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Spin waves in a strong tight-binding itinerant ferromagnet with a (100) surface

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The surface spin-wave problem for a simple-cubic tight-binding ferromagnet is formulated in terms of a spin-wave Green's function. The effect of the surface is treated as a perturbation to the bulk problem. The spin-wave Green's function of a semi-infinite ferromagnet satisfies a Dyson equation with the bulk Green's function as a kernel. Both the bulk spin-wave Green's function and the surface perturbation are parametrized in terms of Heisenberg-like effective exchange integrals. The effective exchange integrals are expressed in terms of one-electron Hartree-Fock (HF) propagators and evaluated. The bulk effective exchange integrals and the surface perturbation for a strong ferromagnet are shown to be negligible beyond the range of electron hopping. The effect of the surface is separated into a geometric effect and a surface renormalizaton of the bulk exchange integrals due to the surface core shift, HF corrections, and Friedel oscillations. It is shown that the renormalization of the effective exchange integrals in the first two atomic planes is sufficient for a strong ferromagnet. The dependences of the renormalized surface exchange integrals on the occupation of the surface layer n_s are computed. For a neutral (100) surface ($n_s=n$), the surface exchange integrals are very close to their bulk values. For $n_s/n<0.88$, there is a surface mode above the continuum of bulk spin waves but there are no surface modes for $n_s/n>0.88$. Acoustic surface modes can exist for other surfaces, e.g., (110).

I. INTRODUCTION

There is renewed interest in the magnetic surface problem stimulated by recent measurements of the surface magnetization[1] and by self-consistent band calculations for surfaces of ferromagnetic transition metals (see, e.g., Ref. 2). Although self-consistent band calculations are very successful in predicting the ground-state properties, they cannot be easily generalized to finite temperatures. The functional-integral method for bulk ferromagnetic metals at finite temperatures was applied recently by Hasegawa[3] to metal surfaces using a tight-binding model. However, his calculation is of mean-field type and is clearly not a good approximation at low temperatures since it ignores completely the spin waves which dominate the low-temperature magnetization. Unfortunately, there are no calculations of the effect of the surface on bulk spin waves for metals and information on surface spin waves is very limited. On the other hand, the surface problem for magnetic insulators is quite well understood. The Heisenberg model of a magnetic insulator assumes a localized spin S on each site and the spins on sites i,j are coupled by an exchange interaction $-\frac{1}{2}J_{ij}S_iS_j$. When a planar surface is introduced, all the exchange bonds across the surface are cut and the exchange integrals in the first few planes may be modified. For nearest-neighbor exchange in a simple-cubic ferromagnet the problem was solved exactly within the random-phase approximation (RPA) by De Wames and Wolfram.[4] They found that surface spin waves appear for a (100) surface provided the exchange integrals coupling nearest neighbors in the first layer $J_{\parallel}$, and in the first and second layers $J_{\perp}$, are different from J^{bulk}. Depending on $J_{\parallel}$ and $J_{\perp}$, surface spin waves may appear either below or above the bulk magnon band. Similar results are obtained in a model which includes nearest-neighbor and second-nearest-neighbor exchange interaction.[5]

However, the measurements made on metallic ferromagnets[1] (nickel, iron, or metallic glasses) require interpretation in terms of the itinerant model of ferromagnetism. Previous studies of surface spin waves in itinerant ferromagnets[6–8] were based directly on the random-phase approximation (RPA) dynamic susceptibility $\chi(q,\omega)$. Griffin and Gumbs[6,7] calculated $\chi(q,\omega)$, neglecting the Friedel oscillations and Hartree-Fock (HF) corrections to the surface susceptibility. This approximation leads to a spurious gap in the spin-wave spectrum and was criticized in Ref. 8. Localization of spin waves on a plane of impurities in an infinite strong ferromagnet was studied in Ref. 8 using a self-consistent approximation to the susceptibility, but there is no real surface in this model since electrons are allowed to hop across the impurity plane. Moreover, none of these calculations was concerned with the effect of the surface on bulk spin waves.

In this paper we describe a new real-space approach to the problem of spin waves in a simple-cubic tight-binding itinerant ferromagnet with a (100) surface. As in the Heisenberg model,[4,5] we set out to calculate surface corrections to the bulk spin-wave Green's function in real space. In Sec. II the bulk spin-wave Green's function of an itinerant ferromagnet is first cast into a Heisenberg-like form and the required effective exchange integrals are evaluated in the tight-binding approximation. Next, the surface corrections to the bulk effective exchange integrals are determined and then the whole problem is mapped onto an equivalent problem of surface in a magnetic insulator. This approach has the great advantage that formulation in terms of effective exchange integrals is physically simple and preserves automatically the spin-rotational symmetry of the surface problem. Also, the surface exchange integrals are directly related to the surface electronic structure which is known from self-consistent band calculations.[2] Finally, in Sec. III the model is used to discuss the location and dispersion of surface spin waves.

