Inelastic scattering of neutrons by surface spin waves on ferromagnets

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We present a theoretical analysis of the inelastic scattering of thermal neutrons from the surface of a ferromagnetic crystal, under conditions where the angle of incidence of the neutron exceeds the critical angle and its wave function attenuates exponentially as one moves into the crystal. Under these conditions, we evaluate and compare the cross section for scattering off surface and bulk spin waves, for a model of a localized-spin ferromagnet. The formalism we use here should prove useful for analysis of a variety of similar problems.

I. INTRODUCTION

For a number of years, the influence of a surface on the magnetic properties of crystals has been an active area of theoretical study, at temperatures well below the bulk ordering temperature where surface spin waves appear under a variety of circumstances,[1] and near the bulk ordering temperature where the influence of the surface on critical behavior may be explored.[2] However, there are few experiments that probe surface magnetism in a microscopic fashion, yielding data that may be placed in direct contact with theory. Spin-polarized electron scattering is a potentially powerful probe of these issues, and we have data from two excellent experiments in hand at the time of this writing.[3]

In a recent Communication, Felcher[4] suggested that neutron scattering may be used to probe the magnetic environment near the surface. At first glance, this suggestion is surprising, since the mean free path of neutrons in most crystals is very long; consequently the scattered neutrons give information primarily on bulk properties of the crystal. However, Felcher points out that in many substances, the sign of the average nuclear scattering length is such that the effective index of refraction of the crystal for neutron propagation is less than unity. Then, just as in crystal optics, there is a critical angle of incidence θ_c beyond which the neutron wave is totally reflected from the crystal surface. The neutron wave function penetrates into the crystal interior, but is exponentially attenuated as one moves into the crystal interior.

A consequence is that neutrons scattered off the surface give information only about the near vicinity of the surface if the incoming beam strikes the surface at grazing incidence with the angle of incidence greater than the critical angle θ_c. We have the intriguing possibility that the neutron scattering method, which has proved to be such a powerful probe of bulk magnetic properties, may be used also to examine the near vicinity of the surface. It is interesting to note that inelastic light scattering experiments (Raman scattering) have been carried out under conditions similar to those just described.[5]

While Felcher's Communication explored only the possibility of examining the spatial variation of the average magnetization, it was suggested that inelastic scattering experiments may be carried out in such a geometry to observe excitation of surface spin waves by a neutron beam that strikes the crystal at grazing incidence.[6] The purpose of this paper is to present a formalism in which such experiments may be analyzed, and to report numerical calculations of the cross sections with the use of the method described below. The standard discussion of the scattering of neutrons by spin waves[7] considers the wave function of the particle to be a plane wave, assumes that the neutron interacts with the spins only while it is within the crystal, and supposes that the spin waves themselves are simple plane waves. In the scattering geometry of present interest, the neutron wave function is more complex, as outlined above. Also, spin fluctuations near the surface produce fluctuating magnetic fields in the vacuum above the crystal surface, so the neutron interacts with the electronic spins in the material not only when it is within the crystal, but also while it is in the vacuum above the crystal, either approaching it or exiting from it. Finally, due account must be taken of the influence of the surface on the spin dynamics in its near vicinity. This is obvious if one wishes to examine the scattering of neutrons by surface spin waves, but it is important to note that the surface affects the nature of the spin fluctuations nearby, produced by thermally excited bulk spin waves.[8]

A theory that incorporates all these effects necessarily leads to final expressions for the inelastic cross section that are more cumbersome and less elegant than the familiar Van Hove formulas encountered in the literature of neutron scattering from bulk spin-wave excitations. But for the picture of the surface scattering experiment we use here, which we believe is sufficiently realistic for the results to be quantitatively reliable, one may obtain closed algebraic expressions for the various contributions to the inelastic cross section. While the basic approach we use here is an adaptation of earlier theories of small-angle inelastic scattering of electrons from surface excitations,[9] the modifications required for the discussion of neutron scattering are nontrivial in nature.

II. THEORETICAL ANALYSIS

We consider a semi-infinite lattice of localized spins, with $\vec{S}_i$ the magnitude of the spin on lattice site i, and suppose that a neutron is incident on the crystal from above. The surface of the crystal coincides with the x-y plane of a Cartesian coordinate system, and the lattice of spins occupies the half space $z \geq 0$. The Hamiltonian is thus

$$H = H_n + H_{nS} + H_S \ , \tag{2.1}$$

where

$$H_n = \frac{P_n}{2M_n} + V_0(\vec{x}_{||}, z) \ , \tag{2.2}$$

where $\vec{P}$ is the momentum of the neutron, M_n is its mass, and $V_0(\vec{x}_{||}, z)$ describes the interaction of the neutron with the array of nuclei. The second term in the Hamiltonian describes the interaction of the neutrons with the electronic spins,[10] here regarded as highly localized.[11] We have, with $\vec{r}$ the position of the neutron and $\vec{s}$ its spin,

$$H_{nS}(\vec{r}) = -g\mu_B\mu_n \sum_i \left[\vec{s}\cdot\vec{\nabla}_r(\vec{S}_i\cdot\vec{\nabla}_{\vec{r}})\frac{1}{|\vec{r}-\vec{R}_i|} + 4\pi\vec{s}\cdot\vec{S}_i\delta(\vec{r}-\vec{R}_1) \right] . \tag{2.3}$$

In Eq. (2.3), $\vec{R}_i$ is the location of spin $\vec{S}_i$, the electronic moment associated with the site is $g\mu_B\vec{S}_i$ with μ_B the Bohr magneton, and μ_n is the neutron magnetic moment. Finally, H_S describes the spin-spin interactions in the crystal. We shall be content to consider the following Heisenberg spin system with nearest-neighbor exchange:

$$H_S = -\tfrac{1}{2}J \sum_{\vec{l}} \sum_{\vec{\delta}} \vec{S}(\vec{l})\cdot\vec{S}(\vec{l}+\vec{\delta}) \ . \tag{2.4}$$

We ignore changes in the exchange near the surface, since they will play no essential role in our discussion. The influence of altered-surface exchange constants is readily incorporated into the discussion through use of appropriate Green's functions which enter the discussion below.

The principal approximation we make is the following. The potential $V_0(\vec{x}_{||}, z)$ is formed by summing over the interaction of the neutron with the array of nuclei in the crystal. We shall replace this potential by a spatially averaged (possibly complex) optical potential V_0. Since the crystal occupies the half space $z > 0$, we have

$$V_0(\vec{x}_{||}, z) = V_0\Theta(+z)$$

within this scheme, with $\Theta(x)$ the step function that equals unity for positive values of its argument and that vanishes for negative values. A consequence of this smearing out of the crystal potential is that we obtain a neutron beam specularly reflected off the surface, but no Bragg beams. The description of the inelastic scattering includes "N processes" for which wave-vector components (parallel to the surface) are conserved, but not "U processes" where wave-vector components parallel to the surface are conserved only to within a nonzero reciprocal-lattice vector (parallel to the surface). To carry out the analysis within a scheme that fully includes the Bragg beams in the semi-infinite geometry can surely be done, but the increase in algebraic complexity is substantial. The approximation outlined above allows us to explore a number of questions of interest, within the framework of a tractable analysis; for example, the breakdown of wave-vector conservation in the direction normal to the surface that is a consequence of the attenuation of the neutron beam into the medium is fully incorporated.

