Spin Waves in a Model Ferromagnetic Metal

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Calculations of the coefficient of q^2 in the expression for the energy ϵ of a long-wavelength spin wave have been performed for a model of a ferromagnetic metal with short-range particle interactions in the low-density limit. A single s-like energy band of tight-binding form is considered in a face-centered cubic crystal. First- and second-neighbor interaction integrals are included in $\epsilon(\mathbf{k})$ as arbitrary parameters. In contrast to previous work, the effective electron interaction which enters the spin-wave calculation is not the bare potential, but is closely related to the two-particle t matrix. It is found to be possible to satisfy the spin-wave stability criterion for the ferromagnetic state as well as the t-matrix criterion for the occurrence of ferromagnetism at reasonably low particle densities for a wide range of values of the band parameters, and for interaction strengths of the order of the bandwidth.

I. INTRODUCTION

IT is now well understood that the itinerant electron theory of ferromagnetism predicts the existence of spin waves as low-lying excitations in a ferromagnetic metal when proper account is taken of electron correlation.[1] However, the computation of spin-wave energies is still quite difficult and requires the use of simplified models. It follows from general considerations that when the wavelength of a spin wave is long, its energy E must be related to the wave number q by

$$E=Dq^2, \tag{1.1}$$

in which D is a constant. Experiments have adequately confirmed the validity of this expression for ferromagnetic metals,[2] and values of D have been determined in numerous cases.

We shall focus our attention on the calculation of D, this calculation being considerably easier than that of the entire dispersion relation. Edwards has recently given an exact general expression for this quantity which is valid for arbitrary band structure and for any assumed interaction between electrons.[3] This expression cannot be evaluated practically in the general case, so we shall discuss here a particular model for which definite results can be obtained.

This model considers only a single energy band, with electrons which interact only when they are on the same lattice site. The model is precisely defined by the Hamiltonian

$$H=\sum_{\mathbf{k}\sigma}\epsilon(\mathbf{k})c_{\mathbf{k}\sigma}^{\dagger}c_{\mathbf{k}\sigma}+V_0\sum_i n_{i\uparrow}n_{i\downarrow}, \tag{1.2}$$

where $\epsilon(\mathbf{k})$ is the band energy, the $c_{\mathbf{k}\sigma'}^{\dagger}c_{\mathbf{k}\sigma}$ are creation and annihilation operators for a Bloch state of wave vector $\mathbf{k}$ and spin σ; V_0 is the assumed matrix element of the electron interaction, and the $n_{i\uparrow(\downarrow)}$ are the number operators for electrons with up (down) spin in localized (Wannier) states on lattice site $\mathbf{R}_i$.

This Hamiltonian has been studied by many authors. A few basic references are listed below.[4–6] Equation (1.2) is certainly a gross oversimplification if applications to real materials are contemplated. It does, however, furnish a situation in which many approximation schemes which may be applied to actual metals can be tested by comparison with exact results for the model. In addition, it is possible to extend the model either by including other bands, or by extending the range of the electron interaction to include nearest-neighbor lattice sites, while retaining some of the solvable characteristics of the simple expression.[7]

The properties of the eigenstates of the Hamiltonian (1.2) have been the subject of considerable controversy. In the next section, we review some of the discussions concerning the possibility of a ferromagnetic ground state, with emphasis on techniques which are applicable when the density of particles is low. One of the major objectives of this paper is to attempt to answer the question as to whether the ferromagnetic state of the system can be, in the low-density regime, stable against spin-wave excitations. We answer this question affirmatively through the procedure of making an explicit numerical calculation of D for a specific model of a ferromagnetic metal. The essential results of Edwards's theory, on which our calculations are based are also summarized in Sec. II. The model we employ is described in Sec. III. The numerical computations and their results are presented in Sec. IV. In Sec. V, certain approximations made in the calculations are evaluated, and shown not to lead to serious error. The conclusions are summarized in Sec. VI.

II. SPIN WAVES AND THE t MATRIX

The question as to whether, for arbitrarily strong interaction strength V_0, the Hamiltonian of Eq. (1.2) possesses a ferromagnetic ground state has provoked much discussion. Nagaoka showed, for the case of a nearly half-filled band, which was of the simplest tight-binding form, that for some lattices and in the

[1] For a critical review of itinerant electron theory, see C. Herring, in *Magnetism*, edited by G. Rado and H. Suhl (Academic Press Inc., New York, 1966), Vol. 4.
[2] T. G. Phillips and H. M. Rosenberg, Rept. Progr. Phys. **29**, 285 (1966).
[3] D. M. Edwards, Proc. Roy. Soc. (London) **A300**, 373 (1967).
[4] J. Hubbard, Proc. Roy. Soc. (London) **A276**, 238 (1963).
[5] J. Kanamori, Progr. Theoret. Phys. (Kyoto) **30**, 275 (1963).
[6] M. C. Gutzwiller, Phys. Rev. **134**, A923 (1964).
[7] J. Callaway, Phys. Rev. **140**, A618 (1965).

limit $V_0 \to \infty$, a ferromagnetic ground state is obtained.[8] Edwards has, however, expressed doubts as to the generality of Nagaoka proof: Is it actually restricted to the case of only one electron more or less than required to give a band exactly half-full?[9] Penn[10] and Alexander and Horowitz[11] have found that configurations with magnetic order, but of a nonferromagnetic type can, in some ranges of the interaction strength, be the ground state of the system when the energy of this state is evaluated in the Hartree-Fock approximation.