II. SPIN-WAVE GREEN'S FUNCTION OF AN ITINERANT FERROMAGNET

As in previous calculations of surface spin waves,[7,8] we consider a simple-cubic tight-binding ferromagnet described by the Hubbard Hamiltonian

$$H=\sum_{i,j,\sigma} t_{ij}c_{i\sigma}^{\dagger}c_{j\sigma}+\sum_{i} U_i n_{i+}n_{i-}+\sum_{i,\sigma} E_i n_{i\sigma} , \quad (1)$$

where $c_i^{\dagger},c_j$ are the creation and annihilation operators of electrons in atomic orbitals, U_i is the effective intra-atomic repulsion (Hubbard U), and t_{ij} are the hopping integrals. The parameters U_i, t_{ij}, and the total number of electrons in the band are chosen so that the Hartree-Fock (HF) ground state is ferromagnetic. The core energies E_i are assumed to be zero in the bulk and E_0 in the surface plane. This allows for adjustments of the surface magnetization which can be either fitted to the results of self-consistent band calculations or treated as a parameter to simulate interface effects. All U_i are assumed to have the bulk value U_0. Changes in U_i at the surface are not considered since they can be mimicked by core shifts E_0. As in Ref. 9, the surface is introduced by cutting all the hopping integrals across a cleavage plane.

Consider now the effect of the surface on the transverse susceptibility χ^{+-} whose poles determine the spin-wave energies. The Fourier transform of the susceptibility matrix in the Wannier representation satisfies a matrix equation (see Ref. 8)

$$\chi_{ij}^{+-}(\omega)=\chi_{ij}(\omega)+\sum_{m}\chi_{im}(\omega)U_0\chi_{mj}^{+-}(\omega) \quad (2)$$

which is exact in the random-phase approximation (RPA) both for bulk and semi-infinite ferromagnets. The kernel χ_{ij} is the transverse unenhanced susceptibility of noninteracting electrons moving in the HF potential

$$V_{i\sigma}=E_i+U_0\langle n_{i,-\sigma}\rangle . \quad (3)$$

For a semi-infinite ferromagnet, $V_{i\sigma}$ is inhomogeneous since both E_i and $\langle n_{i,-\sigma}\rangle$ vary near the surface. The kernel χ is expressed quite generally in terms of the HF one-particle propagators $G_{ij\sigma}$:

$$\chi_{ij}(\omega)=-\pi^{-1}\mathrm{Im}\int_{-\infty}^{E_F}G_{ij-}(E+\omega)G_{ij+}(E)dE , \quad (4)$$

where E_F is the Fermi energy.

Direct solution of Eq. (2) for a spatially inhomogeneous system is impossible since the kernel χ is an off-diagonal matrix both in the Bloch and Wannier representations. More promising and physically appealing is to treat the surface as a perturbation to the bulk problem. Following Mills and Maradudin,[5] we define the spin-wave Green's function of an itinerant ferromagnet Γ by

$$\Gamma=(I-U_0\chi)^{-1} , \quad (5)$$

where I is a unit matrix. Using Eqs. (2) and (5), it is easy to show that the spin-wave Green's function of a semi-infinite ferromagnet Γ^s satisfies the following Dyson equation:

$$\Gamma^s=\Gamma^b+\Gamma^b W\Gamma^s , \quad (6)$$

where Γ^b is the bulk spin-wave Green's function and the surface perturbation W is given by

$$W=U_0(\chi^s-\chi^b) . \quad (7)$$

Here, χ^s and χ^b are the surface and bulk kernels defined by Eq. (4). Equation (6) is equivalent to Eq. (2) and has the same form as for a conventional Heisenberg ferromagnet (see Ref. 5). This suggests that it should be possible to map the itinerant surface problem on an effective Heisenberg problem.

A. Bulk spin-wave Green's function

Consider first the bulk spin-wave Green's function Γ^b. It was shown in Ref. 10 that Γ^b in the Wannier representation is equivalent to the spin-wave Green's function of an effective Heisenberg Hamiltonian with exchange integrals

$$sJ_{ij}^{\mathrm{eff}}=U_0\Delta\chi_{ij}^{b} , \quad (8)$$

where s is the spin, Δ is the exchange splitting, and χ_{ij}^b is given by Eq. (4) with the bulk one-electron propagators. This result is exact in RPA for long-wavelength spin waves. For a strong ferromagnet ($\Delta>E_F$), J_{ij}^{eff} decay exponentially with distance and we shall demonstrate this analytically in the limit $\Delta/E_F\gg 1$.