Once the approximate form for $V_0(\vec{x}_{||}, z)$ is chosen, we proceed by treating H_{nS} as a small perturbation. The neutron encounters the spin system in the eigenstate $|M\rangle$ of H_S, its incoming wave function is $|\psi_n^I\rangle$, so the wave function of the whole system in its initial state is $|\psi_0\rangle = |\psi_n^I\rangle|M\rangle$. Then, in the presence of H_{nS}, the wave function becomes $|\psi\rangle = |\psi_0\rangle + |\psi_S\rangle$, where to first order in

H_{nS} the Schrödinger equation gives

$$|\psi_S\rangle = -\frac{1}{(P_n^2/2M_n)+V_0+H_S-E}H_{nS}|\psi_0\rangle \ , \tag{2.5}$$

with E the total energy of the system, $E=\epsilon_n^I+E_M$, with ϵ_n^I the kinetic energy of the incoming neutron, and E_M the energy of the spin system. By using the identity operator

$$I_{\rm op}=\sum_N \int d^3r' \, |N\rangle \, |\vec{r}\,'\rangle\langle\vec{r}\,'| \, \langle N| \tag{2.6}$$

with $|N\rangle$ once again an eigenstate of H_S, one may write for the probability amplitude $\langle\vec{r}\,|\,\langle N|\psi_S\rangle$ for finding the crystal in eigenstate $|N\rangle$ of H_S, with the neutron at position $\vec{r}$, the result

$$\langle\vec{r}\,|\,\langle N|\psi_S\rangle = -\int d^3r' \left\langle \vec{r} \left| \frac{1}{(P_n^2/2M_n)+V_0-\epsilon_n^S} \right| \vec{r}\,' \right\rangle \langle N|H_{nS}(\vec{r}\,')|M\rangle \psi_n^I(\vec{r}\,') \ , \tag{2.7}$$

where $\psi_n^I(\vec{r}\,')$ is the wave function of the incoming neutron. It is not a plane wave, but rather the appropriate eigenfunction of H_n defined in Eq. (2.2). It thus consists of an incoming plane wave in the vacuum above the crystal, a specularly reflected wave, and, if the neutron angle of incidence is greater than the critical angle discussed in Sec. I, a piece which penetrates into the crystal, but which decays exponentially as one moves into the crystal interior. The explicit form of $\psi_n^I(\vec{r})$ will be given below. In Eq. (2.7), $\epsilon_n^S=E_M-E_n+\epsilon_n^I$ will be the energy with which the inelastically scattered neutron emerges from the crystal.

The quantity

$$G(\vec{r},\vec{r}\,';\epsilon) = \left\langle \vec{r} \left| \frac{1}{(P_n^2/2M_n)+V_0-\epsilon} \right| \vec{r}\,' \right\rangle \tag{2.8}$$

is the Green's function for the neutron in the presence of V_0. This function may be constructed straightforwardly for our approximate form of V_0 by noting that it satisfies the differential equation

$$\left[\frac{P_n^2}{2M_n}+V_0-\epsilon\right] G(\vec{r},\vec{r}\,';\epsilon)=\delta(\vec{r}-\vec{r}\,') \ , \tag{2.9}$$

which is subject to the outgoing boundary conditions relevant to the present problem. It is convenient to Fourier transform this function. Let the z axis be normal to the surface, $\vec{r}_{||}$ and $\vec{K}_{||}$ the projection of $\vec{r}$ and $\vec{K}$ onto the x-y plane, and write (we use units with $\hbar=1$)

$$G(\vec{r},\vec{r}\,';\epsilon) = \int \frac{d^2K_{||}}{(2\pi)^2} g(z,z';\vec{K}_{||},\epsilon) \times \exp[i\vec{K}_{||}\cdot(\vec{r}_{||}-\vec{r}\,'_{||})] \ . \tag{2.10}$$

Then $g(z,z';\vec{K}_{||}\epsilon)$ may be shown to have the following form:

$$g(z,z';\vec{K}_{||},\epsilon) = \frac{2iM_n}{K_\perp^> + K_\perp^<}[\psi^>(z;\vec{K}_{||},\epsilon)\psi^<(z';\vec{K}_{||}\epsilon)\Theta(z-z')+\psi^<(z;\vec{K}_{||},\epsilon)\psi^>(z';\vec{K}_{||},\epsilon)\Theta(z'-z)] \ , \tag{2.11}$$

where, with $\epsilon_\perp=\epsilon-K_{||}^2/2M_n$, we have $K_\perp^<=(2M_n)^{1/2}\epsilon_\perp^{1/2}$, $K_\perp^>=(2M_n)^{1/2}(\epsilon_\perp-V_0)^{1/2}$ with the square-root convention such that $K_\perp^<>0$ (we shall only consider scattering geometries where $\epsilon_\perp$ is positive), and we have $\mathrm{Im}(K_\perp^>)>0$. The functions $\psi^>(z;\vec{K}_{||},\epsilon)$ and $\psi^<(z;\vec{K}_\perp,\epsilon)$ that enter Eq. (2.11) are given by

$$\psi^>(z;\vec{K}_{||},\epsilon) = \begin{cases} \exp(iK_\perp^> z), & z>0 \\ A_1\exp(iK_\perp^> z)+A_2\exp(-iK_\perp^< z), & z<0 \ , \end{cases} \tag{2.12a}$$

and also

$$\psi^<(z;\vec{K}_{||},\epsilon) = \begin{cases} A_2\exp(iK_\perp^> z)+A_1\exp(-iK_\perp^> z), & z>0 \\ \exp(-iK_\perp^< z), & z>0 \ . \end{cases} \tag{2.12b}$$

One finds that $A_1=(K_\perp^> + K_\perp^<)/2K_\perp^<$ and $A_2=(K_\perp^> - K_\perp^<)/2K_\perp^<$.

