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THEORY OF SPIN WAVES AND THE TEMPERATURE DEPENDENCE OF THE LOCAL MAGNETIZATION FOR FERROMAGNETIC SURFACES, OVERLAYERS AND INTERFACES

by

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ABSTRACT

The Bloch's law for the bulk magnetization $M(T)/M(0)=1-B_B T^{3/2}$ holds up to temperatures $T \simeq T_c/3$. One of the classical results of surface magnetism is that the Bloch's law holds also for the surface magnetization $M_S(T)$ but with prefactor $B_S=2B_B$. Measurements of $M_S(T)$ for ferromagnetic metals confirm that $M_S(T)$ obeys $T^{3/2}$ law but with prefactor B_S at least three times as large as the bulk value B_S and depending on the type of surface. The classical spin wave theory thus fails to explain the much faster decrease of $M_S(T)$ observed in metals. The main objective of this thesis was to determine whether a softening of surface exchange can explain the observed larger prefactor B_S whilst preserving the Bloch's law. To this purpose, a general recursion method (method of adlayers) for calculating the exact Green's function in an arbitrary overlayer was developed. The method applies to an overlayer deposited above the (100) surface of a simple cubic semi-infinite Heisenberg ferromagnet with exchange interaction between nearest-neighbours. The surface density of spin wave states of an overlayer of different thickness and weaker surface exchanges are calculated. The classical result on $M_S(T)$ which contradicts experiment breaks down at temperatures as low as 1% T_c. The principal results of surface density of states and $M_S(T)$ beyond this temperatures are briefly discussed and determined by exchange interactions in the overlayer. It is shown that the method of adlayers can be used to calculate the exact Green's function for subsurface layers. The computed results of spin wave density of states and subsurface magnetization are presented. At very low temperatures the $M_{ss}(T)$ decreases with temperature twice as fast as in the bulk and this initial result breaks down immediately at higher temperatures. Further, the application of the method of adlayers to the general interfaces problem is also presented. The exact Green's function for such interface is derived and used to evaluate the density of spin wave states at interface layers. The temperature dependence of interface magnetization is briefly discussed and is shown as obeying the $T^{3/2}$ law with the prefactor depending strongly on exchange integral.

Chapter 1

1.1. Introduction

In terms of the history of solid state physics, the concept of spin waves has been established a long time, dating from Bloch's (1930) work, but in the past the ideas have generally proved to be of theoretical rather than of experimental interest. There is now, however, sound body of experimental work, some of a direct and some of a less direct nature, which can be said to demonstrate that spin waves really do "exist" in magnetic materials and that they are more than merely a mathematical entity.

The spin waves theory is a method for investigating low-temperature properties of magnetic materials with ordered magnetic moments. The method consists essentially in the description of low-lying energy levels of a system of an enormous number of strongly interacting spin moments in terms of spin waves or magnons. If the total number of spin waves present in a system is relatively small, and this so at low temperatures, interactions between spin waves are insignificant and thus low-lying energy eigenvalues of the system are additively obtained from the energies of the spin waves. If the energies of free spin waves and their mutual interactions are known, it is possible to calculate with high accuracy the thermodynamic properties of the system at low temperatures such as the spontaneous magnetization.

The physical basis for spin wave theory described here is the Heisenberg or localized model of ferromagnetic crystals. The model assumes that ferromagnetism is due to electrons which are localized on each atom in the crystal. There is also another model of spin waves in a ferromagnetic crystal. The model is known as an itinerant model and is based on the assumption that magnetic electrons are band electrons which travel through the crystal as running waves. It is found experimentally that the d-electrons in transition metals have properties characteristic of both the itinerant model and the localized model.

However, for long-wavelength spin waves we can map the spin wave problem for a metallic ferromagnet described by the itinerant model onto an equivalent problem described by Heisenberg model of a ferromagnetic insulator (See J. Mathon, 1983).

Since we are only interested in long-wavelength spin waves, we shall assume throughout this thesis that the Heisenberg model is applicable.

1.2. Introduction to Spin Waves

In ordered magnetic crystals such as ferromagnets or antiferromagnets, at temperatures well below the ordering temperature, elementary excitations of the spin system are called spin waves, or magnons.

Consider a spin with spin quantum number S and the Z component S_i^z ($\hbar = 1$), localized at each lattice site in a ferromagnet. A spin wave is a sinusiodal disturbance of such spins.

It was first shown by Bloch that states near the ground state of a ferromagnet (where it is generally assumed that all spins are lined up) can be approximated by superposition of these sinusoidal spin waves.

This was discussed on the basis of the Heisenberg model for magnetic insulator, with Hamiltonian

$$H = - \sum_{i,j} J_{ij} S_i S_j, \quad J_{ij} \geq 0 \qquad (1.2.1)$$

where the summation is taken over all combinations of nearest-neighbour spins S_i and S_j and J_{ij} is the exchange integral between nearest-neighbour spins.

We now define two new operators S_i^+ and S_j^- for spin $S_i = (S_i^x, S_i^y, S_i^z)$ such that

$$S^+ = S_i^x + i\, S_i^y$$

and (1.2.2)

$$S_i^- = S_i^x - i\, S_i^y.$$

The operator S_i^+ corresponds to the destruction of a particle with ↓-spin and replaces it by a particle with ↑-spin; the operator S_i^- has the opposite effect. These operators are called spin-deviation operators.

Substituting Eq.(1.2.2) into Eq.(1.2.1), we obtain

$$H = - \sum_{i,j} J_{ij} \left[\tfrac{1}{2} \left(S_i^+ S_j^- + S_j^- S_i^+ \right) + S_i^z S_j^z \right] \qquad (1.2.3)$$

We now make a further substitution and replace the spin deviation operators by the spin-raising and lowering operators C_i^+ and C_i respectively, i.e.

$$S_i^+ = (2S)^{1/2}\, C_i^+ (1 - 1/2S\; C_i^+\, C_i)^{1/2}$$

$$S_i^- = (2S)^{1/2}\, (1 - 1/2S\; C_i^+\, C_i)^{1/2}\, C_i \qquad (1.2.4)$$

$$S_i^z = S - C_i^+\, C_i$$

where C_i^+ and C_i obey the Bose commutation rules:

$$[C_i, C_j^+] = C_i C_j^+ - C_j^+ C_i = \delta_{ij}$$

and (1.2.5)

$$[C_i, C_j] = [C_i^+, C_j^+] = 0$$

At low temperatures the thermal average of the operator $C_i^+C_i/2S$ which is equal to one half of the relative deviation of the spontaneous magnetization from its saturation value, is very small compared to unity. It is thus reasonable to expand the square root in Eq.(1.2.4) in powers of $C_i^+C_i/2S$,

$$(1 - \frac{1}{2S} C_i^+ C_i)^{1/2} \simeq 1 - \frac{1}{4S} C_i^+ C_i + \ldots\ldots \qquad (1.2.6)$$

In the lowest approximation, we can replace the square root in Eq.(1.2.6) by unity which yields

$$S_i^+ = C_i^+ (2S)^{1/2}$$

$$S_i^- = C_i (2S)^{1/2} \qquad (1.2.7)$$

writing C_i^+ and C_i in the Bloch representation, i.e.

$$C_i^+ = \sqrt{\frac{1}{N}} \sum_{\underline{q}} C_{\underline{q}}^+ e^{i\underline{q}.i}$$

(1.2.8)

$$C_i = \sqrt{\frac{1}{N}} \sum_{\underline{q}} C_{\underline{q}} e^{-i\underline{q}.i}$$

the Hamiltonian (1.2.3) becomes

$$H = \sum_{\underline{q}} \{ \sum_{\underline{r}} 2S\ J(\underline{r})\ (1 - e^{-i\underline{q}.\underline{r}}) \}\ C^{+}_{\underline{q}}\ C_{\underline{q}} \qquad (1.2.9)$$

where $\underline{r} = \underline{r}_i - \underline{r}_j$, $i \neq j$

(See J. M. Ziman, 1972).

If we denote the ground-state of a ferromagnet by ψ_0, then an excited state with one spin reversed, is given by

$$\psi_{\underline{q}} = \frac{1}{N} \sum_{i} e^{i\underline{q}.\underline{r}_i}\ C^{+}_i\ \psi_0 \qquad (1.2.10)$$

Using the Hamiltonian (1.2.9), the spin wave energy $E_{\underline{q}}$ of such a state $H\ \psi_{\underline{q}} = E_{\underline{q}}\ \psi_{\underline{q}}$ is given by

$$E_{\underline{q}} = \hbar\ \omega_{\underline{q}} = \sum_{\underline{r}} 2S\ J(\underline{r})\ (1 - e^{-i\underline{q}.\underline{r}}) \qquad (1.2.11)$$

For a simple cubic lattice with only nearest neighbour interaction and $\underline{q}.\underline{r} \ll 1$, Eq.(1.2.11) becomes

$$E_{\underline{q}} = \hbar\ \omega_{\underline{q}} = 2SJ\ a^2\ q^2 \qquad (1.2.12)$$

where $\omega_{\underline{q}}$ is the spin wave frequency corresponding to a wave vector $\underline{q}$, a is the lattice constant and $J = J(\underline{r})$ is taken to be a constant for any nearest neighbour pair of spins. Direct solution of the eigenvalue problem for spin waves is possible only in some simple cases. A much more general approach is based on the Green's function method which is explained in the next section.

1.3. Green's functions and Resolvents

The application of Green's functions (resolvents) is widespread in Solid State Theory and Quantum Mechanics. The importance of Green's function arises from the fact that exact expressions for many physical properties such as density of states can be derived in term of them. They contain the imformation necessary to explain the physical behaviour of the system. For example if we look at the poles of Green's function we can determine the energy excitations of the system.

We shall here give a brief discussion on some properties of the Green's function. However, the reader is referred to Zubarev (1960) for detailed account.