The down-spin propagators in Eq. (4) are real for a strong ferromagnet and can be expanded in powers of E_F/Δ:

$$G_{0m-}^{b}=N^{-1}\sum_{q}\exp(iqR_m)(E-E_q-\Delta)^{-1}$$
$$\simeq\Delta^{-1}\delta_{m,0}(1+E/\Delta)-\Delta^{-2}t_m+O((E_F/\Delta)^3) , \quad (9)$$

where $E_q=-\sum_m t_m\exp(iqR_m)$ is the tight-binding energy and $\delta_{m,0}$ is the Kronecker delta. We recall that G_{0m+}^b is independent of Δ and the factor $U_0\Delta$ is proportional to Δ^2. It follows that the effective exchange integrals within the range of electron hopping tend to a finite limit for $\Delta/E_F\gg 1$ and all the other exchange integrals tend to zero. For a simple-nearest-neighbor hopping s band considered here, only the nearest neighbor J^{eff} is nonzero. It is given by

$$sJ^{\mathrm{eff}}=-(6n)^{-1}\int_{-\infty}^{E_F}EN_0(E)dE , \quad (10)$$

where $N_0(E)$ is the bulk electron density of states, n is the number of carriers per atom.

Another important property that follows from Eqs. (4) and (10) is that the off-diagonal elements of χ^b and, therefore, the exchange integrals J_{ij}^{eff} are *independent* of the frequency ω in the limit $\Delta/E_F\gg 1$.

The validity of the nearest-neighbor approximation for a strong ferromagnet with finite Δ/E_F such as nickel can be easily tested. The most stringent test is to calculate the spin-wave stiffness $D^{\rm eff}$ from the effective nearest-neighbor exchange integral defined by Eqs. (8) and (4) and compare it with the usual band RPA result for a simple-cubic tight-binding ferromagnet (see, e.g., Ref. 11). We used in this comparison the values $\Delta/E_F=2$ and $n=0.2$ to model nickel assuming that three degenerate t_{2g} bands form the top of nickel d band. The effective stiffness $D^{\rm eff}$ is given by the usual formula $D^{\rm eff}=sJ^{\rm eff}a^2$. We obtain remarkably good agreement. $D^{\rm eff}$ calculated by this method is 94% of the exact RPA stiffness D. As an additional check, the second-nearest neighbor $J_2^{\rm eff}$ was computed from Eqs. (8) and (4). We find $J_2^{\rm eff}/J^{\rm eff}=0.06$, i.e., $J_2^{\rm eff}$ is very small. These results show that a ferromagnet with $\Delta/E_F\simeq 2$ such as nickel is very close to the limit $\Delta/E_F \gg 1$ and its bulk spin-wave Green's function can be taken in the nearest-neighbor approximation.

B. Surface corrections to the bulk spin-wave Green's function

We shall determine in this section the surface perturbation W. It can be seen from Eq. (7) that W is just the difference between the surface χ^s and bulk χ^b kernels. Both kernels are determined by the one-electron propagators via Eq. (4). The surface propagators for a simple-cubic tight-binding band were obtained by Kalkstein and Soven.[9] To be specific, we consider the (100) surface. The propagators $G_{ij\sigma}(q,E)$ in the mixed Bloch-Wannier representation neglecting the core shift and HF corrections are given by[9]

$$G_{ij\sigma}(q,E)=G_\sigma^b(\,|\,i-j\,|\,,q,E)-G_\sigma^b(i+j,q,E)\;, \qquad (11)$$

where G_σ^b are the bulk propagators, i,j label atomic planes parallel to the surface located at $i=1$, and q is the component of the wave vector parallel to the surface.

The effect of the core shift E_0 and of the HF corrections is included by solving the Dyson equation $G^s=G+GVG^s$ for G^s, where G is given by Eq. (11) and

$$V_{m\sigma}=E_0\delta_{m,1}+(\langle n_{m,-\sigma}\rangle - n_{-\sigma}^{\rm bulk})$$

is the HF potential in the mth atomic plane. Since there are no minority carriers in a strong ferromagnet, G_{ij+}^s can be determined exactly. To obtain G_{ij-}^s, we assume that $\langle n_{m+}\rangle$ deviates from $n_+^{\rm bulk}$ only in the surface plane. The Dyson equation for G_-^s can then be also solved analytically. Since the perturbation matrix W is determined by G_+^s and G_-^s, our model of surface is now well defined and the rest of the paper revolves about various approximations to W that are required to render the Dyson equation (6) solvable.

