Surface spin waves in the Hubbard model

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A general random-phase-approximation (RPA) equation for the surface susceptibility of an itinerant ferromagnet is derived. The surface is treated as a perturbation to the bulk problem. It is shown that the resulting secular equation for surface spin waves has the same structure as for magnetic insulators. It is demonstrated that the spin-rotational invariance of the Hubbard Hamiltonian imposes an important self-consistency condition on the surface perturbation to the bulk susceptibility. The previous calculations which do not satisfy this self-consistency condition are critically reviewed. The secular equation for surface spin waves is solved explicitly for a strong itinerant ferromagnet containing a plane of impurities with an excess intra-atomic repulsion ΔU modeling the surface. The unenhanced surface susceptibility is treated exactly in the surface plane and approximated by the bulk susceptibility outside the plane. This approximation is shown to be asymptotically exact within RPA for a ferromagnet with exchange splitting much larger than the bandwidth. Surface spin waves in this model split off the bottom of the bulk spin-wave band for a magnetically weaker surface ($\Delta U < 0$) and they deviate downward from the bulk band only to the order $q_{\parallel}^4$ ($q_{\parallel}$ is the wave vector parallel to the surface). The attenuation of long-wavelength surface spin waves is exponential and their attenuation length is proportional to the square of the wavelength. All these properties are in qualitative agreement with the properties of surface spin waves in magnetic insulators. The similarities and differences between surface spin waves in metals and insulators are discussed in the light of the modern approach to magnetic excitations in bulk itinerant ferromagnets.

I. INTRODUCTION

Surface spin waves in ferromagnetic insulators have been studied extensively.[1,2] In the simplest model, nearest-neighbor exchange interaction is assumed and the exchange integral J_s in the surface plane is chosen to be smaller than the bulk value J. A well-defined surface mode then splits off the bottom of the bulk magnon band. It is also found[1,2] that to the order of $q_{\parallel}^2$ ($q_{\parallel}$ is the wave vector parallel to the surface) the dispersion of surface magnons is the same as the dispersion of the bulk modes and the surface branch only deviates from the bulk band to the order of $q_{\parallel}^4$. The attenuation of long-wavelength surface magnons increases as the square of the wavelength, which indicates that they penetrate very deeply into the crystal.

No such detailed microscopic information is available for surface spin waves in metals. The only theoretical study of surface spin waves in the itinerant model of ferromagnetism applicable to transition metals is due to Griffin and Gumbs.[3,4] In contrast to magnetic insulators, Griffin and Gumbs find that surface spin waves in metals always split off the top of the bulk spin-wave band and they claim that this property is a characteristic feature of the itinerant model of ferromagnetism. To obtain surface spin waves, Griffin and Gumbs were forced (by the complexity of the surface problem in metals) to adopt the classical infinite barrier model (CIBM) which assumes that the static electron density in a metal remains constant right up to its surface. However, recent band-structure calculations[5] indicate that this assumption is not valid in transition metals such as Ni. Moreover, it has been pointed out[6] and acknowledged by Griffin and Gumbs[4] that CIBM breaks the spin rotational symmetry of the problem and Griffin and Gumbs thus loose the Goldstone mode $\omega=0$, $q_{\parallel}=0$. This casts serious doubts on the validity of CIBM and the fundamental problem whether surface spin waves in the itinerant model exist and, in particular, whether they split off the top or bottom of the bulk band remains unresolved.

In this paper we shall study the simplest one-band Hubbard model of an itinerant ferromagnet with surface in the random phase approximation (RPA) and show quite conclusively that surface spin waves split off the bottom of the bulk magnon band provided the intra-atomic Coulomb integral (Hubbard's U) in the surface plane is smaller than in the bulk. The dispersion and penetration depth of surface spin waves will be also determined. No adjustable parameters are used and the present results are asymptotically exact within RPA for a strong ferromagnet with exchange splitting Δ much greater than the bandwidth.

II. RPA SECULAR EQUATION FOR SURFACE SPIN WAVES

We consider a simple cubic ferromagnet described by the standard one-band Hubbard model[7]

$$H = \sum_{i,j,\sigma} t_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} + \sum_{i} U_i n_{i\uparrow} n_{i\downarrow} + V \quad , \tag{1}$$

where $c_{i\sigma}^{\dagger}, c_{j\sigma}$ are the creation and annihilation operators in Wannier states, $n_{i\sigma} = c_{i\sigma}^{\dagger} c_{i\sigma}$, U_i is the effective intra-atomic repulsion (Hubbard's U), and t_{ij} is the hopping integral. The potential V modeling the surface will be specified later. Since the screening by the conduction electrons and the correlations in the narrow band itself may be modified near the surface[8] we allow U_i to vary in the direction perpendicular to the surface. 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. As is well known, the bulk ($V=0$) transverse spin susceptibility χ calculated in RPA exhibits an isolated bulk spin-wave pole which is separated from the Stoner (electron-hole) excitation spectrum. To obtain surface spin waves we require χ in RPA for ferromagnetic electrons that are scattered from the surface potential V. The transverse susceptibility matrix in the Wannier representation is defined by $\chi_{ij}(t) = \langle\langle S_i^{+}(t); S_j^{-}(0) \rangle\rangle$, where $S_i^{+} = c_{i\uparrow}^{\dagger} c_{i\downarrow}$, $S_j^{-} = c_{j\downarrow}^{\dagger} c_{j\uparrow}$, and $\langle\langle\, ;\, \rangle\rangle$ denotes the retarded Green's function. Since the wave vector parallel to the surface $q_{\parallel}$ remains a good quantum number it is more convenient to use mixed Bloch-Wannier representation[8] $\chi_{ij} \equiv \chi_{ij}(q_{\parallel}, \omega)$, where i,j label atomic planes parallel to the surface. We can now write the standard equation of motion for χ_{ij} and solve it in RPA. It is straightforward to show[4,8–10] that $\chi_{ij}(q_{\parallel}, \omega)$ satisfies the following matrix equation which is exact in RPA:

$$\chi_{ij}(q_{\parallel}, \omega) = \chi_{ij}^{0}(q_{\parallel}, \omega) + \sum_{l} \chi_{il}^{0}(q_{\parallel}, \omega) U_l \chi_{lj}(q_{\parallel}, \omega) \quad . \tag{2}$$

The kernel $\chi_{ij}^{0}(q_{\parallel}, \omega)$ is the transverse susceptibility of noninteracting electrons moving in a spin-dependent HF potential $V_{i\sigma} = V_i + U_i \langle n_{i,-\sigma} \rangle$. Here, V_i is the surface potential V in the ith atomic plane and $U_i \langle n_{i,-\sigma} \rangle$ is the HF exchange potential which is highly inhomogeneous since both U_i and $\langle n_{i,-\sigma} \rangle$ vary near the surface. The kernel $\chi_{ij}^{0}(q_{\parallel}, \omega)$ can be quite generally expressed[9] in RPA in terms of HF one-electron Green's functions $G_{ij\sigma}(t)$

$$\chi_{ij}^{0}(t) = \langle c_{i\uparrow}^{\dagger}(t) c_{j\uparrow}(0) \rangle G_{ij\downarrow}(t) + \langle c_{j\downarrow}^{\dagger}(0) c_{i\downarrow}(t) \rangle G_{ij\uparrow}^{*}(t) \quad , \tag{3}$$

where $\langle \cdots \rangle$ denotes the thermal averaging. Assuming that the solution of the one-electron HF problem is known, the spin-wave problem reduces to the solution of the key equation (2). All the previous attempts at solving it without drastic approximations have failed since, unlike the bulk problem, the kernel χ_{ij}^{0} is an essentially off-diagonal matrix both in the Wannier and Bloch representations. Direct solution of Eq. (2) with the exact kernel χ_{ij}^{0} is equivalent to the inversion of an infinite matrix and is thus not feasible.

To avoid this problem, we shall treat the surface as a perturbation to the bulk problem. It is convenient to write first Eq. (2) in an operator form,

$$\chi = \chi^{0} + \chi^{0} U \chi \tag{4}$$

and set $\chi^{0} = \Gamma + \Lambda$, where Γ is the standard unenhanced susceptibility of a bulk ferromagnet and Λ is the surface correction which can be determined from Eq. (3). In the mixed Bloch-Wannier representation, Γ is given by

$$\Gamma_{ij}(q_{\parallel}, \omega) = N_{\perp}^{-1} \sum_{q_{\perp}} \exp[i q_{\perp}(i-j)] \Gamma(q, \omega) \quad , \tag{5}$$

where

$$\Gamma(q, \omega) = N^{-1} \sum_{k} \frac{f_{k\uparrow} - f_{k+q\downarrow}}{\epsilon_{k+q\downarrow} - \epsilon_{k\uparrow} - \omega} \quad ,$$

$N_{\perp}$ is the number of atomic planes parallel to the surface, and $\epsilon_{k\sigma}$ are the bulk HF electron energies. We shall also write explicitly the surface correction to U by setting $U = U_0 + \Delta U$, where U_0 is the bulk value of U and ΔU is a diagonal matrix in the Bloch-Wannier representation with nonzero elements only for atomic planes i near the surface. The formal solution of Eq. (4) for the dynamic susceptibility χ is then given by

$$\chi = [I - G(\Gamma \Delta U + \Lambda U_0 + \Lambda \Delta U)]^{-1} G(\Gamma + \Lambda) \quad , \tag{6}$$

where I is the unit operator and G is the bulk susceptibility denominator

$$G = (I - U_0 \Gamma)^{-1} \quad . \tag{7}$$

Clearly the poles of $[I - G(\Gamma \Delta U + \Lambda U_0 + \Lambda \Delta U)]^{-1}$ determine the spin-wave energies in a ferromagnet with surface. In the Bloch-Wannier representation, the spin-wave poles are thus obtained from the following secular equation:

$$\mathrm{Det}[I - G(\Gamma \Delta U + \Lambda U_0 + \Lambda \Delta U)]_{ij} = 0 \quad , \tag{8}$$

where i,j label atomic planes parallel to the surface. Equation (8) which is still exact in RPA is the most convenient starting point for the study of surface spin waves. We note that Γ, G, and U_0 are the characteristics of a bulk ferromagnet and ΔU, Λ are surface corrections. It is also interesting to note that the secular equation (8) has exactly the same structure as the secular equation obtained by Mills and Maradudin[1] for a Heisenberg ferromanget. The operator G is the unperturbed spin-wave Green's function and

$\Gamma \Delta U + \Lambda U_0 + \Lambda \Delta U$ is the surface perturbation. As shown by Mills and Maradudin the surface perturbation in the Heisenberg model is strictly localized. This suggests that a truncation of the (in general extended) perturbation $\Gamma \Delta U + \Lambda U_0 + \Lambda \Delta U$ should be possible and physically plausible.