1.3.1. The Density of States

Let $|n>$ be the eigenfunction of the time-independent Hamiltonian operator H and E_n its corresponding eigenvalue. We can now write

$$H|n> = E_n|n> \tag{1.3.1}$$

For the time-independent Schrödinger operator (E - H), we can expand in terms of the eigenfunctions of H, provided that zero is not an eigenvalue of H (See P. T. Lansberg, 1969). We define Green's function G as

$$G = (E - H)^{-1}|n><n|$$

$$= \sum_n \frac{|n><n|}{E - E_n} \tag{1.3.2}$$

where $|n>$ satisfies

$$(E - H)|n> = 0 \tag{1.3.3}$$

We can now define the Green's operators $G^{(\pm)}$ by the equation

$$G^{(\pm)}(E) = \frac{1}{E - H \pm i\varepsilon}$$

$$= \sum_n \frac{|n><n|}{E - E_n \pm i\varepsilon} \tag{1.3.4}$$

Using the following definitions for the delta function and the principle value respectively

$$\delta(x) = \frac{1}{\pi} \lim_{\varepsilon \to 0} \frac{\varepsilon}{x^2 + \varepsilon^2} \tag{1.3.5}$$

$$P(x) = \lim_{\varepsilon \ 0} \frac{x}{x^2 + \varepsilon^2}$$

we obtain

$$G^{(\pm)}(E) = \sum_n |n\rangle\langle n| \; [P(E - E_n) \mp i\,\pi\,\delta(E - E_n)] \tag{1.3.7}$$

then

$$G^{(+)}(E) - G^{(-)}(E) = -\,2\pi i \sum_n |n\rangle\langle n| \, \delta(E - E_n) \tag{1.3.8}$$

Now we consider Eq.(1.3.8) in a particular representation $|\ell\rangle$, then

$$\langle \ell | G^{(+)} - G^{(-)} | \ell' \rangle = -\,2\pi i \sum_n \langle \ell | n \rangle\langle n | \ell' \rangle \, \delta(E - E_n) \tag{1.3.9}$$

The diagonal elements in Eq.(1.3.9) are

$$\langle \ell | G^{(+)} - G^{(-)} | \ell \rangle = -\,2\pi i \sum_n \langle \ell | n \rangle\langle n | \ell \rangle \, \delta(E - E_n) \tag{1.3.10}$$

Summing over all the states ℓ and interchanging the order of summation on the R.H.S of Eq.(1.3.10), we have

$$\sum_{\ell} \langle \ell | G^{(+)} - G^{(-)} | \ell \rangle = -2\pi i \sum_{n} \sum_{\ell} \langle \ell | n \rangle\langle n | \ell \rangle \, \delta(E - E_n)$$

$$= -2\pi i \sum_{n} \delta(E - E_n) \qquad (1.3.11)$$

For a system with a continuous spectrum, $\sum_n \delta(E - E_n)$ is the sum of a large number of energy levels in the neighbourhood of E. The number of such levels per unit energy interval dE is defined to be the density of states $\rho(E)$. Since the two function $G^{(+)}$ and $G^{(-)}$ are complex conjugates, we have from Eqs.(1.3.11) and

$$G^{(+)} - G^{(-)} = 2i \, \mathrm{Im}\, G^{(+)}, \qquad (1.3.12)$$

$$-2\pi i \, \rho(E) = 2i \sum_{\ell} \mathrm{Im}\, G_{\ell\ell}^{(+)}(E)$$

i.e. $\rho(E) = -\frac{1}{\pi} \sum_{\ell} \mathrm{Im}\, G_{\ell\ell}^{(+)}(E)$

$$= -\frac{1}{\pi} \, \mathrm{Tr}(\mathrm{Im}\, G^{(+)}) \qquad (1.3.13)$$

The density of states per atom, where N is the number of particles in the system is then given by

$$\rho^{(n)}(E) = \frac{1}{N} \rho(E). \qquad (1.3.14)$$

1.4. Bulk Spin Wave Green's function of The Heisenberg Ferromagnet

In this section, we shall determine the matrix elements of the bulk spin wave Green's function $\frac{1}{(E - H^0)}$, where H^0 is given by Eq.(1.2.1).

Our model is an infinite simple cubic crystal with lattice constant a, such that the lattice sites are given by the translation vector x_n defined by

$$x_n = n_1 a_1 + n_2 a_2 + n_3 a_3 \qquad (1.4.1)$$

where

$$a_1 = (1,0,0)$$

$$a_2 = (0,1,0) \qquad (1.4.2)$$

$$a_3 = (0,0,1)$$

and n_1, n_2 and n_3 are three integers which can be positive, negative or zero; and to which we refer collectively as n.

We now introduce a real, symmetric (N x N) matrix H^0, whose elements are

$$H^0_{nm} = -(S_n S_m)^{1/2} J_{nm}, \quad n \neq m$$

$$H^0_{nn} = -\sum_{n \neq m} H^0_{nm} \tag{1.4.3}$$

Eq.(1.2.3) can now be written as

$$H^0 = \sum_{n,m} H^0_{nm} C^+_n C_m \tag{1.4.4}$$

We now set out to solve for G^b_{nm}, the matrix elements of bulk spin wave Green's function. Let $\{\psi_n^{(S)}\}$ represent the complete set of real eigenvectors of the matrix H^0 and $\{\omega_S\}$ ($\hbar = 1$) its corresponding set of eigenvalues i.e.

$$\sum_m H^0_{nm} \psi_m^{(S)} = \omega_S \psi_n^{(S)} \tag{1.4.5}$$

with $\{\psi_n^{(S)}\}$ satisfying the orthonormality and closure condition,

$$\sum_n \psi_n^{(S)} \psi_n^{(S')} = \delta_{SS'},$$

$$\sum_s \psi_n^{(S)} \psi_m^{(S)} = \delta_{nm} \tag{1.4.6}$$

$\{\psi_n^{(S)}\}$ can now be taken as the basis for a new set of eigenvectors which correspond to new operators a^+_s and a_s, such that

$$C_n^+ = \sum_s \psi_n^{(S)} a_s^+$$

$$C_n = \sum_s \psi_n^{(s)} a_s \qquad (1.4.7)$$

$$(\psi^+ = \psi)$$

Substituting Eqs.(1.4.9) into Eq.(1.4.4), we have

$$H^0 = \sum_{n,m} H_{nm}^0 \sum_s \psi_n^{(S)} C_s^+ \sum_{s'} \psi_m^{(S')} C_{s'}$$

$$= \sum_s \omega_s C_s^+ C_s \qquad (1.4.8)$$

Thus, we have formally diagonalized the Heisenberg Hamiltonian H^0.

The bulk spin wave Green's function $G_{nm}^b(\omega)$ for the infinite Heisenberg ferromagnet can now be defined as

$$G_{nm}^b(\omega) = [\omega\, \delta_{nm} - H_{nm}^0\,]^{-1} \qquad (1.4.9)$$

which when expanded in terms of the eigenfunctions of H^0, takes the form

$$G_{nm}^b(\omega) = \sum_s \frac{\psi_n^{(s)}\ \psi_m^{(s)}}{\omega - \omega_s} \qquad (1.4.10)$$

provided that zero is not an eigenvalue of it.

If the wave vector $\underline{q}$ is determined by the cyclic boundary condition and is uniformly distributed throughout the first Brillouin zone of the crystal, then the eigenvectors are imaginary exponentials and Eq.(1.4.12) may be written in the form

$$G^{b}_{nm}(\omega) = \frac{1}{N} \sum_{\underline{q}} \frac{\underline{e}^{i\underline{q}.(\underline{x}_n - \underline{x}_m)}}{\omega - \omega_{\underline{q}}} \qquad (1.4.11)$$

where $\omega_{\underline{q}}$ is the bulk spin wave excitation energy given by

$$\omega_{\underline{q}} = \sum_{n} 2S\, J_n \,(1 - \cos(\underline{q}.\underline{x}_n)) \quad , \; n \neq 0.$$

1.5. Classical Law for The Temperature Dependence of Magnetization

Bloch introduced spin waves in order to explain the experimental observation that the magnetization M(T) of a ferromagnet decreased when its temperature was raised from the absolute zero.

We shall now reproduce his argument to derive the relation between the magnetization M(T) and temperature T. We start from quantization of spin waves which proceeds exactly as for photons and phonons. The energy of a mode of frequency ω_q with n_q spin waves is given by

$$E_q = (n_q + \tfrac{1}{2})\, \hbar\, \omega_q \tag{1.5.1}$$

The excitation of a spin wave corresponds to the reversal of one spin $\frac{1}{2}$.

In thermal equilibrium the average value of n_q is given by

$$\langle n_q \rangle = \frac{1}{\exp(\hbar\omega_q/k_B T) - 1} \tag{1.5.2}$$

The total number of spin waves excited at a temperature T is

$$\sum_q n_q = \int d\omega\, N(\omega)\, \langle n(\omega) \rangle \tag{1.5.3}$$

where $N(\omega)$ is the number of spin wave mode per unit frequency range. The integral is taken over the allowed range of $\underline{q}$, which is the first Brillouin zone. At sufficiently low temperatures we may carry the integral between 0 and ∞ because $<n(\omega)> \rightarrow 0$ exponentially as $\omega \rightarrow \infty$.

Spin waves have a single polarization for each value of $\underline{q}$. In three dimensions the number of modes of wavevector less than q is $(1/2\pi)^3(4\pi q^3/3)$ per unit volume. The number of spin waves $N(\omega)d\omega$ with frequency in $d\omega$ at ω is is then $(1/2\pi)^3(4\pi q^2)(dq/d\omega)d\omega$.

From Eq.(1.2.12), we obtain

$$\frac{d\omega}{dq} = \frac{4SJa^2q}{\hbar} = \left(\frac{2JSa^2}{\hbar}\right)^{\frac{1}{2}} \omega^{1/2} \tag{1.5.4}$$

Thus the density of states for spin waves is

$$N(\omega) = \frac{1}{4\pi^2} \left(\frac{\hbar}{2JSa^2}\right)^{3/2} \omega^{1/2} \tag{1.5.5}$$

Equation (1.5.2) thus becomes

$$\sum_{\underline{q}} n_{\underline{q}} = 1/4\pi^2 \left(\frac{\hbar}{2JSa^2}\right)^{3/2} \int_0^\infty d\omega \, \frac{\omega}{e^{\beta\hbar\omega} - 1}$$

$$= 1/4\pi^2 \left(k_b T/2SJa^2\right)^{3/2} \int_0^\infty dx \, \frac{x^{1/2}}{e^x - 1} \tag{1.5.6}$$

The definite integral is found in tables and has the value $(0.0587)(4\pi^2)$.

The number N of atoms per unit volume is Q/a^3, where Q = 1, 2, 3 for sc, bcc, fcc lattices, respectively.

Now the quantity $(\sum n_q)/NS$ is equal to the fractional change of magnetization $\Delta M/M(0)$, whence

$$\Delta M/M(0) = \frac{0.0587}{SQ} \left(k_B T/2JS \right)^{3/2} \qquad (1.5.7)$$

or

$$\frac{M(T)}{M(0)} = (1 - \alpha T^{3/2}) \qquad (1.5.8)$$

where M(0) is the saturation magnetization at T=0 and $\Delta M \equiv M(0) - M(T)$ is the magnetization deviation and

$$\alpha = \frac{0.0587}{SQ} (k_B/2JS)^{3/2}.$$

This result due to Felix Bloch is known as the Bloch $T^{3/2}$ law for bulk ferromagnets and it has been confirmed experimentally.

1.6. Spin Wave Green's function for a Geometric Surface

There are many theoretical studies of the effect of surface on spin waves in a ferromagnet (See Mills and Maradudin, 1967, De Wames and Wolfram, 1969 and Mills, 1984). Here we shall consider the Heisenberg model described in section 1.2, where the spins on sites n and m are coupled by an exchange interaction $J_{nm} S_n . S_m$.