In this work we study the properties of the system when the density of particles is low. In this limit, t-matrix techniques can be applied,[5,7] and it has been shown that the paramagnetic state of the system will be unstable with regard to an unsaturated ferromagnetic state provided that a certain inequality is satisfied

$$G(\epsilon_F) t_0 \geq 1, \tag{2.1}$$

where $G(\epsilon_F)$ is the density of states at the (paramagnetic) Fermi energy and t_0 is the low-energy limit of a two-particle t-matrix element defined by

$$t_0 = \lim_{E \to 0, \mathbf{K} \to 0} t(E, \mathbf{K}), \tag{2.2}$$

$$t(E, \mathbf{K}) = V_0 [1 - V_0 \mathcal{G}(E, \mathbf{K})]^{-1}, \tag{2.3}$$

$$\mathcal{G}(E, \mathbf{K}) = \frac{\Omega}{(2\pi)^3} \int \frac{\eta[E(\mathbf{K}/2+\mathbf{k}) - \epsilon_F] \eta[\epsilon(\mathbf{K}/2-\mathbf{k}) - \epsilon_F]}{E - \epsilon(\mathbf{K}/2+\mathbf{k}) - \epsilon(\mathbf{K}/2-\mathbf{k})} d^3k. \tag{2.4}$$

Here $\eta(x)$ is a unit step function. The integral is restricted to values of the wave vector such that states $\mathbf{K}/2+\mathbf{k}$ and $\mathbf{K}/2-\mathbf{k}$ are both unoccupied.

The t-matrix method furnishes an exact low-density treatment of a system of fermions with short-range repulsive interactions in the following sense: If a is the scattering length associated with the interaction, the t matrix gives correctly all the terms in the total energy of the system of order k_F^2, $k_F^3 a$, and $k_F^4 a^2$. Terms of higher order than $k_F^2 (k_F a)^2$ are present in the t matrix, but the complete perturbation series for the energy contains additional terms which are not included in the t matrix.

The first interaction term in the total energy, that of order $k_F^2 (k_F a)$ may be found correctly by neglecting $\mathbf{K}$ and E in (2.4). In this case,

$$\mathcal{G}(0, 0) = -\tfrac{1}{2} I(\epsilon_F), \tag{2.5}$$

where

$$I(\epsilon_F) = \frac{\Omega}{(2\pi)^3} \int \frac{\eta[\epsilon(\mathbf{k}) - \epsilon_F]}{\epsilon(\mathbf{k})} d^3k = \int_{\epsilon_F} \frac{G(E)}{\epsilon} d\epsilon. \tag{2.6}$$

We may, in the same limit, allow ϵ_F to approach zero in Eq. (2.6):

$$I(\epsilon_F) \to I(0) = \int_0 \frac{G(\epsilon)}{\epsilon} d\epsilon.$$

$I(0)$ is the average value of $1/\epsilon$ over the entire band. It is, however, useful to retain the ϵ_F dependence in Eqs. (2.5) and (2.6) since the use of this $\mathcal{G}$ appears to give a rather good approximation to the total energy, at least in the case of a parabolic band, at higher densities where the calculation is more complicated.[12] Use of the exact expression for the Green's function $\mathcal{G}$ [Eq. (2.4)] enables one to obtain correctly the second interaction term in the total energy, which is of order $k_F^2 (k_F a)^2$. The principal physical effect incorporated in this term is exclusion: The interaction of two particles in the system is subject to the restriction that they can scatter only to unoccupied states.

Equation (2.5) leads to the following approximate expression for t_0:

$$t_0 = V_0 [1 + \tfrac{1}{2} V_0 I(\epsilon_F)]^{-1}, \tag{2.7}$$

which may be used in the criterion for a ferromagnetic instability. It is particularly to be noted that when V_0 becomes large, t_0 becomes independent of V_0. This result must occur, since in the limit of very large V_0, the system being described is essentially a hard-sphere Fermi gas, in which the interaction strength is irrelevant, and the low-density properties of the system are described by the scattering length. It may also be shown that in the large-V_0 limit, the criterion for ferromagnetism, which then takes the form

$$2G(\epsilon_F)/I(\epsilon_F) \geq 1, \tag{2.8}$$

is independent of a multiplicative factor in $\epsilon(\mathbf{k})$, for example the total bandwidth, and depends therefore only on the shape of the band.

It is possible to construct artificial band structures, defined by postulating a density of states, in which the criterion for ferromagnetism (2.8) is satisfied, even in the strong form in which $I(\epsilon_F)$ is replaced by $I(0)$. However, the question as to under what circumstances, if any, it if possible to satisfy the inequalities (2.7) and (2.8) for realistic band structures has not been studied in much detail. We will return to this question below in Sec. IV.

