In the derivation of (5.18) we have implicitly assumed that, as the localized spin coordinates $\mathbf{S}_n$ slowly change in time, the conduction-electron ensemble reestablishes the thermal equilibrium almost instantaneously, following adiabatically and very closely the variations of $\mathbf{S}_n$. This corresponds to assume that the conduction-electron relaxation time τ_{ce} is very short compared to T_d, where T_d should be the shortest characteristic period required to describe the time dependence of the $\mathbf{S}_n$ coordinates. This point is also discussed by Hasegawa.[13]

Now, the hyperfine field seen by a nuclear spin is proportional to the total electron spin polarization at the nuclear site. If $\rho(\mathbf{r}=0)$ undergoes fluctuations produced by the fluctuations in the $\mathbf{S}_n$ coordinates [see expression (5.18)], then we can expect these fluctuations of the conduction-electron polarization to be detectable. This type of effect is studied in Sec. VII.

The thermal average of $\rho(\mathbf{r})$ in (5.18) is given by

$$\langle\rho(\mathbf{r})\rangle=\langle S_n^z\rangle\sum_n P(\mathbf{r}-\mathbf{R}_n)\,, \qquad (5.20)$$

where the average $\langle\mathcal{O}\rangle$ of an operator $\mathcal{O}(\mathbf{S}_1,\mathbf{S}_2,\cdots,\mathbf{S}_N)$ is

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[13] H. Hasegawa, Progr. Theoret. Phys. (Kyoto) **21**, 483 (1959).

to be calculated by taking into account the fluctuations in the localized spin coordinates $\mathbf{S}_n$ (see Sec. VII). In (5.20) we note that $\langle S_n^z\rangle$ is independent of n from invariance under translation.

From (5.19) one can see that

$$\sum_n P(\mathbf{r}-\mathbf{R}_n)=\frac{2}{N}\sum_{\mathbf{q}} j(\mathbf{q})F(\mathbf{q})\sum_n e^{i\mathbf{q}\cdot(\mathbf{r}-\mathbf{R}_n)} \times U_{\mathbf{q}}(\mathbf{r}-\mathbf{R}_n)+\text{c.c.} \qquad (5.21)$$

is periodic from cell to cell of the crystal. Noting that $U_{\mathbf{q}}(\mathbf{r})$ is itself periodic in $\mathbf{r}$, it follows that

$$\sum_n e^{i\mathbf{q}\cdot(\mathbf{r}-\mathbf{R}_n)}U_{\mathbf{q}}(\mathbf{r}-\mathbf{R}_n)=U_{\mathbf{q}}(\mathbf{r})e^{i\mathbf{q}\cdot\mathbf{r}}N\delta_{\mathbf{q},0}, \qquad (5.22)$$

and consequently

$$\langle\rho(\mathbf{r})\rangle=4j(\mathbf{0})U_0(\mathbf{r})F(\mathbf{0})\langle S_n^z\rangle. \qquad (5.23)$$

In the ferromagnetic state, for $\mathbf{r}=0$ at the nucleus,

$$\langle\rho(\mathbf{r}=0)\rangle=2j(0)U_0(0)\rho(\epsilon_F)SM_s(T)/M_s(0), \qquad (5.24)$$

or more precisely

$$\langle\rho(\mathbf{r}=0)\rangle=2\langle j(\mathbf{k},\mathbf{k})|u_{\mathbf{k}}(0)|^2\rangle_F \times\rho(\epsilon_F)SM_s(T)/M_s(0), \qquad (5.25)$$

where we have used the property $F(0)=\frac{1}{2}\rho(\epsilon_F)$. The average over the Fermi surface is defined in (5.5) and (5.6), and $M_s(T)$ is the over-all spontaneous magnetization of the localized spins. S is the value of the local spin.

The quantity $\langle\rho(0)\rangle$ is of importance in NMR and Mossbauer experiments. This term, through the hyperfine interaction, contributes to the shift of the NMR frequency and to the separation of the Mossbauer spectral lines. In terms of hyperfine fields, this is the field produced by the conduction electrons polarized by the d electrons. There is another hyperfine field produced by the core s electrons when these become polarized by the d-orbit electrons.[14] As we see these two terms have an indirect origin.

It is likely that the core polarization represents an important or major contribution to the total hyperfine field. On the other hand, the Mossbauer experimental data obtained by Stearns and Wilson[15] in Al:Fe have been interpreted in terms of spatial oscillations of the long-range polarization function $P(\mathbf{r})$ and this seems to indicate a substantial contribution coming from the conduction-electron polarization.

In those cases where the conduction-band polarization provides a substantial contribution to the hyperfine field, we can expect, according to the present model, a number of relations between different measurable quantities. Now, the expression

$$\sum_{\mathbf{R}} e^{i\mathbf{q}\cdot\mathbf{R}}=N\delta_{\mathbf{q},0} \qquad (5.26)$$

is valid when we neglect the interband transitions, or being more specific, is valid for a vector $\mathbf{q}$ limited in a certain region of the momentum space as in (6.11) (see discussion in Sec. VI). Using (5.26), one can easily prove that

$$\sum_n P(\mathbf{R}_n)=4\langle j(\mathbf{k},\mathbf{k})|u_{\mathbf{k}}(0)|^2\rangle_F F(0), \qquad (5.27)$$

and

$$\sum_n \mathbf{R}_n^2P(\mathbf{R}_n)=-4\lim_{\mathbf{q}\to 0}\nabla_{\mathbf{q}}^2[j(\mathbf{q})U_{\mathbf{q}}(\mathbf{0})F(\mathbf{q})]. \qquad (5.28)$$

In some cases, these sums can be obtained approximately from experimental data. In the Stearns and Wilson experiment a plot for $P(\mathbf{r})$ was obtained and from that plot one could calculate the sums (5.27) and (5.28) if one cut the above lattice sums at the seventh neighbor.

The continuous integrals corresponding to (5.27) and (5.28) are given by

$$\int_V P(\mathbf{r})d\mathbf{r}=\frac{4}{N}\langle j(\mathbf{k},\mathbf{k})\rangle_F F(0), \qquad (5.29)$$

and

$$\int_V \mathbf{r}^2P(\mathbf{r})d\mathbf{r}=-\frac{4}{N}\lim_{\mathbf{q}\to 0}\nabla_{\mathbf{q}}^2[j(\mathbf{q})F(\mathbf{q})] +\frac{4}{N}\langle\mathbf{r}_s^2\rangle j(0)F(0), \qquad (5.30)$$

where

$$\langle\mathbf{r}_s^2\rangle=\int_V \mathbf{r}^2|\phi_s(\mathbf{r})|^2d\mathbf{r}. \qquad (5.31)$$

We note that in some of the above expressions, wherever possible we are relaxing the restriction $j(\mathbf{k},\mathbf{k}')u_{\mathbf{k}}^*(\mathbf{r})u_{\mathbf{k}'}(\mathbf{r})\approx j(\mathbf{k}-\mathbf{k}')U_{\mathbf{q}}(\mathbf{r})$; for example, we believe that (5.27) and (5.29) should be valid quite generally. This is no longer true in (5.28) and (5.30), where the assumption $j(\mathbf{k},\mathbf{k}')\approx j(\mathbf{k}-\mathbf{k}')$ is necessary.

In (5.30) we expect the first term to produce the major contribution, due to the long-range character of the conduction-electron polarization. The quantity $\langle\mathbf{r}_s^2\rangle^{1/2}$ is of the order of a lattice distance whereas the first term is expected to correspond to a distance of the order of several lattice distances. For example, in Fe, the Mossbauer data[15] were sensitive enough to direct a conduction-electron polarization as far as the seventh-neighbor shell.

In Ni, if we can consider the range of the exchange interactions[16] between different d spins as related to the range of the conduction-electron polarization, then we obtain a range about the same as in Fe.

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[14] D. A. Goodings and V. Heine, Phys. Rev. Letters **5**, 370 (1960).

[15] M. B. Stearns and S. S. Wilson, Phys. Rev. Letters **13**, 313 (1964); M. B. Stearns, J. Appl. Phys. **36**, 913 (1965).

[16] R. Weber and P. E. Tannenwald, J. Phys. Chem. Solids **24**, 1357 (1963); Phys. Rev. **140**, A498 (1965); J. Appl. Phys. **37**, 1058 (1966).

If we compare the lattice sums (5.27) and (5.28) with the corresponding integrals (5.29) and (5.30) we note the absence of the charge factor $U_{\mathbf{q}}$ in (5.29) and (5.30), where this factor becomes replaced by $1/N$. This fact is due to the normalization of $U_{\mathbf{q}}(\mathbf{r})$. We also note that the absence of the factor $U_{\mathbf{q}}$ in (5.29) and (5.30) seems to indicate their validity even without the assumption (3.4).

The ratio between

$$\frac{1}{N}\sum_n P(\mathbf{R}_n) \quad \text{and} \quad \frac{1}{V}\int_V P(\mathbf{r})d\mathbf{r}$$

is given by

$$(V/N)\sum_n P(\mathbf{R}_n)\Big/\int_V P(\mathbf{r})d\mathbf{r}$$
$$=\langle j(k,k)|u_{\mathbf{k}}(0)|^2\rangle_F/\langle j(\mathbf{k},\mathbf{k})(1/V)\rangle_F, \quad (5.32)$$

and, in this way, we could obtain information on the amount of departure of $|u_{\mathbf{k}}(0)|^2$ from its uniform value $1/V$. If we interpolate the Mossbauer data[15] in Fe for $P(\mathbf{r})$, and assume that $P(\mathbf{r})$ is spherically symmetric, then one could obtain some information about the integrals (5.29) and (5.30). The difficulty here is that in Fe, the Anderson-Clogston[7] effect seems to play an important role, so that the effective $j(\mathbf{k},\mathbf{k})$ is negative instead of positive as one obtains from (1.2).

The integrals (5.29) and (5.30) contribute to the cross section in the elastic neutron scattering[17] at small momentum transfer. In this case the problem is that the cross section is mainly determined by the d-electron spin form-factor. In the future, it may become possible to subtract this contribution by studying the same process in the ferromagnetic metal containing diamagnetic impurities.

Another point to be observed is that if the indirect exchange becomes really effective, then, as we will see in the next section, the quantities (5.27) and (5.29) are related to the paramagnetic temperature, whereas (5.28) and (5.30) are related to the exchange stiffness parameter

$$D=\tfrac{1}{3}S\sum_m \mathbf{R}_{lm}{}^2 J_{lm}.$$

The dependence of some of the measurable parameters on $\rho(\epsilon_F)$ can be observed in some cases. A good material for a test of these model-independent relations seems to be $\mathrm{Eu}_{(1-x)}\mathrm{Gd}_x\mathrm{Se}$. These metallic compounds have been studied by Holtzberg *et al.*[18] The effect of replacing one Eu atom by Gd seems to be only the addition of two more conduction electrons without changing the f sites too much. A variation of the paramagnetic temperature with electron concentration has been interpreted in terms of the RKKY spherical model.

VI. EFFECTIVE HEISENBERG SPIN HAMILTONIAN

We now turn our attention to the last term in (4.5). We note that $|0\rangle$ and $|n\rangle$ are eigenstates of $\mathcal{H}_0{}'$ with eigenvalues E_0 and E_n. With an error of the order j^3 we can replace $|0\rangle$ and $|n\rangle$ by the corresponding eigenstates of $\mathcal{H}_0$. Without introducing a new notation for this replacement, we note that the excitations allowed by the off-diagonal part of $\mathcal{H}_{sd}$ [Eq. (1.9)] are the states involving a particle-hole pair of the form

$$|n\rangle=a_{\mathbf{k}'\sigma'}{}^{\dagger}a_{\mathbf{k}\sigma}|0\rangle, \quad (6.1)$$

where $(\mathbf{k}'\sigma')\neq(\mathbf{k}\sigma)$, with $\epsilon_{\mathbf{k}}$ and $\epsilon_{\mathbf{k}'}$ below and above the chemical potential ϵ_F, respectively. The matrix elements of $\mathcal{H}_{sd}{}'$ can be shown to be

$$\begin{aligned}\langle 0|\mathcal{H}_{sd}{}'|n\rangle=&-j(\mathbf{k}-\mathbf{k}')n_{\mathbf{k}}(1-n_{\mathbf{k}'})\\&\times[(1-\delta_{\mathbf{k}\mathbf{k}'})\delta_{\sigma\sigma'}S_{\sigma\sigma}(\mathbf{k}'-\mathbf{k})\\&+(1-\delta_{\sigma\sigma'})S_{\sigma\sigma'}(\mathbf{k}'-\mathbf{k})], \quad (6.2)\end{aligned}$$

where we have replaced the square Fermi distribution by the corresponding distribution $n_{\mathbf{k}}$ at a given temperature.