We follow the method of Kalkstein and Soven (1971) which applies to an equivalent tight-binding problem. We introduce a surface by cutting the exchange integrals J_{nm} across a cleavage plane, i.e. we set equal to zero all the J_{nm} between spins on atoms which are on adjacent sides of the plane $z = 1/2\ a$, so that all the J_{nm}'s between atoms in the planes $z = 0$ and $z = a$ are zero. This procedure is referred to as the geometric effect of a surface.

We begin with the Hamiltonian for a simple cubic semi-infinite ferromagnetic crystal with a (001) geometric surface

$$H = H^0 + V \qquad (1.6.1)$$

where H^0 is the bulk exchange Hamiltonian defined by Eq.(1.4.4) and V is a perturbation describing the geometric effect of a surface.

We shall use the one dimensional index n to denote the various spin layers parallel to the surface. We recall that all the exchange integral are given by

$$J_{nm} = J \tag{1.6.2}$$

In treating the bulk properties of a ferromagnet it is advantageous to use the translational symmetry and transform from the site representation C^+_n to the spin wave representation $C^+_{\underline{q}}$, where $\underline{q}$ is the corresponding wave vector, confined to the first Brillouin zone. For the surface considered in the present work only translations parallel to the surface are symmetry operation. As a result of this symmetry, the crystal momentum parallel to the surface, $q_{\parallel}$, is still a good quantum number. $q_{\parallel}$ spans the two dimensional Brillouin zone defined by the crystal parallel to the surface. Owing to reduced symmetry of the surface problem it is convenient to work in a mixed representation.

We now define spin deviation operators on a given plane n with a given transverse crystal momentum $\underline{q}_{\parallel}$ by

$$C^+_{\underline{q}_{\parallel},n} = \frac{1}{\sqrt{N_{\parallel}}} \sum_{n_{\parallel}} C^+_{\underline{q}_n} e^{-i\underline{q}_{\parallel}\cdot n_{\parallel}}$$

$$(1.6.3)$$

$$C_{\underline{q}_{\parallel},n} = \frac{1}{\sqrt{N_{\parallel}}} \sum_{n_{\parallel}} C_{\underline{q}_n} e^{i\underline{q}_{\parallel}\cdot n_{\parallel}}$$

where n and $n_{\parallel}$ denote the perpendicular and the parallel components of $\underline{n}$ relative to the surface respectively. Since $\underline{q}_{\parallel}$ is a good quantum number both V and H^0 are diagonal in $\underline{q}_{\parallel}$. Therefore, we can suppress the explicit $\underline{q}_{\parallel}$ dependence of various quantities. In this way we define the set $\{|\underline{q}_{\parallel},n>\}$, localized around the plane $\{n\}$, as a set of states obtained from the ferromagnetic ground state by application of the spin deviation creation operators $C^{+}_{\underline{q}_{\parallel},n}$ with a given $\underline{q}_{\parallel}$. Therefore, we can write

$$<n,\underline{q}_{\parallel}|G^0|m,\underline{q}'_{\parallel}> = G^0(n-m,\underline{q}_{\parallel})\ \delta_{\underline{q}_{\parallel},\underline{q}'_{\parallel}} \qquad (1.6.4)$$

$$<n,\underline{q}_{\parallel}|G|m,\underline{q}'_{\parallel}> = G(n,m,\underline{q}_{\parallel})\ \delta_{\underline{q}_{\parallel},\underline{q}'_{\parallel}} \qquad (1.6.5)$$

$$<n,\underline{q}_{\parallel}|V|m,\underline{q}'_{\parallel}> = V(n,m,\underline{q}_{\parallel})\ \delta_{\underline{q}_{\parallel},\underline{q}'_{\parallel}} \qquad (1.6.6)$$

where

$G^0 = (E - H^0 - i\delta)^{-1}$ is the Green's function operator for infinite ferromagnetic crystal defined by Eq.(1.4.13) and

$G = (E - H^0 - V - i\delta)^{-1}$ is the Green's function operator for semi-infinite ferromagnet.

To obtain the Green's function G for a semi-infinite ferromagnet from the known G^0 for the bulk problem, we can use Dyson's equation

$$G = G^0 + G^0\ V\ G \qquad (1.6.7)$$

where the perturbation V is a (2 x 2) matrix $\begin{pmatrix} V_{00} & V_{01} \\ V_{10} & V_{11} \end{pmatrix}$.

The off-diagonal elements $V_{01} = V_{10} = SJ$, which can be obtained from Eq.(1.4.3), arise from cutting of the exchange J between neighbouring spin S on the planes n = 0 and n = 1. The diagonal elements $V_{00} = V_{11} = -SJ$ come from the matrix H^0 in Eq.(1.4.3) whose elements are the sum of the off-diagonal elements H^0.

To obtain the Green's function G for m, n ≥ 1, it is convenient to consider first the effect of the off-diagonal elements V_{01} and V_{10}. Because this problem is equivalent to the problem considered by Kalkstein and Soven (1971) for a tight-binding Hamiltonian, we can use their result:

$$\bar{G}(m,n;\underline{q}_{\parallel}) = G^0(|m-n|;\underline{q}_{\parallel}) - G^0(m+n;\underline{q}_{\parallel}) \qquad (1.6.9)$$

for m, n ≥ 1.

Here, $\bar{G}$ is only an intermediate (auxillary) Green's function for geometric surface neglecting the effect of the diagonal elements V_{00} and V_{11}.

The only purpose of ignoring first the matrix element V_{11} is that we can express $\bar{G}$ simply in terms of the bulk Green's function G^0. It is now easy to include this diagonal element using again the Dyson's Equation. The exact Green's function G is then given by

$$G(m,n) = \bar{G}(m,n) + \bar{G}(m,1)\ V(1,1)\ G(1,n) \tag{1.6.10}$$

Now we set m = 1 in Eq.(1.6.10) which gives

$$G(1,n) = \bar{G}(1,n) + \bar{G}(1,1)\ V(1,1)\ G(1,n) \tag{1.6.11}$$

The solution of Eq.(1.6.11) is

$$G(1,n) = \frac{\bar{G}(1,n)}{1 - \bar{G}(1,1)\ V(1,1)} \tag{1.6.12}$$

Combining Eqs.(1.6.10) and (1.6.12) we find that the Green's function for the semi-infinite ferromagnet is given by

$$G(m,n) = \bar{G}(m,n) + \frac{\bar{G}(m,1)\ V(1,1)\ \bar{G}(1,n)}{1 - \bar{G}(1,1)\ V(1,1)} \tag{1.6.13}$$

To obtain G(m,n) in Eq.(1.6.13), we have to solve first for the Green's function G^0 from Eq.(1.4.13).

The Green's function G^0 in the mixed representation between states localized around the planes m and n is given by

$$G^0(m,n;\underline{q}_\parallel) = (N_\perp)^{-1} \sum_{\underline{q}_\perp} e^{i(m-n)\underline{q}_\perp a}\ [E - i\delta - E_0(\underline{q})]^{-1} \tag{1.6.14}$$

where

$$E_0(\underline{q}) = 6JS + 2JS\,[\cos(q_z a) + \Lambda(\underline{q}_{\parallel})] \qquad (1.6.15)$$

is the energy of bulk spin waves for infinite ferromagnet which can be obtained from Eq.(1.2.11)

$$\text{with } \Lambda(\underline{q}_{\parallel}) = \cos(q_x a) + \cos(q_y a) \qquad (1.6.16)$$

and a is the lattice constant.

Transforming the sum over $\underline{q}_{\perp}$ to an integral over the first Brillouin zone, i.e.

$$\sum_{\underline{q}_{\perp}} \rightarrow (N_{\perp} a / 2\pi) \int_{-\pi/a}^{\pi/a} d\underline{q}_{\perp} \qquad (1.6.17)$$

then Eq.(1.6.14) becomes

$$G^0(m-n) = (a / 2\pi) \int_{-\pi/a}^{\pi/a} e^{iq_{\perp}(m-n)a}\, [E - E_0(\underline{q}) - i\delta]^{-1}\, d\underline{q}_{\perp} \qquad (1.6.18)$$

Setting $\underline{q}_{\perp} a = t$ then Eq.(1.6.18) becomes

$$G^0(m-n) = (1/2\pi) \int_{-\pi}^{\pi} e^{i(m-n)t}\, [E' - W - i\delta - \{2SJ\cos(t)\}]^{-1} dt \qquad (1.6.19)$$

where $E' = E - 6SJ$ and $W = 2SJ\,\Lambda$.

Equation (1.6.19) can be integrated in the complex plane (See Appendix A) and we obtain

$$G^0(n) = i\mu^{-1}\gamma^{|n|}, \qquad (1.6.20)$$

where

$$\omega = E - 6SJ - 2SJ\Lambda,$$

$$\gamma = \left(\frac{\omega + i\mu}{2SJ}\right),$$

$$\mu = \begin{cases} (4S^2J^2 - \omega^2)^{1/2} \text{ for } \omega^2 \le 4S^2J^2 \\ i \text{ sign}(\omega)(\omega^2 - 4S^2J^2)^{1/2} \end{cases} \qquad (1.6.21)$$

and

$$\text{sgn}(\omega) = \begin{cases} +1, & \omega > 0 \\ -1, & \omega < 0 \end{cases}$$

We can rewrite Eq.(1.6.9) in terms of γ and simplify the notation by omitting the explicit $\underline{q}_{\parallel}$ dependence as

$$\overline{G}(m,n) = i\mu^{-1}\left(\gamma^{|m-n|} - \gamma^{|m+n|}\right) \; ; \text{ for } m, n \ge 1 \qquad (1.6.22)$$

Using Eq.(1.6.22) we obtain

$$\overline{G}(m,1) = i\mu^{-1}\left(\gamma^{|m-1|} - \gamma^{|m+1|}\right), \qquad (1.6.23)$$

$$\overline{G}(1,m) = i\mu^{-1}\left(\gamma^{|1-m|} - \gamma^{|1+m|}\right), \qquad (1.6.24)$$

$$\overline{G}(1,1) = i\mu^{-1} (1 - \gamma^{2}). \tag{1.6.25}$$

It is clear from the above relations that

$$\overline{G}(m,1) = \overline{G}(1,m) \tag{1.6.26}$$

Combining Eqs.(1.6.13), (1.6.23), (1.6.24), (1.6.25) and (1.6.26) and setting m = n, we find

$$G(m,m) = i\mu^{-1} [1 + \gamma^{2m-2} (\frac{\mu - i[\omega + 2SJ]}{\mu + i[\omega + 2SJ]})] \tag{1.6.27}$$

for $m \geq 1$.

The spin wave Green's function G(m,m) in (1.6.27) is a starting point for evaluating the spin wave density of states in a semi-infinite ferromagnet, ferromagnetic overlayer, subsurface layers and interface layers. All these problems will be discussed in chapter2 and chapter 3.

