Temperature Dependence of Spin-Wave Energy in the t-Matrix Approximation*

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A Green's-function method is used to determine the spin-wave energy at finite temperatures in the itinerant model for a ferromagnet. The formalism, which was developed in a previous paper, is based on the t-matrix approximation in a one-band model, using the Hubbard Hamiltonian. Within this approximation, a formal expression is obtained for the spin-wave dispersion relation valid for all values of the wave vector $\vec{q}$ in the low-density limit. From this, the spin-wave energy at low temperatures, expressed in the form $C_0 = C_T T^2$, is evaluated for a fcc lattice with first- and second-neighbor interactions. The value obtained for C_T, using a reasonable set of band parameters, is consistent with that obtained experimentally.

I. INTRODUCTION

In a previous paper[1] (hereafter referred to as I), the formalism for calculating the transverse spin susceptibility was developed for the case of a one-band Hamiltonian given by

$$H = \sum_{\vec{k}\sigma} \epsilon_{\vec{k}} a_{\vec{k}\sigma}^\dagger a_{\vec{k}\sigma} + V \sum_{\vec{k}_1, \vec{k}_2, \vec{q}} a_{\vec{k}_1 + \vec{q}\uparrow}^\dagger a_{\vec{k}_1 \uparrow} a_{\vec{k}_2 - \vec{q}\downarrow}^\dagger a_{\vec{k}_2 \downarrow}. \quad (1.1)$$

Here the operators $a_{\vec{k}\sigma}^\dagger$, $a_{\vec{k}\sigma}$ create or annihilate an electron in a band state of wave vector $\vec{k}$ and spin σ, whose energy is $\epsilon_{\vec{k}}$. The quantity V describes an interaction between electrons of opposite spin on the same site. It is positive and may be large. There we summed up all the relevant diagrams within the t-matrix approximation for the self-energy $\sum$ and the transverse susceptibility $\chi(\vec{q}, t)$ defined by

$$\chi(\vec{q}, t) = -\langle\langle T[s^\dagger(\vec{q}t), s(\vec{q})]\rangle\rangle , \quad (1.2)$$

where $\quad s(\vec{q}) = \sum_{\vec{k}} a_{\vec{k}+\vec{q}\downarrow}^\dagger a_{\vec{k}\uparrow}$,

and the double angular brackets denote expectation value with respect to a grand canonical ensemble. The pole of the Fourier transform of χ gives the spin-wave energy. We also gave an explicit expression for the spin-wave energy at zero temperature under the assumption that the t matrix was constant and indicated the procedure for the finite temperature case. In this paper we shall carry out the calculation for the finite temperature case in detail and shall apply our formalism to the case of a model band structure described in Sec. III.

The Hubbard Hamiltonian[2] given in Eq. (1.1) has been studied by many authors[3-4]; the merits and disadvantages of this Hamiltonian within the itinerant model are discussed by Herring.[5] Recently, Roth[6] used a decoupling technique to calculate the self-energy. In the low-density limit our result obtained in Sec. II is very similar to that obtained from Roth's improved approximation.[7] Also Roth's

result appears to have a self-consistency which we omit for the sake of simplicity. As pointed out by Roth, the self-energy is really energy dependent; one of the purposes of this paper is to calculate this energy dependence and to see how much the spin-wave energy is modified by this dependence.

The spin-wave energy has been calculated by several authors. Izuyama and Kubo[8] derived an expression for the spin-wave energy within the random-phase approximation (RPA), and Mathon and Wohlfarth[9] evaluated it for a simple cubic lattice. However, as discussed in I, the RPA encounters serious difficulties when the interaction constant V becomes large. Callaway[10] has calculated the spin-wave energy using an expression derived by Edwards.[11] However, Edwards's expression is only valid for absolute zero; one of the goals of this paper is to extend Callaway's calculation to finite temperatures.

Experimentally, Phillips[12] has measured the temperature dependence of the spin wave in iron using a spin-wave resonance technique, and more recently Stringfellow[13] measured the spin-wave energy of both iron and nickel by means of neutron scattering. For iron, he obtained the following numbers for C:

$$C = (314 \pm 10) - (1.6 \pm 0.5) \times 10^{-3} T^2$$
$$+ (5.7 \pm 2.2) \times 10^{-5} T^{5/2} \text{ meV Å}^2 ; \quad (1.3)$$

for nickel the numbers are a factor of 1.75 higher. The term in $T^{5/2}$ arises from spin-wave interaction effects (see, e.g., Ref. 8) and is beyond the scope of this paper. However, it appears from Eq. (1.3) that this term is two orders of magnitude smaller than the T^2 term. Since there is no T^2 in the Heisenberg model, it would appear that a reasonable prediction of the coefficient C_T of T^2 should provide good support for the itinerant model. Since the actual band structure of nickel or iron consists of several complicated overlapping bands, one

should not hope to obtain strict agreement between our one-band model and experiment. However, we shall see that the model band structure we have chosen is not too unrealistic, since we shall be able to predict the sign and the right order of magnitude of C_T.

In Sec. II we review the Green's-function technique given in I and calculate a general expression for the spin-wave energy. In Sec. III we calculate the various quantities by introducing a model band structure. Section IV deals with the calculation of the spin-wave energy and its temperature dependence. Finally, in Sec. V we discuss the results obtained in the calculation.

II. GREEN'S-FUNCTION TECHNIQUES

The transverse spin susceptibility and hence the spin-wave energy is calculated using the temperature Green's functions developed by Abrikosov, Gor'kov, and Dzyaloshinski.[14] The results for the absolute zero case and the prescription for generalizing them to the finite temperature case were given in I. Following this prescription and the notation of I, we have for the self-energy $\Sigma(k)$ the expression

$$\Sigma \downarrow(k) = t(k + l_1)G \uparrow(l_1) , \qquad (2.1)$$

where $t(K) = [(1/V) - \mathcal{G}(K)]^{-1}$ $\qquad (2.2)$

and $\qquad \mathcal{G}(K) = - G \downarrow(k_1)G \uparrow(K - k_1) . \qquad (2.3)$

The variables k, K now denote the four vectors $(\vec{k}, i\omega)$ and $(\vec{K}, i\Omega)$, respectively, where $\vec{k}$ and $\vec{K}$ are wave vectors in the Brillouin zone and $\omega = (2n + 1)\pi T$ and $\Omega = 2n\pi T$ are the frequency variables. We have chosen units so that Boltzmann's constant is unity and measured all our energies from the Fermi level. Also, as in I, all subscripted variables are to be summed over.