Adding over all possible intermediary states, and noting that $E_n=E_0+\epsilon_{\mathbf{k}'}-\epsilon_{\mathbf{k}}$, one obtains

$$\begin{aligned}\sum_n\frac{|\langle 0|\mathcal{H}_{sd}{}'|n\rangle|^2}{E_0-E_n}=&2\sum_{\mathbf{k}'\mathbf{k}}\frac{j^2(\mathbf{k}-\mathbf{k}')n_{\mathbf{k}}(1-n_{\mathbf{k}'})}{\epsilon_{\mathbf{k}}-\epsilon_{\mathbf{k}'}}\\&\times[|S_x(\mathbf{k}-\mathbf{k}')|^2+|S_y(\mathbf{k}-\mathbf{k}')|^2]\\&+2\sum_{\mathbf{k}'\neq\mathbf{k}}\frac{j^2(\mathbf{k}-\mathbf{k}')n_{\mathbf{k}}(1-n_{\mathbf{k}'})}{\epsilon_{\mathbf{k}}-\epsilon_{\mathbf{k}'}}|S_z(\mathbf{k}-\mathbf{k}')|^2. \quad (6.3)\end{aligned}$$

The term $\mathbf{k}'=\mathbf{k}$ lacking in the second summation in (6.3) can be shown to be exactly the term $-A^2\rho(\epsilon_F)=-j^2(0)|S_z(0)|^2\rho(\epsilon_F)$ coming from the diagonal part of $\mathcal{H}_{sd}$ [see (4.16)]. Adding together all the second-order terms we obtain the result

$$\mathcal{H}_{SS}{}^{(2)}=-\sum_{lm}J_{lm}\mathbf{S}_l\cdot\mathbf{S}_m, \quad (6.4)$$

where

$$J_{lm}\equiv J(\mathbf{R}_{lm})=+\frac{2}{N^2}\sum_{\mathbf{q}}j^2(\mathbf{q})e^{i\mathbf{q}\cdot\mathbf{R}_{lm}}F(\mathbf{q}). \quad (6.5)$$

We note in (6.5) the absence of $U_{\mathbf{q}}(\mathbf{r})$. The reason for this is that the effect of non-plane-wave character of $\phi_{\mathbf{k}}(\mathbf{r})$ is already taken into account through the appropriate single-particle energies $\epsilon_{\mathbf{k}}$, which are present in the expression for $F(\mathbf{q})$. We also note that the summation (6.5) is real since $j(-\mathbf{q})=j(\mathbf{q})$ and $F(-\mathbf{q})=F(\mathbf{q})$.

Another point to be observed is that instead of $j^2(\mathbf{q})F^2(\mathbf{q})$, we have $j^2(\mathbf{q})F(\mathbf{q})$ in (6.5). This is easy to understand if we remember that each factor $(\epsilon_{\mathbf{k}}-\epsilon_{\mathbf{k}'})^{-1}$

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[17] See, for example, *Thermal Neutron Scattering*, edited by P. A. Egelstaff (Academic Press Inc., New York, 1965).

[18] F. Holtzberg, T. R. McGuire, S. Methfessel, and J. C. Suits, Phys. Rev. Letters **13**, 18 (1964).

in a perturbation expansion gives rise to a factor $F(\mathbf{q})$, as in the expression for the polarization.

The indirect-exchange interaction in finite at $\mathbf{R}_{lm}=0$, as well as is the electronic polarization $P(\mathbf{r})$ at $\mathbf{r}=0$. This fact is related to the neglect of interband transitions which introduces a cutoff in $F(\mathbf{q})$ for large values of $|\mathbf{q}|$. The self-energy contained in (6.4) is a constant given by

$$\mathcal{H}_{\text{self}}=-NJ(\mathbf{R}=0)S(S+1). \tag{6.6}$$

The type of periodic ordering resulting from the Hamiltonian (6.4) is determined[19,20] by the vector $\mathbf{k}_0$ for which the quantity

$$J_{\mathbf{k}}=2S\sum_{\mathbf{R}\neq0} J(\mathbf{R})e^{i\mathbf{k}\cdot\mathbf{R}} \tag{6.7}$$

is a maximum.

Assuming ferromagnetic order and applying the Holstein-Primakoff[21] approximation, we obtain at low temperatures

$$\mathcal{H}_{SS}^{(2)}-\mathcal{H}_{\text{self}}=-S^2NJ_0+\sum_{\mathbf{k}} \hbar\omega_{\mathbf{k}}b_{\mathbf{k}}^\dagger b_{\mathbf{k}}, \tag{6.8}$$

where $b_{\mathbf{k}}^\dagger b_{\mathbf{k}}$ is the number operator for a spin wave and

$$\hbar\omega_{\mathbf{k}}=2S\sum_{\mathbf{R}\neq0} J(\mathbf{R})[1-e^{i\mathbf{k}\cdot\mathbf{R}}]. \tag{6.9}$$

In (6.9) we can include the term $\mathbf{R}=0$, since only the difference $J_0-J_{\mathbf{k}}$ appears. One can show that

$$\hbar\omega_{\mathbf{k}}=(4S/N)[j^2(0)F(0)-j^2(\mathbf{k})F(\mathbf{k})], \tag{6.10}$$

where the vector $\mathbf{k}$ belongs to the first Brillouin zone. We note that $F(\mathbf{q})$ is defined in a region larger then the first Brillouin zone. With the neglect of interband transitions this region becomes finite. In the spherical model[1-3] the field of definition for the function $F(\mathbf{q})$ becomes extended to infinity.

When we compare expression (6.10) with the corresponding quantity obtained by Kasuya[1] [Sec. V, Eq. (3)], we note in (6.10) the absence of terms involving $\mathbf{K}\neq0$, $\mathbf{K}$ being a vector of the reciprocal lattice. We will call these $\mathbf{K}\neq0$ terms "umklapp terms." It is our opinion that in a model where indirect exchange is mediated by the conduction electrons, these umklapp terms are related to the interband transitions.

This point becomes even more evident when we note that in the spherical model[1-3] the expression $\epsilon_{\mathbf{k}}=\hbar^2\mathbf{k}^2/2m$ has its validity extended to the whole momentum space; this corresponds to the extended zone scheme where $\epsilon_{\mathbf{k}+\mathbf{K}}=\hbar^2(\mathbf{k}+\mathbf{K})^2/2m$. The object $\mathbf{K}$ corresponds to our band index l.

Another argument in favor of the absence of umklapp terms in (6.10)—when we neglect interband transitions—is obtained if in the expression (6.9) we replace $J(\mathbf{R})$ by its expression (6.5); in the particular case of simple cubic structure the vector $\mathbf{q}$ in (6.5) is restricted to a cube given by

$$-2\pi< aq_j< 2\pi, \tag{6.11}$$

where the equality sign is not allowed since $-\pi< ak_j\leqslant\pi$ and $-\pi< ak_j'\leqslant\pi$. Another way to understand that (6.11) is the correct field of definition for the vector $\mathbf{q}$ is to replace the sum (6.5) by its corresponding integral

$$\frac{2}{N^2}\frac{V}{8\pi^3}\int_{-2\pi/a}^{+2\pi/a} F(\mathbf{q})j^2(\mathbf{q})e^{-i\mathbf{q}\cdot\mathbf{R}}d\mathbf{q}, \tag{6.12}$$

whose boundary contains, for example, the point $\mathbf{K}=(2\pi/a,0,0)$ where $F(\mathbf{K})$ is not defined, although we could extend the definition by taking

$$F(\mathbf{K})\equiv\lim_{\mathbf{k}\to0} F(\mathbf{K}+\mathbf{k})=\tfrac{1}{2}\rho(\epsilon_F).$$

Consequently the Van Vleck[12] requirement by which we must replace $(\epsilon_{\mathbf{k}'}-\epsilon_{\mathbf{k}})^{-1}$ by its principal part makes it necessary to define the integrals

$$\int_{-2\pi/a}^{2\pi/a} dq_x\cdots \tag{6.13}$$

as

$$\lim_{\epsilon\to0}\int_{-2\pi/a+\epsilon}^{2\pi/a-\epsilon} dq_x\cdots, \tag{6.14}$$

so that the surface of the cube (6.11) must be excluded. It is shown in Appendix B that the exclusion of the surface in these sums may also be related directly to the Bragg condition.

The above discussion, restricted to simple cubic structure, can be generalized immediately to other structures, so that in this sense, expression (6.10) is model-independent. The absence of the factor $U_{\mathbf{q}}(\mathbf{r})$ in (6.5) and (6.10) seems to indicate that the assumption (3.4) can be partially relaxed, whereas the assumption $j(\mathbf{k},\mathbf{k}')=j(\mathbf{k}-\mathbf{k}')$ continues to be necessary.

VII. SPIN-DENSITY FLUCTUATIONS

The thermal average of an operator $\mathcal{O}(\mathbf{S}_1,\mathbf{S}_2,\cdots,\mathbf{S}_N)$ is here defined by

$$\langle\mathcal{O}(\mathbf{S}_1,\mathbf{S}_2,\cdots,\mathbf{S}_N)\rangle =\frac{\mathrm{Tr}[\mathcal{O}(\mathbf{S}_1,\mathbf{S}_2,\cdots,\mathbf{S}_N)\exp(-\beta\mathcal{H}_{SS}^{(2)})]}{\mathrm{Tr}[\exp(-\beta\mathcal{H}_{SS}^{(2)})]}, \tag{7.1}$$

where $\mathcal{H}_{SS}^{(2)}$ is the effective indirect-exchange Hamiltonian (6.4), and $\beta=1/\kappa_BT$, where κ_B is the Boltzman constant.

From (5.18) we obtain

$$\langle[\rho(0)-\langle\rho(0)\rangle]^2\rangle=\sum_{mn} \kappa^{(z)}(\mathbf{R}_{mn})P(\mathbf{R}_m)P(\mathbf{R}_n), \tag{7.2}$$

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[19] D. H. Lyons and T. A. Kaplan, Phys. Rev. **120**, 1580 (1960).

[20] T. A. Kaplan, K. Dwight, D. Lyons, and N. Menyuk, J. Appl. Phys. **32**, 13S (1961); D. H. Lyons, Phys. Rev. **126**, 540 (1962); N. Menyuk, *ibid.* **127**, 1983 (1962).

[21] T. Holstein and H. Primakoff, Phys. Rev. **58**, 1098 (1940).

where $\kappa^{(z)}(\mathbf{R}_{mn})$ is the spin correlation function between the spin at site m and that in site n, defined by

$$\kappa^{z}(\mathbf{R}_{mn})=\langle S_m{}^z S_n{}^z\rangle-\langle S_n{}^z\rangle\langle S_m{}^z\rangle. \qquad (7.3)$$

This is the proper correlation function in the ferromagnetic state, where z is a well-defined direction along the easy axis of spontaneous magnetization; in the paramagnetic region it would be more appropriate to replace $\kappa^{(z)}$ by $\frac{1}{3}\kappa(\mathbf{R})$, where

$$\kappa(\mathbf{R})=\langle\mathbf{S}(0)\cdot\mathbf{S}(\mathbf{R})\rangle-\langle\mathbf{S}(\mathbf{0})\rangle\cdot\langle\mathbf{S}(\mathbf{R})\rangle \qquad (7.4)$$

is the correlation function studied by Van Hove[22] in connection with critical neutron scattering.

In the ferromagnetic state, using the spin-wave approximation[21] we obtain

$$\langle S_m{}^z S_n{}^z\rangle=S^2-2S\frac{1}{N}\sum_{\mathbf{k}\mathbf{k}'}\langle b_{\mathbf{k}}{}^\dagger b_{\mathbf{k}'}\rangle$$
$$+\frac{1}{N^2}\sum_{\mathbf{k}\mathbf{k}'}\sum_{\mathbf{q}\mathbf{q}'}\langle b_{\mathbf{k}}{}^\dagger b_{\mathbf{k}'} b_{\mathbf{q}}{}^\dagger b_{\mathbf{q}'}\rangle e^{i(\mathbf{q}'-\mathbf{q})\mathbf{R}}, \qquad (7.5)$$

where $b_{\mathbf{k}}{}^\dagger$ is the creation operator for a spin wave of momentum **k**.