Chapter 2. Spin Wave Green's function for a Heisenberg ferromagnet with softened Surface Exchange

2.1. Experimental Situation

There has been a shift in research activity in magnetism in recent years from bulk to surfaces and thin films. One of the factors behind this development is the dramatic improvement in the experimental methods, the preparation of good thin films and surfaces (See Arrott et al; 1987) and progress in theoretical and computational methods (See for review Mathon, 1988; Freeman et al.,1985; Mathon and Ahmad, 1988). Many techniques familiar in solid state technology, such as molecular or atom beam epitaxy, are being transferred to surface magnetism (See Bader, 1985; Moog, 1987) and this has had a great impact on the subject.

Another important factor is that fundamental processes in magnetic materials are increasingly being studied by surface methods. For example, most of the imformation about the ferromagnetic band structure, the effect of correlations and finite-temperature magnetism is currently obtained from photoemission data (See Feder, 1985) and secondary electron polarization (See Mauri et al., 1988; Siegmann et al., 1988). Proper understanding of the role of the surface is paramount in correct interpretation of these data.

One development which served as an impetus in surface magnetism was the observation of magnetically 'dead' surface layers by Liebermann et al. (1969, 1970). Their work stimulated the development of new theoretical and experimental methods for studying magnetic surfaces. The work of Liebermann et al. thus highlighted one of the fundamental problems of surface magnetism, i.e. the effect of surface on the ground state magnetization. The other two central questions are concerned with the nature of magnetic excitations at surfaces and the way the magnetization disorders near a surface at finite temperatures.

Unlike the ground state problem, the effect of surface on the excited states is less well understood; for example, the effect of softening of the exchange interactions near a magnetic surface on the temperature dependence of surface magnetization has not been investigated.

One of the classical results of surface magnetism is the prediction of Rado (1957) and of Mills and Maradudin (1967) that the surface magnetization in the spin wave regime decreases following the usual $T^{3/2}$ law

$$M_s(T) / M_s(0) = 1 - k B_B T^{3/2} \qquad (2.1.1)$$

where B_B is the constant describing the decrease of the bulk magnetization due to spin waves and k = 2. The factor 2 arises because spin waves at the surface have always an antinode (the surface represents a free end). It is only recently that this prediction could be tested experimentally. Pierce et al. (1982) measured the surface magnetization $M_s(T)$ for $Ni_{40}Fe_{40}B_{20}$ amorphous ferromagnet using spin-polarized low-energy electron diffraction (SPLEED) and Walker et al. (1984) and Korecki and Gradmann (1985, 1986) measured $M_s(T)$ for Fe(110) surface using Mössbauer spectroscopy. All these measurements confirm that $M_s(T)$ decreases following a $T^{3/2}$ law but the exprimental value of k obtained both for $Ni_{40}Fe_{40}B_{20}$ and Fe(110) is $k \geq 3$.

This large discrepancy between the theoretical and experimental values of factor k casts serious doubts on the validity of the classical result of Rado and Mills and Maradudin. The existing spin wave theories thus cannot explain the observed much faster decrease of $M_s(T)$. This is not surprising since they apply only to a semi-infinite ferromagnet with a magnetization which remains uniform right up to the surface and assume exchange interactions which are not perturbed in the surface region. We now know that neither of these assumptions is valid for ferromagnetic metals (Freeman et at., 1985; Mathon, 1986). For example, it is predicted (Freeman et al., 1985) that the surface magnetization is enhanced by 30% for Fe(100) surface and by 20% for Ni(100) surface. Surface enhancement of the magnetization leads inevitably to a softening of surface exchange (Mathon, 1986) (at least for strong ferromagnets). It is, therefore, essential to investigate the effect of both these factors on $M_s(T)$. Although Mills (1970) pointed out that a softening of exchange in the surface plane has no effect on initial $T^{3/2}$ law, we shall see that his result holds only at temperatures so low that they are of academic interest only.

We shall determine $M_s(T)$ in the most general case of a ferromagnet with spin S_n and exchange integrals J_{nm} which may deviate from the bulk spin S and bulk exchange J in an arbitrary number of atomic planes parallel to the surface using a recursion method for adlayers we have developed (See Mathon and Ahmad 1988, Mathon 1988 and Mathon 1989). We shall show that deviations of surface exchange parameters from their bulk values have profound effect on the surface magnetization $M_S(T)$.

Since spin waves are bosons, the surface magnetization deviation $\Delta M_S(T)$ is given by

$$\Delta M_S(T) = \int_0^\infty 2\mu_B \; N_S(E)[\exp(E/kT) - 1]^{-1} \, dE \qquad (2.1.2)$$

where μ_B is the Bohr magneton and $N_S(E)$ is the surface density of spin wave states.

It is, therefore, clear that the problem reduces to the calculation of $N_S(E)$ which; in turn, is expressed in terms of the spin wave Green's function.

2.2. General Formulation of The Method of Adlayers

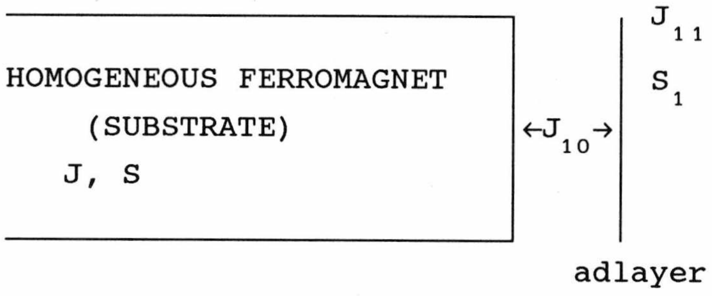

Fig. 2.1. Semi-infinite homogeneous ferromagnetic substrate with one adlayer.

We shall begin with a simple magnetic overlayer consisting of one atomic plane labeled by n = 1 (See fig.2.1). The overlayer is located above the (100) surface of a sc ferromagnet occupying the half-space $z < 0$. The exchange Hamiltonian of the system (see Eq.(1.4.5)) can be written in terms of the Bose spin raising and lowering operators C_n^+, C_n as

$$H = E_0 + \sum_{n,m} H_{nm} C_n^+ C_m \tag{2.2.1}$$

where

$$\begin{aligned} H_{nm} &= -(S_n S_m)^{1/2} J_{nm}, \quad n \neq m \\ H_{nn} &= - \sum_{m \neq n} H_{nm} \end{aligned} \tag{2.2.2}$$

and n, m label the lattice sites.

The Hamiltonian (2.2.1) applies obviously to insulators but is also exact within the random-phase approximation for long wavelength spin waves in metal (See Mathon, 1981). The effective exchange integrals at the surface of a metal (and in the bulk) can be computed from the ground state band structure (See Mathon, 1986) but such ab initio calculations are yet to be done. However, for the purpose of calculating $M_s(T)$, the only result we require is that the Hamiltonian (2.2.1) is valid for metals. The exchange integrals J_{nm} and the local spin S_n can be treated as parameters.

We have $J_{nn+1} = J$, $J_{nn} = J$ and $S_n = S$ in the substrate but the exchange integrals between neighbouring atomic planes and within the plane of the overlayer are arbitrary. The local spin S_n in the atomic plane n of the overlayer is also arbitrary (ferromagnetic).

The spin wave Green's function of the Hamiltonian (2.2.1) is defined by

$$G = (E - H)^{-1}. \qquad (2.2.3)$$

To calculate the Green function G^1_{11} in the new surface, we first assume that the overlayer is physically removed from the substrate. The matrix element of the exact spin wave Green's function $G^0_{00}(\underset{\sim}{q},E)$ in the exposed surface plane of the substrate (n=0) is known (refer to Eq.(1.6.27)).

As a next step, we reinstate the atomic plane of the overlayer n = 1 and give a prescription for calculating the matrix element G^1_{11} of the Green's function in the new surface plane n = 1 in terms of the old G^0_{00}. The superscript "1" indicates that G^1 refers to the substrate covered with one "adlayer".

The matrix elements of G^1 for an overlayer of one atomic layer are related to G^0 for the semi-infinite substrate by a Dyson equation

$$G^1 = G^0 + G^0 W G^1, \tag{2.2.4}$$

where the perturbation W due to the deposition of an adlayer n = 1 can be determined from Eq.(2.2.2), i.e

$$W_{00} = J_{01} S_1 \tag{2.2.5}$$

and

$$W_{10} = W_{01} = - J_{01} (S_0 S_1)^{1/2} \tag{2.2.6}$$

Here, J_{01} is the exchange integral between layers 0, 1 and J_{00} is the exchange integral and S_0 the local spin in the layer 0.

Before Eq.(2.2.4) can be applied, G^0 must be extended to a space of dimension one higher than the space in which it is originally defined (all the matrices in Eq. (2.2.4) must be of the same size). This means that G^0 acquires an additional matrix element

$$G^0_{11} = [E - H_{11}(\underline{q})]^{-1}, \qquad (2.2.7)$$

where

$$H_{11} = H^0_{11} + \overline{W}_{11},$$

$\overline{W}_{11} = S_0 J_{10}$ is the perturbation because each atom in the new surface layer gets one new neighbour in the old surface layer

and

$$H^0_{11} = 4J_{11}S_1 + 2J_{11}S_1\ [\cos(q_x a) + \cos(q_y a)],$$
for $-\pi/a < q_x,\ q_y < \pi/a$,

is the Hamiltonian of a two-dimensional layer of spins forming the 1-st atomic plane of the semi-infinite crystal and a is the lattice constant.

All the other matrix elements connecting the adlayer 1 to the crystal are

$$G^0_{1i} = G^0_{i1} = 0, \quad i \neq 1$$

$$\underset{(N+1 \times N+1)}{G^0_{ij}} = \underset{(N \times N)}{G^0_{ij}}, \quad i, j \neq 1 \tag{2.2.8}$$

where N is the number of at. planes.

Now we try to solve Eq. (2.2.4).

$$G^1_{ij} = G^0_{ij} + G^0_{i1} W_{10} G^1_{0j} + G^0_{i0} W_{01} G^1_{1j} + G^0_{i0} W_{00} G^1_{0j}$$

for $i, j = 1, 0, -1, -2, \ldots\ldots\ldots$ (2.2.9)

Using Eq. (2.2.8) we obtain

$$G^1_{11} = G^0_{11} + G^0_{11} W_{10} G^1_{01} \tag{2.2.10}$$

From Eqs. (2.2.4) and (2.2.8) we also get

$$G^1_{01} = G^0_{00} W_{01} G^1_{11} + G^0_{00} W_{00} G^1_{01} \tag{2.2.11}$$

Substituting Eq.(2.2.11) into Eq.(2.2.10), G^1_{11} becomes

$$G^1_{11} = [E - H_{11} - (W_{01})^2 G^0_{00} [1 - W_{00} G^0_{00}]^{-1}]^{-1} \tag{2.2.12}$$

where

$E = 6JS + 2JS [\cos(q_x a) + \cos(q_y a) + \cos(q_z a)]$

for $-\pi/a < q_x, q_y, q_z < \pi/a$.