C. Geometric effect of surface

Since the surface propagators G^s have no matrix elements across the cleavage plane, all such matrix elements of χ^s must also vanish. It follows that $W_{ij}=-U_0\chi_{ij}^b$ across the cleavage plane, which is equivalent in the terminology of Sec. I to cutting all the effective exchange integrals across the surface. This simple geometric effect of surface is exactly the same as for the conventional Heisenberg ferromagnet. The crudest approximation to W is to assume that all the matrix elements of χ_{ij}^s for $i,j\geq 1$ are equal to the elements of the bulk χ^b. This approximation is equivalent to the classical infinite-barrier model (CIBM) of Griffin and Gumbs.[6,7] It is clear that CIBM is not a realistic model for metals since, even if one neglects the HF corrections, the kernel χ^s is determined by the propagators G which differ from G^b because of the quantum interference effect of the surface (Friedel oscillations). Nevertheless, it is instructive to discuss the consequences of the geometric effect. The situation in the limit $\Delta/E_F\gg 1$ is clear-cut. The approximation of an effective nearest-neighbor exchange becomes exact in this limit and we have the geometric effect for a conventional nearest-neighbor Heisenberg model discussed in Ref. 5. There are no surface spin waves for a (100) surface but they exist for other surfaces, e.g., (110) provided non normal effective exchange integrals are cut in constructing the surface.

For finite Δ/E_F, the effect of the second-nearest-neighbor exchange $J_2^{\rm eff}$ needs to be considered. For the model described in Sec. I, $J_2^{\rm eff}$ is positive (ferromagnetic). We then have the same problem as for a magnetic insulator with nearest-neighbor and second-nearest-neighbor exchange which was solved by Mills and Maradudin.[5] They showed that there is an acoustic surface mode as long as $J_2>0$. This is satisfied by $J_2^{\rm eff}$, and the present model thus predicts an acoustic surface mode for a (100) surface. However, since $J_z^{\rm eff}$ is very small, the surface mode is almost indistinguishable from the bulk spin waves. The effect of Friedel oscillations and HF corrections on W will be discussed next.

D. Friedel oscillations and HF corrections

It can be seen from Eq. (7) that the effect of Friedel oscillations and HF corrections can be regarded as a renormalization of the bulk effective-exchange integrals near the surface. The simplest approximation is to include such renormalization only in the first two atomic planes. Generalization to a surface perturbation of arbitrary size is straightforward but it will be seen that a 2×2 matrix W gives already results asymptotically exact in the limit $\Delta/E_F\gg 1$. For a 2×2 W, the Dyson equation (6) is similar to the Dyson equation for the Green's function of a conventional Heisenberg ferromagnet with exchange integrals in the surface plane $J_{\|}$ and between the surface and adjacent plane $J_\perp$ different from $J^{\rm bulk}$. This problem was solved by DeWames and Wolfram[4] in the mixed Bloch-Wannier representation and we shall apply the same method to the itinerant surface problem. As in Ref. 4, we define a kernel $\Gamma_{ij}(q,\omega)$ by

$$\Gamma_{ij}(q,\omega)=\Gamma^b(\,|\,i-j\,|\,,q,\omega)-\Gamma^b(i+j,q,\omega)\;,$$

where Γ^b is the bulk spin-wave Green's function (5) in the mixed Bloch-Wannier representation. It can be easily shown[4] that the solution of Eq. (6) with the kernel Γ and with a perturbation matrix $W_{11}=-U_0\chi_{10}^b$, $W_{ij}=0$ for $i\neq j\neq 0$ is the spin-wave Green's function for the geometric effect of surface. It follows that Γ^s, including the effects of Friedel oscillations and HF corrections, satisfies a Dyson equation

$$\Gamma^s = \Gamma + \Gamma W \Gamma^s , \tag{12}$$

where W now includes all the surface corrections except for the geometric effect which is already incorporated in Γ. The spin-wave energies are then obtained from the usual secular equation