For boson operators[23]

$$\langle b_{\mathbf{k}}{}^\dagger b_{\mathbf{k}'}\rangle=\delta_{\mathbf{k}\mathbf{k}'}N_{\mathbf{k}}, \qquad (7.6)$$

where

$$N_{\mathbf{k}}=(e^{\beta h\omega_{\mathbf{k}}}-1)^{-1}. \qquad (7.7)$$

Using Wick's theorem,[23] the thermal average in the third term of (7.5) can be shown to be

$$\delta_{\mathbf{k}\mathbf{k}'}\delta_{\mathbf{q}\mathbf{q}'}N_{\mathbf{k}}N_{\mathbf{q}}+\delta_{\mathbf{k}\mathbf{q}'}\delta_{\mathbf{q}\mathbf{k}'}(N_{\mathbf{q}}+1)N_{\mathbf{k}}. \qquad (7.8)$$

Applying the same procedure for $\langle S^z(\mathbf{0})\rangle=\langle S^z(\mathbf{R})\rangle$, we obtain

$$\kappa^{(z)}(\mathbf{R})=\frac{1}{N^2}\sum_{\mathbf{k}\mathbf{k}'}N_{\mathbf{k}}(N_{\mathbf{k}'}+1)e^{i(\mathbf{k}'-\mathbf{k})\cdot\mathbf{R}}. \qquad (7.9)$$

Noting that

$$\sum_n e^{i\mathbf{k}\cdot\mathbf{R}_n}P(\mathbf{R}_n)=4j(\mathbf{k})U_{\mathbf{k}}(0)F(\mathbf{k}), \qquad (7.10)$$

the expression for the fluctuations in $\rho(0)$ can be written as

$$\langle[\rho(0)-\langle\rho(0)\rangle]^2\rangle=\frac{16}{N^2}\sum_{\mathbf{k}\mathbf{k}'}N_{\mathbf{k}}(N_{\mathbf{k}'}+1)$$
$$\times[j(\mathbf{k}-\mathbf{k}')U_{\mathbf{k}-\mathbf{k}'}(0)F(\mathbf{k}-\mathbf{k}')]^2. \qquad (7.11)$$

Assuming that the major contribution comes from $\mathbf{k}\approx\mathbf{k}'\approx0$, due to the factor $N_{\mathbf{k}}N_{\mathbf{k}'}$ we obtain for $T\ll T_c$

$$\langle[\rho(0)-\langle\rho(0)\rangle]^2\rangle$$
$$\approx[(2C/\pi)\zeta(\tfrac{3}{2})j(0)U_0(0)F(0)]^2(\kappa_B Ta^2/D)^3, \qquad (7.12)$$

where

$$C=\int_0^\infty e^{-x^2}x^2dx=\tfrac{1}{4}\sqrt{\pi}.$$

These fluctuations in the conduction-electron spin polarization give rise to a broadening of the linewidth in NMR and Mossbauer spectra. To this contribution we have to add other terms, as, for example, the Korringa[24] linear term in T associated with the pure hyperfine interaction between the nuclei and the conduction electrons.

In the paramagnetic region the correlation function becomes nearly a δ function for $T\rightarrow\infty$, since different spins are uncorrelated. In this case we can write

$$\langle[\rho(0)-\langle\rho(0)\rangle]^2\rangle\approx\tfrac{1}{3}\kappa(0)\sum_{\mathbf{R}}P^2(\mathbf{R}), \qquad (7.13)$$

where $\kappa(0)=S(S+1)$. At finite temperatures one should include a correction factor

$$T\chi/C\approx T/(T-\theta),$$

where χ is the magnetic susceptibility and C is the Curie constant. The final expression becomes

$$\langle[\rho(0)-\langle\rho(0)\rangle]^2\rangle\approx\tfrac{1}{3}S(S+1)\frac{T}{T-\theta}\sum_{\mathbf{R}}P^2(\mathbf{R}), \qquad (7.14)$$

so that near the transition region we should expect a maximum in linewidth, as it is well known.

We note that a quantity similar to $\sum_{\mathbf{R}}P^2(\mathbf{R})$ appears in the high-temperature expansion of the paramagnetic susceptibility, i.e., the coefficient B' in (8.1) (see Sec. VIII) is proportional to

$$\sum_{\mathbf{R}\neq0}J^2(\mathbf{R}).$$

VIII. PARAMAGNETIC AND CRITICAL TEMPERATURE

A. Paramagnetic Temperature

In the paramagnetic region we can expand the magnetic susceptibility in a power series[25] of $1/T$ of the form

$$\frac{1}{\chi}=\frac{T}{C}\left(1-\frac{\theta}{T}+\frac{B'}{T^2}+\cdots\right), \qquad (8.1)$$

where C is the Curie constant and θ is the paramagnetic temperature.

From the Heisenberg Hamiltonian (6.4) one can derive[26,27] the result

$$\kappa_B\theta=\tfrac{2}{3}S(S+1)\sum_{\mathbf{R}\neq0}J(\mathbf{R}), \qquad (8.2)$$

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[22] L. van Hove, Phys. Rev. **95**, 1374 (1954).

[23] See, for example, A. A. Abrikosov, L. P. Gorkov, and I. E. Dzyaloshinski, *Methods of Quantum Field Theory in Statistical Physics* (Prentice-Hall, Inc., Englewood Cliffs, N. J., 1963).

[24] J. Korringa, Physica **16**, 601 (1950).

[25] W. Opechowski, Physica **4**, 181 (1937).

[26] A. Blandin and J. Friedel, J. Phys. Radium **20**, 160 (1959).

[27] A. W. Sáenz, Phys. Rev. **119**, 1542 (1960).

where we can see immediately that, except for a term involving $J(\mathbf{R}=0)$, the paramagnetic temperature is related to the quantities $\sum_n P(\mathbf{R}_n)$ and $\int_V P(\mathbf{r})d\mathbf{r}$ in (5.27) and (5.29). The expression for θ can be shown to be

$$\kappa_B\theta=\tfrac{2}{3}S(S+1)\left[\frac{2}{N}j^2(0)F(0)-J(\mathbf{R}=0)\right], \quad (8.3)$$

where we have only assumed that $j(\mathbf{k},\mathbf{k}')=j(\mathbf{k}-\mathbf{k}')$. We believe, without proof, that the correct expression in the more general case can be obtained with the replacement

$$j^2(0)\rightarrow\langle j^2(\mathbf{k},\mathbf{k})\rangle_F, \quad (8.4)$$

in the first term of the bracket in (8.3).

In the particular case of the simple cubic structure, and with the help of the assumption $j(\mathbf{k},\mathbf{k}')=\text{const}$, we will be able in Sec. IX to obtain explicit expressions for $J(\mathbf{R}=0)$ [see (9.30)], as well as for θ [see (9.32)], both as functions of ϵ_F in terms of tabulated functions. We also obtain numerical values for the paramagnetic temperature as well as for other parameters, as functions of ϵ_F. In this way we can study the problem mentioned in the Introduction and obtain the dependence of the magnetic properties on the electron concentration.

B. Effect of the Temperature Dependence of the Indirect Exchange on T_c

Another point to be observed is that in the above expressions we are assuming that the temperature is sufficiently low compared with T_F, the Fermi temperature. Otherwise a correction factor of the form

$$[1-b(T/T_F)^2]\approx e^{-b(T/T_F)^2} \quad (8.5)$$

must be taken into account.

In the molecular-field approximation the critical temperature is also given by

$$\kappa_B T_0=\tfrac{2}{3}S(S+1)\sum_{\mathbf{R}\neq 0}J(\mathbf{R}), \quad (8.6)$$

where T_0 is a well-defined temperature; here $J(\mathbf{R})$ is to be evaluated at $T=0°\mathrm{K}$.

If T_0 is not so small as compared to T_F, then we must include the correction (8.5). In this case T_c must be obtained self-consistently through an equation of the type $T_c=\text{function}(T)=\text{function}(T_c)$. Then we obtain

$$T_c=T_0e^{-b(T_c/T_F)^2}. \quad (8.7)$$

In the case $T_0\ll T_F$, we can solve this equation by an iteration procedure with the result

$$T_c\approx T_0e^{-b(T_0/T_F)^2}. \quad (8.8)$$

This is the appropriate expression for our model, since $T_0\ll T_F$ is a necessary condition for the validity of perturbation theory; it is plausible that (8.8) may become useful even in cases where the conduction band involves non-s-character. If the dominant Heisenberg Hamiltonian comes about as a consequence of indirect interactions mediated by the conduction band, then (8.8) may become a not bad approximation. This case seems to be of some interest since most of rare-earth and transition metals have a Fermi temperature relatively low compared to that in noble metals.

C. Critical Temperature in Dilute Magnetic Alloys

In the case of dilute disordered alloys, it has been customary[26] to replace in (8.6) the sum $\sum_{\mathbf{R}\neq 0}J(\mathbf{R})$ by

$$\sum_{\mathbf{R}\neq 0}p(\mathbf{R})J(\mathbf{R})=c\sum_{\mathbf{R}\neq 0}J(\mathbf{R}), \quad (8.9)$$

where $p(\mathbf{R})$ is the probability of finding a magnetic impurity at site $\mathbf{R}_n=\mathbf{R}$, and $c=N_0/N$ is the atomic concentration of magnetic impurities. The above result (8.9) is valid only at low concentrations for $c\ll 1$; in other words there are corrections involving terms in c^2, etc.

Now, if we accept (8.9), then in (8.8) we must replace T_0 by cT_0, and in this case—for a disordered alloy as Fe:Au and possibly Gd:Pd or Fe:Pd—we obtain the following expression for T_c:

$$T_c=cT_0e^{-bc^2(T_0/T_F)^2}, \quad (8.10)$$

where T_0, as given by (8.6), is nearly independent of concentration.

As we see in (8.10), T_c/c is no longer a constant independent of concentration. That is, for $b>0$, the slope of the curve T_c versus c tends to decrease with increasing concentration. It seems that a number of alloys follow this rule not only with respect to the critical temperature T_c but also for the paramagnetic temperature θ.[28,29] This effect should be more noticeable in materials for which T_0/T_F is not so small. The dependence on T_0/T_F could provide another check for the formula (8.10).

Evidently, in a careful study we have to include in (8.9) corrections involving c^2 and c^3. We must note furthermore that T_0 and T_F may change somewhat with alloying, but this change is probably small at low concentrations. Some applications of formula (8.10) are being prepared.

For the pure metal case we can write (8.6) in the form

$$\kappa_B T_c=\tfrac{2}{3}S(S+1)[(2/N)j^2(0)F(0)-J(\mathbf{R}=0)]. \quad (8.11)$$

We note in (8.11) that $F(0)=\frac{1}{2}\rho(\epsilon_F)\sim N/4B$, where $2B$ is the width of the conduction band.

The quantity $J(\mathbf{R}=0)$ may be shown to depend on the level-density function not only near the Fermi surface, but over the whole bandwidth.

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[28] R. J. Borg, R. Booth, and C. E. Violet, Phys. Rev. Letters **11**, 464 (1963); J. Crangle, *ibid.* **13**, 569 (1964).

[29] R. M. Bozorth, P. A. Wolff, D. D. Davis, V. B. Compton, and J. H. Wernick, Phys. Rev. **122**, 1157 (1961); J. Crangle and W. R. Scott, J. Appl. Phys. **36**, 921 (1965).

D. Pressure Dependence of T_c

The pressure dependence of T_c has been studied by a number of authors.[30,31] A part of the pressure dependence of T_c is associated with the quantity

$$\frac{\partial J(\mathbf{R}=0)}{\partial p}=\frac{\partial J(\mathbf{R}=0)}{\partial \epsilon_F}\frac{\partial \epsilon_F}{\partial p}; \tag{8.12}$$

for this reason we now consider the derivative of $J(\mathbf{R}=0)$ with respect to ϵ_F.

With the assumption $j^2(\mathbf{q})=j^2(0)=\text{const}$, and using (6.5) and (3.10), we obtain

$$\frac{\partial J(\mathbf{R}=0)}{\partial \epsilon_F}=\frac{2}{N^2}j^2(0)\left[\frac{V}{8\pi^3}\int_{\mathrm{BZ}} d\mathbf{k}\,\delta(\epsilon_F-\epsilon_{\mathbf{k}})\right]\times\left[\frac{V}{8\pi^3}\int_{\mathrm{BZ}} d\mathbf{k}'P\frac{1}{\epsilon_{\mathbf{k}'}-\epsilon_F}\right]. \tag{8.13}$$

Noting that

$$\frac{1}{i\pi}\frac{1}{\epsilon-\epsilon_{\mathbf{k}}-i\lambda}=\delta(\epsilon-\epsilon_{\mathbf{k}})+\frac{1}{i\pi}P\frac{1}{\epsilon-\epsilon_{\mathbf{k}}}, \tag{8.14}$$

we can define[32] a complex level-density function whose real part is just the usual $\rho(\epsilon)$. In this way we can write (8.13) in the form

$$\frac{\partial J(\mathbf{R}=0)}{\partial \epsilon_F}=\frac{2\pi}{N^2}j^2(0)\rho_R(\epsilon_F)\rho_I(\epsilon_F), \tag{8.15}$$

where

$$\rho_R(\epsilon_F)=\frac{V}{(2\pi)^3}\int_{\mathrm{BZ}}\delta(\epsilon_F-\epsilon_{\mathbf{k}})d\mathbf{k} \tag{8.16}$$

and

$$\rho_I(\epsilon_F)=\frac{V}{(2\pi)^3}\frac{1}{\pi}\int_{\mathrm{BZ}}P\frac{1}{\epsilon_{\mathbf{k}}-\epsilon_F}d\mathbf{k}. \tag{8.17}$$

We note in (8.15) the presence of the level density $\rho(\epsilon_F)$ at the Fermi level. This is an indication that the quantity $\partial J(0)/\partial\epsilon_F$ is now less sensitive to the details of the conduction-electron energy spectrum. For this reason, we believe that a relaxation on the assumption $j(\mathbf{k},\mathbf{k}')=j(\mathbf{k}-\mathbf{k}')=j(0)$ seems possible, in this case; a reasonable guess seems to be the replacement, in (8.15),

$$j^2(0)\rightarrow\langle j(\mathbf{k},\mathbf{k})\rangle_F\langle j(\mathbf{k},\mathbf{k})\rangle_{F'}, \tag{8.18}$$

where the first factor is defined in (5.5) and the second average is defined by

$$\langle j(\mathbf{k},\mathbf{k})\rangle_{F'}=\int_{\mathrm{BZ}}j(\mathbf{k},\mathbf{k})P\frac{1}{\epsilon_{\mathbf{k}}-\epsilon_F}d\mathbf{k}\bigg/\int_{\mathrm{BZ}}P\frac{1}{\epsilon_{\mathbf{k}}-\epsilon_F}d\mathbf{k}, \tag{8.19}$$

in analogy with (5.5).