To complete our discussion, we require the wave function of the incoming neutron. If ϵ now refers to the energy of the incoming neutron, and $\vec{K}_{||}$ refers to the projection of its wave vector onto the x-y plane, then

$$\psi_n^I(\vec{r})=e^{i\vec{K}_{||}\cdot\vec{r}_{||}}\psi^{(I)}(z;\vec{K}_{||},\epsilon)=\frac{1}{A_1}e^{i\vec{K}_{||}\cdot\vec{r}_{||}}\psi^{>}(z';\vec{K}_{||},\epsilon)$$

$$=\begin{cases}\dfrac{2K_\perp^<}{K_\perp^> + K_\perp^<}\exp(iK_\perp^> z), & z>0\\[2ex] \exp(iK_\perp^< z)+\dfrac{K_\perp^< - K_\perp^>}{K_\perp^< + K_\perp^>}\exp(-iK_\perp^< z), & z<0\,.\end{cases} \tag{2.13}$$

With these results, the scattered wave function can be written in the form, in the vacuum below the crystal,

$$\langle\vec{r}\,|\langle N\,|\,\psi_S\rangle=\int\frac{d^2K_{||}^{(S)}}{(2\pi)^2 i}e^{i\vec{K}_{||}^{(S)}\cdot\vec{r}_{||}}\frac{M_n e^{-iK_\perp^{(S<)}z}}{K_\perp^{(S<)}}\langle N;S\,|\,H_{nS}\,|\,M;I\rangle\,, \tag{2.14}$$

where, here and in what follows, the superscript S or I means that the quantity involved is to be evaluated at the energy ϵ and $\vec{K}_{||}$ appropriate to the scattered or the incoming neutron. In Eq. (2.14) we have defined

$$\langle N;S\,|\,H_{nS}\,|\,M;I\rangle=\int d^2r'_{||}\,dz'\exp[i(\vec{K}_{||}^{(I)}-\vec{K}_{||}^{(S)})\cdot\vec{r}\,'_{||}]\times\psi^{(In)}(z';\vec{K}_{||}^{(S)},\epsilon^S)\psi^{(In)}(z';\vec{K}^{(I)},\epsilon^I)\langle N\,|\,H_{nS}(\vec{r}\,')\,|\,M\rangle\,. \tag{2.15}$$

In order to evaluate the scattering cross section (more precisely, the scattering efficiency to be defined below), we require the behavior of the neutron wave function far from the crystal. If $\vec{K}=\vec{K}_{||}+\hat{z}K_\perp$, with $K_\perp=(2M_n\epsilon-K_{||}^2)^{1/2}$, and $\Phi(\vec{K})$ is a slowly varying function of $\vec{K}$, then with the method of steepest descents one may show that if[12]

$$\psi(\vec{r})=\int d^2K_{||}\Phi(\vec{K})e^{i\vec{K}\cdot\vec{r}}\,, \tag{2.16}$$

one has

$$\lim_{|\vec{r}|\to\infty}\psi(\vec{r})=-2\pi i\Phi(K\hat{r})\frac{K\cos\theta}{r}e^{iKr}\,, \tag{2.17}$$

where $\cos\theta$ is the angle between the z axis and $\hat{r}$. With this result one finds that the total neutron current which passes through the area $r^2 d\Omega(\hat{K}_S)$, and hence which is scattered into the solid angle $d\Omega(\hat{K}_S)$, is given by

$$\vec{j}_S\cdot d\vec{A}=\frac{M_n K^S}{(2\pi)^2}\,|\langle N;S\,|\,H_{nS}\,|\,M;I\rangle|^2 d\Omega(\hat{K}_S)\,, \tag{2.18}$$

and we write

$$\langle N;S\,|\,H_{nS}\,|\,M;I\rangle=\sum_i\langle N\,|\,V(I,S;\vec{S}_i)\,|\,M\rangle\,, \tag{2.19}$$

where $\langle N\,|\,V(I,S;\vec{S}_i)\,|\,M\rangle$ is the contribution to the matrix element from the interaction of the neutron with the particular spin $\vec{S}_i$. If we then sum over all final states of the crystal, and average over the initial states with P_M, the probability of finding state $|M\rangle$ in the statistical ensemble that describes the crystal, then the total current per unit solid angle $dj_S/d\Omega(\hat{K}_S)$, is given by

$$\frac{dj_S}{d\Omega(\hat{K}_S)}=\frac{M_n K^S}{(2\pi)^2}\sum_{M,N}P_M\left\langle M\left|\sum_i V^*(I,S;\vec{S}_i)\right|N\right\rangle\times\left\langle N\left|\sum_j V(I,S;\vec{S}_j)\right|M\right\rangle\,. \tag{2.20}$$

We want the scattered neutron current per unit solid angle, per unit energy range, to discuss the inelastic scattering cross section. If we use the identity

$$\int d\epsilon_S\delta(\epsilon^S+E_n-\epsilon^I-E_M)=1\,, \tag{2.21}$$

and then use the well-known Fourier transform form of the delta function, one may extract the contribution to Eq. (2.20) from neutrons with scattered energies in the range from ϵ_S to $\epsilon_S+d\epsilon_S$. If we define

$$V(t)=\sum_i V(I,S;\vec{S}_i(t))\,, \tag{2.22}$$

where the spin operator in Eq. (2.22) is in the Heisenberg representation formed with the operator H_S, then for the scattered current per unit solid angle, per unit energy, we have

$$\frac{d^2 j_S}{d\Omega(\hat{K}_S)d\epsilon_S}=\frac{M_n K^S}{(2\pi)^3}\int_{-\infty}^{+\infty} dt\, e^{-i\Omega t}\langle V^\dagger(t)V(0)\rangle , \tag{2.23}$$

where $\Omega=\epsilon_S-\epsilon_I$ is the difference in energy between the scattered and the incident neutron.

We shall evaluate the scattering efficiency per unit solid angle, per unit energy range, $d^2\mathscr{S}/d\Omega(\hat{K}_S)d\epsilon_S$. The quantity

$$[d^2\mathscr{S}/d\Omega(\hat{K}_S)d\epsilon_S]d\Omega(\hat{K}_S)d\epsilon_S$$

is dimensionless, and equal to the probability that the neutron is scattered into the solid angle $d\Omega(\hat{K}_S)$ with energy between ϵ_S and $\epsilon_S+d\epsilon_S$. This is found by dividing Eq. (2.23) by the total neutron current which strikes the crystal, which is $[A(K^{(I)}/M_n]\cos\theta_I$, where A is the surface area of the crystal, and θ_I is the angle of incidence measured from the normal. Thus with factors of $\hbar$ inserted, our basic formula becomes

$$\frac{d^2\mathscr{S}}{d\Omega(\hat{K}_S)d\epsilon_S}=\frac{M_n^2 K^S}{(2\pi)^3\hbar^5 K^I\cos\theta_I}\times\int_{-\infty}^{+\infty} d\Omega\, e^{-i\Omega t}\langle V^\dagger(t)V(0)\rangle_T . \tag{2.24}$$