$$\det | I - \Gamma W | = 0 . \tag{13}$$

For the exact (infinite) matrix W, the spin-rotational symmetry of the problem requires that Eq. (13) has always a solution $\omega = 0$, $q = 0$ (the Goldstone mode). This condition may not be satisfied for a truncated 2×2 matrix W and has to be imposed on the elements of W. The correct form of W in the limit $\omega = 0$ $q = 0$ is clearly that for a Heisenberg ferromagnet. We shall, therefore, map the surface perturbation for an itinerant ferromagnet on a Heisenberg-like matrix W and show in the Appendix that such mapping is exact within RPA for $\Delta/E_F \gg 1$. The matrix W for a Heisenberg ferromagnet is given by[4]

$$\begin{aligned} W_{11} &= -4\Lambda(q)(1-\epsilon_{\parallel}) - (2-\epsilon_{\perp}) , \\ W_{12} &= 1-\epsilon_{\perp}, \quad W_{22} = -W_{12} , \end{aligned} \tag{14}$$

where $\epsilon_{\parallel} = J_{\parallel}/J^b$, $\epsilon_{\perp} = J_{\perp}/J^b$, and

$$\Lambda(q) = 1 - [\cos(q_x a) + \cos(q_y a)]/2 .$$

We now require only the values of $\epsilon_{\parallel}$ and $\epsilon_{\perp}$ for an itinerant ferromagnet. They are expressed in terms of the matrix elements of the unenhanced surface susceptibility

$$\begin{aligned} \epsilon_{\parallel} &= \lim_{\omega\to 0} \sum_q \chi^s_{11}(q,\omega)\exp(i\delta q) \Big/ \sum_q \chi^b_{12}(q,\omega) \\ &= J^{\text{eff}}_{\parallel}/J^{\text{eff}} , \\ \epsilon_{\perp} &= \lim_{\omega\to 0} \sum_q \chi^s_{12}(q,\omega) \Big/ \sum_q \chi^b_{12}(q,\omega) \\ &= J^{\text{eff}}_{\perp}/J^{\text{eff}} , \end{aligned} \tag{15}$$

where J^{eff} is given by Eq. (8), q is the wave vector in the surface plane, and δ is a vector connecting nearest neighbors in the surface plane. Both $\epsilon_{\parallel}$ and $\epsilon_{\perp}$ can be easily computed from the surface one-electron propagators. For given n and Δ, they depend only on the core shift E_0 or, equivalently, on the occupation of the surface layer n_s. The dependences of $\epsilon_{\parallel}$ and $\epsilon_{\perp}$ on n_s/n are shown in Fig. 1 for the filling of the band $n = 0.2$ appropriate to nickel. Solid curves are for large exchange splitting $\Delta/E_F \gg 1$ and dashed curves are for a splitting $\Delta/E_F = 2$, as expected in nickel. The range of n_s/n corresponds to E_0 such that there are no surface electron states. The qualitative behavior of the surface exchange integrals for $\Delta/E_F \gg 1$ and $\Delta/E_F = 2$ is similar. Most importantly, $J^{\text{eff}}_{\parallel}$ and $J^{\text{eff}}_{\perp}$ for a neutral surface ($n_s = n$) are very close to the bulk J^{eff}. Since $n \propto M$ and $n_s \propto M_s$, where M and M_s are the bulk and surface magnetizations, it follows from Fig. 1 that a (100) surface can be magnetically "softer" ($\epsilon_{\parallel}, \epsilon_{\perp} < 1$) for $M_s > M$ and "harder" for $M_s < M$.

The secular equation (13) for spin waves can be now solved as in Ref. 4. However, before it can be applied to surface spin waves it needs to be demonstrated that the effective exchange integrals in Eq. (15) which are taken in the limit $\omega = 0$ are good approximations to the frequency-dependent itinerant W.