An additional criterion for ferromagnetism is furnished by the condition that the ferromagnetic state must be stable with result to the formation of spin deviations. This can be conveniently expressed by the requirement, with regard to Eq. (1.1), that D must be greater than zero. Calculations of spin-wave energies based on the Hamiltonian of Eq. (1.2) have been made

[8] Y. Nagaoka, Phys. Rev. **147**, 392 (1966).
[9] D. M. Edwards, J. Appl. Phys. **39**, 481 (1968).
[10] D. R. Penn, Phys. Rev. **142**, 350 (1966).
[11] S. Alexander and G. Horowitz, Phys. Rev. **164**, 642 (1967).
[12] J. Callaway and R. K. M. Chow, Phys. Rev. **145**, 412 (1966).

by several authors.[3,13–16] These calculations are quite easy if the random-phase approximation (RPA) or an equivalent is used, and they yield the result

$$D(\mathrm{RPA}) = (1/6n)\sum_{\mathbf{k}}^{(0)} \{\nabla^2\epsilon(\mathbf{k}) - 2\,|\,\nabla\epsilon(\mathbf{k})\,|^2/V_0\rho\}. \tag{2.9}$$

The superscript (0) on the summation indicates that only states occupied in the ground state (here considered to be the completely ferromagnetic state) are included in the sum. The quantity n is the number of electrons in the system ($n \leq 2N$, where there are N lattice sites), and $\rho = n/N$.

This result has some desirable properties: For instance, ferromagnetism will not be obtained for an exactly filled or half-filled band, in agreement with Nagaoka.[8] However, except in these cases, the ferromagnetic state will always be stable if V_0 is sufficiently large. This result is inconsistent with the results of the t-matrix approach we have previously described. This inconsistency is serious, and would be expected to lead to an overestimate of spin-wave energies for all V_0. We are lead to the conclusion that Eq. (2.9) must be wrong, and that probably, at least at low densities, V_0 in Eq. (2.9) should be replaced by t_0.

Roth has shown that Eq. (2.9) can be improved by a variational method, in which a trial wave function is assumed for the ferromagnetic system containing a spin deviation.[16] This wave function makes some allowance for electron correlation beyond that incorporated in the RPA. We will, however, work with Edwards's theory of spin waves in ferromagnetic metals in which, as was mentioned above, an exact general expression for D is obtained.[3] When applied to Eq. (1.2), Edwards's theory yields an expression for D resembling Eq. (2.9) except that V_0 is replaced by a $\mathbf{k}$-dependent effective interaction $U(\mathbf{k})$ which reduces to t_0 as it should in the limit of a low-density system.

Edwards's theory yields the following expression for D for the one-band Hamiltonian of Eq. (1.2):

$$D = (1/6n)\sum_{\mathbf{k}}^{(0)} \{\nabla^2\epsilon(\mathbf{k}) - 2\,|\,\nabla\epsilon(\mathbf{k})\,|^2/U(\mathbf{k}) - 2\sum_{\mathbf{k}'}^{(0)} T(\mathbf{k},\mathbf{k}')\nabla_{\mathbf{k}}\epsilon(\mathbf{k})\cdot\nabla_{\mathbf{k}'}\epsilon(\mathbf{k}')\}. \tag{2.10}$$

As in regard to Eq. (2.9), the superscript (0) indicates that only occupied states are included in the sum. $U(\mathbf{k})$ is the $\mathbf{k}$-dependent effective interaction which will be studied in detail below. The third term represents the contribution of so-called nondiagonal diagrams. This will be estimated subsequently, and shown to be entirely negligible for the densities of interest here.

The effective interaction $U(\mathrm{Z})$ is given in the low-density limit by

$$U(\mathbf{k}) = (1/N)\sum_{\mathbf{p}}^{(0)} f(\mathbf{k},\mathbf{p}), \tag{2.11}$$

with

$$f(\mathbf{k},\mathbf{p}) = V_0\{1+(V_0/N)\sum_{\mathbf{q}}{}' [\epsilon_F+\epsilon(\mathbf{k}+\mathbf{p}-\mathbf{q}) +\epsilon(\mathbf{q})-\epsilon(\mathbf{k})-\epsilon(\mathbf{p})]^{-1}\}^{-1}. \tag{2.12}$$

It is particularly to be noted that the sum on $\mathbf{q}$ in Eq. (2.12) includes only unoccupied states (we use a prime on the summation to indicate this), while the sum on $\mathbf{p}$ in (2.11) is restricted to occupied states. In this expression ϵ_F is the Fermi energy in the ferromagnetic state.