The next step is to evaluate the matrix element in the definition of $V(t)$. The algebra is tedious, but straightforward, so we only quote the result. If we let

$$\vec{Q}_{||}=\vec{K}_{||}^{(S)}-\vec{K}_{||}^{(I)} , \tag{2.25}$$

with $\vec{K}_{||}^{(S)}$ and $\vec{K}_{||}^{(I)}$ the projection of the wave vector of the scattered and incident neutron onto the xy plane, then the quantity $V(I,S;\vec{S}_i)$ defined in Eq. (2.19) is given by

$$\begin{aligned}V(I,S;\vec{S}_i)=\Gamma_1^{(i)}[i\vec{Q}_{||}\cdot\vec{S}_{||}^{(i)}+Q_{||}S_z^{(i)}][i\vec{Q}_{||}\cdot\vec{s}_{||}+Q_{||}s_z]\\+\Gamma_2^{(i)}[-i\vec{Q}_{||}\cdot\vec{S}_{||}^{(i)}+Q_{||}S_z^{(i)}][-i\vec{Q}_{||}\cdot\vec{s}_{||}+Q_{||}s_z]+\Gamma_3^{(I)}\vec{S}^{(i)}\cdot\vec{s} ,\end{aligned} \tag{2.26}$$

where $\vec{s}$ is the spin of the neutron, and $Q_{||}=|\vec{Q}_{||}|$. The quantities $\Gamma_j^{(i)}$ are given by

$$\begin{aligned}\Gamma_1^{(i)}=-\frac{2\pi g\mu_B\mu_n}{Q_{||}}\exp(-i\vec{Q}_{||}\cdot\vec{R}_{||}^{(i)})\Bigg\{&\frac{e^{-Q_{||}z_i}}{Q_{||}+i(K_\perp^{S<}+K_\perp^{I<})}+\frac{A_r^I e^{-Q_{||}z_i}}{Q_{||}+i(K_\perp^{S<}-K_\perp^{I>})}\\&+A_r^S\frac{e^{-Q_{||}z_i}}{Q_{||}+i(K^{I<}-K^{S<})}+A_r^S A_r^I\frac{e^{-Q_{||}z_i}}{Q_{||}-i(K_\perp^{S>}+K_\perp^{I>})}\\&+A_t^S A_t^I\frac{(e^{i(K_\perp^{S>}+K_\perp^{I>})z_i}-e^{-Q_{||}z_i})}{Q_{||}+i(K_\perp^{S>}+K_\perp^{I>})}\Bigg\} ,\end{aligned} \tag{2.27a}$$

$$\Gamma_2^{(i)}=-\frac{2\pi g\mu_B\mu_n}{Q_{||}}A_t^S A_t^I\frac{e^{i(K_\perp^{S>}+K_\perp^{I>})z_i}e^{-i\vec{Q}_{||}\cdot\vec{R}_{||}^{(i)}}}{Q_{||}-i(K_\perp^{S>}+K_\perp^{I>})} , \tag{2.27b}$$

and

$$\Gamma_3^{(i)}=-4\pi g\mu_B\mu_n A_t^S A_t^I e^{-i\vec{Q}_{||}\cdot\vec{R}_{||}^{(i)}}e^{i(K_\perp^{S>}+K_\perp^{I>})z_i} . \tag{2.27c}$$

The quantity

$$A_t=2K_\perp^{<}/(K_\perp^{>}+K_\perp^{<}) \tag{2.28a}$$

is the amplitude of the neutron wave function transmitted through the surface into the crystal interior, while

$$A_r=(K_\perp^{<}-K_\perp^{>})/(K_\perp^{>}+K_\perp^{<}) \tag{2.28b}$$

is the amplitude of the reflected wave. The first four terms in Eq. (2.27a) have their physical origin in the interaction of the neutron with the fluctuating magnetic field in the vacuum above the crystal as it either approaches or exits from the vacuum. These terms are very similar to those which control small-angle electron scattering from surface interactions, where coupling of the electron to the oscillating electric dipole moment of the surface species dominates the cross section. We refer the reader elsewhere[9] for a discussion of these terms, most particularly at very small scattering angles where the incoming or exiting particle feels the fluctuating field when it is quite far from the surface. The remaining terms in Eq. (2.27) describe contributions to the matrix element that come when the neutron is inside the crystal. In what follows, we introduce

$$\gamma = i(K_\perp^{S>} + K_\perp^{I>}) , \tag{2.29}$$

a quantity with a negative real part (recall $\mathrm{Im}K_\perp^{>} > 0$), and we write the above expressions in the forms

$$\Gamma_1^{(i)} = e^{-i\vec{Q}_\parallel \cdot \vec{R}_\parallel^{(i)}} (\Gamma_{11} e^{\gamma z_i} + \Gamma_{12} e^{-Q_\parallel z_i}) , \tag{2.30a}$$

$$\Gamma_2^{(i)} = e^{-i\vec{Q}_\parallel \cdot \vec{R}_\parallel^{(i)}} \Gamma_{21} e^{\gamma z_i} , \tag{2.30b}$$

$$\Gamma_3^{(i)} = e^{-i\vec{Q}_\parallel \cdot \vec{R}_\parallel^{(i)}} \Gamma_{31} e^{\gamma z_i} . \tag{2.30c}$$

The next step is to calculate the expectation value

$$\langle V^\dagger(I,S;\vec{S}_i(t)) V(I,S{:}S_j(0)) \rangle ,$$

and to express it in terms of the quantities defined above. We do this, and retain only those terms which contribute to the energy-loss cross-section peaks from either creation or absorption of spin waves by the neutron, i.e., we ignore elastic scattering from the spatial inhomogeneity of the magnetization near the surface. For this purpose we orient the saturation magnetization of the crystal along the z axis (normal to the surface). Then, the terms which contribute to this portion of the cross section are those proportional to the correlation functions $\langle S_x^i(t) S_x^j(0) \rangle$, $\langle S_x^i(t) S_y^j(0) \rangle$, $\langle S_y^i(t) S_x^j(0) \rangle$, and finally $\langle S_y^i(t) S_y^j(0) \rangle$. One may show that the contributions from $\langle S_x^i(t) S_y^j(0) \rangle$ and $\langle S_y^i(t) S_x^j(0) \rangle$ both vanish for the Heisenberg ferromagnet, while the contribution from $\langle S_y^i(t) S_y^j(0) \rangle$ equals the contribution from $\langle S_x^i(t) S_x^j(0) \rangle$. After some algebra, we find that

$$\int_{-\infty}^{+\infty} \frac{dt\, e^{-i\Omega t}}{2\pi} \langle V^\dagger(I,S;\vec{S}_i(t)) V(I,S;\vec{S}_j(0)) \rangle_T$$
$$= \tfrac{2}{3}[2Q_\parallel^4(\Gamma_1^{i*}\Gamma_1^j + \Gamma_2^{i*}\Gamma_2^j) + 2\Gamma_3^{i*}\Gamma_3^j - Q_\parallel^2(\Gamma_1^{i*}\Gamma_3^j + \Gamma_3^{i*}\Gamma_1^j + \Gamma_2^{i*}\Gamma_3^j + \Gamma_3^{i*}\Gamma_2^j)] \int_{-\infty}^{+\infty} \frac{dt}{2\pi} e^{-i\Omega t} \langle S_x^i(t) S_x^j(0) \rangle . \tag{2.31}$$