III. MODEL OF THE SURFACE AND SOLUTION OF THE SECULAR EQUATION

To discuss the surface perturbation we have to specify the surface potential V. Following Kalkstein and Soven[11] we could introduce (100) surface by setting $t_{ij} = 0$ across the $z = 0$ plane. Further refinement would be to modify t_{ij} for first few atomic planes to take account of the band-structure changes near the surface. However, all the important features of the spin-wave localization at a surface can be obtained in a far simpler model of surface for which analytic solution of Eq. (8) is possible. In this simplified model we assume: (i) strong Stoner ferromagnet; (ii) electrons are allowed to hop freely across the surface ($t_{ij} = t_{ij}^{\text{bulk}}$ for all i,j); and (iii) $U_i = U_0$ for $i \neq 0$ and $U_i = U_0 + \Delta U$ for $i = 0$, where ΔU is a parameter. The combined effect of (ii) and (iii) is that we have replaced the general surface problem by a simpler problem of localization of spin waves at a plane of "impurity" atoms with excess intra-atomic repulsion ΔU. Although such a model of surface may seem crude, it reproduces all the qualitative features of surface spin waves. In fact, we can compare it directly with an infinite Heisenberg ferromagnet in which the exchange between nearest neighbors J in the plane $z = 0$ is set equal to $J' \neq J^{\text{bulk}}$. It can be easily shown by the method of Refs. 1 and 2 that surface spin waves become localized below the bulk band for $J' < J^{\text{bulk}}$ and above the band for $J' > J^{\text{bulk}}$. This can be easily understood since a spin wave localized in the plane $z = 0$ experiences either smaller ($J' < J^{\text{bulk}}$) or greater ($J' > J^{\text{bulk}}$) exchange stiffness than in the bulk. Clearly the condition for spin-wave localization is that the exchange stiffness in the surface plane is different from its bulk value. If, on the other hand, one sets only $J = 0$ across the $z = 0$ surface and thereby creates real surface, the spin wave traveling in the surface plane experiences the same stiffness as in the bulk and no localization occurs. This is the well-known result arrived at analytically in Refs. 1 and 2. It follows that the introduction of a real surface (cleavage) plane only complicates the problem but adds nothing to the physics of the spin-wave localization. The same argument applies to the Hubbard model. By setting $U = U_0 + \Delta U$ in the plane $z = 0$ we change the exchange stiffness in this plane and, therefore, we expect spin waves to become localized below the bulk band when the exchange stiffness is smaller ($\Delta U < 0$) and above the band when it is greater ($\Delta U > 0$). We shall now prove rigorously that surface spin waves split off the bottom of the bulk spin-wave band for $\Delta U < 0$.

We first note that assumption (i) further simplifies the problem since the ground state of a strong ferromagnet is not affected by the plane of impurities with excess potential ΔU [up-spin carriers do not feel the impurity plane potential $V_{0\uparrow} = (U_0 + \Delta U)\langle n_{0\downarrow}\rangle$ since $\langle n_{0\downarrow}\rangle = 0$]. It is also important to note that there are three surface terms in the general secular equation (8), i.e, $\Gamma \Delta U$, ΛU_0, and $\Lambda \Delta U$ and all these terms are preserved in our simplified model of surface. The term $\Gamma \Delta U$ can be called "primary" surface perturbation since it describes the direct effect of ΔU on bulk spin waves. The remaining two terms ΛU_0 and $\Lambda \Delta U$ are "secondary" in the sense that Λ reflects the changes in the one-electron states due to ΔU and these changes influence indirectly spin waves which are collective modes made up of all the one-electron states in the crystal. Although the electron density in a strong ferromagnet is not affected by ΔU, the secondary terms ΛU_0 and $\Lambda \Delta U$ are nonzero in our simplified model of surface since down-spin carriers feel the surface potential ΔU via $V_{0\downarrow} = (U_0 + \Delta U)\langle n_{0\uparrow}\rangle$ and their Green's function which appears in Eq. (3) for Λ is modified near the surface. In fact, it will be seen that the correct treatment of the matrix Λ_{ij} is of central importance. To illustrate this, we shall first solve the secular equation (8) in the classical infinite barrier approximation $\Lambda = 0$ which assumes that the impurity plane has no effect on the one-electron states.