The single-particle Green's function satisfies Dyson's equation:

$$G^{-1}(k) = G_0^{-1}(k) - \Sigma(k) , \qquad (2.4)$$

where $\quad G_0(k) = 1/(i\omega - \epsilon_{\vec{k}}) . \qquad (2.5)$

At finite temperatures we shall also have a self-energy correction to the up-spin electron which is given by an expression similar to Eq. (2.1); however, this correction is small: for simplicity we shall neglect this in our calculation, i.e., we assume $G \uparrow(k) = G_0 \uparrow(k)$.

A first approximation to $\mathcal{G}(K)$ is obtained by substituting G_0 for G in Eq. (2.3). Thus we have

$$\mathcal{G}(K) \simeq - T \sum_{\vec{k}} \sum_{\omega} [1/(i\omega - \epsilon_{\vec{k}})][1/(i\Omega - i\omega - \epsilon_{\vec{K}-\vec{k}})].$$

$$\qquad (2.6)$$

Performing the sum over ω, we obtain

$$\mathcal{G}(K) \simeq \sum_{\vec{k}} \frac{1 - f_{\vec{k}\downarrow} - f_{\vec{K}-\vec{k}\uparrow}}{i\Omega - \epsilon_{\vec{k}} - \epsilon_{\vec{K}-\vec{k}}} . \qquad (2.7)$$

For self-consistency, we should really use the $G \downarrow$ given by Eqs. (2.4) and (2.1) in the calculation of $\mathcal{G}$. This, however, would give a complicated self-consistent set of equations which renders the problem unmanageable. Qualitatively, the self-consistency modifies the single-particle energy $\epsilon_{\vec{k}\downarrow}$ and hence the occupation number $f_{\vec{k}\downarrow}$. A simple calculation in the RPA indicates that the down-spin energies $\epsilon_{\vec{k}\downarrow}$ are raised relative to the up-spin energies and that this spin splitting is of the order of the Fermi energy ϵ_F. We shall therefore assume that the down-spin energy is shifted above the Fermi level and also restrict our temperatures T for which $f_{\vec{k}\downarrow} \sim 0$, i.e., to temperatures smaller than the spin splitting. Within this approximation we have

$$\mathcal{G}(\vec{K}, i\Omega) \simeq \sum_{\epsilon_{\vec{k}} > \epsilon_F} \frac{1 - f_{\vec{K}-\vec{k}}}{i\Omega - \epsilon_{\vec{K}} - \epsilon_{\vec{K}-\vec{k}}} . \qquad (2.8)$$

From this expression for $\mathcal{G}$, we can evaluate $t(K)$ and hence the self-energy $\Sigma(k)$. Writing the summation explicitly for Eq. (2.1), we have

$$\Sigma(k) = T \sum_{k' \omega'} t(\vec{k} + \vec{k}', i\omega + i\omega') \frac{1}{i\omega' - \epsilon_{\vec{k}'}} . \qquad (2.9)$$

The summation over ω' is performed by means of the Poisson summation formula, i.e.,

$$\Sigma(k) = - (1/2\pi i) \sum_{\vec{k}'} \int_c dz$$

$$\times t(\vec{k} + \vec{k}', i\omega + z)[f(z)/(z - \epsilon_{\vec{k}'})] . \qquad (2.10)$$

The contour C encloses the poles of $f(z)$ along the imaginary axis. In the deformation of our contour, we shall pick up the pole at $\epsilon_{\vec{k}'}$ and the singularities of t. The analytic behavior of t is the same as that for $\mathcal{G}$. From Eq. (2.8), we see that $\mathcal{G}(\vec{K}, z)$ has a branch cut along the real axis from 0 to ∞. $t(\vec{K}, z)$ will also have this branch cut. However, because we are at low temperatures, the function $f(z)$ will vanish along this branch out. Hence the only contribution to the integral (2.10) will come from the pole $z = \epsilon_{\vec{k}'}$. Therefore,

$$\Sigma(k) = \sum_{\vec{k}'} t(\vec{k} + \vec{k}', i\omega + \epsilon_{\vec{k}'})f(\epsilon_{\vec{k}'}) . \qquad (2.11)$$

With the expression for $\Sigma(k)$, we can calculate the Green's function G and then the transverse susceptibility $\chi(q)$. From I we have

$$\chi(q) = G \uparrow(k_1)G \downarrow(k_1 + q) - G \uparrow(k_1)G \downarrow(k_1 + q)$$

$$\times \Gamma(k_1, k_1' + q)G \uparrow(k_1')G \downarrow(k_1' + q) , \qquad (2.12)$$

where $\quad \Gamma(k, k' + q) = t(k, k' + q) - t(k, k_1 + q)$

$$\times G \uparrow(k_1)G \downarrow(k_1 + q)\Gamma(k_1, k' + q). \qquad (2.13)$$

We have made the appropriate modifications for finite temperature. If we define

$$\chi_k^{(0)}(q) = G\uparrow(k)G\downarrow(k+q)$$

and $\chi_k(q) = \chi_k^{(0)}(q) - \chi_k^{(0)}(q)\Gamma(k, k_1+q)\chi_{k_1}^{(0)}(q)$,

we may write

$$\chi(q) = \sum_k \chi_k(q) \ .$$

By means of Eq. (2.13) for Γ, we can rewrite the equation for $\chi_k(q)$ as

$$\chi_k(q) = \chi_k^{(0)}(q) - \chi_k^{(0)}(q)t(k+k_1+q)\chi_{k_1}(q) \ . \quad (2.14)$$

However, we can simplify the problem by analyzing what values of k go into Eq. (2.14). We consider the $\chi^{(0)}$ terms. Define

$$\chi^{(0)}(q) = \sum_k \chi_k^{(0)}(q) = (-1/2\pi i)\sum_{\vec{k}} \int_c dz \, G\uparrow(\vec{k}, z)$$

$$\times G\downarrow(\vec{k}+\vec{q}, z+i\Omega_q)f(z) \ . \quad (2.15)$$

In the integral over z we have a contribution from $z = \epsilon_k$. This contribution is proportional to $f(\epsilon_k)$. Since we are in the low-temperature limit we have $\epsilon_k \le \epsilon_F$. A similar argument may be made for the other term in $\chi(q)$. Therefore, we are interested in solution $\chi_k(q)$, whose frequency variable $i\omega_k$ is below the Fermi energy. Now, in the low-density limit, ϵ_F is very small. From Eq. (2.8), we expect that $\mathcal{G}(K)$ and hence $t(K)$ are insensitive to small variations $(< \epsilon_F)$ in the variable $i\Omega$. Therefore, we shall approximate the t matrix in Eq. (2.14) by an average t matrix defined by

