Appearance of quasilocalized surface excitations under the action of a random surface potential in a Heisenberg semi-infinite ferromagnet

Silvia Selzer and Norberto Majlis
Instituto de Física, Universidade Federal Fluminense, Outeiro de São João Batista s/n, Caixa Postal 296, 24210 Niterói, Rio de Janeiro, Brazil

Henryk Puszkarski
Physics Institute, A. Mickiewicz University, Mateijki 48/49, PL-60-679, Poznań, Poland
(Received 8 August 1983)

A calculation is presented, based upon the Green's-function method, of the elementary excitations at low temperatures of a semi-infinite Heisenberg ferromagnet with a single-site anisotropy energy $-D(S_n^z)^2$ with a random distribution of impurities adsorbed on the surface, whose only effect is assumed to be a local modification of the coefficient D of the anisotropy energy on the adsorption site. We obtain an effective Hamiltonian in the spin-wave approximation by including the self-energy renormalization of the configuration-averaged propagator up to first order in the impurity surface concentration c. It is found that virtual surface states can appear, with a lifetime which depends on the wave vector of the excitation. The dispersion relation of this "quasilocal" excitation is obtained in the weak coupling approximation.

I. INTRODUCTION

In this paper we shall consider a system with a free surface on which random perturbations act so as to generate a local self-energy correction to the quasiparticle spectrum, which can be in general complex. We are particularly interested in the case where the imaginary part of the self-energy is not negligible, and we find in this case that under certain conditions we have quasilocalized states, in the sense defined in previous works.[1,2]

We choose as an example a case of localized spins on a semi-infinite simple cubic lattice with a free (100) surface. The spins interact via isotropic Heisenberg exchange, and we assume also a single-ion anisotropy of the form $-D(S_i^z)^2$ acting on each site i ($S>\frac{1}{2}$). The surface is perpendicular to the x axis, and a label $m\geq 0$ denotes each (100) plane. The perturbations acting on the surface are due in our example to the presence of impurities, which are supposed to change only the anisotropy constant D on the nearest surface atom.

II. METHOD OF CALCULATION

Since we want to concentrate upon changes of the low-lying excitations we will consider the low-temperature case only where we can transform the Hamiltonian to a single-particle form through Holstein-Primakoff lowest-order transformation. Then, in units of $2SJ$,

$$\underline{H}=\underline{H}_0+\underline{V}\ , \tag{1}$$

$$\underline{H}_0=\sum_{\substack{m,\vec{n}_{||},\vec{\delta}_{||}\\ m\geq 0}} a^{\dagger}_{m,\vec{n}_{||}}a_{m,\vec{n}_{||}+\vec{\delta}_{||}}+\sum_{\substack{m,\vec{n}_{||}\\ m\geq 0}} a^{\dagger}_{m,\vec{n}_{||}}a_{m+1,\vec{n}_{||}}+\sum_{\substack{m,\vec{n}_{||}\\ m\geq 1}} a^{\dagger}_{m,\vec{n}_{||}}a_{m-1,\vec{n}_{||}}-\left[4+\frac{D}{2SJ}\right]\sum_{\substack{m,\vec{n}_{||}\\ m\geq 0}} a^{\dagger}_{m,\vec{n}_{||}}a_{m,\vec{n}_{||}}\ . \tag{2}$$

Let us call

$$n_{m,\vec{n}_{||}}\equiv a^{\dagger}_{m,\vec{n}_{||}}a_{m,\vec{n}_{||}}$$

the number operator for the spin deviations localized at site $(m,\vec{n}_{||})$. We shall assume that $\underline{V}$ has the form

$$\underline{V}=\lambda\sum_{\{\vec{R}\}}(S^z_{\vec{R}})^2\approx\lambda\sum_{\{\vec{R}\}}n_{\vec{R}}\ ,\quad \lambda\equiv\frac{\Delta D}{J}\ . \tag{3}$$

$\{\vec{R}\}$ denotes the set of impurity positions on the surface. We do not consider, for simplicity, surface variation of the exchange constant J, which is taken everywhere equal to the bulk constant. Let us assume also that the impurities are adsorbed on an atop configuration, which means that the set $\{\vec{R}\}$ is a subset of the lattice points in the (100) surface plane, which contains N_s points as a whole. Let the total number of impurities be N_i. Any measurement will be, in practice, equivalent to performing a configurational average on the impurity sites on the surface. We denote a configuration average of any quantity $\underline{A}$ by $\langle\underline{A}\rangle$. We begin by subtracting the average $\langle\underline{V}\rangle$ from $\underline{V}$, defining the fluctuating potential $\underline{U}$ as

$$\underline{U}\equiv\underline{V}-\langle\underline{V}\rangle\ . \tag{4}$$

The configurational average of $\underline{V}$ is defined by

$$\left\langle \sum_{\{\vec{R}\}} n_{\vec{R}} \right\rangle = \sum_{\{\vec{n}_{||}\}} n_{\vec{n}_{||}} P(\vec{R};\vec{n}_{||}) \ . \tag{5}$$