We can rewrite the term $E - H_{11}$ as

$$E - H_{11} = \omega + W_{11}, \tag{2.2.13}$$

where

$$\omega = E - 6SJ - 2SJ[\cos(q_x a) + \cos(q_y a)]$$

and

$$W_{11} = 2SJ - SJ_{10} + [1 - (S_1/S)(J_{11}/J)](E-\omega - 2SJ) \tag{2.2.14}$$

is now regarded as a perturbation in the plane n = 1, i.e. the overlayer.

Substituting Eq.(2.2.13) into Eq.(2.2.12), we finally get

$$G^1_{11} = [\omega + W_{11} - W^2_{01} \; G^0_{00} \; (1 - W_{00} \; G^0_{00})^{-1}]^{-1} \tag{2.2.15}$$

where G^0_{00} is the Green's function for geometric surface and can be obtained from Eq.(1.6.27) by setting m = n = 0.

Equation (2.2.15) is the exact spin wave Green's function in the surface of an overlayer consisting of a single atomic plane.

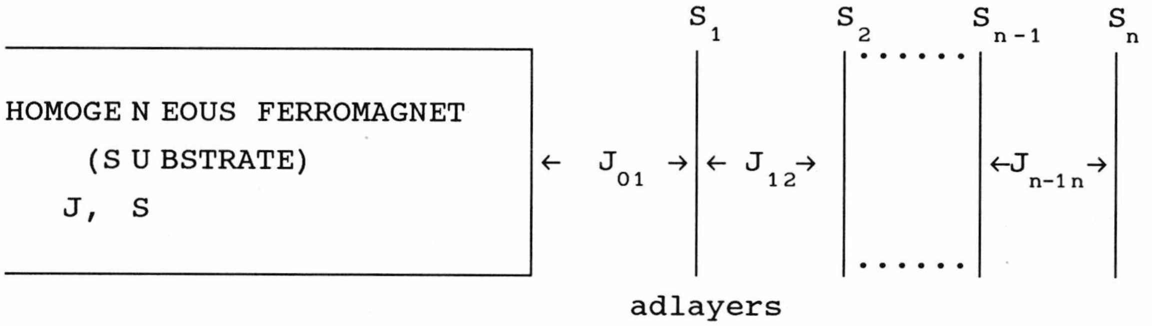

Fig.2.2. Semi-infinite homogeneous ferromagnetic substrate covered with an arbitrary number of adlayers.

The procedure of "depositing an adlayer" can be now repeated and the Green's function G^2_{22} in the new surface at $n = 2$ is again calculated from Eq.(2.2.15) but with G^1_{11} replacing G^0_{00} on the right hand side. In general, after we repeated the process k times, we obtain a general recursion formula

$$G^k_{kk} = [\omega + W_{kk} - \frac{(W_{k-1k})^2 \; G^{k-1k-1}_{k-1k-1}}{1 - W_{k-1k-1} \; G^{k-1k-1}_{k-1k-1}}]^{-1} \qquad (2.2.16)$$

with

$$W_{k-1k-1} = 1/2 \; (J_{k-1k}/J) \; (S_k/S)$$

$$W_{k-1k} = 1/2 \; (J_{k-1k}/J) \; (S_{k-1}/S)^{1/2} \; (S_k/S)^{1/2} \qquad (2.2.17)$$

$$W_{kk} = 1 - 1/2 \; (S_{k-1}/S) \; (J_{k-1k}/J) + (1 - J_{kk}S_k/JS) \; (E-\omega-1)$$

where

$$\omega = E - 3 - [\cos(q_x a) + \cos(q_y a)]$$

and all the energies are measured in units of 2SJ.

Equation (2.2.16) is the basic recursion formula for calculating the density of states (DOS) in the surface of an arbitrary magnetic overlayer. Note that the recursion starts with the exact substrate Green's function G^0_{00} and since there are no approximations involved in the recursion method, the surface Green's function G^N_{NN} obtained after N recursion steps is also exact. In principle, this key matrix element could be calculated by one of the traditional recursion methods for the Green's function (see, e.g. Haydock, 1982 and Lopez Sancho et al., 1985). However, a serious disadvantage of all these methods is that they are iterative and give only an approximate G^N_{NN}. In the calculation of $M_s(T)$ for a ferromagnet the exact surface Green's function G^N_{NN} is required. In fact, we need a very high accuracy for spin waves because spin wave theory is only valid at low temperatures (small energies) and, therefore, we require the surface density of states only at the bottom of the whole spin wave band (in the region of ≃ 10 - 15% of the band width).

In the next section, we shall use the method of adlayers to determine spin wave density of states for one adlayer, which is required in the calculation of the temperature dependence of surface magnetization.

2.3 Surface Density of Spin Wave States for One Adlayer

To obtain Green's function G^1_{11}, we first rewrite Eq.(2.2.14) as

$$G^1_{11} = \frac{1 - W_{00}\, G^0_{00}}{\omega + W_{11} - G^0_{00}\,(\omega\, W_{00} + W_{00}\, W_{11} + (W_{10})^2)} \qquad (2.3.1)$$

Setting $\mathrm{Re}G^0_{00} = R$, $\mathrm{Im}G^0_{00} = I$ and substituting this result in Eq.(2.3.1), we obtain

$$\mathrm{Im}G^1_{11} = \frac{(W_{10})^2\ I}{(\omega + W_{11} - \lambda R)^2 + (\lambda I)^2} \qquad (2.3.2)$$

where

$$\lambda = \omega\, W_{00} + W_{00}\, W_{11} + (W_{10})^2 \qquad (2.3.3)$$

and

$$I = \mathrm{Im}G^0_{00} = \begin{cases} [(1 - \omega)/(1 + \omega)]^{1/2}, & \omega^2 < 1 \\ 0, & \omega^2 > 1 \end{cases}$$

$$R = \mathrm{Re}G^0_{00} = \begin{cases} 1, & \omega^2 < 1 \\ 0, & \omega^2 > 1 \end{cases} \qquad (2.3.4)$$

can be obtained from Eq.(1.6.27).

By combining Eqs. (1.3.14) and (2.3.2), the surface spin wave density of states is given by

$$N_s(E) = \frac{1}{\pi N} \sum_{\underline{q}_{\parallel}} \frac{(W_{10})^2 \, I}{(\omega + W_{11} - \lambda R)^2 + (\lambda I)^2} \qquad (2.3.5)$$

Transforming the sum in Eq.(2.3.5) over $\underline{q}_{\parallel}$ to an integral over first Brillouin zone,

$$\sum_{\underline{q}_{\parallel}} \rightarrow N_{\parallel} \, (a/2\pi)^2 \int_{-\pi/a}^{+\pi/a} \int_{-\pi/a}^{+\pi/a} dq_x \, dq_y \qquad (2.3.6)$$

Eq.(2.3.5) becomes

$$N_s(E) = \frac{a^2}{4\pi^3} \int_{-\pi/a}^{+\pi/a} \int_{-\pi/a}^{+\pi/a} \frac{(W_{10})^2 \, I}{(\omega + W_{11} - \lambda R)^2 + (\lambda I)^2} \, dq_x dq_y$$

$$(2.3.7)$$

and this give us the surface density of spin wave states for one adlayer.

We can now use Eq.(2.3.7) to discuss the analytic behaviour of the surface density of states at the bottom of the spin wave band E ≃ 0.

2.3.1 The Analytic Behaviour of the Spin Wave DOS at the Bottom of the Band $E \simeq 0$

It is convenient to rewrite Eq.(2.2.5), Eq.(2.2.6) and Eq.(2.2.14) as

$$W_{00} = \alpha\varepsilon,\ W_{10} = -\alpha\varepsilon^{1/2} \text{ and } W_{11} = 1 - \rho + (1 - \gamma)(E - \omega - 1) \tag{2.3.8}$$

where

$$\alpha = 1/2\ (J_{10}/J),\ \beta = J_{11}/J\ ,\ \varepsilon = S_1/S,\ \rho = \alpha\varepsilon \text{ and } \gamma = \beta\varepsilon \tag{2.3.9}$$

Substituting now from Eq.(2.3.8) into the denominator of Eq.(2.3.7), we obtain

$$\omega + W_{11} - \lambda = (\omega + 1)(1 - \rho)\gamma + E(\rho\gamma - \rho - \gamma + 1) - \alpha,$$

where

$$\lambda I = -[\rho(1 - \gamma)E + \rho\gamma(1 + \omega)]\ I \tag{2.3.9}$$

The density of spin wave states at the bottom of the band is dominated by the singularity of I at $\omega = -1$ [See Eq.(2.3.4)]. It is clear from Eq.(2.3.9) that the denominator of Eq.(2.3.7) contains only terms proportional to E and $\omega + 1$ and a constants term α. For energy $E \simeq 0$, the leading term of the denominator at the bottom of the band is, clearly, α. To the lowest order in E, we have, therefore, the following exact result:

$$N_S(E) = \frac{a^2}{4\pi^3} \int_{-\pi/a}^{+\pi/a} \int_{-\pi/a}^{+\pi/a} \frac{(W_{10})^2 I}{\alpha^2} \, dq_x \, dq_y$$

(2.3.10)

Substituting for I from Eq.(2.3.4), take the form

$$N_S(E) = \left[\frac{a^2}{4\pi^3} \int_{-\pi/a}^{+\pi/a} \int_{-\pi/a}^{+\pi/a} [(1 - \omega)/(1 + \omega)]^{1/2} \, dq_x \, dq_y \right] \varepsilon$$

(2.3.11)

Equation (2.3.11) should be now integrated numerically to obtain $N_S(E)$.

However, it is clear already from Eqs.(2.3.8) and (2.3.10) that

$$N_s(E) = N_0(E) \, \varepsilon \qquad (2.3.12)$$

holds at the bottom of the spin wave band, where $N_0(E)$ is the density of states for geometric surface.

Using Eq.(2.3.9) and writting $N_0(E)$ in term of $N_B(E)$ (See Appendix B), Eq.(2.3.12) becomes

$$N_s(E) = 2N_B(E)(S_1/S) + O(E^{3/2}) \qquad (2.3.13)$$

where $N_B(E)$ is bulk density of spin wave states.

We have thus proved that the surface density of spin wave states is independent of the deviations of exchange integrals from the bulk J. It follow from Eq.(2.1.2) that the initial temperature dependence of the surface magnetization obeys the classical result of Rado (1959) and Mills and Maradudin (1967), i.e. the surface magnetization decrease initially twice as fast as in the bulk [note that the factor S_1/S in Eq.(2.3.13) is canceled out because $M_s(T)$ is normalized to $M_s(0)$]. This result disagrees with experiment of Pierce et al. (1982) and Walker et al. (1984), and that was the motivation for us to investigate the behaviour of $N_s(E)$ or $M_s(T)$ beyond this initial region where analytic discussion is possible.