IX. EXCHANGE MOMENTS

In connection with the expansion of (6.9) in a power series of $\mathbf{k}^2$, we define the following exchange moments:

$$\langle\mathbf{R}^2\rangle=\sum_{\mathbf{R}}\mathbf{R}^2J(\mathbf{R})/J_E, \tag{9.1}$$

$$\langle\mathbf{R}^4\rangle=\sum_{\mathbf{R}}\mathbf{R}^4J(\mathbf{R})/J_E, \tag{9.2}$$

$$\langle R_x^4+R_y^4+R_z^4\rangle=\sum_{\mathbf{R}}(R_x^4+R_y^4+R_z^4)J(\mathbf{R})/J_E, \tag{9.3}$$

where J_E is a constant with the dimension of an exchange energy to be specified later; in this form $\langle\mathbf{R}^{2n}\rangle$ has the dimension of a^{2n}, where a is a lattice distance.

If the ordering becomes ferromagnetic, then some of these exchange moments can be measured at low temperatures. The T-dependent spin-wave energy has been shown[33,34] to be

$$\hbar\omega_{\mathbf{k}}(T)=D(T)\mathbf{k}^2, \tag{9.4}$$

for $\mathbf{k}^2a^2\ll 1$ in cubic systems; in (9.4),

$$D(T)=D_0(1-ET^{5/2}), \tag{9.5}$$

$$D_0=\tfrac{1}{3}SJ_E\langle\mathbf{R}^2\rangle, \tag{9.6}$$

and

$$E=\frac{\pi\zeta(\frac{5}{2})}{\bar{N}S}\frac{\langle\mathbf{R}^4\rangle}{\langle\mathbf{R}^2\rangle}(\kappa_B/4\pi D_0)^{5/2}. \tag{9.7}$$

The quantities D_0 and E have been measured for some ferromagnetic metals, using spin-wave resonance in thin films,[16,35] so that information about $\langle\mathbf{R}^2\rangle$ and $\langle\mathbf{R}^4\rangle$ has been obtained.

It is our purpose in this section to investigate the effect of a multiply connected Fermi surface on the exchange moments $\langle\mathbf{R}^{2n}\rangle$, or, being more specific, to study what occurs when ϵ_F reaches a critical value ϵ_c for which the Fermi surface touches the Brillouin-zone boundary.

This is evidently a discontinuous process. The discontinuous expansion of the Fermi surface has been shown[36] to be described by a certain singularity in the

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[30] S. H. Liu, Phys. Rev. **127**, 1889 (1962).

[31] D. Bloch and R. Pauthenet, in *Proceedings of the International Conference on Magnetism, Nottingham, 1964* (Institute of Physics and the Physical Society, London, 1965), p. 255.

[32] T. Wolfram and J. Callaway, Phys. Rev. **130**, 2207 (1963); P. Vashista and J. Mahanty, Proc. Phys. Soc. (London) 85, 1215 (1965).

[33] F. Keffer and R. Loudon, J. Appl. Phys. **32**, 2S (1961).

[34] W. Marshal, in *Proceedings of the Eighth International Conference on Low-Temperature Physics, London, 1962*, edited by R. O. Davies (Butterworth Scientific Publications, Ltd., London, 1963).

[35] H. Nosé, J. Phys. Soc. Japan **15**, 1714 (1960); **16**, 342 (1961); **16**, 2475 (1961).

[36] See, for example, N. F. Mott and H. Jones, *The Theory of the Properties of Metals and Alloys* (Dover Publications, Inc., New York, 1936).

level-density function $\rho(\epsilon)$. It seems that these van Hove[37] singularities have never been directly observed, probably because of some smearing out associated with electron-phonon or other interactions. Anyway, it is reasonable to expect a rapid variation of $\rho(\epsilon)$ and its derivatives in the neighborhood of the singularity.

It has been shown[37,38] that these singularities are described by the critical points in the single-particle dispersion relation $\epsilon=\epsilon_{\mathbf{k}}$. With the tight-binding approximation we will be concerned in the simple cubic case with an analytic critical point (saddle point), whereas in the body-centered case the corresponding singularity is a nonanalytic critical point producing a $\ln^2|\epsilon|$ singularity in $\rho(\epsilon)$.

The level-density function and its derivatives are related to the behavior of the function $F(\mathbf{q})$ in the neighborhood of $\mathbf{q}=0$. It seems reasonable to expect that, at least in the neighborhood of the critical points, we can replace

$$j^2(\mathbf{k},\mathbf{k}') \rightarrow j^2(\mathbf{k}_c,\mathbf{k}_c)=\text{const}, \tag{9.8}$$

where $\mathbf{k}_c$ is a critical momentum.

A replacement similar to (9.8) has been employed by many authors in connection with the spherical model, by taking $j^2(\mathbf{k},\mathbf{k}')=j^2(\mathbf{k}-\mathbf{k}')=j^2(0)$. We must note that in the spherical model $\rho(\epsilon)\propto\sqrt{\epsilon}$ is a rapidly varying function of ϵ, for $\epsilon\rightarrow 0$; since in this case $\mathbf{k}_c=0$, the replacement corresponding to (9.8) should read

$$j(\mathbf{k},\mathbf{k}') \rightarrow j(\mathbf{0},\mathbf{0}) \tag{9.9}$$

in the spherical model.

If the magnetic ordering is not ferromagnetic and in (6.7) the maximum in $J_{\mathbf{q}}$ occurs at $\mathbf{q}=\mathbf{q}_0$, it is probable that the proper replacement corresponding to (9.8) would be

$$j^2(\mathbf{k},\mathbf{k}') \rightarrow j^2(\mathbf{k}_c,\ \mathbf{k}_c+\mathbf{q}_0)=\text{const}. \tag{9.10}$$

In the case of $\mathbf{q}_0\neq 0$, i.e., spiral ordering, a study of the quantities $\langle \mathbf{R}^{2n}\rangle$ may help in the determination of the maximum in $J_{\mathbf{q}}$ and its location. It is worthwhile to note that if we compare, for example, $\langle \mathbf{R}^4\rangle$ with $\langle \mathbf{R}^2\rangle$, the quantity $\langle \mathbf{R}^4\rangle$ is, in a sense, of a more important physical significance than $\langle \mathbf{R}^2\rangle$, since in (9.2) the long-range comeponnt of $J(\mathbf{R})$ is more heavily represented than in (9.1). We also note that the cut in $F(\mathbf{q})$ for $|\mathbf{q}|\gtrsim 2\pi/a$ introduced by the neglect of interband transitions does not affect the long-range component of $J(\mathbf{R})$ or of the conduction-electron polarization.

With approximation (9.8) we obtain in (6.5)

$$J(\mathbf{R})=\frac{2}{N^2}j^2(\mathbf{k}_c,\mathbf{k}_c)\frac{V}{(2\pi)^3}\int F(\mathbf{q})e^{-i\mathbf{q}\cdot\mathbf{R}}d\mathbf{q}, \tag{9.11}$$

where we have already replaced the sum in $\mathbf{q}$ by the appropriate integral. We note in (9.11) that $j^2(\mathbf{k}_c,\mathbf{k}_c)$ may change from one singularity to the other.

In (9.11) the function $F(\mathbf{q})$ is zero outside a region about twice as big in each direction as is the Brillouin zone. Consequently, we can develop $F(\mathbf{q})$ in a triple Fourier series. We will see that not all Fourier coefficients of $F(\mathbf{q})$ are described by the integral in (9.11).

We also note that (9.11) may be considered as model-independent in the sense that it could be applicable to arbitrary lattice structure, in materials where interband transitions are known to be irrelevant.

It does not seem to be a simple problem to calculate the integral (9.11) for the face-centered and body-centered structures. In those cases as well as for more complicated structures the best way seems to be some adaptation of the critical-point method.[38] In this paper, we will restrict ourselves to the simple cubic case, since we are interested only in the qualitative features of the model.

At this point, and noting (2.12), it is convenient to define the dimensionless quantity

$$c_{\mathbf{k}}=-\sum_j \cos k_j, \tag{9.12}$$

where we note that for $\mathbf{k}\rightarrow 0$,

$$c_{\mathbf{k}}\approx -3+\tfrac{1}{2}\mathbf{k}^2, \tag{9.13}$$

so that with $B<0$, the bottom of the band is located at $\epsilon_{\mathbf{k}=0}=-|B|$ or $\omega=-3$, where ω as defined in (2.14) describes the location of the Fermi level. Working with dimensionless momenta we obtain from (3.10)

$$F(\mathbf{q})=\frac{3}{|B|}\frac{V/a^3}{(2\pi)^3}f(\mathbf{q}), \tag{9.14}$$

where $2|B|$ is the width of the conduction band and $f(\mathbf{q})$ is a dimensionless function given by

$$f(\mathbf{q})=\int_{-\pi}^{\pi}d\mathbf{k}\,\theta(\omega-c_{\mathbf{k}}) \times\int_{-\pi}^{\pi}d\mathbf{k}'P\frac{1}{c_{\mathbf{k}'}-c_{\mathbf{k}}}\delta(\mathbf{k}'-\mathbf{k}-\mathbf{q}), \tag{9.15}$$

where $d\mathbf{k}=dk_x dk_y dk_z$ and the region of integration is defined by $-\pi\leqslant k_j\leqslant\pi$ and $-\pi\leqslant k_j'\leqslant\pi$.

Noting that $f(\mathbf{q})$ is zero outside the cube

$$-2\pi<q_j<2\pi, \tag{9.16}$$

we can expand $f(\mathbf{q})$ in a tridimensional Fourier series

$$f(\mathbf{q})=\sum_{\mathbf{n}} f(\mathbf{n})e^{i\mathbf{q}\cdot\mathbf{n}/2}, \tag{9.17}$$

where $n_j=0,\ \pm1,\ \pm2,\ \cdots$.

The Fourier coefficients $f(\mathbf{n})$ are given by the triple integral

$$f(\mathbf{n})=\frac{1}{(4\pi)^3}\int_{-2\pi}^{2\pi}f(\mathbf{q})e^{-i\mathbf{q}\cdot\mathbf{n}/2}d\mathbf{q}, \tag{9.18}$$

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[37] L. van Hove, Phys. Rev. **89**, 1189 (1953).

[38] A. A. Maradudin, in *Solid State Physics*, edited by F. Seitz and D. Turnbull (Academic Press Inc., New York, 1963), Suppl. 3.

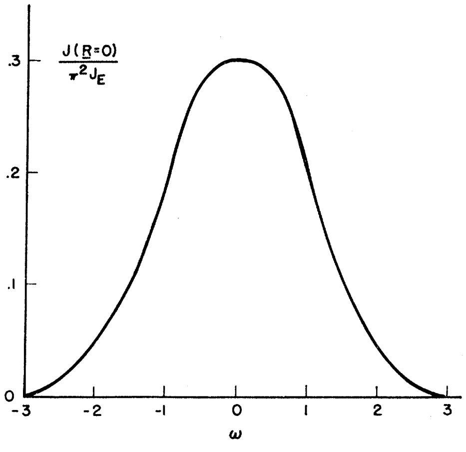

FIG. 1. $J(\mathbf{R}=0)/\pi^2 J_E$ versus ω. In this and in subsequent figures, ω is a measure of the position of the Fermi surface, as defined by (2.14). The conduction band is empty at $\omega=-3$ and full at $\omega=+3$. The symmetry about $\omega=0$ reflects the similarity between the electron surface as developed from $\omega\geqslant -3$ and the hole surface as developed from $\omega\leqslant +3$.

where the factor $\frac{1}{2}$ in the phase is related to the length 4π of the sides in cube (9.16). With these simplifications and using (9.11), (9.14), and (9.18) we obtain

$$J(\mathbf{R})=J_E f(2\mathbf{n}), \tag{9.19}$$

where

$$J_E=\frac{6}{\pi^3}\frac{j^2(\mathbf{k}_c,\mathbf{k}_c)}{B^2}|B|, \tag{9.20}$$

and $R_j=an_j$.