Our next task is to obtain an expression for the spin-correlation function which appears in Eq. (2.31). Some years ago, Maradudin and Mills obtained closed-form expressions for a certain Green's function that describes spin waves in the semi-infinite, simple-cubic Heisenberg ferromagnet with a (100) surface, and with nearest- and next-nearest-neighbor exchange interactions between the spins. This Green's function can be used to evaluate the spin-correlation function that appears in Eq. (2.31) by a prescription quoted below. For the purposes of the present paper we prefer to use a somewhat more general form[14] of the Green's function that may be applied to a variety of crystal structures and surface geometries, so long as the exchange interactions between a given spin and its neighbors extends no farther than one atomic plane above or below the spin. This Green's function contains, as a special case, a number of surface geometries discussed in the theoretical literature, including the one explored by Maradudin and Mills. In Ref. 14 we encounter a certain Green's function of a complex variable z referred to as $G(\vec{1},\vec{1}';z)$, and here we refer to the same function as $G(i,j;z)$. If $n(\Omega) = [\exp(\beta\Omega) - 1]^{-1}$ is the Bose-Einstein function with $\beta = 1/k_B T$, one may obtain the following relation:

$$\int_{-\infty}^{+\infty} \frac{dt\, e^{-i\Omega t}}{2\pi} \langle S_x^i(t) S_x^j(0) \rangle$$
$$= \frac{S}{4\pi i} \{ n(\Omega)[G(i,j;\Omega - i\epsilon) - G(i,j,;\Omega + i\epsilon)] + (1 + n(\Omega))[G(j,i;-\Omega + i\epsilon) - G(j,i;-\Omega - i\epsilon)] \} . \tag{2.32}$$

It will be useful to quote the explicit form of the Green's function; as noted earlier, we ignore changes in exchange constants near the surface, though changes in surface exchange are incorporated in the Green's functions obtained in Ref. 14. The bulk spin-wave spectrum of the material, with the wave vector $\vec{q}=\vec{q}_{\parallel}+\hat{z}q_z$, has the form

$$\Omega_B(\vec{q}_{\parallel},q_z)=A(\vec{q}_{\parallel})-B(\vec{q}_{\parallel})\cos(q_z a_0)\ , \tag{2.33}$$

with a_0 the distance between adjacent planes parallel to the surface. The Green's function of the semi-infinite crystal may then be expressed in terms of the objects, with z a complex frequency

$$g_0(n;\vec{q}_{\parallel},z)=\frac{a_0}{2\pi}\int_{-\pi/a_0}^{+\pi/a_0}\frac{dq_z e^{iq_z n a_0}}{z-\Omega_B(\vec{q}_{\parallel},q_z)}\ . \tag{2.34}$$

If $J(\vec{\delta}_{\parallel}+\hat{z}\delta_z)$ is the strength of the exchange interaction between a given spin and its neighbor located relative to the given spin at the position $\vec{\delta}_{\parallel}+\hat{z}\delta_z$, then we also need

$$B_{l_z}(\vec{q}_{\parallel})=2S\sum_{\vec{\delta}_{\parallel}}J(\vec{\delta}_{\parallel}+a_0 l_z\hat{z})e^{i\vec{q}_{\parallel}\cdot\vec{\delta}_{\parallel}} \tag{2.35a}$$

and

$$\gamma(\vec{q}_{\parallel})=B_1(\vec{q}_{\parallel})/B_1(0)\ . \tag{2.35b}$$

In Eq. (2.35b) the sum over $\vec{\delta}_{\parallel}$ covers all sites in the plane located at $a_0 l_z\hat{z}$ to which a given spin in a reference plane at $l_z=0$ is coupled. For any particular crystal structure and model of the exchange interactions, the quantities $B_0(\vec{q}_{\parallel})$ and $B_{\pm1}(\vec{q}_{\parallel})$ are easily evaluated. The bulk spin-wave dispersion relation may be expressed in terms of the following quantities:

$$A(\vec{q}_{\parallel})=\tfrac{1}{2}[B_0(0)-B_0(\vec{q}_{\parallel})]+B_1(0)\ , \tag{2.36a}$$

$$B(\vec{q}_{\parallel})\equiv B_1(\vec{q}_{\parallel})\ . \tag{2.36b}$$

Then the Green's function for the semi-infinite crystal has the form

$$G(i,j;z)=\frac{1}{N_S}\sum_{\vec{q}_{\parallel}}e^{+i\vec{q}_{\parallel}\cdot[\vec{R}_{\parallel}^{(i)}-\vec{R}_{\parallel}^{(j)}]}\times g(l,l';\vec{q}_{\parallel},z)\ , \tag{2.37}$$

where the position vectors of spin i and spin j are written $\vec{R}^{(i)}=\vec{R}_{\parallel}^{(i)}+\hat{z}a_0 l$, and $\vec{R}^{(j)}=\vec{R}_{\parallel}^{(j)}+\hat{z}a_0 l'$. We have, in terms of the functions $g(n)$ defined in Eq. (2.34),[14]

$$g(l,l';\vec{q}_{\parallel},z)=g_0(l-l';\vec{q}_{\parallel}z)+t(\vec{q}_{\parallel},0)[g_0(l;\vec{q}_{\parallel},z)g_0(l';\vec{q}_{\parallel},z)+g_0(l-1;\vec{q}_{\parallel},z)g_0(l'-1;\vec{q}_{\parallel}.z)]$$
$$+t(\vec{q}_{\parallel},1)[g_0(l-1;\vec{q}_{\parallel},z)g_0(l';\vec{q}_{\parallel}z)+g_0(l;\vec{q}_{\parallel},z)g_0(l'-1;\vec{q}_{\parallel},z)]\ , \tag{2.38}$$

where

$$t(\vec{q}_{\parallel},0)=\frac{[\gamma^2(\vec{q}_{\parallel})-1]g_0(1;\vec{q}_{\parallel},z)-2\gamma^2(q_{\parallel})/B(\vec{q}_{\parallel})}{D(\vec{q}_{\parallel},z)}\ , \tag{2.39a}$$

$$t(\vec{q}_{\parallel},1)=\frac{[1-\gamma^2(\vec{q}_{\parallel})]g_0(0;\vec{q}_{\parallel},z)+2\gamma^2(\vec{q}_{\parallel})/B(\vec{q}_{\parallel})}{D(\vec{q}_{\parallel},z)}\ , \tag{2.39b}$$

and

$$D(\vec{q}_{\parallel},z)=\{[\gamma(\vec{q}_{\parallel})+1][g(0;\vec{q}_{\parallel},z)-g(1;\vec{q}_{\parallel},z)]+2\gamma(\vec{q}_{\parallel})/B(\vec{q}_{\parallel})\}$$
$$\times\{[\gamma(\vec{q}_{\parallel})-1][g(0;\vec{q}_{\parallel},z)-g(1;\vec{q}_{\parallel},z)]-2\gamma(\vec{q}_{\parallel})/B(\vec{q}_{\parallel})\}\ . \tag{2.39c}$$

While the expressions above seem cumbersome, in fact, the sum over i and j in the cross section [Eq. (2.24); note Eq. (2.22)] may be carried out in closed form so that the evaluation of the neutron cross section reduces to the evaluation of an algebraic expression that involves only elementary functions. The expression is cumbersome, and we have evaluated it on a computer as a consequence. We conclude this section, however, by quoting the final form of the cross section.