The secular equation (8) in CIBM assumes the form

$$\operatorname{Det}\left|\delta_{ij} - \sum_n \chi_{in}^{\text{bulk}} \Delta U \delta_{n0} \delta_{j0}\right| = 0 \quad , \tag{9}$$

where $\chi_{in}^{\text{bulk}} = \sum_l G_{il} \Gamma_{ln}$ is the bulk enhanced RPA susceptibility given by

$$\chi_{ij}^{\text{bulk}}(q_\parallel, \omega) = N_\perp^{-1} \sum_{q_\perp} \exp[iq_\perp(i-j)] \times \Gamma(q,\omega)[1 - U_0 \Gamma(q,\omega)]^{-1} \quad . \tag{10}$$

It follows from Eq. (9) that the spin-wave energies are determined by

$$\frac{1}{\Delta U} = \operatorname{Re} \chi_{00}^{\text{bulk}}(q_\parallel, \omega) \quad . \tag{11}$$

For small $q_\parallel$ and ω the susceptibility $\chi_{ij}^{\text{bulk}}(q_\parallel, \omega)$ is dominated by the bulk spin-wave poles, i.e.,

$$\Gamma(q,\omega)[1 - U_0 \Gamma(q,\omega)]^{-1} \approx n_\uparrow [Dq_\perp^2 + (Dq_\parallel^2 - \omega)]^{-1} \quad ,$$

where D is the bulk spin-wave stiffness and $n_\uparrow$ is the number of up-spin electrons per atom. Outside the bulk spin-wave band, i.e., for $\omega < Dq_{\parallel}^2$ the summation over $q_{\perp}$ in Eq. (10) can be replaced by integral and χ_{00}^{bulk} becomes

$$\text{Re}\chi_{00}^{\text{bulk}}(q_{\parallel},\omega) \approx \frac{n_{\uparrow}}{\pi} D^{-1/2} a (Dq_{\parallel}^2-\omega)^{-1/2} \times \tan^{-1}[(Dq_0^2)^{1/2}(Dq_{\parallel}^2-\omega)^{-1/2}] \;, \tag{12}$$

where a is the lattice constant and q_0 is a cutoff wave vector whose magnitude is unimportant since we are only interested in the limit $q_{\parallel}\to 0$, $\omega\to 0$.

When ω approaches the bottom of the bulk spin-wave band from below, $\text{Re}\chi_{00}^{\text{bulk}}(q_{\parallel},\omega)$ tends to $+\infty$ and it follows from Eq. (11) that there is always a bound state (surface spin wave) *below* the bulk band provided $\Delta U > 0$. In the special case $q_{\parallel}=0$, the surface spin-wave energy ω_s is clearly negative, i.e., there is a gap in the spin-wave spectrum. Since impurities with excess potential ΔU do not lower the spin-rotational symmetry of the Hubbard Hamiltonian[12] the Goldstone theorem is violated by the approximation $\Lambda=0$. It can be easily seen that the same argument applies even to more elaborate models of surface (such as adopted by Griffin and Gumbs[4]). Clearly CIBM is not a good approximation in this case and the effect of surface on the unenhanced susceptibility χ^0 has to be evaluated self-consistently.

The next simplest approximation is to treat the surface layer exactly and replace χ^0 outside the surface by the bulk susceptibility Γ. Therefore, we shall set

$$\Lambda_{ij} = \begin{cases} \Lambda_{00} & \text{for } i=j=0 \\ 0 & \text{for } i\neq 0,\ j\neq 0 \;, \end{cases} \tag{13}$$

where Λ_{00} is given by Eq. (3). The approximation (13) is expected to be valid when the hopping term t_{ij} is small compared with U. In fact, it has been demonstrated[13] that it becomes asymptotically exact in the limit $t_{ij}/U\to 0$ in the sense that the Goldstone theorem is exactly satisfied. It follows that the approximation (13) preserves the spin-rotational symmetry of the problem and we may use it to discuss the existence and properties of surface spin waves.

Since both Λ_{ij} and ΔU_{ij} have now nonzero elements only for $i=j=0$, the secular equation (8) becomes

$$1-\chi_{00}^{\text{bulk}}\Delta U - G_{00}\Lambda_{00}(U_0+\Delta U)=0 \;, \tag{14}$$

where $G_{00}=\chi_{00}^{\text{bulk}}U_0+1$ and χ_{00}^{bulk} is defined by Eq. (10). Equation (14) can be easily transformed to the form

$$U_0[1+U_0\chi_{00}^{\text{bulk}}(q_{\parallel},\omega)] = [\Delta U U_0^{-1}(U_0+\Delta U)^{-1}+\Lambda_{00}(q_{\parallel},\omega)]^{-1} \tag{15}$$

which is more convenient for graphical analysis. The bulk susceptibility is again given by Eq. (12) and we only require $\Lambda_{00}(q_{\parallel},\omega)$ for small ω and $q_{\parallel}$. It is easy to evaluate the general expression (3) for Λ_{00} and an explicit formula for Λ_{00} is obtained in the Appendix. As already discussed, the approximation (13) is expected to be valid for a strong ferromagnet with exchange splitting much greater than the bandwidth. In this limit, the expansion of Λ_{00} in powers of ω and $q_{\parallel}$ takes the simple form

$$\Lambda_{00}(q_{\parallel},\omega) = -\Delta U U_0^{-1}(U_0+\Delta U)^{-1} - \text{sgn}(\Delta U)(\alpha\omega-\beta q_{\parallel}^2)+\cdots \;, \tag{16}$$

where α and β are given in the Appendix. In fact, for the discussion of the existence of surface spin waves only the result $\beta/\alpha < D$ is required.