If we compare $J(\mathbf{R})$ and $P(\mathbf{R})$ in (9.19) and (5.19), respectively, we can see that, except for an extra factor $U_{\mathbf{q}}(\mathbf{R}_n)=U_{\mathbf{q}}(0)$ in the integrand (5.19) both quantities are related to $f(2\mathbf{n})$.

From (9.15) and (9.18) it can be shown that the Fourier coefficients $f(\mathbf{n})$ are all real and symmetric, i.e.,

$$f^*(\mathbf{n})=f(\mathbf{n}), \tag{9.21}$$

and

$$f(-\mathbf{n})=f(\mathbf{n}). \tag{9.22}$$

Now, instead of working with the function $f(\mathbf{q})$ in (9.15), it is convenient to define

$$g(\mathbf{q})=\frac{\partial f(\mathbf{q})}{\partial\omega}$$

$$=\int_{-\pi}^{\pi}d\mathbf{k}\,\delta(\omega-c_{\mathbf{k}})\int_{-\pi}^{\pi}d\mathbf{k}'P\frac{1}{c_{\mathbf{k}'}-\omega}\delta(\mathbf{k}'-\mathbf{k}-\mathbf{q}) \tag{9.23}$$

and the corresponding Fourier coefficients

$$g(\mathbf{n})=\frac{1}{(4\pi)^3}\int_{-2\pi}^{2\pi}g(\mathbf{q})e^{i\mathbf{q}\mathbf{n}/2}d\mathbf{q}; \tag{9.24}$$

in order to obtain $f(\mathbf{n})$ we use the property

$$f(\mathbf{n})=\int_{-\infty}^{\omega}g(\mathbf{n})d\omega. \tag{9.25}$$

Using the integral representations

$$\delta(\omega-c_{\mathbf{k}})=\frac{1}{2\pi}\int_{-\infty}^{+\infty}e^{i(\omega-c_{\mathbf{k}})t}dt, \tag{9.26}$$

$$P\frac{1}{c_{\mathbf{k}'}-\omega}=\int_0^{\infty}e^{-\lambda\xi}\sin(c_{\mathbf{k}'}-\omega)\xi d\xi, \tag{9.27}$$

with $\lambda=+0$, we show in Appendix B that

$$g(2\mathbf{n})=-\pi^2(-1)^{n_x+n_y+n_z}C_{\mathbf{n}}(\omega)S_{\mathbf{n}}(\omega), \tag{9.28}$$

where

$$\begin{pmatrix}C_{\mathbf{n}}(\omega)\\ S_{\mathbf{n}}(\omega)\end{pmatrix}=\int_0^{\infty}\begin{pmatrix}\cos\omega t\\ \sin\omega t\end{pmatrix}J_{n_x}(t)J_{n_y}(t)J_{n_z}(t)dt, \tag{9.29}$$

and $J_n(t)$ is the ordinary Bessel function of integer order and real argument.[39]

The Fourier transforms (9.29) have been employed in a paper by Wolfram and Callaway[32] where we can find a table for the first four quantities $C_{\mathbf{n}}(S_{\mathbf{n}})$ as functions of ω. Noting that $C_{\mathbf{n}}(\omega)$ is an even function of ω, whereas $S_{\mathbf{n}}(\omega)$ is odd, with help of their table[32] we have calculated the quantity

$$J(\mathbf{R}=0)/\pi^2 J_E=-\int_{-3}^{\omega}C_0(\omega)S_0(\omega)d\omega, \tag{9.30}$$

with the result shown in Fig. 1.

Figure 2 is a plot of the quantity [see (8.15)]

$$-\frac{\partial J(\mathbf{R}=0)}{\partial\epsilon_F}\Big/\frac{(3\pi^2 J_E)}{|B|}=C_0(\omega)S_0(\omega). \tag{9.31}$$

Using the expression (8.3) for the paramagnetic temperature, combined with (5.7) and the expression (A3)

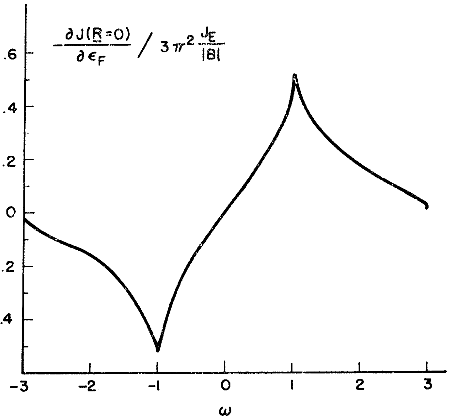

FIG. 2. $-[J(\mathbf{R}=0)/\partial\epsilon_F]/[(3\pi^2 J_E)/|B|]$ versus ω. The electron surface touches the Brillouin-zone cube face centers at $\omega=-1$ and the cube face edges at $\omega=+1$. Correspondingly, the hole surface touches its Brillouin-zone cube face edges at $\omega=-1$ and cube face centers at $\omega=+1$.

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[39] G. N. Watson, *A Treatise on the Theory of Bessel Functions* (Cambridge University Press, Cambridge, England, 1952).

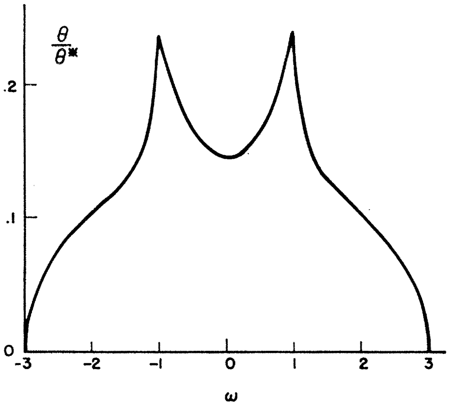

FIG. 3. θ/θ^* versus ω.

for the level-density function, we obtain

$$\frac{\theta}{\theta^*}=\tfrac{1}{2}C_0(\omega)+\int_{-3}^{\omega}C_0(\omega)S_0(\omega)d\omega\,, \tag{9.32}$$

where

$$\kappa_B\theta^*=\tfrac{2}{3}S(S+1)\pi^2J_E\,, \tag{9.33}$$

and J_E is defined in (9.20). In Fig. 3 we plot the quantity θ/θ^* as a function of ω.

For the calculation of the exchange moments, we note that $g(2\mathbf{n})$ in (9.28) can be written in the form

$$g(2\mathbf{n})=-\pi^2(-1)^{n_x+n_y+n_z}\times\int_0^\infty\cos\omega t dt\int_0^\infty\sin\omega\xi d\xi G_{\mathbf{n}}(t)G_{\mathbf{n}}(\xi)\,, \tag{9.34}$$

where

$$G_{\mathbf{n}}(t)=\prod_j J_{n_j}(t)\,, \tag{9.35}$$

so that, for example,

$$\frac{1}{J_E}\frac{\partial}{\partial\omega}\sum_{\mathbf{R}}J(\mathbf{R})=-\pi^2\times\int_0^\infty\cos\omega t dt\int_0^\infty\sin\omega\xi d\xi\sigma_0^3(t,\xi)\,, \tag{9.36}$$

where

$$\sigma_0(\xi,t)=\sum_{n=-\infty}^{+\infty}(-1)^nJ_n(t)J_n(\xi)\,. \tag{9.37}$$

From the addition theorem[39] for Bessel functions, one can show that for $t>0$ and $\xi>0$

$$\sum_{n=-\infty}^{+\infty}(-1)^nJ_n(t)J_n(\xi)=J_0(t+\xi)\,, \tag{9.38}$$

$$\sum_{n=-\infty}^{+\infty}(-1)^nn^2J_n(t)J_n(\xi)=-\frac{t\xi}{t+\xi}J_1(t+\xi)\,, \tag{9.39}$$

and

$$\sum_{n=-\infty}^{+\infty}(-1)^nn^4J_n(t)J_n(\xi)=-\frac{t\xi}{t+\xi}\left[J_1(t+\xi)-\frac{3t\xi}{t+\xi}J_2(t+\xi)\right]. \tag{9.40}$$

In Appendix C we show that using (9.38), (9.39), and (9.40) we can calculate the exchange moments (9.1), (9.2), and (9.3) as well as $\sum_{\mathbf{R}}J(\mathbf{R})$. The results can be written in the form

$$\frac{60}{\pi^2}\langle1\rangle=30C_0(\omega)\,, \tag{9.41}$$

$$\frac{60}{\pi^2}\langle\mathbf{R}^2\rangle/a^2=-5[C_0(\omega)+\omega C_0'(\omega)]\,, \tag{9.42}$$

$$\frac{60}{\pi^2}\langle\mathbf{R}^4\rangle/a^4=2[C_0(\omega)+2\omega C_0'(\omega)+\tfrac{1}{2}(\omega^2+6)C_0''(\omega)]\,, \tag{9.43}$$

$$\frac{60}{\pi^2}\langle R_x^4+R_y^4+R_z^4\rangle/a^4=C_0(\omega)+\omega C_0'(\omega)+9C_0''(\omega)\,, \tag{9.44}$$

where

$$\langle1\rangle=\sum_{\mathbf{R}}J(\mathbf{R})/J_E\,, \tag{9.45}$$

and

$$C_0(\omega)\propto\rho(\epsilon_F) \tag{9.46}$$

is the dimensionless level-density function defined in (A4). In the above expressions, C_0' and C_0'' are the first and second derivatives of $C_0(\omega)$ with respect to ω. A plot of the above level-density function in the simple cubic case as compared to the spherical-model level-density function is given by Mott and Jones.[36]

We note in (9.41)–(9.44) that, since $C_0(-\omega)=C_0(\omega)$ is an even function of ω, the above exchange moments are also even functions of ω, or in other words, the exchange moments are symmetric under particle-hole transformation. This is a model-independent property related to the form of the *s-d* Hamiltonian.

As we can see, with the approximations used in this section, the exchange moments are related to the level-density function $\rho(\epsilon_F)$ and its derivatives at the Fermi level. We have already shown that (9.41) is model-independent, i.e., valid for any lattice structure. We note in (9.42) that $\omega C_0'(\omega)$ is invariant under a change in the scaling of the bandwidth. Using the method of Nitsovich[40] one can show that $\langle\mathbf{R}^2\rangle$ is proportional to $-[\rho(\epsilon_F)+\epsilon_F\rho'(\epsilon_F)]$ for the bcc structure in the tight-binding approximation. Consequently, (9.42) is very probably valid for all lattice structures.

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[40] V. M. Nitsovich, Phys. Metals Metall. **6**, 22 (1958).

TABLE I. Numerical values of various terms in the calculation of (9.30), (9.31), (9.32), and (9.42) in a simple cubic crystal.

ω	$-\int_{-3}^{\omega} C_0S_0 d\omega$	$\frac{1}{2}C_0$	θ/θ^*	C_0S_0	C_0	$-\omega C_0'$	$-(C_0+\omega C_0')$
0.0	0.302	0.448	0.145	0.000	0.895	0.000	−0.895
0.2	0.299	0.449	0.150	0.066	0.898	−0.002	−0.900
0.4	0.289	0.448	0.160	0.137	0.897	0.002	−0.894
0.6	0.271	0.450	0.179	0.217	0.900	−0.010	−0.909
0.8	0.244	0.453	0.209	0.323	0.907	−0.029	−0.934
1.0	0.199	0.435	0.237	0.525	0.871	0.181	−0.689
1.2	0.152	0.308	0.157	0.387	0.617	1.522	0.905
1.4	0.117	0.253	0.136	0.307	0.506	0.776	0.269
1.6	0.090	0.213	0.123	0.252	0.426	0.643	0.217
1.8	0.067	0.180	0.113	0.207	0.360	0.591	0.231
2.0	0.048	0.152	0.104	0.171	0.304	0.562	0.258
2.2	0.033	0.127	0.094	0.139	0.254	0.553	0.300
2.4	0.020	0.103	0.082	0.110	0.205	0.578	0.373
2.6	0.010	0.079	0.068	0.083	0.158	0.611	0.452
2.8	0.004	0.053	0.049	0.055	0.106	0.732	0.626
3.0	0.000	0.000	0.000	0.000	0.000	1.593	1.593

Noting in (9.43) that the width for ω is 6, a generalization of (9.43) can be obtained if we scale the bandwidth in proportion to the coordination number, i.e., the number of nearest neighbors. It seems that, with these adjustments, the expressions for the exchange moments can be generalized for other lattice structures. Calculations for bcc are now in progress.

For the simple cubic system, we have calculated numerical values of the quantity $C_0'(\omega)$ from the first differences in the table for $C_0(\omega)$ given by Wolfram and Callaway.[32] In this way we have determined approximately the quantity

$$-[C_0(\omega)+\omega C_0'(\omega)] \tag{9.47}$$

related to $\langle\mathbf{R}^2\rangle$. In Fig. 4 we plot the result for (9.47).