It is easy to show that in the low-density limit $f(\mathbf{k},\mathbf{p})$ reduces to t_0, the low-density limit of the t matrix. This occurs because in the low-density region $\epsilon(\mathbf{q})$, which refers to an unoccupied state, must be larger than $\epsilon(\mathbf{k})$, $\epsilon(\mathbf{p})$, or ϵ_F; all of which refer to occupied states and also $\epsilon(\mathbf{k}+\mathbf{p}-\mathbf{q})\approx\epsilon(\mathbf{q})$. Then

$$f(\mathbf{k},\mathbf{p}) = V_0/[1+\tfrac{1}{2}V_0I(0)] = t_0. \tag{2.13a}$$

Furthermore, it will be a reasonable approximation, for densities which are not too large, to replace $I(0)$ by $I(\epsilon_F)$, just as was done in Eq. (2.5):

$$f(\mathbf{k},\mathbf{p}) = V_0/[1+\tfrac{1}{2}V_0I(\epsilon_F)]. \tag{2.13b}$$

We have examined the adequacy of this approximation for $f(\mathbf{k},\mathbf{p})$ in two cases in which the results of the calculations to be described below, and which are based on Eq. (2.13b) turn out to predict spin-wave stability ($D>0$). The method of doing will be described in Sec. V; we will, however, anticipate the result here. The corrections to Eq. (2.13) resulting from exact evaluation of Eq. (2.11) are not large at low densities, and (at least in the cases investigated) are such as to favor the stability of the ferromagnetic state. In addition, the corrections due to the inclusion of the third term in (2.10); that is, the portion involving $T(\mathbf{k},\mathbf{k}')$ appear to be completely negligible.

III. MODEL BAND STRUCTURE

We will now describe the model band structure on which the computations of D are based. We assume an s-like band in a face-centered cubic lattice, including second-neighbor interactions. This band is described by the function

$$E(k) = E_0 + E_1(\cos\tfrac{1}{2}k_xa\cos\tfrac{1}{2}k_ya + \cos\tfrac{1}{2}k_xa\cos\tfrac{1}{2}k_za + \cos\tfrac{1}{2}k_ya\cos\tfrac{1}{2}k_za) + E_2(\cos k_xa + \cos k_ya + \cos k_za). \tag{3.1}$$

Equation (3.1) contains three arbitrary coefficients E_0, E_1, and E_2 in addition to the lattice parameter a;

[13] T. Izuyama, Progr. Theoret. Phys. (Kyoto) **23**, 969 (1960).
[14] F. Englert and M. M. Antonoff, Physica **30**, 429 (1964).
[15] A. K. Rajagopal, H. Brooks, and N. R. Ranganathan, Technical Report No. ARPA-11, Harvard University, 1964 (unpublished); A. K. Rajagopal and H. Brooks, in *Proceedings of the International Conference on Magnetism, Nottingham, 1964* (The Institute of Physics and The Physical Society, London, 1965), p. 55.
[16] L. Roth, J. Phys. Chem. Solids **28**, 1549 (1967); J. Appl. Phys. **39**, 474 (1968).

TABLE I. Critical points of the energy band [Eq. (3.1)]. P_1 indicates that the saddle point is a minimum in one direction and a maximum in two; P_2 refers to the opposite situation. Σ or Σ' refer to saddle points located at points of the type $\mathbf{k}=(2\pi/a)$ $(1, y, y)$ or $\mathbf{k}=(\pi/a)$ $(0, z, z)$, where $y=(1/\pi)\cos[1/(4R+1)]$; $z=(1/\pi)\cos[-1/(4R+1)]$, and those obtained by symmetry from the ones listed.

R	$X(1,0,0)$	$W(1,\frac{1}{2},0)$	$L(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	$\Gamma(0,0,0)$	Σ or Σ'
$-0.5<R<0$	Min	Saddle (P_2)	Saddle (P_1)	Max	No
$0<R<0.15$	Saddle (P_1)	Min	Saddle (P_1)	Max	Yes ($12P_2$)
$R>0.25$	Saddle (P_2)	Saddle (P_1)	Min	Max	Yes ($12P_2$)

however, only one parameter is essential. This is the ratio R of second- to first-neighbor interactions,

$$R=E_2/E_1. \tag{3.2}$$

E_0 may be chosen so that $E(\mathbf{k})=0$ at the minimum of the band, and then when R is introduced, D depends explicitly on E_1 only as a multiplying factor (in the limit of large V_0).

Attention is focused on the face-centered cubic lattice and the energy band (3.1) for the following reasons. If $E_1>0$, and R is small in magnitude, the density of states has a peak in the lower portion of the band which results from the presence of closely spaced critical points. If $R=0$, there is actually a logarithmic singularity in the density of states, since there is a line in the zone face connecting W and X on which the energy is constant. (The Brillouin zone for the face-centered cubic lattice is shown in Fig. 1 for reference.) A peak in the density of states near the bottom of an energy band favors ferromagnetism for low particle density. By including the parameter R we avoid the computationally troublesome and physically unrealistic singularity; by varying it we can shift the position of the band minimum and the other critical points.

This position of the critical points is described as a function of R for R in the range from -0.5 to $+0.5$ (with $R=0$ excluded) in Table I. Varying the number and position of the critical points through changes in R alters the density of states. This gives us a convenient method of investigating the effect of changes in band shape on the tendency to ferromagnetism.

Calculations somewhat similar to those we describe here have been performed for a tight-binding band in a simple cubic lattice by Katsuki and Wohlfarth.[17] The band they considered is a special case of Eq. (3.1) obtained by setting $E_1=0$. The present work refers to a situation of greater physical significance; since Eq. (3.1) is a rough approximation to the band structure of nickel near the Fermi energy although real nickel has many addition complications, principally low-lying d bands. In addition, we include the effect of shape alterations, and compute the effective interaction rather than treat it as an arbitrary parameter.