The qualitative behavior of the left- and right-hand sides of Eq. (15) is shown in Fig. 1 both for $\Delta U > 0$

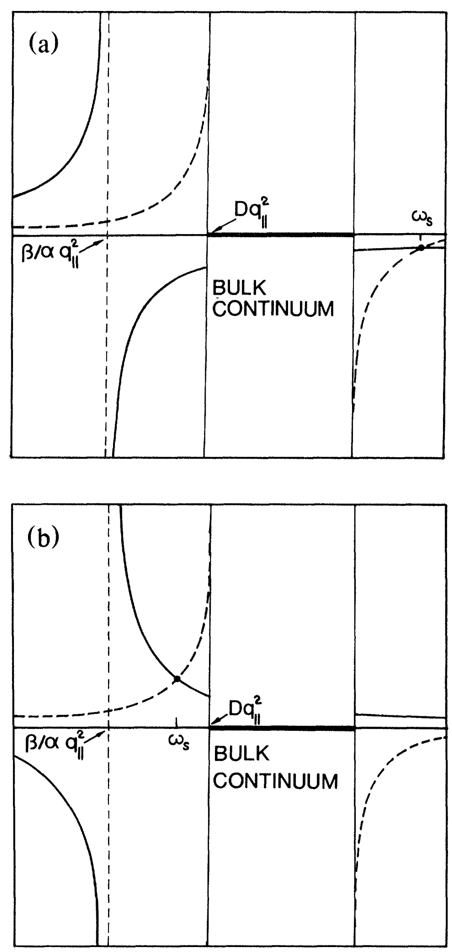

FIG. 1. Schematic plots of the left-hand side (broken curves) and right-hand side (continuous curves) of Eq. (15) as functions of ω for fixed $q_{\parallel}$. (a) corresponds to $\Delta U > 0$ and (b) to $\Delta U < 0$.

and $\Delta U < 0$. It is clear that Eq. (15) has no solution below the bulk spin-wave band for $\Delta U > 0$. On the other hand, there is always a solution for $\Delta U < 0$, i.e., surface spin waves exist and they split off the bottom of the bulk spin-wave band. Moreover, since the surface spin-wave energy ω_s lies between the points $\omega = (\beta/\alpha) q_\parallel^2$ and $\omega = D q_\parallel^2$ it tends to zero continuously in the limit $q_\parallel \to 0$, i.e., the surface mode satisfies the Goldstone theorem. It can be also seen from Fig. 1(a) that for $\Delta U > 0$ the Goldstone theorem is satisfied by the bulk mode.

This behavior of surface spin waves obtained in the self-consistent approximation (13) is in sharp contrast to the behavior of surface spin waves in CIBM. While CIBM predicts surface spin waves below the bulk band for $\Delta U > 0$, the present calculation shows that they appear for $\Delta U < 0$. It follows that CIBM not only violates the Goldstone theorem but also looses completely the acoustic surface mode for $\Delta U < 0$.

IV. DISPERSION AND PENETRATION DEPTH OF SURFACE SPIN WAVES

To determine the dispersion of surface spin waves we have to solve Eq. (15) explicitly. Working to the lowest order in ω and $q_\parallel$ we may use Eq. (12) for $\chi_{00}^{\text{bulk}}(q_\parallel, \omega)$ and the expansion (16) for $\Lambda_{00}(q_\parallel, \omega)$. Because of the symmetry of the problem, the surface spin-wave energy ω_s can be expanded in powers of $q_\parallel$ as

$$\omega_s = A q_\parallel^2 + B q_\parallel^4 + \cdots \quad . \tag{17}$$

Substituting for χ_{00}^{bulk}, Λ_{00}, and ω_s in Eq. (15) and keeping only the lowest powers of $q_\parallel$, we obtain

$$2a^{-1} D^{1/2} U_0^{-2} n_\uparrow^{-1} (D q_\parallel^2 - A q_\parallel^2 + \cdots)^{1/2} = -\mathrm{sgn}(\Delta U)(\alpha A q_\parallel^2 - \beta q_\parallel^2 + \cdots) \quad . \tag{18}$$

In the lowest order in $q_\parallel$, the right-hand side can be neglected and Eq. (18) is clearly satisfied for $A = D$. The surface spin-wave energy is then given by

$$\omega_s = D q_\parallel^2 + B q_\parallel^4 + \cdots \quad , \tag{19}$$

where D is the bulk spin-wave stiffness constant. Hence to the order of $q_\parallel^2$ the surface and bulk spin-wave energies are identical. This result which also holds for the Heisenberg model[1] is quite general since the surface perturbation on the right-hand side of Eq. (18) is always of higher order in $q_\parallel$ than the bulk term on the left-hand side.

The calculation of the coefficient B of the quartic term would require more detailed knowledge of the frequency and wave-vector dependences of Λ_{00} and χ_{00}^{bulk}. Although such a calculation is quite feasible the effort is hardly justified since the present model of surface is too simple for the numerical value of B to be significant. Nevertheless, it is easy to discuss qualitatively the behavior of the quartic term. It follows from Eq. (18) that its right-hand side (i.e., the surface term) contributes to B and, therefore, the surface mode deviates from the bulk band to the order of $q_\parallel^4$. The graphical analysis of Fig. 1(b) indicates that the deviation is downward (which is important since well-defined surface spin waves can exist only outside the bulk band).