2.3.2 Surface DOS for $J_{10}/J < 1$, $J_{11}/J = 1$ and $S_1/S = 1$

It is well known that a two-dimensional isotropic Heisenberg ferromagnet is neither ferromagnetic nor antiferromagnetic at non-zero temperature because there can be no spontaneous magnetization or sublattice magnetization (See Mermin and Wagner, 1966). Weakening the exchange between the surface layer and the bulk, we expect that there must be a transition of the surface density of states from three-dimensional behaviour to two-dimensional behaviour when the adlayer becomes completely decoupled from the substrate. Therefore, it is essential to investigate first the effect of a weaker surface to bulk exchange $J_{10}/J < 1$ while keeping $J_{11}/J = 1$ and also keeping the surface spin equal to its bulk value ($S_1/S = 1$). To obtain the surface density of states, we may set $q_x a = x$ and $q_y a = y$ in Eq.(2.3.7) and use the symmetry of the integrands in the xy-plane. The Eq.(2.3.7) becomes

$$N_s(E) = \frac{1}{\pi^3} \int_{-\pi}^{0} \int_{-\pi}^{0} \frac{(W_{10})^2 \, I}{(\omega + W_{11} - \lambda R)^2 + (\lambda I)^2} \, dx \, dy \tag{2.3.15}$$

The problem is that the integrand is divergent at $\omega = -1$. To remove this divergence , we can use the following trick:

$$N_s(E) = 2N_B(E) + \frac{1}{\pi^3}\iint_{-\pi}^{0}\left\{ \frac{(W_{10})^2\, I}{(\omega + W_{11} - \lambda R)^2 + (\lambda I)^2} - I \right\} dx\, dy \tag{2.3.16}$$

where we have used the result

$$\frac{1}{\pi^3}\iint_{-\pi}^{0} I \quad dx\, dy \simeq 2N_B(E)$$

which holds at the bottom of the spin wave band [See Eq.(2.3.10)].

It is well known (See Appendix C) that $N_B(E)$ near the bottom of the spin wave band is given by

$$N_B(E) = (1/2\pi^2)\ (2E)^{1/2} \tag{2.3.17}$$

It is easy to show that the term in braces in Eq.(2.3.16) is no longer divergent at $\omega = -1$. We can, therefore, set $J_{10}/J = \alpha < 1$, $J_{11}/J = 1$ and $S_1/S = 1$ in Eq.(2.3.16), and compute easily the surface density of states for a range of J_{10}/J. The computed surface density of states is shown in Fig.2.3 with the energy measured in units of k_BT_C ($J/k_BT_C \simeq 0.5$ for a simple cubic lattice and $S = 1/2$).

For small E ($E \simeq 0.00\text{-}0.01k_BT_C$), all DOS curves fall on the universal curve $2N_B(E) \propto E^{1/2}$ as required by Eq.(2.3.13) but the DOS for smaller J_{10} deviate rapidly upward with increasing E. The upward turn is due to an $E^{3/2}$ term which is greatly enhanced for $J_{10} \ll J$. The analytic behaviour of $N_S(E)$ beyond the initial $E^{1/2}$ term can be derived easily from Eq.(2.3.15), where

$$N_s(E) \simeq 1/\pi^2 \left[\sqrt{2}\, E^{1/2} + \frac{\sqrt{2}}{6} \frac{\alpha(1 - 2\alpha)}{\alpha^2} E^{3/2} + \ldots\right] \tag{2.3.18}$$

It is clear that the coefficient of the $E^{3/2}$ term diverges for $J_{10} \rightarrow 0$ and this explains the rapid rise of the curves in Fig.2.3 for small J_{10}. However, the region in which the $E^{3/2}$ term is dominant is very narrow and all the computed density of states curves turn downward again and resemble the initial $E^{1/2}$ dependence. We stress that, for $J_{10}/J \simeq 0.5$ or smaller, the crossover takes place at low temperatures $T < 0.05\text{-}0.1 k_B T_C$. For energies higher than $\simeq 0.1 k_B T_c$, the density of states depends strongly on J_{10}.

If we reduce J_{10} until its value becomes zero, the surface layer becomes completely decoupled from the rest of the crystal and its density of states approaches the density of states of a two-dimensional ferromagnet $N_{2D}(E)$ denoted in Fig.2.3 by a broken curve. Since $N_{2D}(E)$ starts from a constant value $(1/\pi)k_B T_c$ at $E = 0$, the surface density of states for small J_{10} must rise very steeply from zero and then flatten off with a final slope which is smaller than that of $2N_B(E)$ (see Fig. 2.3). For very small J_{10}, the final slope of $N_s(E)$ is close zero.

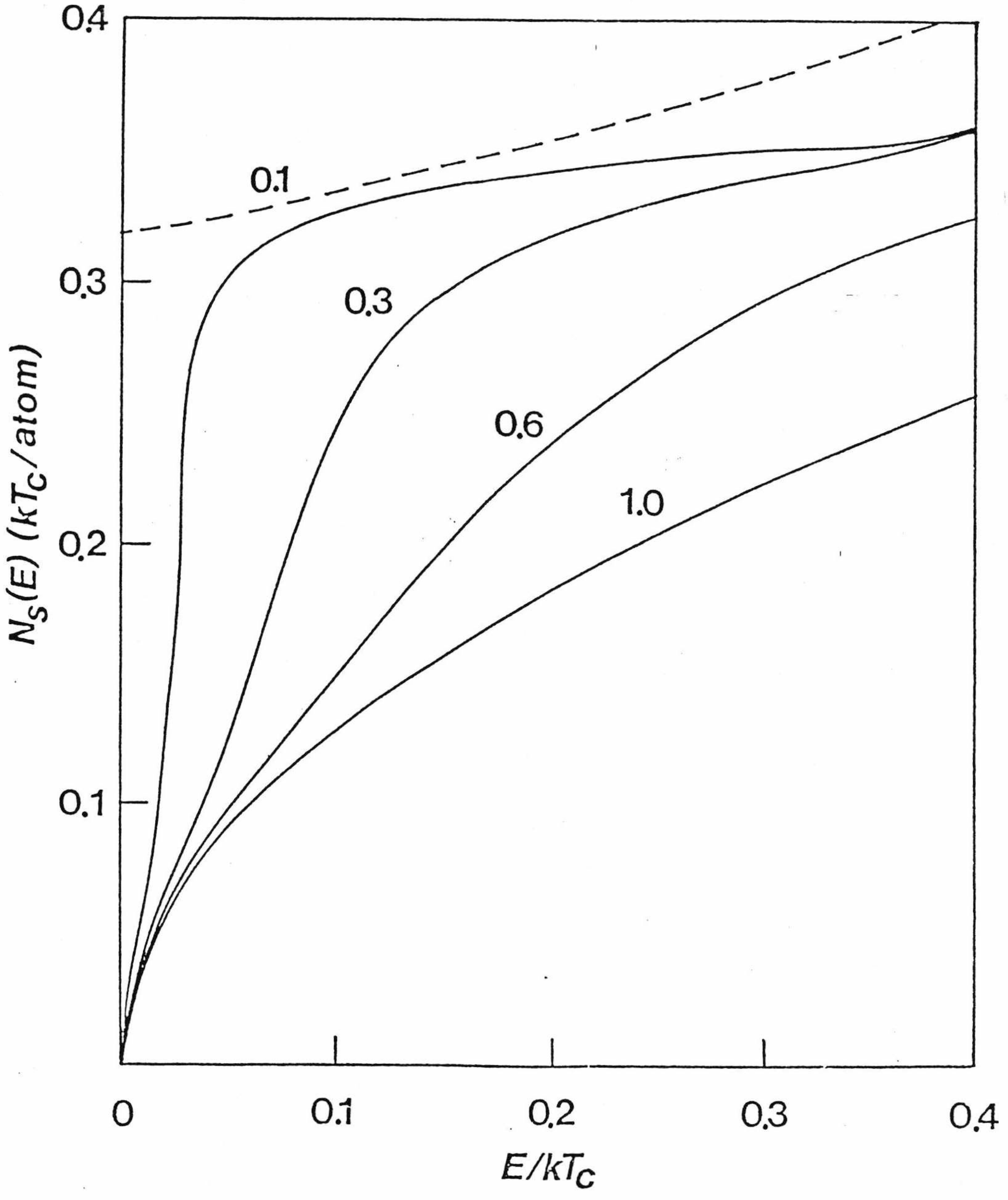

Fig. 2.3 Calculated density of spin wave states $N_s(E)$ in the (100) surface of sc ferromagnet with a softened exchange integral J_{10} perpendicular to the surface. The values of J_{10}/J are 0.1, 0.3, 0.6 and 1.0. The DOS of a two-dimensional ferromagnet is denoted by broken curve.

It is apparent already from the behaviour of the density of states shown in Fig.2.3 that the initial dependence $\propto E^{1/2}$ leading to the classical law for $M_S(T)$ is confined to energies so low that they cannot be of practical interest. This will be discussed in detail in section (2.5). However, apart from the influence of softening of the perpendicular exchange J_{10} on the spin wave density of states , we need to investigate the effect of softening of exchange parallel to the surface J_{11} beyond the classical region. This will be discussed in the next section.

2.3.3 Surface DOS for $J_{11}/J < 1$, $J_{10}/J = 1$ and $S_1/S = 1$

In calculating the effect of J_{10} on the spin wave density of states, we assumed tacitly in section 2.3.2 that J_{10} influences only bulk spin waves. This is justified because it is known from the work De Wames and Wolfram (1969) that there are no surface spin waves present for $J_{10} < J$. However, the situation for $J_{11} \neq J$ is more complicated. It was shown by De Wames and Wolfram (1969) that surface spin waves lying below the bulk spin waves band occur for $J_{11} < J$. Such surface excitations will clearly contribute to the surface density of states and must be included in our calculation. It is, therefore, necessary to consider separately the contributions of bulk and surface spin waves to the surface density of states. The contribution of bulk spin waves can be obtained directly from general formulation of section 2.3 (See Fig.2.4) but the contribution of surface spin waves needs to be discussed separately.