For a comparison of the relative importance of the different terms in these calculations, in Table I we show the numerical results for the simple cubic case.

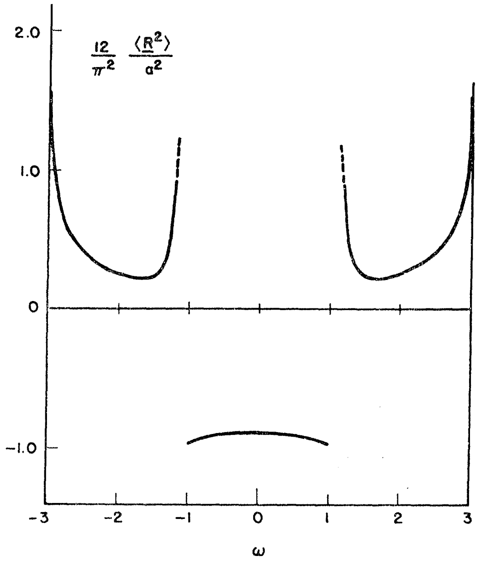

FIG. 4. $(12/\pi^2)\langle\mathbf{R}^2\rangle/a^2$ versus ω.

There is no point in going on to the calculation of $\langle\mathbf{R}^4\rangle$, since the use of second differences in the tabulated values of $C_0(\omega)$ would make the results imprecise. Qualitatively we can say that the discontinuities in $\langle\mathbf{R}^4\rangle$ can be expected to be more dramatic than those for $\langle\mathbf{R}^2\rangle$. Some preliminary calculations indicate that, for the simple cube and for the bcc structures, the over-all behavior of $\langle\mathbf{R}^4\rangle$ as a function of ϵ_F is one following roughly as the derivative of $\langle\mathbf{R}^2\rangle$ with respect to ϵ_F.

We have also examined the behavior of $\langle\mathbf{R}^2\rangle$ and $\langle\mathbf{R}^4\rangle$ in the limit $\omega\rightarrow -3$, where the Fermi surface becomes spherical. Noting (9.13), we can write

$$\Delta\omega\equiv\omega+3\approx\tfrac{1}{2}k_F^2a^2. \tag{9.48}$$

In Appendix D we show that, for $\Delta\omega\rightarrow +0$,

$$C_0(-3+\Delta\omega)\approx\frac{1}{\pi\sqrt{2}}(\Delta\omega)^{1/2}; \tag{9.49}$$

in this way we can determine the first and second derivatives of $C_0(\omega)$. In this region, the major contribution to the exchange moments comes from the last term in (9.42), (9.43), and (9.44). Retaining only the dominant terms we obtain the result

$$\frac{\langle\mathbf{R}^2\rangle}{a^2}\propto +\frac{1}{(\Delta\omega)^{1/2}}, \tag{9.50}$$

$$\frac{\langle\mathbf{R}^4\rangle}{a^4}\propto -\frac{1}{2}\frac{1}{(\Delta\omega)^{3/2}}, \tag{9.51}$$

$$\frac{\langle R_x^4+R_y^4+R_z^4\rangle}{a^4}\propto -\frac{3}{10}\frac{1}{(\Delta\omega)^{3/2}}, \tag{9.52}$$

and consequently, using (9.48) and (9.50)–(9.52),

$$\frac{\langle\mathbf{R}^4\rangle}{a^2\langle\mathbf{R}^2\rangle}\approx -1/k_F^2a^2, \tag{9.53}$$

and

$$\frac{\langle R_x^4+R_y^4+R_z^4\rangle}{\langle \mathbf{R}^4\rangle}\approx+\tfrac{3}{5}. \qquad (9.54)$$

Expression (9.53) is just the result obtained by Kasuya,[1] with the neglect of interband transitions (umklapp terms); (9.54) is a new result. We also note that (9.50)–(9.54) are structure-independent, since they correspond to $k_F{}^2a^2\rightarrow 0$.

Using the critical-point method[38] one can show that, for the sc system, near the first singularity $\omega_b=-1$ (see Sec. II), i.e., for $\omega=-1-\eta$, with $|\eta|\ll 1$, the dimensionless level-density function $C_0(\omega)$ can be written as

$$C_0(\omega)=G(\omega)+S(\omega)\,, \qquad (9.55)$$

where $G(\omega)$ is analytic in the neighborhood of $\omega=-1$, and $S(\omega)$ is the singular part given by

$$\begin{aligned} S(\omega)&=-Q\sqrt{\eta} \quad \text{for} \quad \eta>0\,,\\ &=0 \qquad\quad \text{for} \quad \eta<0; \end{aligned} \qquad (9.56)$$

Q is a positive constant.

Using (9.55), (9.56), and the expressions (9.42)–(9.44) for the exchange moments, and keeping only the dominant terms involving the derivatives of the singular contribution $S(\omega)$, we obtain the results

$$\langle \mathbf{R}^2\rangle/a^2\propto+\frac{5}{2}\frac{1}{\sqrt{\eta}}\,, \qquad (9.57)$$

$$\langle \mathbf{R}^4\rangle/a^4\propto+\frac{7}{4}\frac{1}{\eta\sqrt{\eta}}\,, \qquad (9.58)$$

$$\langle R_x^4+R_y^4+R_z^4\rangle/a^4\propto+\frac{9}{4}\frac{1}{\eta\sqrt{\eta}}\,, \qquad (9.59)$$

valid for the simple cubic structure, for $\omega=-1-\eta$, with $0<\eta\ll 1$; consequently, one obtains

$$\langle \mathbf{R}^4\rangle/a^2\langle \mathbf{R}^2\rangle\approx+(7/10)(1/\eta) \qquad (9.60)$$

and

$$\langle R_x^4+R_y^4+R_z^4\rangle/\langle \mathbf{R}^4\rangle\approx+(9/7)\,. \qquad (9.61)$$

The above results are valid only for $\omega\lesssim-1$, i.e., just before the formation of the multiply connected Fermi surface. In this region, a very small increase of electron concentration is capable of producing relatively large variations in the magnetic properties. This fact seems to rise some doubts on the applicability of the perturbation theory. The same problem seems also to occur in the region corresponding to the spherical model, i.e., for $k_Fa\ll 1$.

For $0<\eta\ll 1$ we can obtain positive values for $\langle \mathbf{R}^2\rangle$ and for $\langle \mathbf{R}^4\rangle$, a result which is consistent with experimental data for some ferromagnetic metals. We also note that relatively large values for the ratio $\langle \mathbf{R}^4\rangle/(a^2\langle \mathbf{R}^2\rangle)$ can be obtained in the region $0<\eta\ll 1$, in contrast with the negative value obtained by Kasuya[1] [see (9.53)] in the spherical model, i.e., for $k_Fa\ll 1$.

As a last comment, the quantity

$$D\propto\sum_{\mathbf{R}\neq 0}\mathbf{R}^2J(\mathbf{R}) \qquad (9.62)$$

can also be calculated from the tables obtained by Mattis[41] for the quantity $J_{\mathbf{k}}$ in (6.7) for the three cubic systems, using the spherical model. The exchange stiffness can be calculated graphically from the appropriate slopes of the curve $J_{\mathbf{q}}$ versus $q_j{}^2$. In this way we can take into account the umklapp terms not included in the expressions (9.50)–(9.54).

We note that the expression used by Mattis for the conduction-electron polarization includes phenomenologically a conduction-electron relaxation time Γ, assumed to be a constant. This procedure introduces a cutoff of the polarization at large distances.

The results for the graphical determination of D are shown in Fig. 5, where the different curves are normalized differently; we are concerned only with their k_F dependence.

One can also plot the above graphically obtained $\langle \mathbf{R}^2\rangle$ versus $(k_Fa)^{-1}$ for a check with (9.50). The result indicates that, with the introduction of Mattis's relaxation time, the quantity $(\Delta\omega)^{1/2}$ in (9.49) should be replaced by $(\Delta\omega+\alpha^2)^{1/2}$, where α is a constant. This indicates that the effect of a finite conduction-electron mean free path is to round off the sharp discontinuities and kinks. A good guess seems to be that the absolute value of the exchange moment $\langle \mathbf{R}^{2n}\rangle$ should be limited by a condition of the type

$$|\langle \mathbf{R}^{2n}\rangle|\leqslant l_e{}^{2n}\,, \qquad (9.63)$$

where l_e is the conduction-electron mean free path.

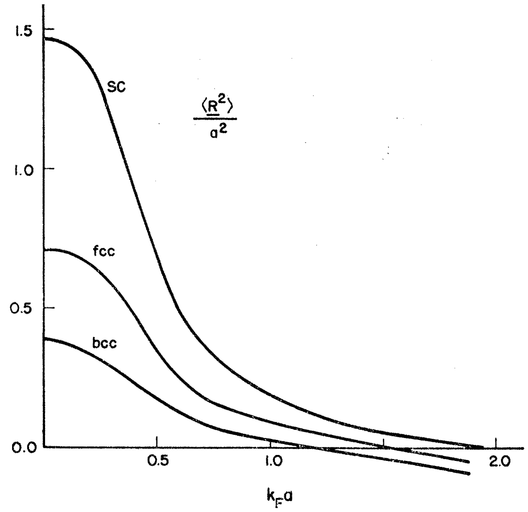

FIG. 5. $\langle \mathbf{R}^2\rangle/a^2$ versus k_Fa. Based on tabulations by Mattis.

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[41] D. C. Mattis, *The Theory of Magnetism* (Harper and Row, New York, 1964), p. 205.

X. APPLICATION TO RARE-EARTH METALLIC COMPOUNDS AND ALLOYS

The quantities discussed in Sec. IX have been plotted in terms of the Fermi energy there described by the parameter ω. If we want these quantities in terms of the conduction-electron concentration we have to calculate the quantity

$$N_e=2\int_{E_b}^{\epsilon_F}\rho(\epsilon)d\epsilon=\frac{2N}{\pi}\int_{-3}^{\omega}C_0(\omega)d\omega\,, \qquad (10.1)$$

and this one could do by numerical integration of the tabulated function $C_0(\omega)$.[32]

The change in electron concentration is usually obtained by alloying.

We have assumed that the spins $\mathbf{S}_n$ are located periodically in the lattice structure. A relaxation in this condition is possible at low concentration when the conduction electrons "see" an almost periodic potential. If we dissolve magnetic ions in a metal, due to the valence difference between the impurity ions and those of the matrix, we can expect a readjustment of the conduction-electron charge distribution as a consequence of the electrostatic potential introduced by the impurity and the Coulomb repulsion among the conduction electrons. This effect is well described by Friedel sum rules.[42] In the present case we can expect a charge and spin polarization. The charge polarization will affect the spin polarization in (5.19) through the factor $U_{\mathbf{q}}(\mathbf{r})$, particularly at points $\mathbf{r}$ close to the impurity. This effect can be made relatively small if the valence difference is not large. Now, at large distances, the potential becomes again nearly periodic, so that, even if the valence difference is not so small, we can take $U_{\mathbf{q}}(\mathbf{r})$ as nearly independent of $\mathbf{r}$, or being more precise, we can take $U_{\mathbf{q}}(\mathbf{r})$ as the periodic quantity appropriate for the pure matrix.

As we see, the problem of charge difference makes necessary a clear distinction between the short-range and long-range effects. The short-range effects are always model-dependent and very sensitive not only to the details of the matrix band structure, but also to the valence difference[43] and local distortion of the lattice.[44]

On the other hand, at low concentrations, the long-range effects are related to the behavior of $F(\mathbf{q})$ in the neighborhood of $\mathbf{q}=0$; consequently they are essentially model-independent in the sense that they depend only on some features of the matrix conduction-electron spectrum in the neighborhood of the Fermi level.

The paramagnetic temperature, as given by (8.3), has been shown to be the sum of two terms, one being model-independent and the other being model-dependent. The quantity $J(\mathbf{R}=0)$ is sensitive to the details of the band structure, as well as to the cutoff introduced in $F(\mathbf{q})$ by the neglect of interband transitions.

In the case of rare-earth metals, due to weak crystal fields, the orbital angular momentum becomes unquenched, so that the appropriate expression for θ is obtained by replacing $\mathbf{S}$ by $(g-1)\,\mathbf{J}$, where $\mathbf{J}$ is the total angular momentum.[45] The equation for θ obtained by deGennes[45] in the spherical model was used by Mattis *et al.*[46] in a calculation of the k_F dependence of the paramagnetic temperature for different lattice structures. We note that among the cubic systems the face-centered structure is the one which more heavily weighs the short-range component of the conduction-electron spin polarization, due to the compactness of the fcc lattice.