There are two distinctly different contributions to the cross section. The first comes from scattering off of surface spin waves. As discussed elsewhere, the Green's function $g(l,l';\vec{q}_{||},z)$ has a pole on the real axis of the complex-frequency plane, at the zero of the denominator $D(\vec{q}_{||},z)$ defined in Eq. (2.39c). This pole, when combined with Eq. (2.32) leads to a Stokes or an anti-Stokes scattering process where the neutron either loses the energy $\Omega_S(\vec{Q}_{||})$ upon suffering the wave-vector transfer $\vec{Q}_{||}$ parallel to the surface, or gains this energy. It also scatters off of bulk spin waves. This contribution, whose form will be the subject of further discussion in Sec. III, comes from a branch cut in the function $g(l,l';\vec{q}_{||},z)$, which also lies on the real axis and extends from $\Omega_m(\vec{q}_{||})$ to $\Omega_M(\vec{q}_{||})$, where $\Omega_m(\vec{q}_{||})$ and $\Omega_M(\vec{q}_{||})$ are the minimum and maximum bulk spin-wave frequencies associated with the wave vector $\vec{q}_{||}$ parallel to the surface. If, in Eq. (2.33) both $A(\vec{q}_{||})$ and $B(\vec{q}_{||})$ are positive, then

$$\Omega_m(\vec{q}_{||})=A(\vec{q}_{||})-B(\vec{q}_{||}) ,$$

while

$$\Omega_M(\vec{q}_{||})=A(\vec{q}_{||})+B(\vec{q}_{||}) .$$

First, consider the scattering of the neutron off of bulk spin waves. It is convenient to introduce the dimensionless measure of energy transfer

$$\Omega'=[\Omega-A(\vec{q}_{||})]/B(\vec{q}_{||}) , \quad (2.40)$$

which lies in the range $-1\leq\Omega'\leq+1$ for a process in which a bulk spin wave is absorbed. [We consider only anti-Stokes scattering, where $\epsilon_S>\epsilon_I$ and $\Omega>0$. The Stokes cross section is obtained from this by simply multiplying the anti-Stokes cross section by $\exp(\hbar|\Omega|/k_BT)$.] For Ω' in the range from -1 to $+1$, it is convenient to introduce the angle θ defined by

$$e^{-i\theta}=\Omega'-i(1-\Omega'^2)^{1/2} , \quad (2.41)$$

the function

$$f(x)=\frac{-1}{1+e^{-x}e^{-i\theta}} , \quad (2.42a)$$

and also

$$F(x,y)=\frac{(e^{x+y}e^{-i2\theta}-1)}{(e^{x+y}-1)(e^{x}e^{-i\theta}+1)(e^{y}e^{-i\theta}+1)} . \quad (2.42b)$$

When the algebra has been completed, the cross section for the anti-Stokes scattering off bulk spin waves is then, with A_0 the area of the two-dimensional unit of a plane of all spins parallel to the surface,

$$\frac{d^2\mathscr{S}}{d\Omega(\hat{k}_S)dE_S}=\frac{M_n^2K^{(S)}n(\Omega)}{(2\pi)^2\hbar^4K^{(I)}A_0\cos\theta_I}(A_1+A_2) , \quad (2.43)$$

where, with $\gamma=i(K_\perp^{S>}+K_\perp^{I>})$ as in Eq. (2.29), one has

$$A_1=\frac{S}{3\pi B(\vec{Q}_{||})(1-\Omega'^2)^{1/2}}\mathrm{Re}\{2Q_{||}^4[|\Gamma_{12}|^2F(Q_{||},Q_{||})+|\Gamma_{11}|^2F(-\gamma^*,-\gamma)+\Gamma_{11}^*\Gamma_{12}F(-\gamma^*,Q_{||})$$
$$+\Gamma_{11}\Gamma_{12}^*F(Q_{||},-\gamma)+|\Gamma_{21}|^2F(-\gamma^*,-\gamma)]$$
$$+2|\Gamma_{31}|^2F(-\gamma^*,-\gamma)-Q_{||}^2\Gamma_{12}^*\Gamma_{31}F(Q_{||},-\gamma)$$
$$-Q_{||}^2\Gamma_{31}^*\Gamma_{12}F(-\gamma^*,Q_{||})-Q_{||}^2\Gamma_{11}^*\Gamma_{31}F(-\gamma^*,-\gamma)$$
$$-Q_{||}^2\Gamma_{11}\Gamma_{31}^*F(-\gamma^*,-\gamma)-Q_{||}^2\Gamma_{21}^*\Gamma_{31}F(-\gamma^*,-\gamma)$$
$$-Q_{||}^2\Gamma_{21}\Gamma_{31}^*F(-\gamma^*,-\gamma)\} , \quad (2.44)$$

$$A_2=\frac{S}{3\pi B(\vec{Q}_{||})(1-\Omega'^2)}\mathrm{Im}(\{2Q_{||}^4[(|\Gamma_{11}|^2+|\Gamma_{21}|^2+|\Gamma_{31}|^2)f(\gamma^*)f(\gamma)+\Gamma_{11}^*\Gamma_{12}f(\gamma^*)f(-Q_{||})$$
$$+\Gamma_{12}^*\Gamma_{11}f(-Q_{||})f(\gamma)+|\Gamma_{12}|^2f(-Q_{||})f(-Q_{||})]$$
$$-Q_{||}^2[(\Gamma_{11}^*\Gamma_{31}+\Gamma_{11}\Gamma_{31}^*+\Gamma_{21}^*\Gamma_{31}+\Gamma_{21}\Gamma_{31}^*)f(\gamma^*)f(\gamma)$$
$$+\Gamma_{12}^*\Gamma_{31}f(-Q_{||})f(\gamma)+\Gamma_{12}\Gamma_{31}^*f(\gamma^*)f(-Q_{||})]\}H)\,, \tag{2.45}$$

where in Eq. (2.45) we have defined

$$H=\frac{(\gamma^2+1)\sin\theta+2\gamma\sin\theta\cos\theta}{(\gamma^2-1)\sin\theta+i[2\gamma+(\gamma^2+1)\cos\theta]}\,. \tag{2.46}$$