We shall now discuss the penetration depth of surface spin waves. It is first necessary to determine the dynamic response $\chi_{nn}(q_\parallel, \omega)$ of a general atomic plane n parallel to the surface. The amplitude of the surface spin wave S_n^+ is then proportional to the residue of χ_{nn} at the pole $\omega = \omega_s$. The susceptibility χ_{nn} can be calculated from Eq. (6) and since the denominator in Eq. (6) is already known [Eq. (15) or (16)], it is straightforward to show that

$$\chi_{nn} = \chi_{nn}^{\text{bulk}} + \frac{[\Delta U + \Lambda_{00} U_0 (U_0 + \Delta U)](\chi_{00}^{\text{bulk}} U_0 + 1)^{-1} \chi_{n0}^{\text{bulk}} \chi_{0n}^{\text{bulk}} U_0}{(U_0 + \Delta U)(\chi_{00}^{\text{bulk}} U_0 + 1)^{-1} - [\Delta U + \Lambda_{00} U_0 (U_0 + \Delta U)]} \quad . \tag{20}$$

It should be noted that χ_{nn}^{bulk} and χ_{n0}^{bulk} remain finite at $\omega = \omega_s$ and the surface spin-wave pole is due entirely to the denominator in Eq. (20). It follows that the amplitude of the surface spin wave in the nth atomic plane is given by

$$S_n^+ \propto \lim_{\omega \to \omega_s} [\Delta U + \Lambda_{00} U_0 (U_0 + \Delta U)] \times (\chi_{00}^{\text{bulk}} U_0 + 1)^{-1} \chi_{n0}^{\text{bulk}} \chi_{0n}^{\text{bulk}} \quad . \tag{21}$$

The only terms in Eq. (21) depending on n are χ_{0n}^{bulk} and χ_{n0}^{bulk} and they clearly determine the penetration depth of surface spin waves. Since ω_s lies outside the bulk spin-wave band, $\chi_{0n}^{\text{bulk}}(q_\parallel, \omega)$ can be expressed from Eqs. (10) and (12) as an integral

$$\chi_{0n}^{\text{bulk}}(q_\parallel, \omega) \propto \int_0^{naq_0} \frac{dx \cos x}{n^2 \kappa^2 + x^2} \quad . \tag{22}$$

Here,

$$\kappa = a (q_\parallel^2 - \omega_s / D)^{1/2} = a(-B/D)^{1/2} q_\parallel^2 + O(q_\parallel^4) \quad , \tag{23}$$

a is the lattice constant, and q_0 is a cutoff momentum whose magnitude is unimportant provided $n\kappa \ll q_0 na$. For long-wavelength surface spin waves this condition is always satisfied and the upper limit in Eq. (22) can be replaced by infinity. It follows that

$$\chi_{0n}^{\text{bulk}} = (\chi_{n0}^{\text{bulk}})^* \propto e^{-n\kappa}/\kappa \quad . \tag{24}$$

Since $\kappa \propto q_{\parallel}^2$, it might seem that S_n^+ diverges for $q_{\parallel} \to 0$ as $q_{\parallel}^{-4}$. However, it can be easily shown that the factor $[\Delta U + \Lambda_{00} U_0 (U_0 + \Delta U](\chi_{00}^{\text{bulk}} U_0 + 1)^{-1}$ removes this divergence and the surface spin-wave amplitude is given by

$$S_n^+ = S_{\text{bulk}}^+ \exp[-2naq_{\parallel}^2(-B/D)^{1/2}] \quad . \tag{25}$$

In the limit $q_{\parallel}=0$ the amplitude S_n^+ is independent of n and the surface spin wave reduces to the homogeneous bulk mode $\omega=0$, $q_{\parallel}=0$. For finite $q_{\parallel}$, the amplitude decays exponentially away from the surface and the attenuation of long-wavelength surface spin waves increases as the square of the wavelength. Both results are in complete agreement with the Heisenberg model for ferromagnetic insulators.[1]