In addition to the parameters contained in the formula for the energy band [Eq. (3.1)], the interaction strength V_0 enters the theory as an arbitrary parameter. However, when we express the band energies in terms of E_1, we may also introduce the dimensionless ratio V_0/E_1. Since the width of the energy band is roughly $4E_1$, this amounts to measuring the interaction strength in terms of the bandwidth. We will, however, eliminate this parameter explicitly by going to the strong-interaction limit: $V_0\gg 4E_1$ in which D becomes independent of V_0. Although this situation is probably unphysical insofar as values of V_0 appropriate to real metals probably do not satisfy this condition,[1] its use will enable us to answer the question of principal interest here: whether for low densities, the ferromagnetic state can be stable with respect to spin-wave excitations for any interaction strength. Anticipating an affirmative answer to this question, it will also follow that the ferromagnetic state is stable for V_0/E_1 greater than some minimum value, which can be estimated rather readily.

IV. COMPUTATIONAL PROCEDURES AND RESULTS

In Eq. (2.10) and similar formulas, we replace

$$(1/N)\sum_{\mathbf{k}}\rightarrow[\Omega/(2\pi)^3]\int d^3k, \tag{4.1}$$

where Ω is the volume of the unit cell ($\frac{1}{4}a^3$ for the face-centered cubic lattice). Also, let

$$\rho=n/N.$$

The quantity ρ is the number of particles per lattice site: We refer to ρ as the particle density from here on; and we consider $\rho\ll 1$. We drop the third term in Eq.

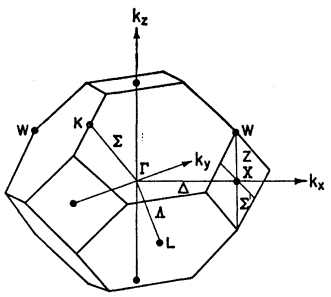

FIG. 1. Brillouin zone for the face-centered cubic lattice. Points and lines of symmetry are indicated.

[17] A. Katsuki and E. P. Wohlfarth, Proc. Roy. Soc. (London) **A295**, 192 (1966).

(2.10), which becomes

$$D=[\Omega/6(2\pi)^3\rho]$$
$$\times\int d^3k\left[\nabla^2\epsilon(\mathbf{k})-\frac{2\,|\,\nabla\epsilon(\mathbf{k})\,|^2}{U(\mathbf{k})}\right]\eta[\epsilon_F-\epsilon(\mathbf{k})]. \quad (4.2)$$

In this equation, the unit step function has the effect of ensuring that only occupied states are included. We also have

$$U(\mathbf{k})=[\Omega/(2\pi)^3]\int d^3p\,\eta[\epsilon_F-\epsilon(\mathbf{p})]f(\mathbf{k},\mathbf{p}). \quad (4.3)$$

In the strong-interaction limit $V_0\gg E_1$, we have

$$\frac{1}{f(\mathbf{k},\mathbf{p})}=\frac{\Omega}{(2\pi)^3}$$
$$\times\int d^3q\,\frac{\eta[\epsilon(\mathbf{q})-\epsilon_F]}{\epsilon_F+\epsilon(\mathbf{k}+\mathbf{p}-\mathbf{q})+\epsilon(\mathbf{q})-\epsilon(\mathbf{k})-\epsilon(\mathbf{p})}. \quad (4.4)$$

For future use, we note some useful symmetry properties of $U(\mathbf{k})$ and $f(\mathbf{k},\mathbf{p})$. These results are not restricted to the large-V_0 limit, but apply whatever is the value of V_0. Let α be any operator in the crystal point group (in this case the cubic point group). We know that $\epsilon(\alpha\mathbf{k})=\epsilon(\mathbf{k})$. It follows that

$$U(\alpha\mathbf{k})=U(\mathbf{k}),$$
$$f(\alpha\mathbf{k},\alpha\mathbf{p})=f(\mathbf{k},\mathbf{p}),$$
$$f(\alpha\mathbf{k},\mathbf{p})=f(\mathbf{k},\alpha^{-1}\mathbf{p}). \quad (4.5)$$

The computation of $U(\mathbf{k})$ is seen to involve a double integral; one part over the unoccupied portion of the Brillouin zone, and the other involving the occupied portion. In the rigorous evaluation of $f(\mathbf{k},\mathbf{p})$, it is necessary also to include the umklapp processes. $U(\mathbf{k})$ must be determined throughout the occupied portion of the zone so that the integral for D [Eq. (4.2)] may be performed. This calculation must be repeated for each value of the Fermi energy ϵ_F and each value of the parameter R considered. However, the evaluation of $U(\mathbf{k})$ for a single value of $\mathbf{k}$ and of the parameters ϵ_F and R requires a very substantial amount of computing time even for a relatively small mesh in the Brillouin zone. We have, therefore, adopted the procedure of approximating $f(\mathbf{k},\mathbf{p})$ as follows:

$$1/f(\mathbf{k},\mathbf{p})=\tfrac{1}{2}I(\epsilon_F) \quad (4.6)$$

in the limit of large V_0. The quantity $I(\epsilon_F)$ is defined by Eq. (2.6). The approximation becomes exact as $\epsilon_F\to 0$. This approximation enables the evaluation of D to be carried out accurately in other respects for a wide range of the parameters ϵ_F and R. Subsequently, we have checked the validity of Eq. (4.6) for a small selection of values of the parameters (in the region in which the ferromagnetic state is predicted to be stable). Those results will be described in more detail in Sec. V; however, the conclusion is that use of Eq. (4.6) is good to about 10 or 15% in the determination of $U(\mathbf{K})$ for densities in the interesting range. In addition the accurate value of U is larger than the approximate value: That is, the corrections favor ferromagnetism.