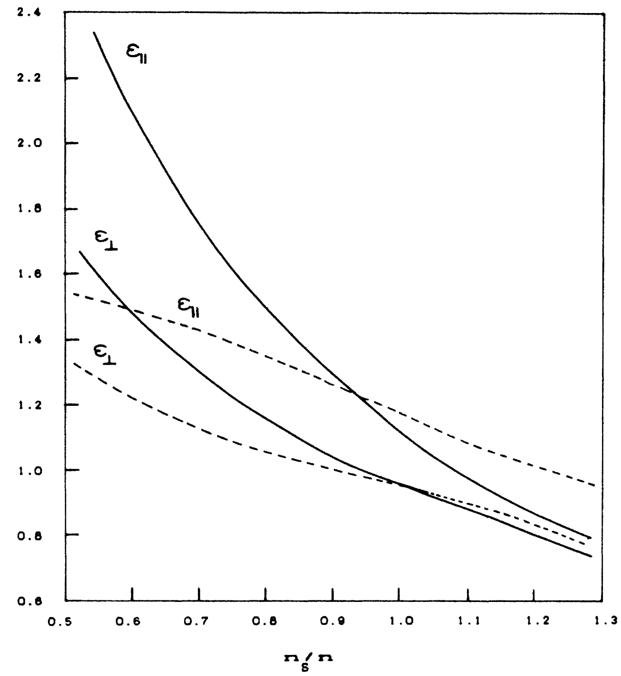

FIG. 1. Dependence of the surface effective-exchange integrals $\epsilon_{\parallel} = J_{\parallel}/J^{\text{eff}}$ and $\epsilon_{\perp} = J_{\perp}/J^{\text{eff}}$ on the occupation of the surface layer n_s/n. Solid curves are for $n = 0.2$ and $\Delta/E_F \gg 1$; dashed curves are for $n = 0.2$ and $\Delta/E_F = 2$.

This problem is addressed in the Appendix where it is shown that the mapping on a frequency-independent Heisenberg W is asymptotically exact for $\Delta/E_F \gg 1$ provided $M_s = M$ (neutral surface). When M_s deviates from M (e.g., for interfaces), W_{11} becomes frequency dependent. This is unimportant for long-wavelength bulk spin waves since such dependence contributes to the spin-wave energy only to the order $O(q^4)$. However, the frequency-dependent term in W_{11} is essential for surface spin waves and they are discussed in the next section.

III. SURFACE SPIN WAVES FOR A (100) SURFACE

Since acoustic surface spin waves deviate from bulk spin waves only to the order $O(q^4)$, the problem of existence of surface modes in an itinerant ferromagnet is unusually subtle and any approximation which is not fully self-consistent is virtually useless. For this reason, we shall discuss surface spin waves only in the limit $\Delta/E_F \gg 1$ where the present formulation is asymptotically exact. The problem is formally equivalent to the surface problem for a Heisenberg ferromagnet solved by DeWames and Wolfram.[4] The only difference is that W_{11} acquires a frequency-dependent term $(\omega/sJ^{\text{eff}})(1-n/n_s)$ for $n_s \neq n$ (see the Appendix). Surface spin waves are solutions of the secular equation (13). As shown in Ref. 4, Eq. (13) is equivalent to a cubic equation

$$x^3+x^2(W_{11}+W_{22})+x(2W_{12}+W_{11}W_{22}-W_{12}^2)+W_{22}=0\ , \quad (16)$$

where the variable x is defined by

$$x+1/x=4\Lambda(q)+2-\omega/sJ^{\mathrm{eff}}\ . \quad (17)$$

In contrast to the conventional Heisenberg ferromagnet, W_{11} now depends on x via the frequency-dependent term in Eq. (17). Nevertheless, Eq. (16) remains cubic and can be easily solved. The roots of the cubic equation (16) which correspond to physical solutions must have $|x|>1$ (see Ref. 4). Since $\epsilon_{\parallel}$ and $\epsilon_{\perp}$ were already evaluated in Sec. II, all the coefficients in Eq. (16) are known and depend only on the ratio $n_s/n=M_s/M$. It follows that the existence and location of surface modes is determined by a single parameter M_s/M.

Solving numerically Eq. (16), we find that there is always a surface mode above the continuum of bulk spin waves for $M_s/M<0.88$. The dispersion of this surface mode is illustrated in Fig. 2 for a range of M_s/M. Since $\epsilon_{\parallel}>1$ and $\epsilon_{\perp}>1$ for $M_s/M<0.88$, the situation here is qualitatively the same as for magnetic insulators with magnetically "harder" surface (see Ref. 4). For $0.88<M_s/M<1.09$, there are no surface spin waves since Eq. (16) has no physical roots in this interval.

The remaining case $M_s/M>1.09$ is very interesting. We have $\epsilon_{\parallel}<1$ and $\epsilon_{\perp}<1$ in this interval, i.e., magnetically "softer" surface. For a magnetic insulator, there is a well-defined acoustic mode in this situation located below the bulk continuum (see Ref. 4). However, for an itinerant ferromagnet, this mode is removed by the frequency-dependent term in W_{11}. We recall that the surface acoustic mode for a magnetic insulator deviates from the bulk continuum only because the element W_{11} of the surface perturbation depends on the component q of the momentum parallel to the surface. We find that the contribution of the momentum-dependent term to the secular equation (16) is exactly compensated by the frequency-dependent term. This result shows again how sensitive the acoustic surface spin waves are to any deviation from self-consistency. Exact compensation is obtained only because we use W_{11} which is exact in RPA.