In terms of the dimensionless measure of energy transfer Ω', the surface spin waves lie in the regime where $|\Omega'|>1$ always holds true. When surface spin waves exist (see Refs. 13 and 14 for a summary of the relevant conditions) their dispersion relation is, in the present notation,

$$\Omega_S(\vec{Q}_{||})=A(Q_{||})-\frac{B(\vec{Q}_{||})}{2\gamma(\vec{Q}_{||})}[1+\gamma(\vec{Q}_{||})^2]\,. \tag{2.47}$$

The expression for the cross section involves the variable

$$\eta=\Omega'+(\Omega'^2-1)^{1/2}\,, \tag{2.48}$$

and the function

$$h(x)=\frac{-\eta}{e^x+\eta}\,. \tag{2.49}$$

The cross section for anti-Stokes scattering is then

$$\frac{d^2\mathscr{S}}{d\Omega(\hat{K}_S)dE_S}=\frac{M_n^2K^Sn(\Omega_S)}{(2\pi)^2\hbar^4A_0\cos\theta_I}\mathscr{A}_3\delta(\Omega-\Omega_S(\vec{Q}_{||}))\,, \tag{2.50}$$

where

$$\mathscr{A}_3=\frac{2S}{3\eta(\Omega'^2-1)}\left[\frac{\gamma^6-3\gamma^4+3\gamma^2-1}{8\gamma^3}\right]\Bigg\{Q_{||}^4[(|\Gamma_{11}|^2+|\Gamma_{21}|^2)h(-\gamma^*)h(-\gamma)$$
$$+\Gamma_{11}^*\Gamma_{12}h(-\gamma^*)h(Q_{||})+\Gamma_{11}\Gamma_{12}^*h(-\gamma)h(Q_{||})]$$
$$-\frac{Q_{||}^2}{2}[(\Gamma_{11}^*\Gamma_{31}+\Gamma_{11}\Gamma_{31}^*+\Gamma_{21}^*\Gamma_{31}+\Gamma_{21}\Gamma_{31}^*)h(-\gamma^*)h(\gamma)$$
$$+\Gamma_{12}^*\Gamma_{31}h(Q_{||})h(-\gamma)+\Gamma_{31}^*\Gamma_{12}h(Q_{||})h(-\gamma^*)]$$
$$+|\Gamma_{31}|^2h(-\gamma^*)h(-\gamma)\Bigg\}\,. \tag{2.51}$$

The purpose of this section has been to develop a method within which inelastic neutron reflection spectroscopy may be tested theoretically, and then to carry the calculation through for the case of inelastic scattering from spin-wave excitations near a ferromagnetic surface. While the calculation may be carried through to the end, and so one is left with only algebraic expressions, the results are quite cumbersome in form. One may ask if these results may be simplified so they become more illuminating. For example, in the theory of small-angle inelastic electron scattering from surfaces, quantitatively useful expressions with a rather simple form emerge from the analysis.[9] We are not aware of a similar limit in the present problem largely because in a typical neutron inelastic scattering experiment the energy transfer is a substantial fraction of the impact energy, and the wave-vector transfer is also not small compared to that of the incoming neutron. In essence, there is no small parameter that enters the kinematics of the scattering process, so one must employ the full formula with all contributions included.

III. CONCLUDING REMARKS AND NUMERICAL CALCULATIONS

We now turn to a brief discussion of the nature of the inelastic scattering event for neutrons incident on the crystal at grazing incidence. Then we summarize our numerical studies of the cross section based on the formalism described in Sec. II.

The scattering geometry we explore is illustrated in Fig. 1. The incident neutron strikes the crystal at a grazing angle of incidence θ_I greater than the critical angle θ_c, and we assume that the scattered neutron exits with polar angle $\theta_S < \theta_c$. The wave function of the incident neutron is thus exponentially attenuated as one moves into the crystal, but that of the scattered neutron has wave-vector components normal to the surface that are real (in the limit in which the optical potential seen by the neutron is real). Recall that we have averaged over the spin direction of both the incident and scattered neutron in our derivation of the cross section.

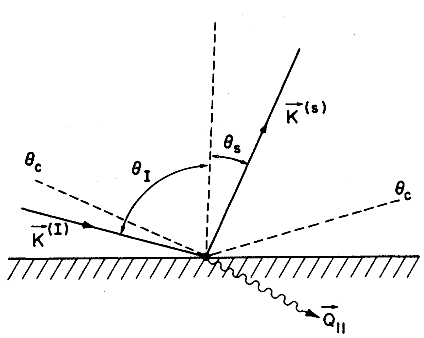

FIG. 1. Scattering geometry explored in Sec. III. The incident neutron has wave vector $\vec{K}^{(I)}$, and strikes the crystal at grazing incidence, with the angle of incidence θ_I larger than the critical angle θ_c. Thus its' wave function is exponentially attenuated as one moves into the crystal. The scattered neutron exits with polar angle $\theta_S < \theta_c$, so its wave function is plane-wave-like in the crystal.

If the neutron scatters by creating or absorbing a spin wave, then wave-vector components parallel to the surface are conserved in the scattering process. Thus the neutron emerges with the wave vector parallel to the surface given by (recall that our treatment does not include umklapp processes)

$$\vec{K}_{\|}^{(S)} = \vec{K}_{\|}^{(I)} \pm \vec{Q}_{\|} . \tag{3.1}$$

Conservation of energy then provides an additional constraint,

$$\epsilon_S = \epsilon_I \pm \hbar\Omega_S(\vec{Q}_{\|}) , \tag{3.2}$$

and these three constraints uniquely determine the direction of the outgoing neutron. Conservation of the wave vector normal to the surface has no meaning here, and the wave vector of the neutron normal to the surface assumes the value necessary to ensure energy conservation once Eq. (3.1) is met.

As we have seen, there are contributions to the cross section for scattering from bulk spin waves also. The same conditions hold here, and since wave-vector components normal to the surface are not conserved, in principle, all bulk spin waves contribute to the cross section. That is, if we imagine scanning the energy spectrum of neutrons scattered inelastically from the surface with the fixed wave-vector transfer parallel to the surface, we shall find a continuous energy loss *band* that extends from $\hbar\Omega_m(\vec{Q}_{\|})$ to $\hbar\Omega_M(\vec{Q}_{\|})$, the minimum and maximum bulk spin-wave frequencies associated with the wave vector $\vec{Q}_{\|}$.