$\{\vec{n}_{||}\}$ is the set of all the lattice points in a (100) plane. $P(\vec{R};\vec{n}_{||})$ is the probability that the impurity site $\vec{R}$ coincides with the lattice point $\vec{n}_{||}$. In Eq. (5) the assumption has been made already that the impurities are distributed independently of each other, which of course is a valid approximation at low coverages of the surface. We also assume that their distribution is uniform, and we shall therefore take

$$P(R;\vec{n}_{||}) = N_i/N_s \equiv c \ . \tag{6}$$

Then

$$\langle \underline{V} \rangle = \lambda c \sum_{\vec{n}_{||}} n_{0,\vec{n}_{||}} \ . \tag{7}$$

Let us call

$$\underline{\tilde{H}}_0 = \underline{H}_0 + \langle \underline{V} \rangle \ . \tag{8}$$

Then

$$\underline{H} = \underline{\tilde{H}}_0 + \underline{U} \ , \tag{9}$$

where $\underline{U}$ was defined in Eq. (4).

Since the Hamiltonian is a quadratic form in the spin deviation operators $\{a^{\dagger}_{m,\vec{n}_{||}}, a_{m',\vec{n}'_{||}}\}$, we can just consider the matrix elements of H and define the Green matrix $G(E)$ as the resolvent matrix for H:

$$\underline{G}(E) = \frac{1}{E + i\epsilon - \underline{H}} \ . \tag{10}$$

The only nonzero elements of the matrix $\underline{U}$ [Eq. (4)] are

$$U_{0\vec{n}_{||},0\vec{n}'_{||}} = \lambda \delta_{\vec{n}_{||},\vec{n}'_{||}} \left[\sum_{\{\vec{R}\}} \delta_{\vec{n}_{||},\vec{R}} - c \right] \ . \tag{11}$$

Let us remark that $\langle \underline{U} \rangle \equiv 0$. We define an unperturbed operator $\underline{G}^0(E)$ as

$$\underline{G}^0(E) = \frac{1}{E + i\epsilon - \underline{\tilde{H}}_0} \ . \tag{12}$$

Now we write the identity

$$\underline{G}(E) \equiv \underline{G}^0(E) + \underline{G}^0(E)\underline{U}\,\underline{G}(E) \ . \tag{13}$$

We calculate now the configurational average of the matrix $\underline{G}$ by first iterating the identity (13) to obtain the series

$$\underline{G} = \underline{G}^0 + \underline{G}^0\underline{U}\,\underline{G}^0 + \underline{G}^0\underline{U}\,\underline{G}^0\underline{U}\,\underline{G}^0 + \underline{G}^0\underline{U}\,\underline{G}^0\underline{U}\,\underline{G}^0\underline{U}\,\underline{G}^0 + \cdots \ . \tag{14}$$

Then

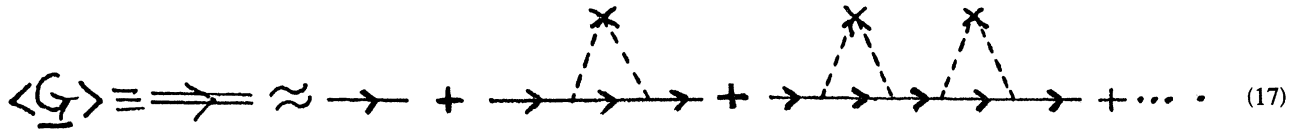
$$\langle \underline{G} \rangle = \underline{G}^0 + \underline{G}^0\langle \underline{U} \rangle \underline{G}^0 + \underline{G}^0\langle \underline{U}\,\underline{G}^0\underline{U} \rangle \underline{G}^0 + \cdots \ . \tag{15}$$