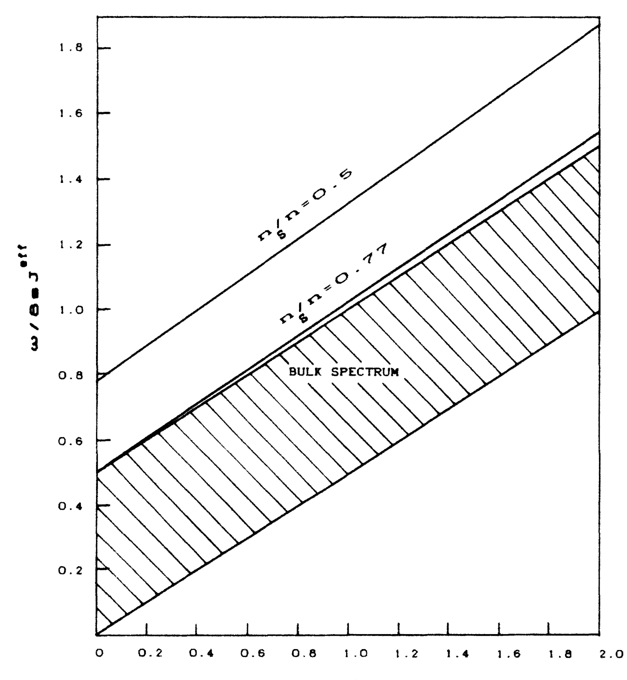

FIG. 2. Dispersion of the surface mode; $\Lambda(q)$ is defined in the text.

Since there are no optical modes for magnetically "softer" surface (as for magnetic insulators[4]), we conclude that there are no surface spin waves for $M_s/M>0.88$. In particular, there are no surface spin waves in this model for a neutral surface $M_s=M$. This completes the discussion of the surface spin-wave problem in the limit $\Delta/E_F\gg1$.

IV. DISCUSSION

The principal result of the paper is the mapping of the spin-wave problem for a semi-infinite metallic ferromagnet on an equivalent problem for an insulator. Such mapping provides a general recipe for solving the surface spin-wave problem in the following steps.

(i) The one-electron surface problem is solved in the HF approximation.

(ii) The bulk effective exchange integrals are computed from the one-electron HF propagators.

(iii) All bulk exchange integrals are set equal to zero across the surface (geometric effect of surface).

(iv) Surface renormalization of the effective exchange integrals is computed from the surface HF one-electron propagators. This determines the surface perturbation.

(v) The surface perturbation matrix is truncated to a manageable size and the Dyson equation for the surface spin-wave Green's function is solved.

All these steps were implemented in the paper for a (100) surface in a simple-cubic tight-binding strong ferromagnet and monitored by going to the limit $\Delta/E_F\gg1$ where all the results are exact in RPA. Such calculation is feasible since both the bulk exchange integrals and the surface perturbation are negligible beyond the range of electron hopping. This result is strictly valid only for a strong ferromagnet but may be a good approximation even for weak ferromagnets (see Ref. 12). It is clear that the above formula is also applicable to a multiband tight-binding band structure. Therefore, the present model calculation can be generalized to any surface for which a reliable self-consistent band calculation is available. One only requires tight-binding parametrizations of both the bulk and surface ferromagnetic band structures. Such parametrization was used recently by Edwards and Munitz[13] to calculate bulk spin-wave energies in Ni and Fe. They obtained correct spin-wave energies in Ni using d bands only and assuming a rigid exchange splitting. In view of that, it is not unreasonable to model the unoccupied minority t_{2g} bands in Ni by a single degenerate band and the present model calculation can be then applied qualitatively to nickel. Self-consistent band calculations for a (100) Ni surface[2] predict an enhancement of the surface magnetization by 8—10%. We can model this by adjusting the core shift E_0 to give $1.08 < n_s/n < 1.10$. It is rather remarkable that both $J_{\parallel}^{\text{eff}}$ and $J_{\perp}^{\text{eff}}$ are then almost exactly equal to the bulk J^{eff} (see Fig. 1). We expect this result to hold more generally for any tight-binding parametrization as long as the layer-by-layer count of magnetic electrons is constant, since the surface exchange integrals are closely related to the local density of states. The effect of surface then reduces to the geometric effect, discussed in Sec. III which is exactly the same as in magnetic insulators. In particular, the result of Mills and Maradudin,[5] that the surface magnetization follows the $T^{3/2}$ law with a prefactor twice as large as for the bulk magnetization, holds for a neutral surface. This has been observed for iron by Gradmann using Mössbauer spectroscopy.[14]