$$\bar{t}(k+q) = (1/\rho)\sum_{\vec{k}'} f(\epsilon_{\vec{k}'})t(\vec{k}'+\vec{k}+\vec{q}, \ \epsilon_{\vec{k}'}+i\omega+i\Omega_q) \ ,$$

$$(2.16)$$

where $\rho = \sum_{\vec{k}} f(\epsilon_{\vec{k}})$ $\quad (2.17)$

is the density. Note that from Eq. (2.11) this average t is related to the self-energy by the equation

$$\bar{t}(k+q) = (1/\rho)\Sigma(k+q) \ . \quad (2.18)$$

Our equation for $\chi_k(q)$ now reads

$$\chi_k(q) = \chi_k^{(0)}(q) - \chi_k^{(0)}(q)[\Sigma(k_1+q)/\rho]\chi_{k_1}(q) \ . \quad (2.19)$$

The solution of this equation is easily obtained. It is given by

$$\chi_k(q) = \frac{\chi_k^{(0)}(q)}{1 + \chi_{k_1}^{(0)}(q)\Sigma(k_1+q)/\rho} \quad .$$

Thus $\chi(q) = \dfrac{\chi^{(0)}(q)}{1 + \chi_{k_1}^{(0)}(q)\Sigma(k_1+q)/\rho}$, $\quad (2.20)$

where $\chi^{(0)}(q)$ is given by Eq. (2.15).

The energy of the spin wave is now given by the

pole of the analytic continuation of $\chi(q)$. We consider the denominator $D(q)$, given by

$$D(q) = 1 + (1/\rho)\chi_{k_1}^{(0)}(q)\Sigma(k_1+q)$$

$$= 1 + \frac{T}{\rho}\sum_{\vec{k}\omega} \frac{1}{i\omega - \epsilon_{\vec{k}}}$$

$$\times \frac{\Sigma(\vec{k}+\vec{q}, \ i\omega + i\Omega_q)}{i\omega + i\Omega_q - \epsilon_{\vec{k}+\vec{q}} - \Sigma(\vec{k}+\vec{q}, \ i\omega + i\Omega_q)} \ .$$

Performing the summation over ω, we have

$$D(q, \ i\Omega_q) = 1 + \frac{1}{\rho}\sum_{\vec{k}} \frac{f(\epsilon_{\vec{k}})\Sigma(\vec{k}+\vec{q}, \ \epsilon_{\vec{k}}+i\Omega_q)}{\epsilon_{\vec{k}} - \epsilon_{\vec{k}+\vec{q}} + i\Omega_q - \Sigma(\vec{k}+\vec{q}, \ \epsilon_{\vec{k}}+i\Omega_q)}$$

The analytic continuation is easily obtained by replacing $i\Omega_q$ by q_0. Putting $D(q, q_0) = 0$, we have

$$\rho = -\sum_{\vec{k}} \frac{f(\epsilon_k)\Sigma(\vec{k}+\vec{q}, \ \epsilon_{\vec{k}}+q_0)}{\epsilon_{\vec{k}} - \epsilon_{\vec{k}+\vec{q}} + q_0 - \Sigma(\vec{k}+\vec{q}, \ \epsilon_{\vec{k}}+q_0)} \ . \quad (2.21)$$

This is the dispersion relation for the spin wave for a general q at finite temperature and is the generalization of Eq. (2.19) in I. For small $\vec{q}$, q_0 we may expand the energies $\epsilon_{\vec{k}+\vec{q}}$ in the usual fashion and, neglecting the q_0 dependence in Σ, we have

$$q_0 = \frac{\sum_{\vec{k}} f(\epsilon_{\vec{k}})[\frac{1}{2}(\vec{q}\cdot\nabla)^2\epsilon_{\vec{k}} - (\vec{q}\cdot\nabla\epsilon_{\vec{k}})^2/\Sigma(\vec{k})]/\Sigma(\vec{k})}{\sum_{\vec{k}} f(\epsilon_{\vec{k}})/\Sigma(\vec{k})} \ , \quad (2.22)$$

where we have written $\Sigma(\vec{k})$ for $\Sigma(\vec{k}, \ \epsilon_{\vec{k}})$. For cubic crystals we may write

$$q_0 = Cq^2 \ ,$$

where

$$C = \frac{1}{6} \frac{\sum_{\vec{k}} f(\epsilon_{\vec{k}})[\nabla^2\epsilon_{\vec{k}} - 2|\nabla\epsilon_{\vec{k}}|^2/\Sigma(\vec{k})]/\Sigma(\vec{k})}{\sum_{\vec{k}} f(\epsilon_k)/\Sigma(\vec{k})} \ . \quad (2.23)$$

This expression reduces, in the limit of $T = 0$ and $\Sigma(\vec{k})$ constant, to that obtained in I. Because of the $\vec{k}$ or energy dependence of $\Sigma(\vec{k})$, the spin-wave energy coefficient appears in a more complicated form.

III. SELF-ENERGY WITHIN MODEL BAND STRUCTURE

From Eq. (2.23) it is seen that the calculation essentially reduces to a calculation of the self-energy $\Sigma(\vec{k})$ given by Eq. (2.11) with $\epsilon_{\vec{k}}$ replacing $i\omega$, i.e.,

$$\Sigma(\vec{k}) = \sum_{\vec{k}'} t(\vec{k}+\vec{k}', \ \epsilon_{\vec{k}}+\epsilon_{\vec{k}'})f(\epsilon_{\vec{k}'}) \ . \quad (3.1)$$

For sufficiently low temperature T we may extract its dependence by the following procedure. Defining the quantity $P(\vec{k}, \epsilon')$ by the relationship

$$P(\vec{k}, \epsilon') = \sum_{\vec{k}'} t(\vec{k}+\vec{k}', \ \epsilon_{\vec{k}}+\epsilon_{\vec{k}'})\delta(\epsilon_{\vec{k}'} - \epsilon') \ , \quad (3.2)$$

we may write

$$\Sigma(\vec{k}) = \int_{-\epsilon_F}^{W} P(\vec{k}, \epsilon')f(\epsilon')d\epsilon' \ , \quad (3.3)$$

where $-\epsilon_F$ and W denote the bottom and top of the band. Assuming $T \ll \epsilon_F$, we may expand the right-

hand side of Eq. (3.3) in powers of T by the standard methods.[15] Thus, we have

$$\Sigma(\vec{k}) = \int_{-\epsilon_F}^{0} P(\vec{k}, \epsilon') d\epsilon' + \frac{(\pi T)^2}{6} \frac{d}{d\epsilon'} P(\vec{k}, \epsilon')\Big|_{\epsilon'=0} \quad .$$

$$(3.4)$$

The lower and upper limits of the integral are, respectively, the bottom of the band and the Fermi level. The zero indicates that we have measured all our energies with respect to the Fermi level.