The paramagnetic temperature of the ordered compounds $\mathrm{Eu}_{1-x}\mathrm{Gd}_x\mathrm{Se}$ has been measured[18] as a function of x. In agreement with these experimental results, the values of θ calculated by Mattis and his collaborators show an initially rapid rise of θ as a function of electron concentration, followed by a region of linear decrease, where θ becomes negative for $x\gtrsim 0.60$. In the present model, θ is positive in the simple cubic case, during the whole process of filling the Brillouin zone; we do not know yet whether it is possible to obtain negative values for the paramagnetic temperature in certain regions of electron concentration, for the body-centered and face-centered structures.

The present model is able to describe the rapid rise of the paramagnetic temperature in the region $-3<\omega\lesssim -2$, where $J(\mathbf{R}=0)$ is relatively small, at least for the simple cubic case, as we can see from Table I. This fact seems to be model-independent, since for $k_Fa\ll 1$, the conduction-electron s-wave function is insensitive to the lattice structure. Consequently, in the limit of small conduction-electron concentration, i.e., for $k_Fa\ll 1$, one can show that the rapid rise of θ with electron concentration is due to a term going as $\bar{N}_e^{1/3}\propto x^{1/3}$.

If we could determine $J(\mathbf{R}=0)$ by some independent measurement through NMR or Mossbauer technique then a check of expression (8.3) might be provided by the measurement of the electronic specific heat or the Pauli electron spin susceptibility (Knight shift).[47] We note that the detection of a kink in θ, in this case, requires only the measurement of the differences in Knight shift as we change the electron concentration.

The main feature of the present model is the prediction of a kink in θ associated to a discontinuity in $\langle\mathbf{R}^2\rangle$ as we increase the electron concentration. As we can see

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[42] J. Friedel, Phil. Mag. **43**, 153 (1952).

[43] E. Daniel, J. Phys. Radium **20**, 51 (1959); L. E. Drain, Phil. Mag. **4**, 484 (1959); W. Kohn and S. H. Vosko, Phys. Rev. **119**, 912 (1960); T. J. Rowland, *ibid.* **125**, 459 (1962).

[44] F. J. Blatt, Phys. Rev. **108**, 285 (1957).

[45] P. G. deGennes, Compt. Rend. **247**, 1836 (1958).

[46] D. Mattis, N. Anthony, and L. Horowitz, IBM Report No. RC-945, 1963 (unpublished); D. Mattis and W. E. Donath, Phys. Rev. **128**, 1618 (1962).

[47] W. D. Knight, in *Solid State Physics*, edited by F. Seitz and D. Turnbull (Academic Press Inc., New York, 1956), Vol. 2.

in Fig. 1, the quantity $J(\mathbf{R}=0)$ is a smooth function of ω. Consequently, the kink in θ is associated with the kink in the level-density function, and so its presence may be considered as a model-independent result. It is worthwhile to note that this Kohn[48] anomaly in θ is expected to be more noticeable in proportion to the number of faces in the Brillouin zone that touch the Fermi surface, or in other words, in proportion to the number of necks in the multiply connected Fermi surface.

We also note that the compounds $Eu_{1-x}Gd_xSe$ are ferromagnetic in the region $x \ll 1$ and antiferromagnetic for $x \approx 1$. In the ferromagnetic region a determination of $\langle \mathbf{R}^2 \rangle$ can be obtained through the temperature dependence of the spontaneous magnetization.[49] Some information about $\langle \mathbf{R}^2 \rangle$ can also be obtained in the antiferromagnetic region by measuring the T dependence of the sublattice magnetization at low temperatures through NMR techniques.[50,51] Our model predicts, for the simple cubic case, a discontinuous change in $\langle \mathbf{R}^2 \rangle$ from positive to negative value.

A kink in the total energy of the system was predicted by Pick and Blandin[52] from somewhat different considerations, although essentially related to the Bragg condition at the Brillouin-zone surface. In that paper[52] they also noted the qualitative validity of the Hume-Rothary[53,36] rules in the determination of the phase boundaries in alloys. In the case of magnetic alloys, a change in crystal structure may be preferred if the gain in energy so obtained is larger than the corresponding gain for a change in magnetic structure.

Even noting that the present model is not applicable in Fe-Ni alloys, it seems worthwhile to observe that a kink in the paramagnetic temperature has been shown recently to be associated with a discontinuity in $\langle \mathbf{R}^2 \rangle$. The kink in θ was observed by Peschard,[54] and the discontinuity in $\langle \mathbf{R}^2 \rangle \propto D$ was detected by means of neutron diffraction by Hatherly *et al.*[55]

Other compounds of interest[56] are $Gd_{2+x}Se_{3-x}$ and $Gd_{2+x}S_{3-x}$. When x is changed from zero to 0.10 the electrical conductivity increases by about four orders of magnitude, without a change in lattice structure; the lattice parameter a_0, for example, does not have any detectable change in this region, whereas the paramagnetic temperature changes from $-10°$K (at $x=0$) to 88°K (at $x=0.10$). No data on $\langle \mathbf{R}^2 \rangle$ seem to exist for these compounds, in this region of electron concentration. If we assume that this region corresponds to $\rho(\epsilon) \propto \sqrt{\epsilon}$, i.e., spherical Fermi surface, then it would be impossible to obtain a negative value for θ, unless some new mechanism is taken into account. The effect of interband transitions in this region is negligible, as we have seen.

Another rare-earth compound studied by Holtzberg *et al.*[56] is $Gd_4(Sb_xBi_{1-x})_3$. The replacement of a Bi ion by its closely related element Sb does not change the electron concentration, as one can conclude from the nearly constant electrical conductivity. These ferromagnetic compounds follow the $T^{3/2}$ Bloch law[57] for the spontaneous magnetization. In this way a plot of the exchange-stiffness parameter D versus the Gd-Gd distance has been obtained. The total increase in D is of the order of 30%, for an increase of only 2% in the Gd-Gd distance. In the spherical model, assuming $N_e=$ const, an increase in the lattice parameter a corresponds to a decrease in k_F, so that $k_F a$ is kept constant. In our model, this situation is described by a change in ϵ_F and a change in $|B|$, in such a way that ω does not change. In this case, if we assume that $J_E = j^2(0)/|B| =$ const, we cannot describe the change in $\langle \mathbf{R}^2 \rangle \propto a^2$. A possibility to be examined is to assume for $|B|$ a different variation compared to that for $j^2(0)$, so that $J_E = J_E(a)$. This corresponds to a change in the band width, or in other words, to a change in the conduction-electron effective mass. This change in effective mass has to be made consistent with the experimental results for the electrical resistivity. We also note that the change in J_E so obtained may be used in a calculation of $a=a(x)$ if we assume, as in the paper by Rocher,[58] that the magnetoelastic energy comes entirely from the distance dependence of the indirect-exchange Hamiltonian (6.4). *Note added in proof.* A paper by L. M. Roth, H. J. Zeiger, and T. A. Kaplan [Phys. Rev. **149**, 519 (1966)], dealing with the same problem, has come to the author's attention. They have studied the asymptotic behavior of the indirect exchange $J(\mathbf{R})$ for $R \to \infty$, and have shown this to be related to the shape of the Fermi surface.

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[48] W. Kohn, Phys. Rev. Letters **2**, 393 (1959).

[49] See, for example, F. Keffer, *Handbuch der Physik* (Springer-Verlag, New York, 1966), Vol. 18/2.

[50] P. R. P. Silva (unpublished).

[51] V. Jaccarino and L. R. Walker, J. Phys. Radium **20**, 341 (1959).

[52] R. Pick and A. Blandin, Physik Kondensierten Materie **3**, 1 (1964).

[53] See, for example, W. Hume-Rothary, G. W. Mabbott, and K. M. Channel-Evans, Phil. Trans. Roy. Soc. **233**, 1 (1934).

[54] M. Peschard, Rev. Metall. **12**, 663 (1925).

[55] M. Hatherly, K. Hirakawa, R. D. Lowde, J. F. Mallet, M. W. Stringfellow, and B. H. Torrie, Proc. Phys. Soc. (London) **84**, 55 (1964).

[56] F. Holtzberg, T. R. McGuire, S. Methfessel, and J. C. Suits, J. Appl. Phys. **35**, 1033 (1964).

[57] F. Bloch, Z. Physik **61**, 206 (1930).

[58] Y. A. Rocher, Advan. Phys. **11**, 233 (1962).

APPENDIX A

In order to show that

$$\lim_{\mathbf{q}\to 0} F(\mathbf{q})=\tfrac{1}{2}\rho(\epsilon_F)$$

in the simple cubic case, let us first calculate the level-density function and then the limit.

Using the dimensionless quantities of (2.14) and (9.12), the expression (4.7) may be written in the form

$$\rho(\epsilon_F')=\frac{3}{|B|}\frac{N}{(2\pi)^3}\int_{-\pi}^{\pi}\delta(\omega-c_{\mathbf{k}})d\mathbf{k}\,, \tag{A1}$$

where we now replace the δ function by its integral representation (9.26) and use expression[59]

$$\int_{-\pi}^{\pi}e^{\pm it\cos k}dk=2\pi J_0(t)\,, \tag{A2}$$

to obtain

$$\rho(\epsilon_F)=\frac{3N}{\pi|B|}C_0(\omega)\,, \tag{A3}$$

where

$$C_0(\omega)=\int_0^{\infty}\cos\omega t J_0^3(t)dt\,, \tag{A4}$$

as in (9.29).

Taking into account (9.15), and replacing the integral representation

$$\theta(\omega-c_{\mathbf{k}})=\tfrac{1}{2}+\frac{1}{\pi}P\int_0^{\infty}\frac{\sin(\omega-c_{\mathbf{k}})t}{t}dt \tag{A5}$$

in the expression (9.15) for $f(\mathbf{q})$ we obtain

$$f(\mathbf{q})=\frac{1}{\pi}\int_0^{\infty}P\frac{dt}{t}\int_{-\pi}^{\pi}d\mathbf{k}\sin(\omega-c_{\mathbf{k}})t$$

$$\times\int_{-\pi}^{\pi}P\frac{1}{c_{\mathbf{k}'}-c_{\mathbf{k}}}\delta(\mathbf{k}'-\mathbf{k}-\mathbf{q})d\mathbf{k}'\,, \tag{A6}$$

since

$$\frac{1}{2}\int_{-\pi}^{\pi}d\mathbf{k}\int_{-\pi}^{\pi}P\frac{1}{c_{\mathbf{k}'}-c_{\mathbf{k}}}\delta(\mathbf{k}'-\mathbf{k}-\mathbf{q})d\mathbf{k}'=0\,, \tag{A7}$$

as one can show easily, if we take into account that $c_{-\mathbf{k}}=c_{\mathbf{k}}$, when we first change the variables of integration $\mathbf{k}\to-\mathbf{k}$, $\mathbf{k}'\to-\mathbf{k}'$ in a first step, and then interchange $\mathbf{k}\leftrightarrow\mathbf{k}'$, in a second step.

With $\mathbf{q}=(0,0,q)$ we can write

$$P\frac{1}{c_{\mathbf{k}'}-c_{\mathbf{k}}}\delta(\mathbf{k}'-\mathbf{k}-\mathbf{q})=-P\frac{1}{\cos(k_z+q)-\cos k_z}$$

$$\times\delta(k_x'-k_x)\delta(k_y'-k_y)\delta(k_z'-k_z-q)\,, \tag{A8}$$

so that in (A6) we obtain

$$f(\mathbf{q})=-\frac{1}{\pi}\int_0^{\infty}P\frac{dt}{t}\int_{-\pi}^{\pi}dk_x\int_{-\pi}^{\pi}dk_y\int_{-\pi}^{\pi}dk_z$$

$$\times\frac{\sin(\omega-c_{\mathbf{k}})t}{\cos(k_z+q)-\cos k_z}\int_{-\pi}^{\pi}\delta(k_z'-k_z-q)dk_z'\,, \tag{A9}$$

where we note that

$$\int_{-\pi}^{\pi}\delta(k_z'-k_z-q)dk_z'$$

$$=\theta(\pi-k_z-q)-\theta(-\pi-k_z-q)\,, \tag{A10}$$

so that k_z is restricted to the common region between

$$-\pi<k_z+q<\pi \tag{A11}$$

and

$$-\pi<k_z<\pi\,; \tag{A12}$$

consequently,

$$f(\mathbf{q})=-\frac{1}{\pi}\int_0^{\infty}\frac{dt}{t}\int_{-\pi}^{\pi}dk_x\int_{-\pi}^{\pi}dk_y\int_{-\pi}^{\pi-q}dk_z$$

$$\times\frac{\sin(\omega-c_{\mathbf{k}})t}{\cos(k_z+q)-\cos k_z}\,, \tag{A13}$$

where we have assumed that $0<q<2\pi$; in (A13) we have dropped the symbol P, with the understanding that $x^{-1}\equiv P(1/x)$.