The second term on the right-hand side of Eq. (15) vanishes by definition. The third term we shall take as our approximate self-energy,

$$\begin{aligned}
\Sigma^{(1)}_{0\vec{n}_{||},0\vec{n}'_{||}}(E) &\equiv \langle (\underline{U}\,\underline{G}^0\underline{U})_{0\vec{n}_{||},0\vec{n}'_{||}} \rangle = \lambda^2 G^0_{0\vec{n}_{||},0\vec{n}'_{||}}(E) \left\langle \left[\sum_{\{\vec{R}\}} \delta_{\vec{n}_{||},\vec{R}} - c \right] \left[\sum_{\{\vec{R}'\}} \delta_{\vec{n}'_{||},\vec{R}'} - c \right] \right\rangle \\
&= \lambda^2 c \delta_{\vec{n}_{||},\vec{n}'_{||}} G^0_{00}(\vec{n}_{||} - \vec{n}'_{||}, E) = \lambda^2 c \delta_{\vec{n}_{||},\vec{n}'_{||}} \frac{1}{N_s} \sum_{\vec{k}_{||}} G^0_{00}(\vec{k}_{||}, E) \\
&= \lambda^2 c \delta_{\vec{n}_{||},\vec{n}'_{||}} \frac{a^2}{4\pi^2} \int_{BZ} d^2\vec{k}_{||} G^0_{00}(\vec{k}_{||}, E + i\epsilon) \equiv \lambda^2 c \delta_{\vec{n}_{||},\vec{n}'_{||}} \mathcal{F}(E + i\epsilon)
\end{aligned} \tag{16}$$

(where BZ is the Brillouin zone).

We shall sum Eq. (15) approximately by neglecting the contribution of simultaneous scattering by more than one impurity and by treating the scattering by each impurity in the lowest Born approximation, which leads to[3]



(17)

In Eq. (17) each dotted line represents a λ; a cross, c; a solid line with arrow, G^0.

The averaged propagator $\langle \underline{G} \rangle$ can be interpreted as the resolvent of an effective, frequency-dependent Hamiltonian which, in the representation where the transverse coordinates have been Fourier transformed, can be defined as

$$[\underline{H}^{\text{eff}}(E,\vec{k}_{||})]_{m,m'} = [\underline{\tilde{H}}_0(\vec{k}_{||})]_{mm'} + \delta_{mm'}\delta_{m0}\Sigma^{(1)}(E) = [\underline{H}_0(\vec{k}_{||})]_{mm'} + [\lambda c + \lambda^2 c \mathcal{F}(E + i\epsilon)]\delta_{m0}\delta_{mm'} \ . \tag{18}$$

In order to obtain the local modes we must study the poles of the matrix element

$$\langle \underline{G}(E+i\epsilon,\vec{k}_{||})\rangle_{00}=\left[\frac{1}{E+i\epsilon-\underline{H}^{\text{eff}}(E,\vec{k}_{||})}\right]_{00}\equiv g \tag{19}$$

in what follows. We introduce the notation[4]

$$2t=E-4\Lambda(\vec{k}_{||})-D/2SJ-2\ , \tag{20}$$

$$\Lambda(\vec{k}_{||})=1-\tfrac{1}{2}[\cos(ak_y)+\cos(ak_z)] \tag{21}$$

[we consider the (100) plane which contains the k_y and k_z axes], and, as in Ref. 4, we define the continuous fraction

$$\xi=\frac{1}{2t-1/(2t-\cdots)}\equiv\frac{1}{2t-\xi}\ . \tag{22}$$

Assuming that $\lambda\ll 1$, we consider the case $\lambda<0$, and neglect at first the contribution proportional to $\mathcal{F}$. Then $g\rightarrow g^0$ defined as

$$g^0=(\xi^{-1}+1-\lambda')^{-1}\ , \tag{23}$$

where $\lambda'=c\lambda$. In the interval $|t|<1$, $|\xi|=1$, and we have a branch cut, where $\mathrm{Im}\langle\underline{G}\rangle$ has a discontinuity on the real axis of E.[4]

There can be a surface state at a pole of g_0, where

$$\xi^{-1}+1-\lambda'=0 \tag{24}$$

with $|\xi|<1$, corresponding to a mode exponentially decaying in space into the bulk.[4] The condition for a surface mode is then

$$|1-\lambda'|>1$$

which is automatically satisfied if $\lambda'<0$.