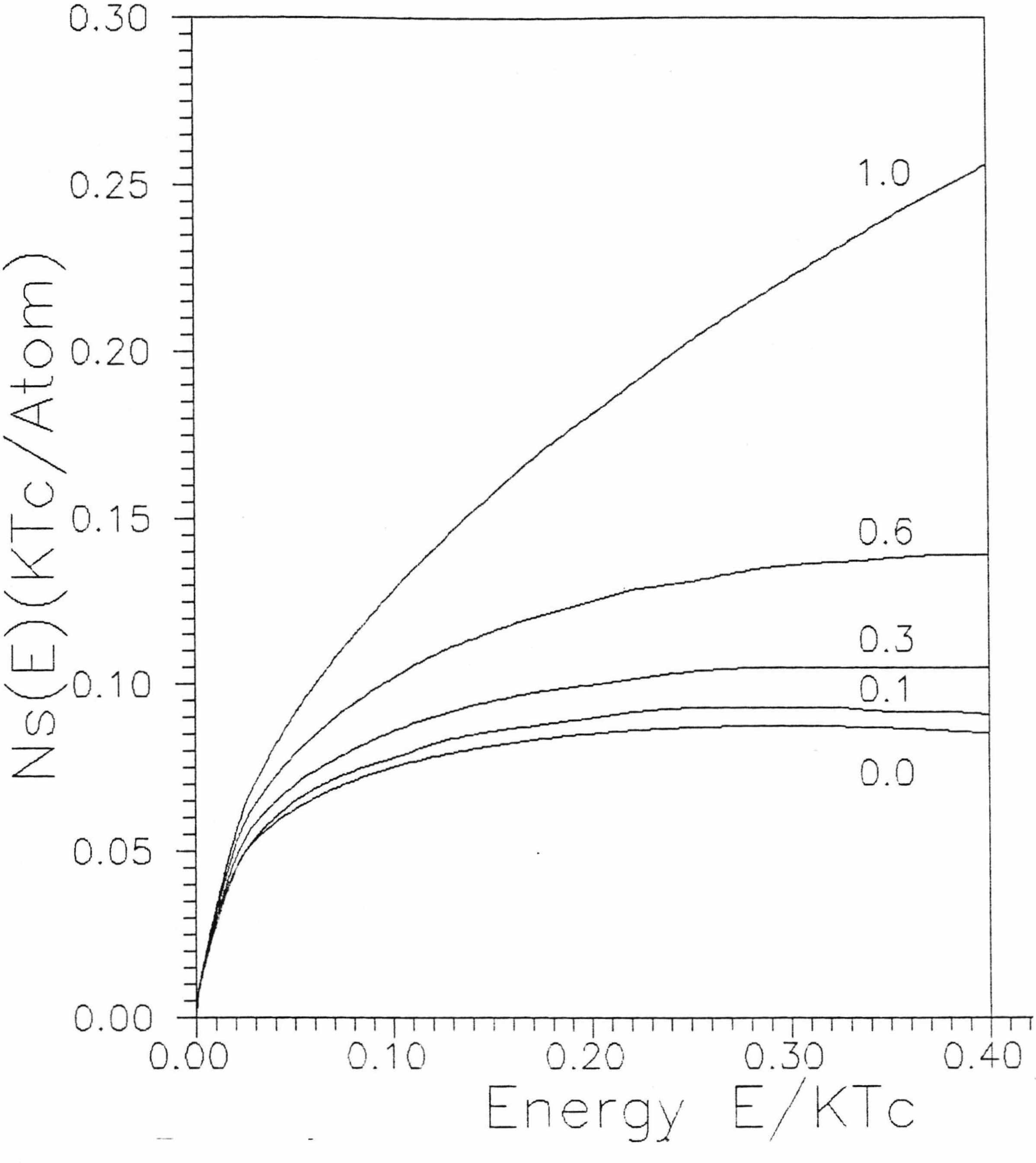

Fig.2.4 The surface density of spin wave states $N_S(E)$ for an atomic overlayer above (100) surface of sc ferromagnet with a softened parallel exchange J_{11}. The values J_{11}/J are 0.0, 0.1, 0.3, 0.6 and 1.0.

2.4 The Effect of Surface Spin Waves on the Surface DOS for One Adlayer

2.4.1 Introduction to Surface Spin Waves

Magnetic surface waves are excitation of the transverse component of the magnetization, whose amplitute is localized near the surface of a magnetically ordered system. These waves are characterized by wave vector $\underline{q}_{\parallel}$ parallel to the surface, and one or more (sometimes complex) attenuation constants, which describe the excitation amplitude as a function of distance into the crystal normal to the surface.

Magnetic surface waves are predicted by both microscopic and macroscopic theories. In the microscopic Heisenberg theory, surface spin waves occur because of abrupt changes in the exchange interactions at and near the surface. In macroscopic magnetostatic theory, they are associated with shape dependent demagnetization fields. In general, dipolar, exchange, crystal orientation, applied magnetic field orientation, size and shape effects influence the magnetic surface wave dispersion (See Mills, 1984).

The name surface magnon or surface spin wave is used for surface waves for which the exchange interaction is the dominant energy at low temperature ($T \simeq 0$). Surface spin waves of ferromagnets have been the subject of extensive study. Most of the discussion have been concerned with one of two types of model, semi-infinite itinerant ferromagnet or semi-infinite Heisenberg ferromagnet. Gumbs and Griffin (1980), Weling (1980) and Mathon (1981 and 1986) have done Hubbard model calculations for itinerant ferromagnet with (001) surface. Mills and Maradudin (1967) first discussed the criteria for the existence of surface states in Heisenberg ferromagnets and their effect on the thermodynamic properties using a simple cubic (001) model of a surface. De Wames and Wolfram (1969) showed that surface states below or above the bulk spectrum can occur with appropriate perturbations at the surface of a Heisenberg ferromagnet. The method of retarded Green's function had been applied by Selzer and Majlis (1982 and 1983) to study the surface spin waves, surface magnetization, and surface Curie temperature of a semi-infinite Heisenberg ferromagnet.

However, none of these authors have studied the effect of surface spin waves on $M_s(T)$ beyond the classical region. Guided by our results for $J_{10} < J$, we expect that, in contrast to the classical region, the behaviour of $M_s(T)$ will be strongly influenced by deviations of J_{11} from J and surface spin waves clearly play an important role. We shall, therefore, apply our method of adlayers to surface spin waves.

2.4.2 Method of Calculation

We know from the work of De Wames and Wolfram (1969), that surface spin waves exist below the bulk band ($\omega < -1$) when parallel surface exchange satisfies $J_{11}/J< 1$. We are only interested in surface spin waves below the bulk band because they influence the $T^{3/2}$ law. Our aim in this section is to obtain the surface spin wave Green's function below the bulk band using the adlayer method in the case of softening of the parallel surface exchange J_{11}.

We can obtain the surface spin wave Green's function G^1_{11}, from Eq.(2.2.15)

$$G^1_{11} = \frac{1}{\omega + W_{11} - \dfrac{(W_{01})^2 G^0_{00}}{1 - W_{00} G^0_{00}}}$$

with perturbations

$W_{00} = 1/2$, $W_{10} = -1/2$ and $W_{11} = 1/2 + (1 - \beta)(E - \omega - 1)$

where $\beta = J_{11}/J < 1$ and G^0_{00} is given by Eq.(2.3.4) .

We note that $\mathrm{Im}G^0_{00} = I$ vanishes for $\omega < -1$ and, therefore, surface spin waves appear as isolated poles of G^1_{11}. To obtain such isolated poles, we have to introduce a small imaginary part to ω, i.e. $\omega \rightarrow \omega + i\delta$. It is then straightfoward to show that the imaginary part of G^1_{11} is given by

$$\underset{\delta\to 0}{Im G^1_{11}} = \pi\, \delta(\omega + 1/2 + (1 - \beta)(E - \omega - 1) - 1/2(\omega^2 - 1)^{1/2})$$

for $\omega < -1$. (2.4.1)

Spin wave poles are, therefore, obtained from

$$\omega + 1/2 + (1 - \beta)(E - \omega - 1) - 1/2\ (\omega^2 - 1)^{1/2} = 0 \quad (2.4.2)$$

We can now define $\Lambda = E - 1 - \omega$ and substitute this new variable in Eq.(2.4.2). This leads to the following results for the surface spin wave energy E:

$$E = \Lambda\, \frac{[1 + 2\beta(1 - \beta)\Lambda]}{[1 + 2(1 - \beta)\Lambda]} \quad (2.4.3)$$

where

$\Lambda = W - 1$ and $W = E - \omega$.

Equation (2.4.3) is valid both for $\beta < 1$ and $\beta > 1$. We are only interested in $\beta < 1$. This equation is identical with the results of De Wames and Wolfram (1969). De Wames and Wolfram showed that there are no surface spin waves in the interval $1 < \beta < 5/4$ for $0 \le \Lambda \le 4$. Fig.2.5 shows the dispersion curves of surface spin waves (acoustical surface branch) below the bulk spectrum for $\beta = 0.5$ and above the bulk spectrum for $\beta = 2.0$ (optical branch). The dispersion curve for the bulk spectrum $E = \Lambda + c$ ($0 \le C \le 2$) is a special case of Eq.(2.4.3) for $\beta = 1$.

By combining Eq.(1.3.14), Eq.(2.3.6) and Eq.(2.4.1), and using symmetry properties of the integrand, we find that the surface spin wave density of states is given by

$$N_s(E) = \frac{a^2}{\pi^2} \iint_{-\pi/a}^{0} \delta\left(\frac{\omega + 1}{2} + (1-\beta)\Lambda - 1/2\ (\omega^2+1)^{1/2} \right) dq_x\ dq_y \tag{2.4.4}$$

To make evaluation of Eq.(2.4.4) easier, we set $q_x a = x$ and $q_y a = y$ and then use the substitution

$$f(x,y) = \frac{\omega + 1}{2} + (1-\beta)\Lambda - 1/2\ (\omega^2+1)^{1/2} = t \text{ and } y = u.$$

The surface spin wave DOS then becomes

$$N_s(E) = (1/\pi)^2 \iint \delta(t)\ |\ J(t,u)\ |\ du\ dt \tag{2.4.5}$$

where the Jacobian J(t,u) is given by

$$J(t,u) = 1/\sin(x) \frac{2}{1 - 2(1 - \beta) - \omega(\omega^2 - 1)^{-1/2}} \tag{2.4.6}$$

Using the delta function in Eq.(2.4.5), we can set $t = 0$ in the Jacobian, which yields

$$Ns(E) = (1/\pi)^2 \int\ |\ J(0,u)\ |\ du \tag{2.4.7}$$

where

$$J(0,u) = 1/\sin(x) \frac{2}{1 - 2(1 - \beta) - \omega\ [(\omega\ \ + 1) + 2(1 - \beta)\Lambda]^{-1}}$$

and the term $(\omega^2 - 1)^{-1/2}$ in Eq. (2.4.6) becomes $(\omega + 1) + 2\,(1 - \beta)\Lambda$.

Therefore, Eq.(2.4.7) becomes

$$N_s(E) = (1/\pi)^2 \int \frac{1}{[1-\cos^2(x)]^{1/2}}\,\frac{2\,du}{1-2(1-\beta)-\omega\,[(\omega+1)+2(1-\beta)\Lambda]^{-1}}$$

subject to the restriction $-1 < \cos(x) = \Lambda - 2 - \cos(u) < 1$.