The situation for interfaces is more interesting since $J_{\parallel}^{\text{eff}}, J_{\perp}^{\text{eff}}$ deviate from the bulk J^{eff}. For example, a Ni surface coated with a Fe layer should be magnetically softer since the number of holes in the surface layer is increased (see Fig. 1). This should lead to a prefactor in the $T^{3/2}$ law greater than two and the more rapid decrease of the surface magnetization should be observable by Mössbauer spectroscopy (see Walker *et al.*[1] and Ref. 14). Assuming an iron-rich surface due to segregation, such a mechanism may also explain the more rapid decrease of the surface magnetization in Ni-Fe glass observed by Pierce *et al.*[1]

APPENDIX

We now show that the surface perturbation matrix W for a strong itinerant ferromagnet with neutral surface ($n_s = n$) reduces exactly in the limit $\Delta/E_F \gg 1$ to the Heisenberg W given by Eq. (14). This is done in the following steps. First, the Dyson equation for the HF surface one-electron propagators is solved, treating exactly the core shift E_0 and HF corrections in the surface plane. Next, the surface propagators are expressed in terms of the bulk propagators $G_{nm\sigma}^{b}$ and all G_{nm-}^{b} are expanded in powers of E_F/Δ as in Eq. (9). Working consistently to the order $O((E_F/\Delta)^2)$, it is easy to show that

$$W_{11} = (\omega/sJ^{\text{eff}})(1 - n/n_s) - 4\Lambda(q)(1-\epsilon_{\parallel}) - (2-\epsilon_{\perp})$$

with

$$\begin{aligned} \epsilon_{\parallel} &= -(n/n_s)^2 t(\pi n N)^{-1} \\ &\quad \times \int_{-\infty}^{E_F} \sum_k \exp(i\delta k) \text{Im} G_{11+}^{s}(k,E)\,dE\ , \\ \epsilon_{\perp} &= 1 - (n/n_s)(\pi n N)^{-1} \\ &\quad \times \int_{-\infty}^{E_F} \sum_k (E + \gamma - E_0) \text{Im} G_{11+}^{s}(k,E)\,dE\ , \end{aligned} \tag{A1}$$

where

$$\gamma = -t \sum_{\delta} \exp[i(k+q)\delta]\ ,$$

δ labels nearest neighbors in the surface plane, and t is the nearest-neighbor hopping integral. Similarly, W_{12} exact to order $O((E_F/\Delta)^2)$ is given by

$$W_{12} = 1 - \epsilon_{\perp}(n_s/n)\ . \tag{A2}$$

It is now clear that the matrix W reduces exactly to W given by Eq. (14) provided the surface core shift is adjusted to make the surface neutral ($n_s = n$).

[1]D. T. Pierce, R. J. Cellota, J. Unguris, and H. C. Siegmann, Phys. Rev. B **26**, 2566 (1982); S. Alvarado, M. Campagna, and H. Hopster, Phys. Rev. Lett. **48**, 51 (1982); J. C. Walker, R. Droste, G. Stern, and J. Tyson, J. Appl. Phys. **55**, 2500 (1984).

[2]Xue-yuan Zhu, J. Hermanson, F. J. Arlinghaus, J. G. Gay, R. Richter, and J. R. Smith, Phys. Rev. B **29**, 4426 (1984); H. Krakauer, A. J. Freeman, and E. Wimmer, *ibid.* **28**, 610 (1983); O. Jepsen, J. Madsen, and O. K. Andersen, *ibid.* **18**, 605 (1978).

[3]H. Hasegawa, J. Phys. F **16**, 347 (1986).

[4]R. E. De Wames and T. Wolfram, Phys. Rev. **185**, 721 (1969).

[5]D. L. Mills and A. A. Maradudin, J. Phys. Chem. Solids **28**, 1855 (1967).

[6]A. Griffin and G. Gumbs, Phys. Rev. Lett. **37**, 371 (1976).

[7]G. Gumbs and A. Griffin, Surf. Sci. **91**, 669 (1980).

[8]J. Mathon, Phys. Rev. B **24**, 6588 (1981).

[9]D. Kalkstein and P. Soven, Surf. Sci. **26**, 85 (1971).

[10]J. Mathon, Phys. Rev. B **27**, 1916 (1983).

[11]D. M. Edwards, Phys. Lett. **24** A, 350 (1967).

[12]M. W. Finnis, K. L. Kear, and D. G. Pettifor, Phys. Rev. Lett. **52**, 291 (1984).

[13]D. M. Edwards and R. B. Munitz, J. Phys. F **15**, 2339 (1985).

[14]U. Gradmann (private communication).