Antiferromagnetic Magnon States Near Stepped Surfaces

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We present results for the partial and total spectral density of one-
-magnon states near the (105) surface of a bcc Heisenberg antiferromag-
net. Both surface states and resonances are identified for the surface
without relaxation or reconstruction.

Apresentamos resultados para o cálculo da densidade espectral parcial e
total de estados de um magnon perto da superfície (105) de um antifer-
romagneto de Heisenberg de estrutura cúbica de corpo centrado. Identi-
ficamos a presença tanto de estados como de ressonâncias de superfície,
sem incluir relaxação ou reconstrução.

Recently, Salzberg and Gonçalves da Silva [1] studied the spectral density
of one-magnon states near the stepped surface of a Heisenberg ferromag-
net. It was shown in that work that the presence of steps induces the
appearance of both surface states and resonances, the spectral weight of
which is a function of the position of the spin with respect to the step
edges. The aim of the present work is to present a similar calculation
for the case of an antiferromagnet. We consider a bcc structure with
nearest neighbor coupling only, such that in the Néel state any given
spin is surrounded by eight oppositely directed nearest neighbors.

Although the spectrum of excitations near the surfaces of antiferromagnets has been studied before[2], the discussion in these previous works was limited to "flat", low Miller indices, surfaces. It is well known that, from the point of view of catalysis, stepped surfaces play a more consideralble role[3]. Hence it is of great interest to determine the excitation spectrum also for surfaces of high Miller indices.

The Hamiltonian used is:

$$H = 2 \sum_{i,i'} J(i1,i'2) \vec{S}_{i1} \cdot \vec{S}_{i'2} - 2\mu_B H_A \sum_i (S^z_{i1} - S^z_{i2}). \qquad (1)$$

In (1) the sum extends over all sites of a simple cubic lattice, the indices 1 and 2 labelling the two distinct spins in the magnetic primitive cell. The exchange constant $J(i1, i'2)$ is non-zero only between nearest neighbor pairs. The anisotropy field H_A is taken as infinitesimally small in the numerical calculations.

The surface considered is the (105) surface, shown in Figure 1, viewed along the directions (a) $[00\bar{1}]$ and (b) $[0\bar{1}0]$. Notice that the vector $\vec{t}_2$ is parallel to the *average* direction of the surface. The basic repeat unit of this surface is formed by three rows of spins in one sublattice (up) and three rows of spins in the other sublattice (down); up and down spins are separated by a step of height $0.5\dot{a}$, where a is the conventional cubic unit cell lattice parameter. For computational purposes [4] the crystal is viewed as a collection of regularly stacked layers, each of which has a two-dimensional periodicity described by the primitive vectors $\vec{t}_1$ and $\vec{t}_2$. The primitive cell contains 12 atoms; odd-numbered ones belong to one sublattice and even-numbered ones to the other. In the surface layer the coordination number is four for atoms 3, 5, 10 and 12; six for atoms 1 and 8; and eight for all others.

We define local one-spin deviation functions:

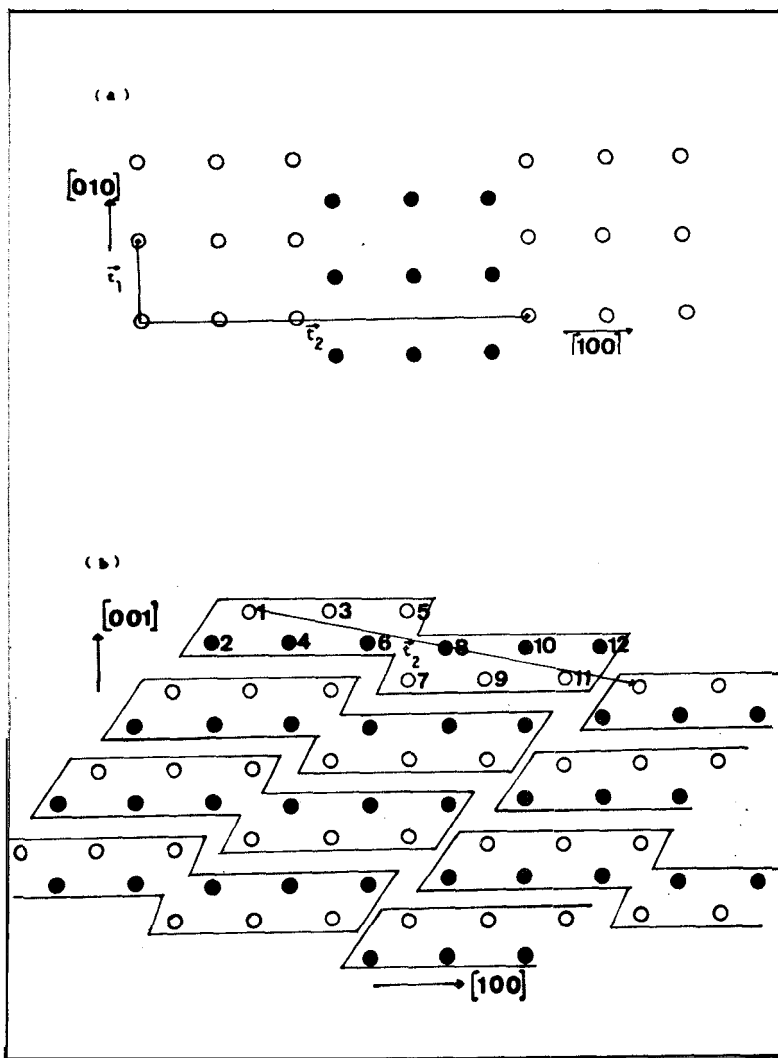$$|n\vec{r}_n\nu\rangle = \frac{1}{\sqrt{2S}} S^{\pm} (n\vec{r}_n\nu) |N\rangle \qquad (2)$$

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Fig.1 - The (105) surface. (a) Viewed along direction $[\bar{0}0\bar{1}]$, i.e., perpendicular *into* the flat portion of the steps. Open circles represent up spin atoms and filled circles represent down spin atoms. Notice that, at every three atomic rows parallel to the direction $[\bar{0}10]$ there is a step of height half a lattice parameter. The vector $\vec{t}_2$ is *not* on the plane of the page. (b) Viewed along the direction $[\bar{0}10]$, i.e., parallel to the steps direction. The primitive cell containing 12 atoms is indicated. The atomic layers considered in the calculation are parallel to the *average* direction of the surface, which coincides with rhe direction of vector $\vec{t}_2$.

where n is the layer label, $\vec{r}_n$ is a two-dimensional vector of the Bravais lattice defined by $\vec{t}_1$ and $\vec{t}_2$ and v = 1,2,..., 12 labels the spins in the primitive cell. The Néel state is indicated by $|N>$ and S^- (S^+) is used for spins in the up (down) sublattice. We also define Bloch-like spin wave excitations in two dimensions in the usual way[4-6]

$$\rho_n(\vec{k},\omega) = -\frac{1}{\pi} I_m \sum_\nu <n\vec{k}\nu|G(\omega+i0^+)|n\vec{k}\nu> \tag{3}$$

where $\vec{k}$ is a two-dimensional wavevector and $G(\omega+i0^+)$ is the one-magnon Green's function associated with the hamiltonian (1). We can also compute partial spectral density of states by restricting the sum in (3) over pairs of oppositely directed spins. The method of calculation of the spectral density is based on the transfer matrix formalism and is discussed in detail elsewhere[4-6]; for this reason we present here only our results.