Use of Eq. (4.6) gives

$$U(\mathbf{k})=2\rho/I(\epsilon_F). \quad (4.7)$$

This result is independent of $\mathbf{k}$. We thereupon obtain

$$D=[\Omega/6(2\pi)^3\rho]$$
$$\times\int d^3k[\nabla^2\epsilon(\mathbf{k})-(I(\epsilon_F)/\rho)\,|\,\nabla\epsilon(\mathbf{k})\,|^2]\eta[\epsilon_F-\epsilon(\mathbf{k})]. \quad (4.8)$$

We have computed D for a selection of values of R; and for a given R, as a function of Fermi energy ϵ_F. Since the Fermi energy is determined by the particle density through

$$\rho=[\Omega/(2\pi)^3]\int d^3k\,\eta[\epsilon_F-\epsilon(\mathbf{k})], \quad (4.9)$$

this amounts to determining D as a function of particle density. At the same time, it is possible to check whether the t-matrix criterion for ferromagnetism in the strong-interaction limit, Eq. (2.8) is satisfied. Since this pertains to unsaturated ferromagnetism, we would expect that it would be somewhat easier to satisfy Eq. (2.8) than the spin-wave stability criterion; since $I(\epsilon_F)$ is a decreasing function of ϵ_F, this means that Eq. (2.8) would be satisfied at lower densities.

Calculations were performed by numerically integrating Eq. (4.8) using a cubic mesh inside 1/48 of the Brillouin zone. Each mesh point was assigned an appropriate weight according to symmetry. The computer program was constructed so that $I(\epsilon_F)$ and $G(\epsilon_F)$ were determined at the same time. The accuracy of the numerical calculations is determined by the number of mesh points at which the integrands were evaluated. It was found to be feasible to use a mesh of unit cubes in which the point X (see Fig. 1) was assigned coordinates (64, 0, 0). This mesh contains 24 225 nonequivalent points in the basic 1/48 of the zone. This mesh is not adequate for very small values of R ($|R|<0.01$) and some calculations were also made in these cases using a mesh containing approximately 8 times as many points in which X was assigned coordinates (128, 0, 0).

Some indication of what can be accomplished with the mesh size chosen is indicated in Fig. 2, where the density of states is shown for $R=0.1$, as constructed using the mesh containing 24 225 points. The density of states is essentially a differential quantity and tends to fluctuate significantly if an inadequately large number of mesh points are used. While some statistical noise obviously is present in the results, the critical points show clearly. An integrated quantity, such as $I(\epsilon_F)$ should be given quite adequately. It was found to be possible to satisfy both criteria for ferromagnetism at reasonably low densities ($\rho<0.15$) for R within each of the three ranges of values listed in Table I. The value

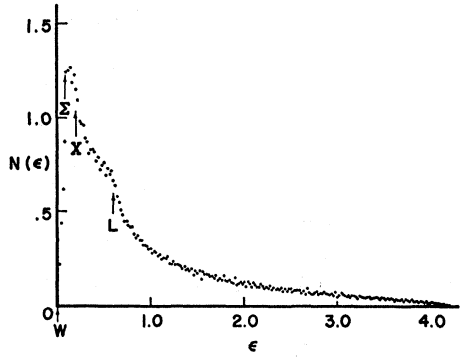

FIG. 2. Density of states for a tight-binding s band in a face-centered cubic lattice [Eq. (3.1)], with $R=0.1$. These results were obtained by numerical sampling, using 24 225 points in 1/48 of the Brillouin zone. The position of critical points in the band structure is indicated.

of the density for which the spin-wave stability criterion is shown is in Fig. 3. These results are in accord with expectations based on Ref. 7, and are summarized below.

(1) There is a minimum value of ρ below which (for each R) it is impossible to satisfy either criterion. (2) The criteria become satisfied for values of ϵ_F which lie near a peak of the density of states. (3) The spin-wave stability criterion is, in each case we have investigated, satisfied for a higher value of ϵ_F [and smaller $I(\epsilon_F)$] than is Eq. (2.8). (4) If we turn the band around, that is, choose E_1 in Eq. (3.1) to be negative so that the band minimum is at Γ, it is found to be impossible to satisfy either criterion until somewhat higher densities are achieved. The difference illustrates the fact that ferromagnetism at low densities is favored by a peak close to the bottom of a band. However, the case of $R=0$, in which there is a logarithmic singularity at $\epsilon=0$ (with $E_1>0$), is somewhat anomalous. We do not find this to be a particularly favorable case; and in fact the singularity in $G(\epsilon_F)$ causes $I(\epsilon_F)$ to diverge as $\epsilon_F\to 0$ so that ferromagnetism is not obtained at very low densities in this case either. (5) If the limiting value of $I(\epsilon_F)$, $I(0)$, is used in Eqs. (4.8) and (2.8), it is still possible to satisfy the t-matrix criterion for a ferromagnetic instability for some values of ϵ_F and R,