The function P is still temperature dependent through t. By an analogous procedure, we can expand t as a power series in T. For if we define the quantity $Q(\vec{K}, z, \epsilon)$ by the equation

$$Q(\vec{K}, z, \epsilon) = \sum_{\vec{k}} \frac{\delta(\epsilon_{\vec{k}} - \epsilon)\theta(\epsilon_{\vec{K}-\vec{k}})}{z - \epsilon_{\vec{k}} - \epsilon_{\vec{K}-\vec{k}}} \quad , \qquad (3.5)$$

where we have restricted the energies $\epsilon_{\vec{K}-\vec{k}}$ to above the Fermi level by means of the θ function given by

$$\theta(x) = 1 \quad \text{for} \quad x > 0$$
$$= 0 \quad \text{for} \quad x < 0,$$

we have from Eq. (2.9)

$$\mathcal{G}(\vec{K}, \vec{z}) = \mathcal{G}_0(\vec{K}, \vec{z}) - \frac{(\pi T)^2}{6} \frac{d}{d\epsilon} Q(\vec{K}, z, \epsilon)\Big|_{\epsilon=0} \quad .$$

Substituting this into Eq. (2.2) and expanding to second order in T, we have

$$t(\vec{K}, z) = t_0(\vec{K}, z) - \frac{(\pi T)^2}{6} t_0^2(\vec{K}, z) \frac{d}{d\epsilon} Q(\vec{K}, z, \epsilon)\Big|_{\epsilon=0} \cdot$$

$$(3.6)$$

In the above and the following, the subscript 0 denotes the value of the quantity at absolute zero. This expression for t may now be substituted into Eq. (3.2) to give

$$P(\vec{k}, \epsilon') = P_0(\vec{k}, \epsilon')$$

$$- \tfrac{1}{6} (\pi T)^2 \sum_{k'} \delta(\epsilon_{\vec{k}'} - \epsilon') t_0^2(\vec{k} + \vec{k}', \epsilon_{\vec{k}} + \epsilon_{\vec{k}'})$$

$$\times \frac{d}{d\epsilon} Q(\vec{k} + \vec{k}', \epsilon_{\vec{k}} + \epsilon_{\vec{k}'}, \epsilon)\Big|_{\epsilon=0} \quad . \quad (3.7)$$

The self-energy may now be written as

$$\Sigma(\vec{k}) = \Sigma_0(\vec{k}) + \tfrac{1}{6} (\pi T)^2 S(\vec{k}) \, , \qquad (3.8)$$

where $\quad S(\vec{k}) = \dfrac{d}{d\epsilon} P_0(\vec{k}, \epsilon')\Big|_{\epsilon=0}$

$$- \sum_{\epsilon_{k'} < 0} t_0^2(\vec{k} + \vec{k}', \epsilon_{\vec{k}} + \epsilon_{\vec{k}'})$$

$$\times \frac{d}{d\epsilon} Q(\vec{k} + \vec{k}', \epsilon_k + \epsilon_{k'}, \epsilon)\Big|_{\epsilon=0} \quad . \quad (3.9)$$

Expressions (3.8) and (3.9) are quite general for the one-band model. However, the expressions themselves, let alone their computation, are be-

coming unwieldy. It is appropriate at this point to introduce a model band structure and to see whether any simplifications may be obtained within this model energy band.

The band energy $\epsilon_{\vec{k}}$ is assumed to be of the form

$$\epsilon_{\vec{k}} = E_0 + E_1(\cos\tfrac{1}{2}k_x a \, \cos\tfrac{1}{2}k_y a$$

$$+ \cos\tfrac{1}{2}k_y a \, \cos\tfrac{1}{2}k_z a + \cos\tfrac{1}{2}k_z a \, \cos\tfrac{1}{2}k_x a)$$

$$+ E_2(\cos k_x a + \cos k_y a + \cos k_z a) - \epsilon_F \, . \quad (3.10)$$

This describes an s-like band which includes first- and second-neighbor interactions in a fcc lattice (Fig. 1). This model band structure, which has been used by Callaway,[10] contains three arbitrary coefficients E_0, E_1, E_2 as well as the lattice constant a and Fermi level ϵ_F. However, only the ratio $R = E_2/E_1$ and ϵ_F are essential to the calculation since E_0 may be chosen so that $\epsilon_k + \epsilon_F = 0$ at the minimum of the bands, i.e., $-\epsilon_F$ is the bottom of the band. The structure of the above band structure and its dependence on R is discussed in detail in Ref. 10, which also shows a typical curve for the density-of-states function $N(\epsilon)$. This curve, which corresponds to $R = 0.1$, is reproduced in Fig. 2. The unit of energy in this figure and in all our calculations is taken to be E_1. Since the bandwidth is about $4E_1$, we are essentially measuring all our energies with respect to the bandwidth W.

Since we are dealing with a low-density system, i.e., a system for which $\epsilon_F \ll W$, we are mainly interested in the behavior of $N(\epsilon)$ for small ϵ. From Fig. 2 it is seen that $N(\epsilon)$ starts from zero at the bottom of the band and increases linearly to a peak at a point about 0.1–0.2 from the bottom of the band. In his calculation, Callaway[10] concluded that ferromagnetism is favored when the Fermi level is near the peak of the curve $N(\epsilon)$ and that this band structure should be a fairly good representation of the actual state of affairs in Ni.

Even though we can do our calculation for a range of values for the parameters R, ϵ_F, and V, it is not now feasible because of the large amount of computer time required. This is apparent from an expression like that for $S(\vec{k})$. Therefore, we shall use a representative set of values of these parameters which we hope will give a good indication of the band-structure effects. Based on the calculation done by Callaway we choose $R = 0.1$, $\epsilon_F = 0.15$, and $V = 5$.