V. DISCUSSION

The principal result of Sec. II is the derivation of a general RPA secular equation for spin-wave energies in a crystal with surface. The surface is treated as a perturbation to the bulk problem and the structure of the secular equation (8) is found to be exactly the same as in the Heisenberg model of magnetic insulators. It follows that the physical condition for the existence of surface spin waves in metals is also the same, i.e., spin waves become localized at the surface provided the surface exchange stiffness differs from the bulk. Although the secular equation for surface spin waves has the same structure, there are important differences between surface spin waves in metals and insulators. First, the range of the surface perturbation in Eq. (8) is infinite but the surface perturbation in the Heisenberg model extends only over 1–2 atomic planes. As a result, the introduction of a cleavage plane in the Hubbard model (without any other changes in the surface parameters) modifies the HF exchange potential in several adjacent atomic planes, which changes the exchange stiffness. Hence the cleavage plane should lead to the surface localization of spin waves. No such localization occurs in the analogous Heisenberg model with nearest-neighbor exchange if only the bonds normal to the surface are cut. The Hubbard model behaves in this respect as a Heisenberg Hamiltonian with a long-range exchange. The second important difference is the frequency dependence of the surface perturbation in the Hubbard model. In magnetic insulators, the surface perturbation depends only on the wave vector $q_{\parallel}$. This is the most important feature of an itinerant ferromagnet. To see what effect these properties of the surface perturbation have on surface spin waves in metals, we have examined in Sec. III the simplest model of spin-wave localization at a plane of impurities with excess intra-atomic repulsion ΔU. The main approximation of Sec. III is the truncation of the range of the "secondary" surface perturbation Λ_{ij} in Eq. (8). The correct treatment of this term is crucial in any surface (and impurity!) problem. When the secondary perturbation Λ_{ij} is completely neglected, one gets the infinite classical barrier approximation (CIBM) of Refs. 3 and 4. We find that, at least for the present model of surface, CIBM is quite inadequate. The reason for its failure is that the dependence of the surface perturbation on the wave vector $q_{\parallel}$ and frequency ω is completely lost in CIBM. As a result, CIBM does not satisfy the important self-consistency condition that the surface perturbation should vanish in the limit $\omega \to 0$, $q_{\parallel} \to 0$. This condition is imposed by the spin-rotational symmetry of the problem and must be satisfied both in the Heisenberg and Hubbard models (in the Heisenberg model, the surface perturbation is independent of ω). Although Gumbs and Griffin[4] recognize that CIBM fails in the limit $\omega \to 0$, they argue that it predicts correctly the position and properties of the surface mode *above* the bulk spin-wave band. We find that this is not the case. In the present model of surface, CIBM predicts the surface mode *above* the bulk band for $\Delta U < 0$. This is clearly unphysical result since the exchange stiffness is reduced in a magnetically weaker layer ($\Delta U < 0$). In Sec. III, the secondary perturbation Λ_{ij} is treated exactly in the surface layer and it is shown that the surface mode splits off the bottom of the bulk band. Our result is asymptotically exact in RPA for a strong ferromagnet with exchange splitting much larger than the bandwidth. For weaker ferromagnets, the surface perturbation is clearly more delocalized and its effect on several atomic planes would have to be considered. This can be easily done and our preliminary results indicate that such a delocalization does not change qualitatively the results obtained in the present model.

The most striking feature of the acoustic surface spin waves obtained in the present self-consistent approximation is their remarkable similarity to the surface spin waves in magnetic insulators. For a magnetically weaker surface $\Delta U < 0$ (analogous to $J^{\text{surface}} < J^{\text{bulk}}$ in the Heisenberg model), we find that surface spin waves split off the bottom of the bulk band (as in the Heisenberg model), they deviate downward from the bulk band only to the order of $q_{\parallel}^4$ (as in the Heisenberg ferromagnet), and their attenuation is proportional to the square of the wavelength (again as in the Heisenberg ferromagnet). Such a similarity is clearly not accidental and can be explained if one adopts the view that magnetic excitations in an itinerant ferromagnet involving rotations of the magnetic moment only (such as spin waves) are qualitatively the same as in magnetic insulators described by the Heisenberg Hamiltonian. This is in line with the current approach to ferromagnetism[14–16] in transition metals as exemplified by the Hubbard's theory of iron.[14] According to Hubbard an effective interatomic exchange can be defined in an itinerant ferromagnet and the present calculation shows that such an effective localized model remains valid even when a surface (or impurity) is introduced. One expects this model to work well when the intra-atomic integral U is large compared with the bandwidth. This explains the success of our truncation of the surface perturbation Λ_{ij} to a very short-range Heisenberg-like perturbation.

Finally, we may speculate about the position of the surface mode for $\Delta U > 0$ (magnetically stronger surface). The graphical analysis of Fig. 1 indicates that the surface mode should split off the top of the bulk spin-wave band (as in the Heisenberg model with $J^{\text{surface}} > J^{\text{bulk}}$). We expect this result to hold for itinerant ferromagnets similar to iron for which the Hubbard's effective localized model is believed to be valid. For weaker ferromagnets, the effective localized model becomes progressively worse at higher excitation energies (e.g., above the bulk spin-wave band), and detailed numerical analysis is required since no simple expansions of χ_{ij}^{bulk} and Λ_{ij} are possible near the top of the bulk spin-wave band. However, we wish to emphasize that our qualitative results for the *acoustic* surface branch ($q_\parallel \to 0$, $\omega \to 0$) are valid for any itinerant ferromagnet including the weak one. The case of a weak itinerant ferromagnet is even more interesting since other surface modes at higher energies might exist *in addition* to the Heisenberg-like acoustic mode discussed in the present paper. Such high-energy modes could be more easily resolved in low-energy electron diffraction (LEED) experiments. Work is now in progress to obtain the whole excitation spectrum of an itinerant ferromagnet by the present self-consistent method.

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APPENDIX

In the mixed Bloch-Wannier representation, Eq. (3) for the kernel $\chi_{ij}^0(q_\parallel, \omega)$ assumes the form

$$\chi_{ij}^0 = -N_\parallel^{-1} \sum_{k_\parallel} \int_{-\infty}^{\epsilon_F} [\operatorname{Im} G_{\uparrow ji}(k_\parallel, \Omega) \times \operatorname{Re} G_{\downarrow ij}(k_\parallel + q_\parallel, \Omega + \omega)]\, d\Omega \ . \tag{A1}$$