The calculation was performed for the central point in the two-dimensional Brillouin zone covering the range of positive frequencies. Because of time reversal symmetry it is true that:

$$\rho^{(1,2)}(\omega) = \rho^{(7,8)}(-\omega)$$
$$\rho^{(3,4)}(\omega) = \rho^{(9,10)}(-\omega) \tag{4}$$
$$\rho^{(5,6)}(\omega) = \rho^{(11,12)}(-\omega)$$

where $p^{(\nu,\nu')}(\omega)$ is the partial spectral density mentioned above for the pair (ν,ν'). In Figure 2 we show the total spectral density for the first three layers nearest to and including the surface. The presence of a surface state at ω_s = 2.43 (2JS) and of a surface resonance at ω_r = 3.44 (2JS) can be clearly seen. The large peak at ω = 8 (2JS) is the characteriistic divergence of the density of antiferromagnetic magnon states at the maximum excitation energy. In Figure 3 we show the partial spectral density of states for the different pairs of atoms in the primitive cell at the surface. As we move from the inside of the step (pair (1,2)) to the edge (pair (5,6)) the weights of the surface state and resonance increase, reducing the weight of the continuum. No divergence of $p(\omega)$ is observed at ω = 8 (2JS). This is in accord with the reduced
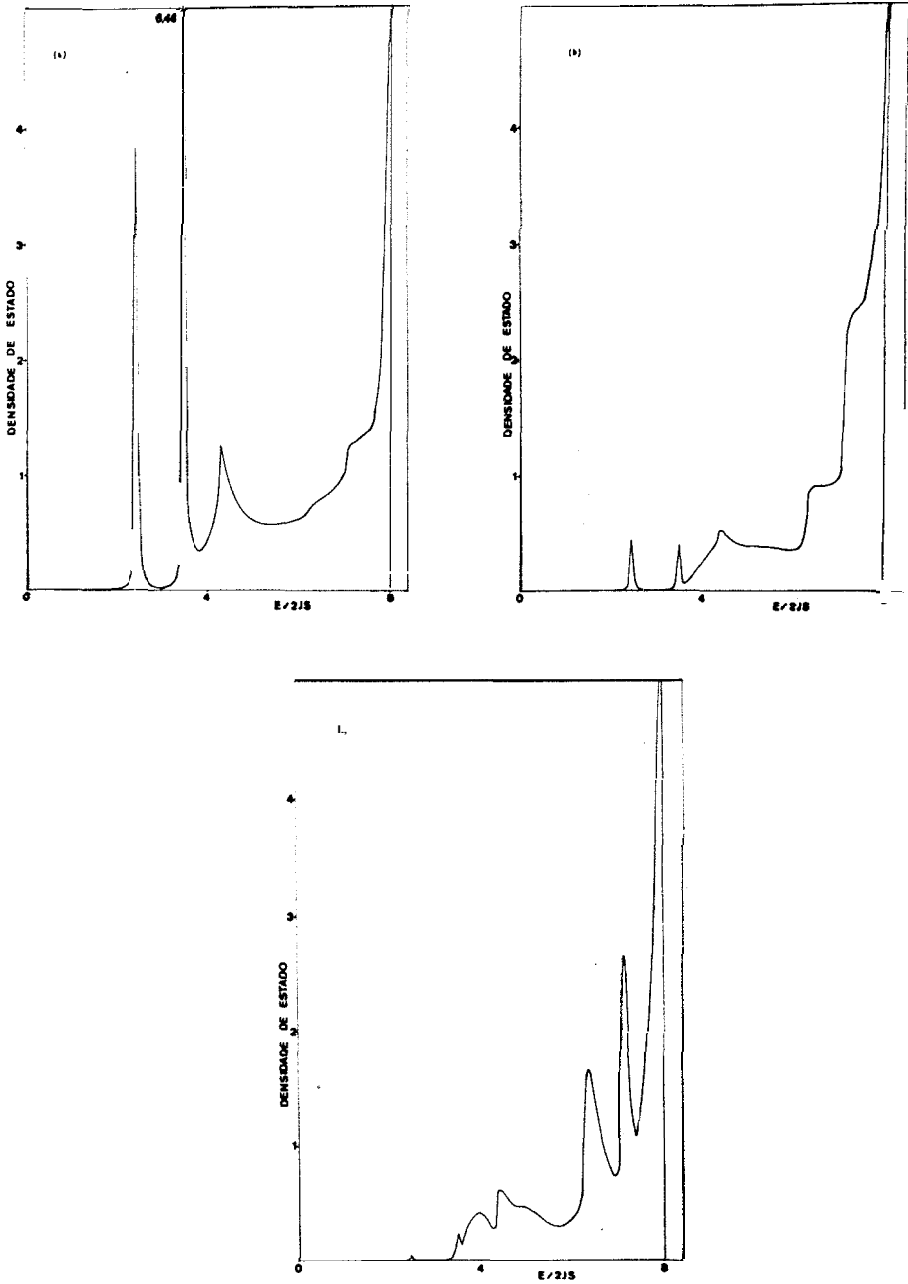
Fig.2 ⁻ Total spectral density of states on (a) surface layer; (b) layer
immediately below it; (c) second layer below surface. Motice disappea-
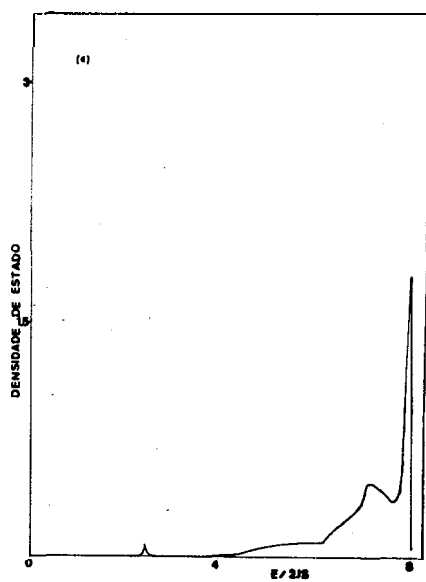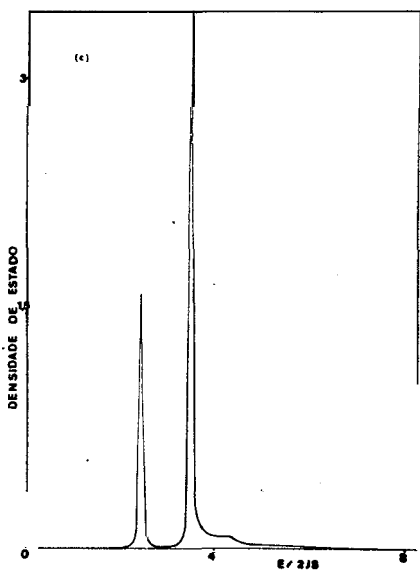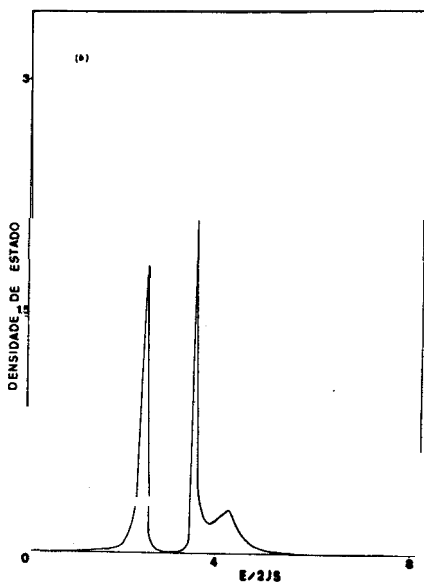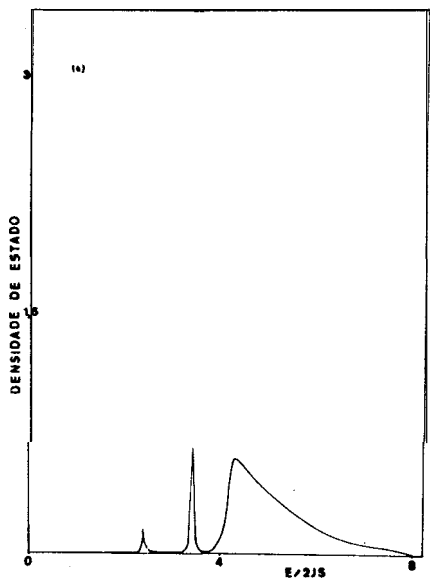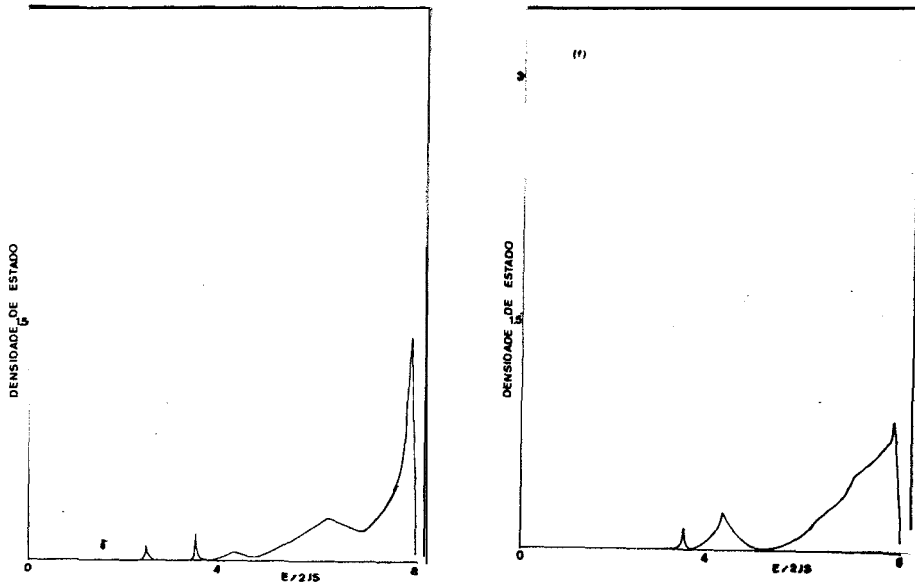rance of surface structures below the edge of the continuum.