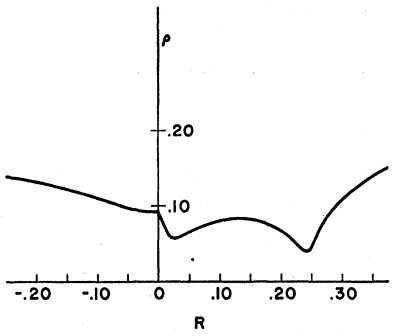

FIG. 3. The lowest value of the particle density for which the spin-wave stability criterion ($D>0$) is satisfied is shown as a function of R. The changing position of critical points with R (see Table I) is seen to produce substantial changes in this value.

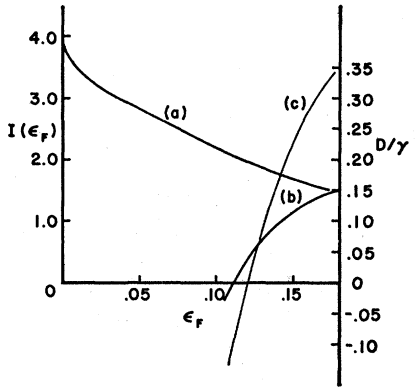

FIG. 4. Curve (a): $I(\epsilon_F)$ is shown as a function of ϵ_F for $R=0.1$ (left-hand scale). Curve (b): Ratio (D/γ) of spin-wave effective mass to band effective mass at W is shown for $R=0.1$ as a function of ϵ_F as determined from detailed numerical calculations. Curve (c): Same as (b) except that the approximate formula of Eq. (4.11) is used.

but the spin-wave stability criterion apparently can not be satisfied. The value of I obtained in this way is large compared to a reciprical bandwidth. This situation results from the dominance of the low-energy peak in the density of states in the computation of $I(0)$. That a similar conclusion holds in the case of a tight-binding s band in a simple cubic lattice may be deduced from the calculations of Katsuki and Wohlfarth[17] using the value of $I(0)$ given in Ref. 7 for this case.

The value of the coefficient D can be compared with the corresponding quantity for the electron energy band. In the case of the random-phase approximation one has,[18] for a parabolic band for which $\epsilon=\gamma\mathbf{k}^2$,

$$D/\gamma=1-4\epsilon_F/5V_0\rho. \tag{4.10}$$

Our approach leads to a similar result for a parabolic

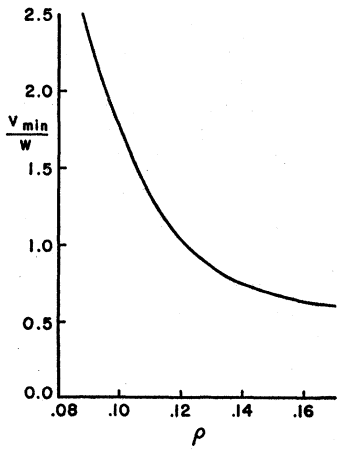

FIG. 5. Ratio of minimum value of the interaction strength $V_{\min}$, to the bandwidth W, for which the spin-wave stability criterion is satisfied is shown as a function of particle density for $R=0.1$.

[18] C. Herring, in *Magnetism*, edited by G. Rado and H. Suhl (Academic Press Inc., New York, 1966), Vol. 4, p. 370.

band in which V_0 is replaced by $2/I(\epsilon_F)$:

$$D/\gamma = 1 - 2I(\epsilon_F)\epsilon_F/5\rho. \quad (4.11)$$

Equation (4.11) will be only a rough approximation in our case since the energy band [Eq. (3.1)] with $E_1<0$ is not parabolic for the energies of interest to us. Quantitatively, Eq. (4.11) furnishes a reasonable estimate of the value of ϵ_F at which $D=0$, but the values of the ratio D/γ tend to be high by a factor of 2, if we take γ from the behavior of $\epsilon(\mathbf{k})$ at the band minimum. In Fig. 4 we show as an example, D compared with the density-of-states effective mass at the symmetry point W (which is the band minimum) for the case $R=0.1$. $I(\epsilon_F)$ is also shown.

We can also use our results to determine the minimum value of V_0 such that the system is stable against excitation of spin waves. This is easily done using Eq. (2.13b) to determine $f(\mathbf{k}, \mathbf{p})$. Let us denote this value of V_0 by $V_{\min}$. Since by definition, if $V_0=V_{\min}$, $D=0$, we have from Eq. (4.2)

$$\frac{V_{\min}}{1+\frac{1}{2}V_{\min}I(\epsilon_F)} = \frac{2}{\rho}\frac{\int d^3k \mid \nabla\epsilon(\mathbf{k}) \mid^2 \eta[\epsilon_F-\epsilon(\mathbf{k})]}{\int d^3k\, \nabla^2\epsilon(\mathbf{k})\, \eta[\epsilon_F-\epsilon(\mathbf{k})]}. \quad (4.12)$$

This equation is easily solved for $V_{\min}$. It is convenient to express the results in terms of the dimensionless ratio of $V_{\min}$ to the width of the band W. For example, if $0<R<0.25$, the bandwidth $W=E_1(4+2R)$ and formulas for W for other values of R are easily obtained. Typically V_0/W is a number reasonably close to 1. Results in one interesting case ($R=0.1$) are shown in Fig. 5.