With these parameters one can proceed to calculate numerically the various quantities like $t_0(\vec{K}, z)$ and $\Sigma_0(\vec{k})$. The calculations were done on an IBM 360 computer model 65. They were done in the standard fashion, using a cubic mesh inside $\frac{1}{48}$ of the Brillouin zone. Each mesh point was assigned an appropriate weight according to symmetry. The accuracy of the numerical calculations
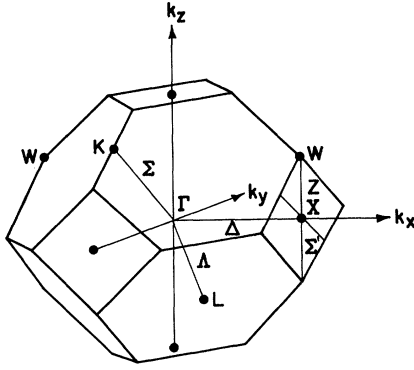
FIG. 1. Brillouin zone for the fcc lattice. Points and lines of symmetry are indicated.

is determined by the number of mesh points at which the integrals were evaluated. Although the density of states $N(\epsilon)$, the Laplacian, and the square of the gradient function can be done with a mesh in which the point X (see Fig. 1) was assigned the coordinates (64, 0, 0) and which contains 24 225 points in the basic $\frac{1}{48}$ of the zone, it is impractical to calculate t and Σ with the same large number of inequivalent points because of their momentum dependence. For these, a mesh with 89, or whenever practical, 505 equivalent points were used.

Because of the above computing difficulty and the need for some simple expressions for t and Σ, some approximations must be made. From a detailed calculation of the t matrix at absolute zero,
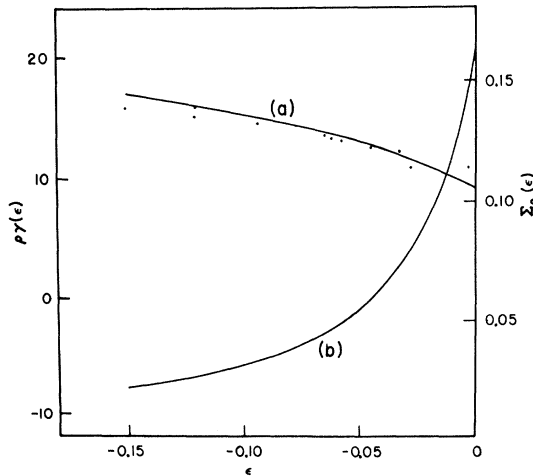

FIG. 2. Density-of-states function for model band structure. The energies are measured from the bottom of the band. The position of critical points in the band structure is indicated. This figure is taken from Ref. 10.

it is found that $t(\vec{K}, z)$ varies very slowly with the total momentum $\vec{K}$, and that the self-energy $\Sigma(\vec{k})$ is fairly insensitive to the values of $\vec{K}$ in $t(\vec{K}, z)$. This is not very surprising since $\vec{K}$ is the sum of two momenta $\vec{k}_1$ and $\vec{k}_2$ which must both lie under the Fermi level. Because of the low density, most of the values of $\vec{k}$ are centered around $\vec{k}$ for which $\epsilon_{\vec{k}}$ is a minimum.

Therefore, we make the approximation

$$t(\vec{K}, z) \simeq t(\vec{\overline{K}}, z) = t(z) \quad \text{for all } \vec{K}, \tag{3.11}$$

where $\vec{\overline{K}}$ denotes some average total momentum $\vec{\overline{K}}$. The value we shall use for $\vec{\overline{K}}$ is the value corresponding to the point X for want of a better guess. A similar approximation is made for the quantity $Q(\vec{K}, z, \epsilon)$, i.e.,

$$Q(\vec{K}, z, \epsilon) \simeq Q(z, \epsilon) . \tag{3.12}$$

With this approximation, our formulas simplify. Our functions P, Σ will depend only on $\vec{k}$ through the energy $\epsilon_{\vec{k}}$. Thus we abbreviate:

$$\Sigma(\vec{k}) = \Sigma(\epsilon_{\vec{k}}) = \Sigma(\epsilon) = \Sigma_0(\epsilon) + \tfrac{1}{6}(\pi T)^2 S(\epsilon), \tag{3.8'}$$

where $\quad \Sigma_0(\epsilon) = \int t_0(\epsilon + \epsilon') N(\epsilon') d\epsilon' \tag{3.13}$

and $\quad S(\epsilon) = \dfrac{d}{d\epsilon'}[t_0(\epsilon + \epsilon')N(\epsilon')]_{\epsilon'=0}$

$$- \int d\epsilon' N(\epsilon') t_0^2(\epsilon + \epsilon')$$

$$\times \frac{d}{d\epsilon''} Q(\epsilon + \epsilon', \epsilon'')\Big|_{\epsilon''=0} . \tag{3.9'}$$

The calculation for $\Sigma(\epsilon)$ and hence for the spin-wave energy is still not practicable unless one has analytic expressions for the various quantities since one needs to take derivatives. In other words, one needs to fit these quantities to some simple functions.

We consider the quantity $Q(z, \epsilon)$ given by

$$Q(z, \epsilon) = \sum_{\vec{k}} \frac{\delta(\epsilon_{\vec{k}} - \epsilon)\theta(\epsilon_{\vec{K}-\vec{k}})}{z - \epsilon_{\vec{k}} - \epsilon_{\vec{K}-\vec{k}}} . \tag{3.5'}$$

Since we have chosen $\vec{\overline{K}}$ to be $\vec{X} = (2\pi/a)$ (1, 0, 0), we have

$$\epsilon_{\vec{K}-\vec{k}} = \epsilon_{\vec{k}} - 2E_1 \cos\tfrac{1}{2}k_x a(\cos\tfrac{1}{2}k_y a + \cos\tfrac{1}{2}k_z a) .$$

Thus the denominator has a dependence of $z - 2\epsilon - c$, where c is a correction term. Because of the strong restrictions on $\epsilon_{\vec{k}}$ and $\epsilon_{\vec{K}-\vec{k}}$ this correction is expected to be small. Therefore, we should expect

$$Q(z, \epsilon) \simeq 2b/(z - 2\epsilon - c) , \tag{3.14}$$

where b and c are to be determined from a detailed calculation. An accurate determination of $Q(z, \epsilon)$ demands a huge amount of computer storage and time. However, a rough computation of Q using

505 nonequivalent points in the $\frac{1}{48}$ of the basic Brillouin zone did indeed show the desired dependence although the values for b and c were not very reliable because of fluctuations and noise.