Fig.3

Fig.3 - Partial spectral density of states for (a) pair (1,2); (b) pair (3,4); (c) pair (5,6); (d) pair (7,8); (e) pair (9,10); (f) pair (11,12). Notice the predominance of the surface features for pair (5,6), which is at the edge of the step.

coordination number of the atoms on the surface. The spectral density for pairs (7,8), (9,10) and (11,12) does not show prominent surface features, but shows a divergence at the top of the band. This is due to' the fact that excitations with positive frequencies have a much larger weight on the up spin sublattice. For these pairs, however, the up spin atoms do not lie on the surface and have the bulk coordination number of eight. The information concerning the surface scate is summarized in Table 1. We see from it that this state is concentrated on the first three layers, to within the precision of our numerical calculation.

In conclusion, we have reported results for the spectral density of one magnon states near the (105) surface of a bcc antiferromagnet. Even without relaxation or reconstruction, stepped surfaces present a much richer variety of surface associated features than flat ones. In magnetic systems this is due mainly to the existence of atoms with different coordination numbers on the surface. In a future work we will report on the effect of anisotropy, relaxation and reconstruction on the spectral

	$\rho^{(1,2)}$	$\rho^{(3,4)}$	$\rho^{(5,6)}$	$\rho^{(7,8)}$	$\rho^{(9,10)}$	$\rho^{(11,12)}$	ρ
$n = 0$	0.04	0.38	0.43	0.02	0.02	0.00	0.89
$n = 1$	0.00	0.07	0.03	0.00	0.00	0.00	0.10
$n = 2$	0.00	0.01	0.00	0.00	0.00	0.00	0.01

Table 1 - Weight of the delta function (surface state) at $\omega_s = 2.425$ (2JS) at various pairs of atoms and layers. The total weight inside the primitive cell is also shown.

density of states. Unfortunately, contrary to the situation of electronic states, theoretical investigations of magnetic surfaces seem to be more abundiint than experimental ones. We hope that this situation will be corrected in the near future.

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