The dispersion relation of the surface mode is

$$\nu_s^{(0)}=4\Lambda(\vec{k}_{||})+D-\lambda'^2/(1-\lambda')\ . \tag{25}$$

The surface is therefore stable, with a ferromagnetic ground state, if $-(\lambda'^2/1-\lambda')+D\geq 0$, which gives a critical value $\lambda'^*<0$ such that

$$(\lambda'^*)^2/(1-\lambda'^*)=D\ . \tag{26}$$

Including now the $\lambda^2 c\mathcal{F}(E)$ term in the Hamiltonian, or in the denominator of g, we look for the zeros of

$$g^{-1}=[2t-\xi+1-\lambda c-\lambda^2 c\mathcal{F}(E+i\epsilon)]\ . \tag{27}$$

The calculation of $\mathcal{F}(E+i\epsilon)$ for the square lattice proceeds along standard procedures, so we leave the details for the Appendix. Let us write

$$\mathcal{F}(E+i\epsilon)\equiv\Delta(E)-i\gamma(E)\ . \tag{28}$$

Combining Eq. (27) with Eq. (21), we see that the local-mode frequencies will be complex, and γ must be negative to ensure that we obtain the branch of G which is analytic in the upper half-plane. The modes are therefore resonances or metastable states. However, if $|\gamma|$ is small they will not be very different from the ordinary stable modes for a perfect surface. We discuss now the numerical results for the quasi-local-mode dispersion relation.

III. RESULTS

Neglecting the self-energy we find a pole at the frequency [Eq. (25)]:

$$\nu_s^{(0)}(\vec{k}_{||})=\nu_-^b(\vec{k}_{||})-\lambda^2c^2/(1-\lambda c)\ . \tag{29}$$

Here $\nu_-^b(\vec{k}_{||})\equiv 4\Lambda(\vec{k}_{||})+D$ is the lower limit of the continuum spectrum. The weak coupling limit solution is obtained, as indicated in the preceding section, by substituting $E=\nu_s^{(0)}$ as the argument of $\mathcal{F}(E)$, and calculating

$$\nu_s^{(1)}=\nu_s^{(0)}+\lambda^2 c\mathcal{F}(\nu_s^0+i\epsilon)\ . \tag{30}$$

Let us call

$$\delta(\vec{k}_{||})\equiv\nu_s^{(1)}(\vec{k}_{||})-\nu_b^-(\vec{k}_{||})\ . \tag{31}$$

In Fig. 1 we plot $\mathrm{Re}\delta$ and $\mathrm{Im}\delta$ vs $\Lambda(\vec{k}_{||})$. The calculations were made for the case $\lambda=-0.5$, $c=0.2$, which yields $\lambda^2 c=0.05$ for the effective coupling constant.

From Fig. 1 it can be seen that $\mathrm{Im}\delta$ attains its minimum near $\Lambda=2$, on the zone boundary. The real part of $\nu_s^{(1)}$ reaches the lower limit of the continuum for $\Lambda\simeq 1.3$, near the van Hove singularity in the density of states, which occurs for $\Lambda=1$.

For $1.3\leq\Lambda\leq 2$ the local mode remains inside the continuum, becoming a resonance proper. One verifies that the poles of g appear on the lower half of the complex plane, as they should, since $\gamma<0$. The time evolution of the quasi-local-mode, in the terminology of Refs. 1 and 2, is dominated by this pole, and it is therefore exponentially damped for $t>0$, as required for a metastable state. We remark that in the middle of the band, where $\nu_s^{(1)}\sim 4$ in our units, $\gamma\simeq -0.1$, which describes a reasonably acute resonance. Near the point Γ (center of the zone) the local-mode frequency is well separated from the lower edge of the continuum band and its width $|\gamma|\rightarrow 0$ as $\Lambda\rightarrow 0$.

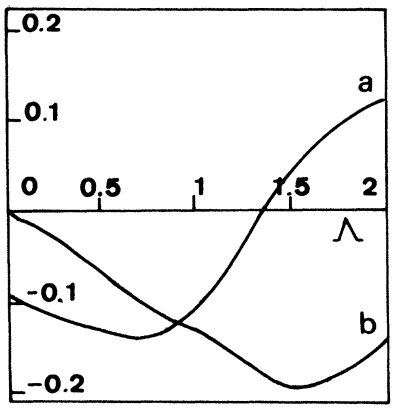


FIG. 1. Curve a depicts the difference $\mathrm{Re}\delta=\mathrm{Re}\nu_s^{(1)}-\nu_b^-$ between the surface magnon frequency $\nu_s^{(1)}$ and the lower limit of the continuum spectrum ν_b^-, vs the two-dimensional structure factor $\Lambda(\vec{k}_{||})$ defined in Eq. (21). In curve b the imaginary part of the self-energy is plotted vs $\Lambda(\vec{k}_{||})$. $c=0.2$, $\lambda=-0.5$. Energies are expressed in terms of $2SJ$.