We assume that we do have this dependence for Q and compute the t matrix. From Eq. (2.2) we have

$$t_0(z) = [1/V - \mathcal{G}_0(z)]^{-1} , \qquad (2.2')$$

where $\quad G_0(z) = \int_0^W Q(z, \epsilon) d\epsilon = 2b \int_0^W \frac{d\epsilon}{z - 2\epsilon - c}$

$$= -b \ln \frac{2W + c - z}{c - z} \simeq -b \ln \frac{2W}{c - z} ,$$

where the last equality is obtained by neglecting $c - z$ with respect to the bandwidth W. Thus, $t_0(z)$ becomes

$$t_0(z) = \{1/V + b \ln[2W/(c - z)]\}^{-1} . \qquad (3.15a)$$

From Eq. (3.15a) we verify that $t_0(z)$ does indeed have a branch cut along the real axis from c to ∞, where $c \sim 0$.

Because $t_0(z)$ is an integrated quantity it is less susceptible to fluctuations and noise arising from using too coarse a mesh in the numerical computations. In Fig. 3 is shown a plot of the computed t matrix using a mesh with 505 nonequivalent points. This is drawn as a full line. Also shown is a dashed curve, which represents Eq. (3.15a) with appropriate values for b and c. The values found for b and c which fit the computed curve best are

$$b = 0.1925, \qquad c = 0.03. \qquad (3.15b)$$
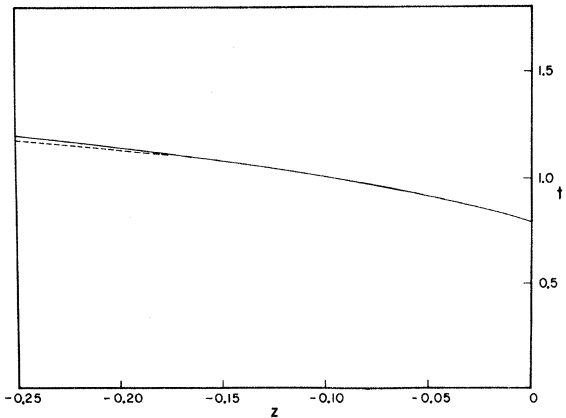
Therefore, the almost exact fit between the com-

FIG. 3. t matrix as a function of energy z. The full line is the curve obtained from an exact numerical calculation whereas the dashed line denotes the curve obtained from Eq. (3.15a). The dashed line coincides with full line where only the full line is shown.
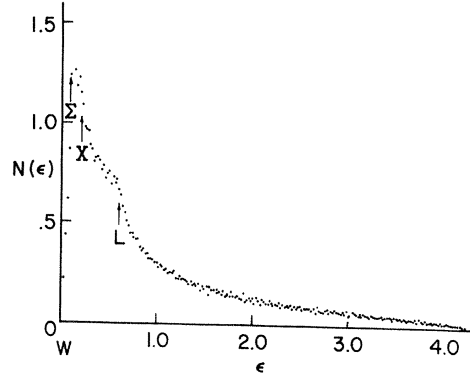

FIG. 4. (a) Full line represents Σ_0 and was drawn from Eq. (3.16). The points represent values obtained from an exact numerical calculation. (b) $\gamma(\epsilon)$, the temperature-dependent part of $\Sigma(\epsilon)$.

puted t matrix and approximate t matrix given by Eq. (3.15a) shows that the exact t matrix does have the behavior given in (3.15a) and that the cutoff c, which allows for the finite total momentum, is indeed small. To convince ourselves that this fit is not accidental we calculated the t matrix for a different value of ϵ_F; there again we found the predicted behavior. We shall therefore use Eq. (3.15a) as a faithful representation of the actual t matrix.

We also observe that although there is a definite dependence of the t matrix on energy, this dependence is very slow, as can be seen from the figure. In I it was actually assumed that the t matrix was constant. It will be shown in Sec. IV that this approximation is very good for the spin-wave energy at absolute zero since the t matrix occurs as part of integrals where the other factors multiplying it are very rapidly varying. For instance, with expression (3.15a) for the t matrix we may now evaluate the self-energy at zero temperature by substituting for t_0 into Eq. (3.13). From Figs. 2 and 3 we see that $N(\epsilon)$ is very rapidly varying compared to t_0, and we may take the latter out of the integral. Thus

$$\Sigma_0(\epsilon) = \int t_0(\epsilon + \epsilon') N(\epsilon') d\epsilon' \simeq t_0(\epsilon) \int N(\epsilon') d\epsilon' = t_0(\epsilon) \rho,$$

$$(3.16)$$

where ρ is the density. Figure 4 gives the comparison between the actually computed $\Sigma_0(\vec{k})$ and that obtained from (3.15a) and (3.16). This figure confirms (i) that the self-energy is dependent only on energy and (ii) that our approximate form [(3.15a)] for t is correct.

From Eqs. (3.15a) and (3.14) for t_0 and Q we may now compute the temperature correction to $\Sigma(\epsilon)$. Substituting for Q and differentiating, we have from Eq. (3.9')

$$S(\epsilon) = t_0(\epsilon)N'(0) + N(0)t'(\epsilon) - 4b \int \frac{t_0^2(\epsilon + \epsilon')N(\epsilon')\,d\epsilon'}{(c - \epsilon - \epsilon')^2}$$

$$\simeq t_0(\epsilon)N'(0) + N(0)t'(\epsilon) - 4bt_0^2 \int \frac{N(\epsilon')\,d\epsilon'}{(c - \epsilon - \epsilon')^2}$$

when the second equality is obtained by taking t_0^2 out of the integral because of its slow variation compared to the other functions. With the expression (3.16) for $\Sigma_0(\epsilon)$ we may write

$$\Sigma(\epsilon) = \Sigma_0(\epsilon)[1 - \tfrac{1}{6}(\pi T)^2 \gamma(\epsilon)] \; , \tag{3.17}$$

where

$$\gamma(\epsilon) = \frac{1}{\rho}\left(4bt_0(\epsilon)\int \frac{N(\epsilon')\,d\epsilon'}{(c - \epsilon - \epsilon')^2} - N'(0) - N(0)\frac{t_0'(\epsilon)}{t_0}\right) , \tag{3.18}$$

where $N(0)$ and $N'(0)$ denote the density of states and its derivative at the Fermi level.

With the assumed form of the density of states given by Eq. (4.3) the function $\gamma(\epsilon)$ may be evaluated and is shown in Fig. 4. We note that although $\Sigma_0(\epsilon)$ is slowly varying with respect to ϵ, the function $\gamma(\epsilon)$ is very rapidly varying and cannot be taken from under an integral sign.