The second term in Eq. (3) vanishes for a strong ferromagnet since $\operatorname{Im} G_{\downarrow ij} = 0$ above the Fermi level ϵ_F. The majority carriers in a strong ferromagnet do not feel the exchange potential of the impurity plane and their Green's function $G_{\uparrow ji}(k_\parallel, \Omega)$ is just the bulk HF Green's function, i.e.,

$$\operatorname{Im} G_{\uparrow ji}(k_\parallel, \Omega) = N_\perp^{-1} \sum_{k_\perp} \delta(\Omega - \epsilon_{k\uparrow}) \exp[ik(j-i)] \ , \tag{A2}$$

where $\epsilon_{k\uparrow}$ is the HF bulk electron energy. To obtain $G_{\downarrow ij}(k_\parallel, \Omega)$, we have to solve the quasi-one-dimensional Slater-Koster problem

$$G_{\downarrow ij} = G_{\downarrow ij}^0 + \Delta U n_\uparrow G_{\downarrow i0}^0 G_{\downarrow 0j} \tag{A3}$$

for the minority carriers scattered from the exchange potential $\Delta U n_\uparrow$ localized in the plane $i = 0$. Here, $G_{\downarrow ij}^0$ is the bulk HF Green's function. It follows that

$$G_{\downarrow ij} = G_{\downarrow ij}^0 + \Delta U n_\uparrow G_{\downarrow i0}^0 G_{\downarrow 0j}^0 (1 - \Delta U n_\uparrow G_{\downarrow 00}^0)^{-1} \ , \tag{A4}$$

where

$$G_{\downarrow 00}^0 = N_\perp^{-1} \sum_{k_\perp} (\Omega - \epsilon_{k\downarrow})^{-1} \ . \tag{A5}$$

It should be noted that there is always a bound state below the minority band for $\Delta U < 0$. However, since we consider only strong ferromagnets with exchange splitting much larger than the band width the bound state lies above the Fermi level and has no effect on the majority carriers. When Eq. (A4) is substituted in Eq. (A1) the first term in Eq. (A4) yields the bulk kernel Γ_{ij} and the second term gives Λ_{ij}. The matrix element Λ_{00} is given by

$$\Lambda_{00}(q_\parallel, \omega) = -n_\uparrow \Delta U N^{-1} \sum_k f_{k\uparrow} [G_{\downarrow 00}^0(k, q_\parallel, \omega)]^2 \times [1 - n_\uparrow \Delta U G_{\downarrow 00}^0(k, q_\parallel, \omega)]^{-1} \ , \tag{A6}$$

where

$$G_{\downarrow 00}^0(k, q_\parallel, \omega) = N_\perp^{-1} \sum_{k_\perp'} (\epsilon_{k\uparrow} - \epsilon_{k_\perp', k_\parallel + q_\parallel \downarrow} + \omega)^{-1} \ . \tag{A7}$$

To evaluate Λ_{00}, we take the limit $W/\Delta \to 0$ in Eq. (A6), where W is the bandwidth and $\Delta = \epsilon_{k\downarrow} - \epsilon_{k\uparrow}$ is the exchange splitting. In this limit, the dispersion of $\epsilon_{k\sigma}$ is small compared with Δ and we may approximate $G_{\downarrow 00}^0 \approx -\Delta^{-1}$. Hence $\Lambda_{00}(0,0)$ is given by

$$\Lambda_{00}(0,0) = -\Delta U [U_0(U_0 + \Delta U)]^{-1} \ . \tag{A8}$$

Expanding $\Lambda_{00}(q_\parallel, \omega)$ as

$$\Lambda_{00}(q_\parallel, \omega) = \Lambda_{00}(0,0) - \operatorname{sgn}(\Delta U)(\alpha\omega - \beta q_\parallel^2) + \cdots \tag{A9}$$

and setting $\beta = \beta_1 + \beta_2 + \beta_3$, we obtain in the same limit the following expressions for α and β_i valid for a cubic crystal:

$$\alpha=\frac{|\Delta U|(2U_0+\Delta U)}{\Delta(U_0+\Delta U)^2 U_0} ,$$

$$\begin{aligned}\beta_1&=\frac{|\Delta U|(2U_0+\Delta U)}{6\Delta^2(U_0+\Delta U)^2}N^{-1}\sum_k f_{k\uparrow}\nabla_k^2\epsilon_{k\uparrow} ,\\ \beta_2&=-\frac{|\Delta U|(2U_0+\Delta U)}{3\Delta^3(U_0+\Delta U)^2}N^{-1}\sum_k f_{k\uparrow}(\nabla_k\epsilon_{k\uparrow})^2 ,\\ \beta_3&=-\frac{|\Delta U|U_0^2}{3\Delta^3(U_0+\Delta U)^3}N^{-1}\sum_k f_{k\uparrow}(\nabla_k\epsilon_{k\uparrow})^2 .\end{aligned} \tag{A10}$$

We now recall that the bulk RPA exchange stiffness of a strong cubic ferromagnet is given by the standard formula (see, for example, Ref. 12)

$$D=\frac{U_0}{6N\Delta}\sum_k f_{k\uparrow}\left[\nabla_k^2\epsilon_{k\uparrow}-\frac{2}{\Delta}(\nabla_k\epsilon_{k\uparrow})^2\right] . \tag{A11}$$

It follows that the important ratio β/α which governs the existence of surface spin waves is given by

$$\frac{\beta}{\alpha}=D-\frac{U_0^3}{\Delta^2(U_0+\Delta U)(2U_0+\Delta U)}\times N^{-1}\sum_k f_{k\uparrow}(\nabla_k\epsilon_{k\uparrow})^2 . \tag{A12}$$

Since the second term in Eq. (A12) is manifestly negative the condition $\beta/\alpha < D$ used in Sec. III is always satisfied.

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