The present work can be seen as a theoretical proposal for a physical realization of a system whose effective Hamiltonian is not Hermitian, of a type which was discussed in Refs. 1 and 2. It should be possible to find these phenomena by performing experiments which allow one to detect the presence of surface modes on a clean surface, and on the same surface with some small coverage of adsorbates. As can be seen from Eq. (25), the net effect of the average potential $\langle V \rangle$ is to produce an effective anisotropy at the surface which is modified with respect to the bulk value. Since we assume a ferromagnetic surface, we are limiting the values of λ' so that $|\lambda'| < \lambda'^{*}$. For reasonable values of $(D/2SJ) \sim 0.1$, this implies $|\lambda| c \lesssim 0.2$–0.3.

A variation of the local anisotropy at the surface plane can give rise, as it has been found in Ref. 4, to profound alterations in the critical behavior of the surface. For small values of λ and c we expect an effective decrease in the anisotropy at the surface, and this will make it less stable. Therefore, in case the ferromagnetic substrate already had a surface anisotropy strong enough to produce a surface critical temperature higher than the bulk substrate,[4] one might expect to find a disappearance of the surface magnetism above the bulk critical temperature, upon adsorbing atoms that interact with the adsorbate in such a way as to modify the surface anisotropy. Any quantitative predictions will require the self-consistent solution of Eq. (27), and the extension of the theory to finite temperatures, a program with which we are already working.

ACKNOWLEDGMENTS

The authors gratefully acknowledge hospitality at the International Centre for Theoretical Physics of Trieste (ICTP), during the first part of this work. S. S. and N. M. acknowledge financial support by Financiadora Nacional de Estudos e Projetos (FINEP) and Conselho Nacional de Desenvolvimento Científico e Tecnológico (CNPq) of Brazil.

APPENDIX

We must perform the integral, over the first Brillouin zone of the square reciprocal lattice, of the function $G^0(E,\vec{k}_{||})$ which depends upon $\vec{k}_{||}$ only through the function $\Lambda(\vec{k}_{||})$ defined in the text [(Eq. (21)]. It turns out to be convenient to define new coordinates ξ and η:

$$k_y a \equiv \xi + \eta \ ,$$

$$k_z a \equiv \xi - \eta \ ,$$

so that, calling $b = \cos\xi \cos\eta$, we have

$$\Lambda = 1 - b \ . \tag{A1}$$

Now

$$\mathcal{F} = \frac{a^2}{\pi^2} \int dk_y dk_z g^0[E,(\vec{k}_{||})] = \frac{1}{2\pi^2} \int d\xi \, d\eta \, g^0(E, 1-b)$$

$$= \frac{1}{\pi^2} \int_0^1 db \, g^0(E,1-b) \int_0^{\cos^{-1}(b)} d\xi (\cos^2\xi - b^2)^{-1/2} \ , \tag{A2}$$

$$\cos\xi = t \ ,$$

$$\mathcal{F} = \frac{1}{\pi^2} \int_{-1}^1 db \, g^0(E,1-b) \int_{|b|}^1 \frac{dt}{(1-t^2)^{1/2}(t^2-b^2)^{1/2}} \ . \tag{A3}$$

Making now the transformation

$$m = 1 - b^2 \ ,$$

$$\sin^2\theta = \frac{1}{t^2} \frac{t^2 - b^2}{1 - b^2} \ .$$

We find

$$\mathcal{F} = \frac{1}{\pi^2} \int_0^1 \frac{dm}{2} [g^0(E, 1-\sqrt{1-m}$$

$$+ g^0(E, 1+\sqrt{1+m}\,)] \frac{K(m)}{\sqrt{1-m}} \ , \tag{A4}$$

where

$$K(m) = \int_0^{\pi/2} (1 - m \sin^2\theta)^{-1/2} d\theta \ .$$

The function $K(m)$ is the complete elliptic integral of the first kind.[5] We have performed the final integration in Eq. (A4) over the variable m, by Simpson's method. The values of $K(m)$ at the discrete set of points involved (19 points were sufficient) were taken from Ref. 5. Care must be taken to evaluate Cauchy's principal value of the integral whenever a local mode exists for that particular energy, in which case $g^0(E + i\epsilon, \Lambda)$ has a pole on the real axis.

[1] H. Puszkarski, Solid State Commun. 33, 757 (1980).

[2] N. Majlis, S. Selzer, Diep-The-Hung, and H. Puszkarski, Report No. IC/82/231 International Centre for Theoretical Physics (Trieste), 1981 (unpublished).

[3] S. Doniach and E. H. Sondheimer, *Green's Functions for Solid State Physicists* (Benjamin, Reading, Massachusetts, 1974).

[4] S. Selzer and N. Majlis, Phys. Rev. B 27, 544 (1983).

[5] *Handbook of Mathematical Functions*, edited by M. Abramowitz and I. A. Stegun (Dover, New York, 1965).