IV. CALCULATION OF SPIN-WAVE ENERGY

We shall now return to the evaluation of the spin-wave energy q_0 given by Eq. (2.23). The self-energy function $\Sigma(\vec{k}) = \Sigma(\epsilon_{\vec{k}})$ has been calculated in Sec. III. We still need the functions $l(\epsilon)$ and $g(\epsilon)$ defined by

$$l(\epsilon) = \sum_{\vec{k}} \nabla^2 \epsilon_{\vec{k}} \delta(\epsilon_{\vec{k}} - \epsilon) \; , \tag{4.1}$$

and

$$g(\epsilon) = \sum_{\vec{k}} 2\,|\nabla \epsilon_{\vec{k}}|^2 \delta(\epsilon_{\vec{k}} - \epsilon) \; . \tag{4.2}$$

The functions are evaluated with essentially the same program that is used for $N(\epsilon)$. Since the expression for the spin-wave energy is dominated by the functions $N(\epsilon)$, $l(\epsilon)$, and $g(\epsilon)$, these must be evaluated very accurately. Therefore, a mesh containing 24 225 nonequivalent points was used.

It is found that for the range of energies between the bottom of the energy band and the Fermi level, the functions $N(\epsilon)$, $l(\epsilon)$, and $g(\epsilon)$ may be fitted by simple algebraic functions:

$$N(\epsilon) = N(0)(1 + \epsilon/\epsilon_F) \; , \tag{4.3}$$

$$l(\epsilon) = \lambda a^2(\epsilon + \epsilon_F) \; , \tag{4.4}$$

$$g(\epsilon) = \eta a^2(\epsilon + \epsilon_F)^2 \; , \tag{4.5}$$

where a is the lattice constant and the constants $N(0)$, λ, and η turned out to be 1.8, 4.6, and 4.4, respectively, for the value of the parameter R chosen. Compared to $\Sigma_0(\epsilon)$, these functions are very rapidly varying. We may therefore take $\Sigma_0(\epsilon)$ out of the integral sign whenever it occurs

with one of these in the integrand without any appreciable error. We shall use this approximation in the following calculation.

In terms of the above functions we write the spin-wave energy constant C given in Eq. (2.23) as

$$C = \frac{1}{6}\int_{-\epsilon_F}^{W}\left(f(\epsilon)\frac{l(\epsilon) - g(\epsilon)/\Sigma(\epsilon)}{\Sigma(\epsilon)}\right) \Big/ \int_{-\epsilon_F}^{W}\frac{f(\epsilon)N(\epsilon)}{\Sigma(\epsilon)}\,d\epsilon\right)d\epsilon. \tag{4.6}$$

At absolute zero we substitute Σ_0 for Σ in Eq. (4.6) and replace the Fermi function $f(\epsilon)$ by an ordinary step function at the Fermi level, and using the argument of slow variation above we have

$$C_0 = (1/6\rho)(I_l - I_g/\Sigma_0) \; , \tag{4.7}$$

where $\quad I_l = \int l(\epsilon)\,d\epsilon, \quad I_g = \int g(\epsilon)\,d\epsilon \; . \tag{4.8}$

This is exactly the same result as found in I. Note that for the rest of this section we shall omit the limits in the integrals for brevity, it being understood that the integrals are taken from the bottom of the band $-\epsilon_F$ to the Fermi level 0.

For finite temperatures we use Eq. (3.17) for Σ and using the same procedure for expanding the expressions in powers of T, we have

$$C = [A_0 + A_T \tfrac{1}{6}(\pi T)^2]/[B_0 + B_T \tfrac{1}{6}(\pi T)^2] \; , \tag{4.9}$$

where $\quad A_0 = (1/\Sigma_0)(I_l - I_g/\Sigma_0),$ \tag{4.10}

$$A_T = \int \frac{l(\epsilon)\gamma(\epsilon)}{\Sigma_0(\epsilon)} - 2\int \frac{g(\epsilon)\gamma(\epsilon)}{\Sigma_0^2(\epsilon)}$$
$$+ \frac{d}{d\epsilon}\left(\frac{l(\epsilon)}{\Sigma_0(\epsilon)} - \frac{g(\epsilon)}{\Sigma_0^2(\epsilon)}\right)_{\epsilon = 0} \; , \tag{4.11}$$

$$B_0 = 6\rho/\Sigma_0 \; , \tag{4.12}$$

and $\quad B_T = 6\int \frac{N(\epsilon)\gamma(\epsilon)}{\Sigma_0(\epsilon)} + 6\frac{d}{d\epsilon}\left(\frac{N(\epsilon)}{\Sigma_0(\epsilon)}\right)_{\epsilon = 0} \; . \tag{4.13}$

Again expanding C to the second power in T, we have

$$C = C_0 + C_T T^2 \; , \tag{4.14}$$

where $\quad C_T = (\pi^2/6B_0)(A_T - C_0 B_T) \; . \tag{4.15}$

If we substitute (4.10)–(4.13) into Eq. (4.15) we shall obtain a very complicated expression for C_T. However, the expression simplifies somewhat if we assume that $l(\epsilon)$ and $N(\epsilon)$ are proportional, as implied in Eqs. (4.3) and (4.4). Also, we may remove the Σ_0 from the integrals because of its slow variation. After some algebra we obtain

$$C_T = (\pi^2/36\rho\Sigma_0)\{C^{(1)} + C^{(2)} + C^{(3)}\} \; , \tag{4.16}$$

where $\quad C^{(1)} = -g'(0) + I_g N'(0)/\rho \; , \tag{4.17}$

$$C^{(2)} = \Sigma_0'[2g(0) - I_g N(0)/\rho]\Sigma_0 \; , \tag{4.18}$$

$$C^{(3)} = -2I_1 + I_g I_2/\rho \; ; \tag{4.19}$$

$$I_1 = \int g(\epsilon)\gamma(\epsilon)\,d\epsilon, \quad I_2 = \int N(\epsilon)\gamma(\epsilon)\,d\epsilon; \tag{4.20}$$

and the primes denote differentiation. The argument zero shows that the function is to be evaluated at the Fermi level. The contribution coming from $C^{(1)}$ is that which will be obtained if the self-energy is constant and independent of temperature. $C^{(2)}$ gives the contribution coming explicitly from the energy variation of Σ_0. It is noted that although we may neglect the energy variation of Σ_0 in calculating integrals, we cannot neglect this variation within a derivative. The contribution $C^{(3)}$ comes from the temperature dependence of Σ.