The numerical calculation presented below shows, however, that instead of a broad band that extends from $\hbar\Omega_m(\vec{Q}_{\|})$ to $\hbar\Omega_M(\vec{Q}_{\|})$, one does see a well-defined loss peak in the energy spectrum of the scattered neutrons. Its origin is as follows. If, for simplicity, we once again regard the optical potential in the crystal as real, then the neutron wave function in the crystal has the form $\exp[-\gamma^{(I)}z]$, where the attenuation constant

$$\gamma^{(I)} = K^{(I)}(\cos^2\theta_c - \cos^2\theta_I)^{1/2} ,$$

or with

$$\theta_c = \pi/2 - \epsilon_c, \quad \theta_I = \pi/2 - \epsilon_I ,$$

and

$$\gamma^{(I)} \cong K^{(I)}(\epsilon_c^2 - \epsilon_I^2)^{1/2} .$$

We may write

$$e^{-\gamma^{(I)}z}=\int_{-\infty}^{+\infty}\frac{dk_{\perp}^{(I)}}{2\pi i}\frac{e^{ik_{\perp}^{(I)}z}}{k_{\perp}^{(I)}-i\gamma^{(I)}}\ , \tag{3.3}$$

so that the incident neutron wave function may be regarded as a linear superposition of plane waves with a range of wave vectors in the range from $-\gamma^{(I)}$ to $+\gamma^{(I)}$, very roughly. When θ_I and θ_c are both very near $\pi/2$ and thus close to each other, $\gamma^{(I)}$ is rather small compared to $K^{(I)}$. To first approximation the wave function of the incoming neutron is thus a plane wave parallel to the surface, i.e., the z dependence of its wave function is controlled by spatial Fourier components of the small wave vector. The scattered neutron is a plane wave in the material with wave vector $K_{\perp}^{(S>)}$ normal to the surface, which is large compared to $\gamma^{(I)}$, under conditions illustrated in Fig. (1), so we expect "near wave-vector conserving" interactions with spin waves that have a wave vector normal to the surface Q_z equal to $K_{\perp}^{(S>)}$. That is, a neutron moving parallel to the surface, if it absorbs a spin wave of wave vector Q_z, will be scattered into a final-state wave vector normal to the surface $K_{\perp}^{(S>)}=Q_z$. Equation (3.3) implies that wave-vector components normal to the surface are conserved only to within $\pm\gamma^{(I)}$ on the average, so the bulk spin-wave loss feature is spread out into a line whose width is controlled by the decay constant of the neutron's wave function normal to the surface. (Our calculation ignores the finite lifetime of the spin waves, but in practice, the spin-wave lifetime should be sufficiently long for the uncertainty in the wave vector normal to the surface to be the controlling factor in the bulk spin-wave loss feature.)

Our numerical calculations have been carried out for scattering from a (100) surface of a fcc Heisenberg ferromagnet, with nearest-neighbor exchange. In order to crudely mimic ferromagnetic EuS, we have chosen $S=\frac{7}{2}$ for the spin, and set the strength of the nearest-neighbor exchange so the Curie temperature is 100 K. None of our conclusions depend sensitively on this choice of parameters. Finally, the critical angle has been chosen equal to 1°. The results of the numerical calculations can be summarized briefly, since the magnitude of the calculated cross section does not vary greatly with scattering angle.

In Fig. 2 we show $d^2\mathscr{S}/d\Omega(\hat{K}_S)dE_S$ for scattering from bulk spin waves. The cross section is for absorption of a bulk spin wave; with the neutron incident at 89.9° the scattered neutron emerges with an angle of 57° from the normal, with its wave vector in the same plane as the incident neutron. Finally, the scattering plane is aligned along the [100] direction. We see an energy-loss peak, as described earlier, with width controlled by $\gamma^{(I)}$, the amount of "wave-vector smearing" provided by the attenuation of the neutron wave function in the material. The position of the peak is given quite accurately by taking the component of the wave vector of the bulk spin wave normal to the surface equal to $K_{\perp}^{(S>)}$, as discussed earlier, with the parallel components of the wave vector controlled by the scattering kinematics. In this example, the integrated strength of the loss peak is given by

$$\frac{d\mathscr{S}}{d\Omega(\hat{K}_S)}=\int dE_S\frac{d^2\mathscr{S}}{d\Omega(\hat{K}_S)dE_S}=4\times10^{-3}\ . \tag{3.4}$$

Below, we shall comment briefly on the significance of this number; we have carried out a number of calculations for different scattering geometries, and this seems to be a typical number for the integrated strength of the bulk spin-wave peak.

Our calculations give an integrated strength for scattering from surface spin waves smaller than the result quoted in Eq. (3.4) by a factor of 10 to 20, typically. This suggests that one should employ a scattering geometry in which the surface spin-wave loss or gain feature is well separated from the bulk loss peak, so that the surface spin-wave feature is not obscured by the low-frequency wing of the bulk spin-wave feature. We have not explored the question of choosing an optimum scattering geometry,

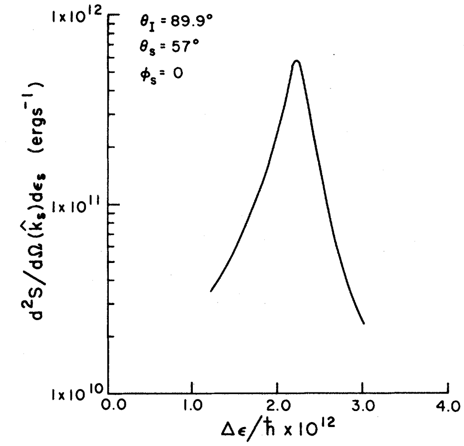

FIG. 2. Cross section, as a function of energy transfer, for scattering of a thermal neutron (kinetic energy 300 K) from the surface of a model ferromagnetic crystal. We show the energy-gain feature produced by scattering by absorbing bulk spin waves. The scattering efficiency is plotted against $\Delta E/\hbar$, with ΔE the energy transfer.

since any conclusions we have reached are specific to our particular model crystal, and hence, are of little general interest.

In a typical neutron scattering study we understand that the detector subtends a solid angle of roughly 10^{-4} sr. Thus the scattering efficiency per unit solid estimated in Eq. (3.4) suggests the fraction of neutrons in the incident beam that strike the crystal, and determined that the detector in the bulk spin-wave loss peak will be roughly 4×10^{-7}, with a signal 10 or 20 times weaker for scattering from surface spin waves. Such signals should be detectable, in principle, though experiments of this sort may prove difficult for a variety of reasons.

Calculations such as those described here may be carried out within the present formalism for scattering of neutrons from a variety of surface excitations, and we hope our discussion of scattering from spin waves near surfaces will prove helpful to those interested in this class of experiments. It is our understanding that analysis similar in spirit to the present one has been undertaken by Rakhecha.[15] Unfortunately, we have not seen a detailed description of his work, and so we are unable to comment on the comparison between the two calculations at this time.

Note added in proof. We have learned that G. Vineyard has presented a theory of grazing incidence x-ray diffraction from crystals, with the use of a formalism very similar to that used here. Vineyard also treats the crystal as a semi-infinite continuous medium in his description of the reflection and refraction of the incident x ray but, in addition, he checks this approximation by replacing the continuum by a series of stratified layers to find only very small corrections to this picture. We wish to thank Dr. Vineyard for a copy of his paper in advance of publication, and for helpful discussions of the relationship of his work to ours.

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