Replacing in (A13) $\sin(\omega-c_{\mathbf{k}})t$ by its complex exponent form, and noting that $c_{\mathbf{k}}=-\sum_j\cos k_j$, we can factorize the triple integral into a product of three terms, with the result

$$f(\mathbf{q})=-\frac{1}{\pi}(2\pi)^2\int_0^{\infty}\frac{J_0^2(t)}{2it}dt$$

$$\times\left[e^{i\omega t}\int_{-\pi}^{\pi-q}\frac{e^{it\cos k}dk}{\cos(k+q)-\cos k}-\text{c.c.}\right]\,, \tag{A14}$$

where we have made use of (A2).

The second integral in (A14) may be brought into the form

$$-\frac{1}{2}\int_{-(\pi-q/2)}^{(\pi-q/2)}dk\frac{e^{it\cos(k+\frac{1}{2}q)}-e^{it\cos(k-\frac{1}{2}q)}}{\cos(k+\frac{1}{2}q)-\cos(k-\frac{1}{2}q)}\,, \tag{A15}$$

if we change in (A14) the variable of integration to $k'=k+\frac{1}{2}q$ and note the symmetry, $\pm(\pi-\frac{1}{2}q)$, of the new region of integration, so that the replacement $k'\to-k'$ can be applied with the result (A15).

Now we expand $\cos(k\pm\frac{1}{2}q)$ in a power series of q,

$$\cos(k\pm\tfrac{1}{2}q)=\cos k\mp\tfrac{1}{2}q\sin k-\tfrac{1}{8}q^2\cos k+\cdots\,, \tag{A16}$$

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[59] See, for example, *Handbook of Mathematical Functions*, edited by M. Abramowitz and I. A. Stegun (Dover Publications, Inc., New York, 1965), p. 360.

where we keep only the first and second terms, to obtain

$$f(\mathbf{q})\approx 2\pi\int_0^\infty \frac{J_0^2(t)}{t}dt\left[e^{i\omega t}\int_{-(\pi-q/2)}^{(\pi-q/2)} e^{it\cos k}\right.$$
$$\left.\times\frac{\sin(\frac{1}{2}tq\sin k)}{q\sin k}dk+\text{c.c.}\right]. \quad \text{(A17)}$$

Noting the factor $[J_0^2(t)/t]e^{i\omega t}\sim e^{i\omega t}/t^2$, the important values of t will come from the region $t\lesssim 1/\omega$, so that for $q/\omega\longrightarrow 0$, we can replace

$$\sin(\tfrac{1}{2}tq\sin k)/q\sin k\longrightarrow \tfrac{1}{2}t, \quad \text{(A18)}$$

and set $q=0$ in the limits of integration in k. With (A17), (A18), and (A2) we obtain

$$\lim_{q\to 0} f(0,0,q)=(2\pi)^2C_0(\omega), \quad \text{(A19)}$$

and with (9.14) and (A3),

$$\lim_{\mathbf{q}\to 0} F(\mathbf{q})=\tfrac{1}{2}\rho(\epsilon_F). \quad \text{(A20)}$$

APPENDIX B

Replacing in (9.24) the expression (9.23) for $g(\mathbf{q})$ we obtain

$$g(\mathbf{n})=(4\pi)^{-3}\int_{-\pi}^{\pi} d\mathbf{k}e^{i\mathbf{k}\mathbf{n}/2}\delta(\omega-c_{\mathbf{k}})$$
$$\times\int_{-\pi}^{\pi} d\mathbf{k}'e^{-i\mathbf{k}'\mathbf{n}/2}P\frac{1}{c_{\mathbf{k}'}-\omega}, \quad \text{(B1)}$$

so that, with the help of the integral representations (9.26) and (9.27), we can factorize the integrations in $\mathbf{k}$ and $\mathbf{k}'$ into the form

$$g(\mathbf{n})=(4\pi)^{-3}(2\pi)^{-1}$$
$$\times\int_0^\infty e^{-\lambda\xi}d\xi\int_{-\infty}^{+\infty} e^{i\omega t}dt\int_{-\pi}^{\pi} d\mathbf{k}e^{-i(\mathbf{k}\mathbf{n}/2+tc_{\mathbf{k}})}$$
$$\times\frac{1}{2i}\left[e^{-i\omega\xi}\int_{-\pi}^{\pi} e^{i(\mathbf{k}'\mathbf{n}/2+\xi c_{\mathbf{k}'})}-\text{c.c.}\right], \quad \text{(B2)}$$

where we have made use of the transformation $\mathbf{k}'\longrightarrow -\mathbf{k}'$, as a new variable of integration.

Noting that

$$\tfrac{1}{2}\mathbf{k}\mathbf{n}+tc_{\mathbf{k}}=\sum_j(\tfrac{1}{2}k_jn_j-t\cos k_j), \quad \text{(B3)}$$

we obtain

$$\int_{-\pi}^{\pi} d\mathbf{k}e^{i(\mathbf{k}\mathbf{n}/2+tc_{\mathbf{k}})}=\prod_j\int_{-\pi}^{\pi} e^{-i(kn_j/2+t\cos k)}dk. \quad \text{(B4)}$$

The integral

$$\Phi_{\nu_j}(t)=\frac{i^{\nu_j}}{2\pi}\int_{-\pi}^{\pi} e^{i(k\nu_j+t\cos k)}dk \quad \text{(B5)}$$

was studied by Nielsen[60] (1904). For ν_j integer we find[59]

$$\int_{-\pi}^{\pi} e^{i(k\nu_j+t\cos k)}dk=2\pi i^{\nu_j}J_{\nu_j}(t), \quad \text{(B6)}$$

so that, restricting ourselves to the even Fourier coefficient $g(2\mathbf{n})$, we can write

$$\int_{-\pi}^{\pi} e^{i(\mathbf{k}\mathbf{n}+tc_{\mathbf{k}})}d\mathbf{k}=(2\pi)^3(-i)^nG_{\mathbf{n}}(t), \quad \text{(B7)}$$

where

$$G_{\mathbf{n}}(t)=J_{n_x}(t)J_{n_y}(t)J_{n_z}(t) \quad \text{(B8)}$$

and

$$n\equiv n_x+n_y+n_z. \quad \text{(B9)}$$

Taking into account that

$$G_{\mathbf{n}}(-t)=(-1)^nG_{\mathbf{n}}(t), \quad \text{(B10)}$$

one can obtain easily the result (9.28).

We also note that the ordinary Bessel function $J_{n_j}(t)$ can be represented by[61]

$$J_{n_j}(t)=\frac{(\frac{1}{2}t)^{n_j}}{\Gamma(n_j+\frac{1}{2})\Gamma(\frac{1}{2})}\int_{-1}^{1}(1-x^2)^{n_j-\frac{1}{2}}\cos(tx)dx, \quad \text{(B11)}$$

where we observe the presence of a singularity at $x=\pm1$. One can show that this fact occurs also in the spherical model. We note that $x=\pm1$ corresponds to $\cos k=\pm1$, i.e., $k=0$ or $k=\pm\pi$. In one dimension, with $c_{\mathbf{k}}$ replaced by $-\cos k$ we can see immediately that this is a result of the Bragg condition at $k\longrightarrow 0$ and $k\longrightarrow\pm\pi$. We note that at $k\approx 0$, $\cos k\approx 1-\frac{1}{2}k^2$, whereas at $k\longrightarrow\pm\pi$, $\cos k\approx -1+\frac{1}{2}(k\mp\pi)^2$, and in both limits they correspond to spherical Fermi surfaces, as in the spherical model. As we see the Bragg condition makes necessary the exclusion of the surface of the cube (6.11).

APPENDIX C

Let us consider, for example, the calculation of $\langle\mathbf{R}^2\rangle$. Using (9.34), and noting that $\langle\mathbf{R}^2\rangle=3\langle R_z^2\rangle$ from cubic

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[60] N. Nielsen, *Handbuch der Theorie der Zylinderfunctionen* (B. G. Teubner, Leipzig, 1904).

[61] See, for example, I. M. Ryshik and I. S. Gradstein, *Table of Series, Products, and Integrals* (Plenum Press, Inc., New York, 1963), 2nd ed.

symmetry we obtain

$$-\sum_{\mathbf{n}} \mathbf{n}^2 g(2\mathbf{n})/\pi^2 = 3\int_0^\infty \cos\omega t\,dt \int_0^\infty \sin\omega\xi\,d\xi \times\sum_{n_x} (-1)^{n_x} J_{n_x}(t) J_{n_x}(\xi) \sum_{n_y} (-1)^{n_y} J_{n_y}(t) J_{n_y}(\xi) \times\sum_{n_z} (-1)^{n_z} n_z^2 J_{n_z}(t) J_{n_z}(\xi); \quad \text{(C1)}$$

now, using (9.38) and (9.39) we can write

$$-\sum_{\mathbf{n}} \mathbf{n}^2 g(2\mathbf{n})/\pi^2 = -3\int_0^\infty \cos\omega t\,dt \int_0^\infty \sin\omega\xi\,d\xi \times J_0^2(t+\xi)\frac{t\xi}{t+\xi} J_1(t+\xi), \quad \text{(C2)}$$

where we note the symmetry of the factor

$$\frac{t\xi}{t+\xi} J_0^2(t+\xi) J_1(t+\xi) \quad \text{(C3)}$$

under $\xi \leftrightarrow t$. With this property, the replacement

$$\cos\omega t \sin\omega\xi = \tfrac{1}{2}[\sin\omega(t+\xi) + \sin\xi(t-\xi)] \quad \text{(C4)}$$

becomes convenient, since only the first term in (C4) contributes to the integral (C2). Noting that

$$-3J_0^2(x)J_1(x) = 3J_0^2(x)\frac{dJ_0(x)}{dx} = \frac{d}{dx}J_0^3(x), \quad \text{(C5)}$$

we obtain

$$-\sum_{\mathbf{n}} \mathbf{n}^2 g(2\mathbf{n})/\pi^2 = \frac{1}{2}\int_0^\infty dt \int_t^\infty dx \times \sin\omega x \frac{t(x-t)}{x} \frac{d}{dx} J_0^3(x), \quad \text{(C6)}$$

where we have replaced $\xi = x-t$. Using the property

$$\int_t^\infty dx \cdots = \int_0^\infty \theta(x-t)\,dx \cdots, \quad \text{(C7)}$$

valid for $t>0$, and changing the order of integration we obtain

$$-\sum_{\mathbf{n}} \mathbf{n}^2 g(2\mathbf{n})/\pi^2 = -\tfrac{1}{12}(d/d\omega)\int_0^\infty x \times \cos\omega x (dJ_0^3/dx)\,dx. \quad \text{(C8)}$$

The integral in x is now performed by parts with the result

$$-\textstyle\sum_{\mathbf{n}} \mathbf{n}^2 g(2\mathbf{n})/\pi^2 = \tfrac{1}{12}(d/d\omega)[C_0(\omega) + \omega C_0'(\omega)], \quad \text{(C9)}$$

where $C_0(\omega)$ is defined in (A4). Noting that

$$f(2\mathbf{n}) = \int_{-\infty}^{\omega} g(2\mathbf{n})\,d\omega, \quad \text{(C10)}$$

and that[32]

$$C_0(\omega) = C_0'(\omega) = 0, \quad \text{(C11)}$$

for $\omega < -3$ we obtain the result (9.42).

Applying the same procedure one can also prove (9.41), (9.43), and (9.44).

APPENDIX D

Using the Fourier transforms[62] of $J_0(t)$ and $J_0^2(t)$ we obtain for $C_0(\omega)$ in (A4), with $\omega = -3+\Delta\omega$, for $0<\Delta\omega<1$,

$$C_0(-3+\Delta\omega) = \int_{-2}^{-2+\Delta\omega} \frac{L(y)}{[1-(\omega-y)]^{1/2}}\,dy, \quad \text{(D1)}$$

where

$$L(y) = \frac{1}{2\pi} P_{-1/2}(\tfrac{1}{2}y^2 - 1),$$

and $P_{-1/2}(u)$ is a Legendre function. Changing the variable of integration to $x = -2+\Delta\omega - y$, we can write

$$C_0(-3+\Delta\omega) = \int_0^{\Delta\omega} \frac{L(-2+\Delta\omega-x)}{[1-(1-x)^2]^{1/2}}\,dx \quad \text{(D2)}$$

$$= \int_0^{\Delta\omega} \frac{L(-2+\Delta\omega-x)}{(2-x)^{1/2}x^{1/2}}\,dx. \quad \text{(D3)}$$

Noting the singularity at $x \to 0$, and that the other factors are regular at $x \to 0$, we obtain

$$C_0(-3+\Delta\omega) \approx \frac{L(-2+\Delta\omega)}{\sqrt{2}} \int_0^{\Delta\omega} \frac{dx}{\sqrt{x}} \approx \frac{2}{\sqrt{2}} L(-2)(\Delta\omega)^{1/2}, \quad \text{(D4)}$$

where

$$L(-2) = \lim_{\Delta\omega \to +0} L(-2+\Delta\omega) = 1/2\pi.$$

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[62] See, for example, *Table of Integral Transforms*, edited by A. Erdélyi (McGraw-Hill Book Co., Inc., New York, 1953), Vol. 1.