V. ADEQUACY OF APPROXIMATIONS

In this section, we report the results of an investigation into the adequacy of two of the principal approximations made in these calculations. We will first consider the neglect of the $\mathbf{k}$ and $\mathbf{p}$ dependence of $f(\mathbf{k}, \mathbf{p})$ and second, the omission of the terms involving $T(\mathbf{k}, \mathbf{k}')$ in Eq. (2.1).

In order to study the first of these questions, we have used Eq. (4.4) to calculate $U(\mathbf{k})$ for the case of $R=0.1$, $\epsilon_F=0.15$ and $R=0.05$, $\epsilon_F=0.12$. These are situations in which ferromagnetism is predicted by the approximations discussed previously. The calculation of $f(\mathbf{k}, \mathbf{p})$ is, relatively, quite lengthy because of the necessity to take account of umklapp processes. These were included; however, as a result most of the computations had to be done with a mesh containing only 89 points in 1/48 of the Brillouin zone, in which the point X is assigned coordinates (8, 0, 0). A few values of $f(\mathbf{k}, \mathbf{p})$ were determined using a mesh based on $X=(16, 0, 0)$. The essential results were the following: $f(\mathbf{k}, \mathbf{p})$ turns out to be slowly varying in both $\mathbf{k}$ and $\mathbf{p}$. When $U(\mathbf{k})$ is calculated from $f(\mathbf{k}, \mathbf{p})$, the values of this function for the occupied $\mathbf{k}$ in the mesh did not vary from the average value by more than 15% in any instance. The average of $U(\mathbf{k})$ obtained from D as finally computed corresponds to an effective value of $I(\epsilon_F)$ smaller by about 10% than that obtained from Eq. (2.6) using the same size mesh for the integration. It appears, therefore, if the effective interaction is computed exactly according to Edwards's theory, the result tends to favor the stability of the ferromagnetic state at low densities—at least in this example—with respect to our approximation. This result does not apply to a one-dimensional system where use of $I(\epsilon_F)$ exaggerates the tendency to ferromagnetism. Likewise, use of $I(\epsilon_F)$ will probably not be valid at high densities. In a high-density limit, corresponding for instance to a nearly half-filled band, an alternative expression must also be used for $U(\mathbf{k})$[3].

We now consider the correction due to the inclusion of the third term in Eq. (2.1). Let the contribution from this be denoted by ΔD:

$$\Delta D = -(1/3n) \sum_{\mathbf{k},\mathbf{k}'}{}^{(0)}\, T(\mathbf{k}, \mathbf{k}')\nabla_{\mathbf{k}'}\epsilon(\mathbf{k}')\cdot\nabla_{\mathbf{k}}\epsilon(\mathbf{k}). \quad (5.1)$$

In the low-density limit, Edwards obtains for this expression[3]

$$\Delta D = -(1/3n)\sum_{\mathbf{k},\mathbf{k}'}{}^{(0)}\,[f(\mathbf{k}, \mathbf{k}')/U(\mathbf{k})\,U(\mathbf{k}')] \times \nabla_{\mathbf{k}}\epsilon(\mathbf{k})\cdot\nabla_{\mathbf{k}'}\epsilon(\mathbf{k}'), \quad (5.2)$$

where $f(\mathbf{k}, \mathbf{k}')$ and $U(\mathbf{k})$ are the functions previously defined. Edwards points out that ΔD would vanish by symmetry if $f(\mathbf{k}, \mathbf{k}')$ were constant. We have estimated this term using the values of $f(\mathbf{k}, \mathbf{p})$ whose computation was described above. We did not carry the evaluation through to completion because it became apparent that its contribution must be less than 1% of the second term in (2.10) for the parameters considered ($R=0.1$, $\epsilon_F=0.15$). This results because of the large amount of cancellation between positive and negative terms in Eq. (5.2), which in turn occurs because $f(\mathbf{k}, \mathbf{p})$ varies only slowly. We can conclude, therefore, that the neglect of ΔD is an excellent approximation for the low-density region.

VI. CONCLUSIONS

We have numerically evaluated the coefficient of q^2 in the expression for the energy of a long-wavelength spin wave in a model ferromagnet of face-centered cubic lattice structure with a single energy band and short-range interactions. The calculations were performed according to Edwards's theory, in the low-density limit. It was found to be possible to satisfy the criterion for stability against spin-wave excitations for reasonable values of the band parameters and, at the same time, the t-matrix criterion for the occurrence of ferromagnetism. Values for the spin-wave effective mass are obtained which are reasonably consistent with those obtained in simpler theories (RPA with a parabolic band) provided that the unscreened contrast interaction V_0 is replaced by an expression based on the t matrix.