Substituting the expressions (3.16), (3.18), and (4.3)–(4.5) for the functions Σ_0, γ, N, l, and g and performing the integrals, we obtain

$$C^{(1)} = -\tfrac{4}{3}\eta a^2 \epsilon_F \;,$$

$$C^{(2)} = -\tfrac{4}{3}\eta a^2 \epsilon_F bt_0 \epsilon_F/c \;, \tag{4.21}$$

$$C^{(3)} = -\tfrac{4}{3}\eta a^2 \epsilon_F \{[F(c/\epsilon_F) - \epsilon_F/c]bt_0 - \tfrac{11}{2}\} \;,$$

where the function $F(x)$ is given by

$$F(x) = 1/x + (10 + 33x + 25x^2 + 4x^3)\ln[(1+x)/x]$$
$$- \tfrac{11}{2} - 7x - 2(3+2x)(2+x)^2 \ln[(2+x)/(1+x)].$$

Apart from a common factor, the contributions from $C^{(1)}$, $C^{(2)}$, and $C^{(3)}$ are, respectively, 1, $bt_0 \epsilon_F/c$, and $bt_0(F - \epsilon_F/c) - \tfrac{1}{2}$. Substituting the appropriate values for the parameters we have approximately

$$C^{(1)} : C^{(2)} : C^{(3)} : : 1 : 0.8 : 0.25 \;. \tag{4.22}$$

It is apparent from these numbers that the three contributions are comparable in magnitude. Therefore in calculating the temperature dependence of the spin-wave energy the variation of the self-energy with respect to the energy cannot be neglected.

Substituting for $C^{(1)}$, $C^{(2)}$, $C^{(3)}$ in Eq. (4.16) we have finally

$$C_T = -(\pi^2 \eta \epsilon_F a^2/54\rho\Sigma_0)[1 + 2bt_0 F(c/\epsilon_F)] \;. \tag{4.23}$$

We should point out that almost all the integrals may be done exactly with the $\Sigma_0(\epsilon)$ left inside the integral sign. However, the expressions obtained are very cumbersome and do not differ appreciably from the approximate ones given above.

V. RESULTS AND DISCUSSIONS

Although the spin-wave energy has been measured by Stringfellow[13] for the cases of iron and nickel, one cannot strictly compare the results of our calculation with the experimental results since the one-band model is a gross simplification of a real metal. For instance, in nickel the actual

band structure is characterized by a complex system of overlapping bands. However, calculations done by Callaway[10] have shown that the one-band model we have used is not too unreasonable provided that there is a suitable peak in our density of states.

Before comparing the temperature dependence of C with experiment, it is instructive to compare our results with those of Callaway[10] for the absolute zero case. Since we use exactly the same band structure as Callaway, a meaningful comparison would be our self-energy and the quantity $U(k)$ used in his calculation. Callaway based his calculation on an expression given by Edwards,[11] which coincides with our expression if we identify his $U(\vec{k})$ with our $\Sigma(\vec{k})$ and assume slow variation of $\Sigma(\vec{k})$ with energy. In his calculation Callaway assumed a constant t matrix. A look at our Fig. 3 or 4 shows that Callaway's assumption of a constant t matrix is essentially correct. Also Callaway has simplified his calculation to infinite V. With the same set of parameters for R and ϵ_F he obtained a t_0 of about $1.19E_1$. If we put in our value of V into his calculation, his t matrix turns out to be $0.96E_1$. From our figure we see that both of these mumbers lie within our variation of t. We see therefore that it is reasonable to use a constant value for t in the zero temperature calculation. Provided $V > W$, the t matrix varies rather slowly with respect to the interaction constant V.

In all our calculations the energies have been measured in units of E_1. In conventional units, the expressions for C_0 and C_T are

$$C_0 = \frac{1}{6\rho}\epsilon_F^2 \left(\frac{\lambda}{2} - \frac{\eta\epsilon_F}{3\Sigma_0}\right) a^2 E_1 \;, \tag{5.1}$$

$$C_T = -\frac{\pi^2 \eta \epsilon_F}{54\rho\Sigma_0} a^2 \frac{k_B^2}{E_1}(1 + 2btF). \tag{5.2}$$

Therefore $\quad \dfrac{C_T}{C_0} = -\dfrac{\pi^2 \eta}{9\epsilon_F \Sigma_0} \dfrac{(1+2btF)}{(\tfrac{1}{2}\lambda - \eta\epsilon_F/3\Sigma_0)}\left(\dfrac{k_B}{E_1}\right)^2 . \tag{5.3}$

Substitution of our parameters into the expression (5.3) leads to a value of C_T/C_0 given by

$$C_T/C_0 \simeq -400(k_B/E_1)^2 \quad . \tag{5.4}$$

If we take E_1 to be of the order of 1 eV, we obtain $C_T/C_0 \sim -3\times10^{-6}$, which compares reasonably well with the value -5×10^{-6} given by Stringfellow.

Mathon and Wohlfarth[9] also calculated the temperature dependence of C. They used the improved RPA approximation given by Izuyama and Kubo.[8] For the case of a simple cubic lattice they obtained results similar to ours for values of the interaction parameter of the same order of the bandwidth W. This is not too surprising since the difference between the t-matrix approximation and the RPA is only manifested for large values of the interac-

tion parameter V, as we have discussed in I.

We have obtained an expression [Eq. (2.23)] for the coefficient C for the spin-wave energy at finite temperature. In obtaining this we have neglected self-consistency effects. Although this problem has been treated by Roth[7] in the case of a simple cubic lattice, we have not been able to do so with a more realistic band structure like ours. We believe that we have taken the most important effects into account. Because of our band structure with the characteristic peak in the density of states, we have been able to obtain a simple analytic form of the t matrix [Eq. (3.15a)] as a function of energy. It is found that both the t matrix and the self-energy are independent of momentum within our model. Because of this we were able to do the integrals and differentiations to obtain an expression for the temperature-dependent part of C. Although the zero temperature self-energy is slowly varying with respect to energy, its temperature-dependent part is rapidly varying and was taken into account in the calculation of C_T. Also it was shown that the energy dependence of Σ cannot be neglected in the evaluation of C_T. In the final evaluation of C_T the functions $N(\epsilon)$, $l(\epsilon)$, and $g(\epsilon)$ were fitted to simple algebraic functions with which integrals can be done. The final result for C_T turns out to be negative as expected, although it is possible for it to be positive for some other band structure.[9] In this respect, calculations of C_T should be done with other values of the parameters R, ϵ_F, and V. These calculations are fairly straightforward although they involve substantial computation time. Because of the assumption of a single band, there should not be too much emphasis placed on the exact numerical value of C_T, although we have managed to obtain reasonable agreement with experiment. One should follow up this calculation with a many-band calculation. It is hoped that we shall be able to do this in the near future.

ACKNOWLEDGMENTS

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