(2.4.8)

To evaluate the integral in Eq.(2.4.8), we have to determine the values of Λ from Eq.(2.4.3). Λ satisfies a quadratic equation

$$2\beta(1-\beta)\Lambda^2 + [1-2(1-\beta)E]\Lambda - E = 0 \qquad (2.4.9)$$

whose solution is given by

$$\Lambda = \frac{[2(1-\beta)E-1] + [4(1-\beta)^2E^2 + 4(1-\beta)(2\beta-1)E + 1]^{1/2}}{4\beta(1-\beta)} \qquad (2.4.10)$$

(We take the solution for Λ with for + sign only because $\Lambda \geq 0$).

To evaluate the integral in Eq.(2.4.8), we shall make the substitution

$$\cos(x) = \Lambda - 2 - z, \text{ where } z = \cos(u)$$

Equation (2.4.8) then becomes

$$N_s(E) = \frac{-2}{\pi^2} \frac{E+(1-2\beta)\Lambda}{4\beta(1-\beta)\Lambda-2(1-\beta)E+1} \int \frac{dz}{[1-z^2]^{1/2} \quad [1-(\Lambda-2-z)^2]^{1/2}}$$

where z satisfies $-1 < z < \Lambda - 1$. (2.4.11)

To remove a divergence at $z = -1$ in Eq.(2.4.11), we rewrite the integrand as

$$\int_{-1}^{\Lambda-1} \frac{dz}{[1-z^2]^{1/2} \; [1-(\Lambda-2-z)^2]^{1/2}}$$

$$= \int_{-1}^{\Lambda-1} \frac{dz}{[1-z^2]^{1/2} \; [1-(\Lambda-2-(-1))^2]^{1/2}} +$$

$$\int_{-1}^{\Lambda-1} \frac{1}{[1-z^2]^{1/2}} \left[\frac{1}{[1-(\Lambda-2-z)^2]^{1/2}} - \frac{1}{[1-(\Lambda-2-(-1))^2]^{1/2}}\right] dz$$

(2.4.12)

where the second term becomes zero for $z \rightarrow 1$.

The surface DOS computed from Eq.(2.4.12) is shown in Fig.2.6. It is very clear from Fig.2.6, that surface spin wave DOS is much higher than the bulk spin wave DOS (See Fig.2.4). Therefore, large contribution to the total DOS for softening of the parallel exchange comes from the surface spin wave DOS beyond the classical region (See Fig.2.7).

It is very clear that the calculation using Simpson's algorithm for surface spin wave DOS described above is quite complicated. When we come to more complex systems e.g. thick overlayer problem (See section 2.6) or interface problem (See chapter 3) the calculation becomes intractable. Therefore, we have to find another method to avoid this difficulty in calculating spin wave DOS. In the next section we introduce an alternative method using special points in two-dimensional Brillouin zone to get spin wave DOS.

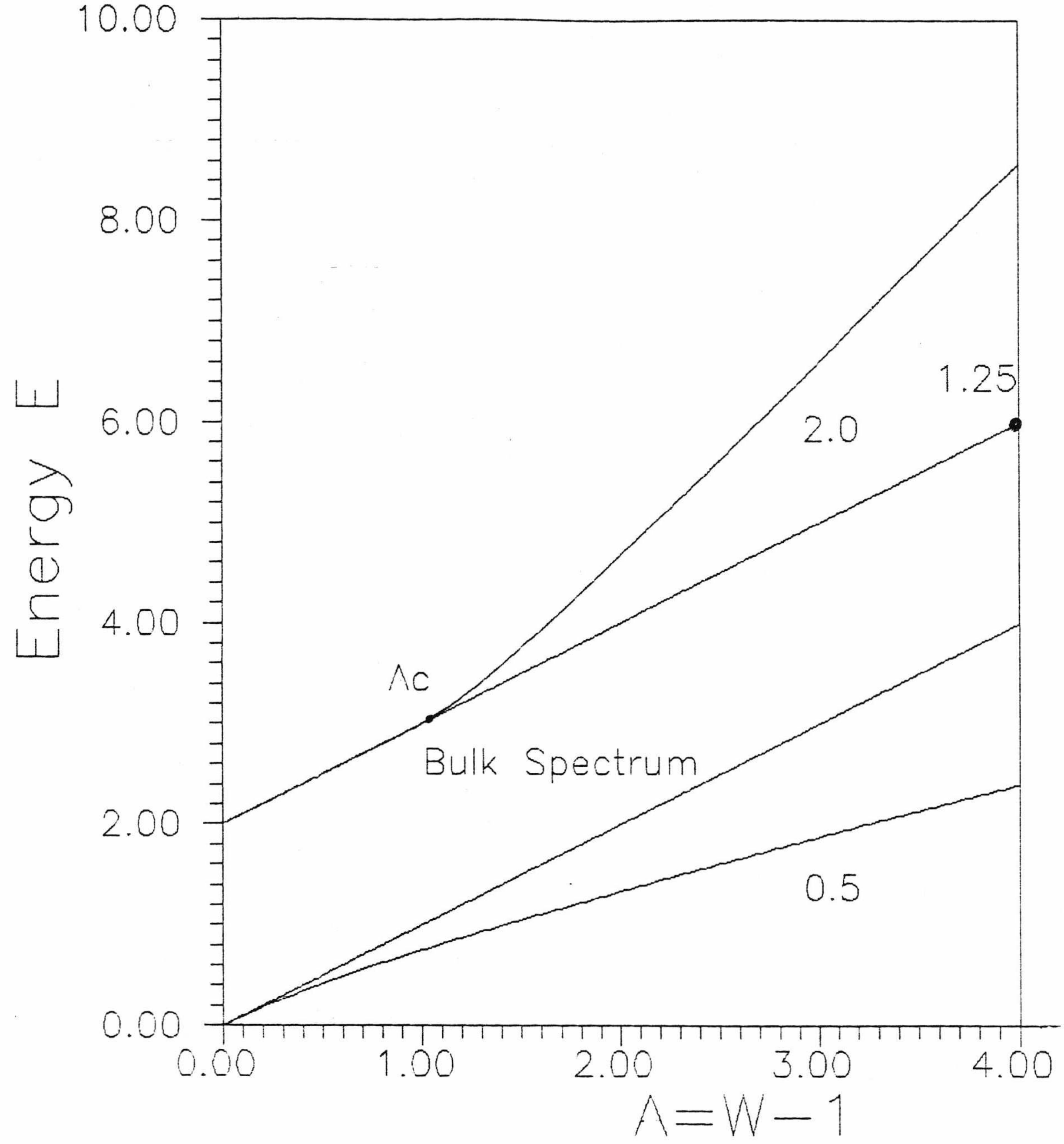

Fig.2.5 Dispersion curves for the (100) surface of sc ferromagnet for $J_{11}/J = 0.5$ and 2.0 with $J_{10}/J = 1.0$.

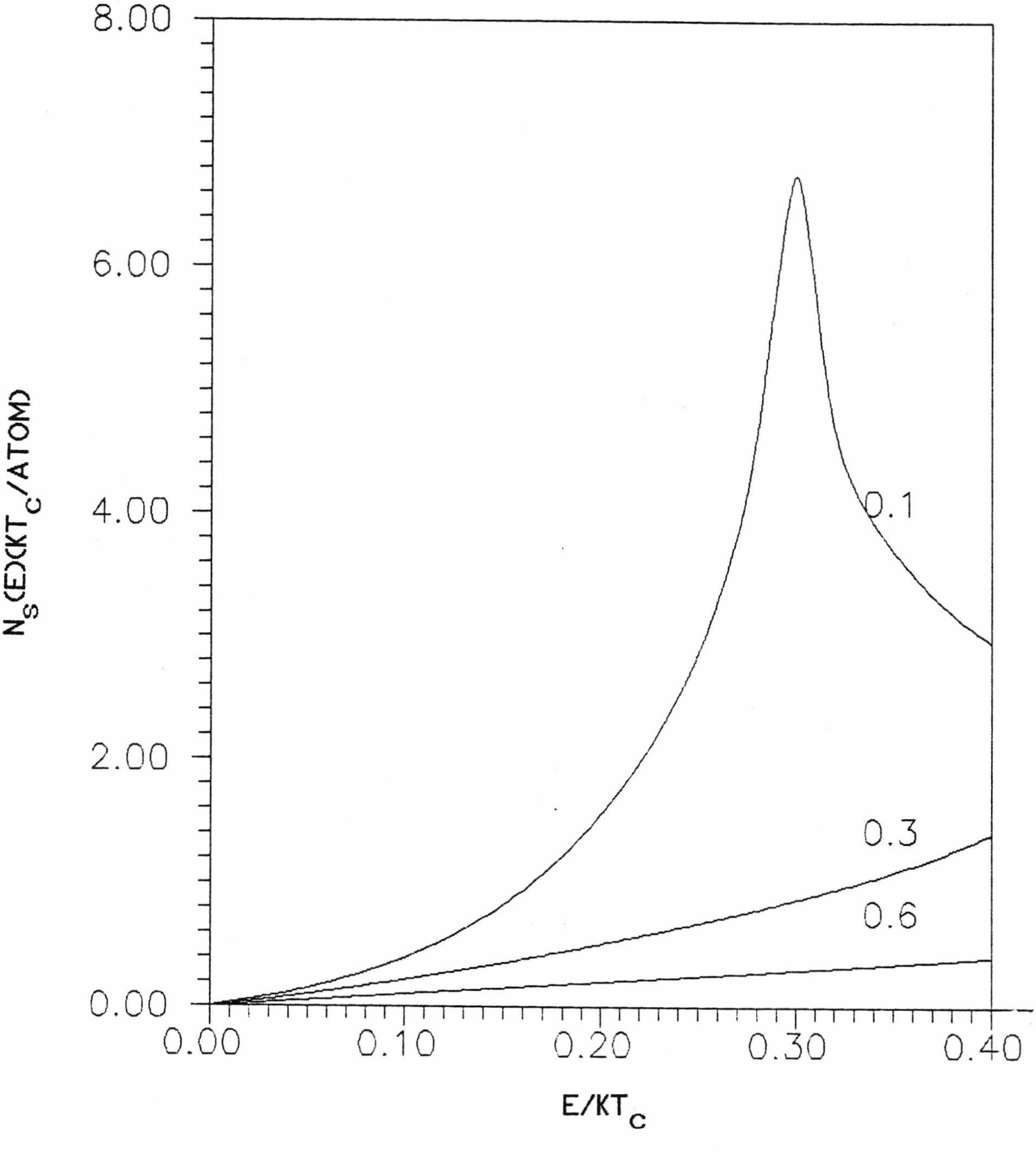

Fig.2.6 The density of states of surface spin waves $N_S(E)$ in the (100) surface of a sc ferromagnet with a softened parallel exchange J_{11} within the surface of overlayer. The values of J_{11}/J are 0.1, 0.3 and 0.6.

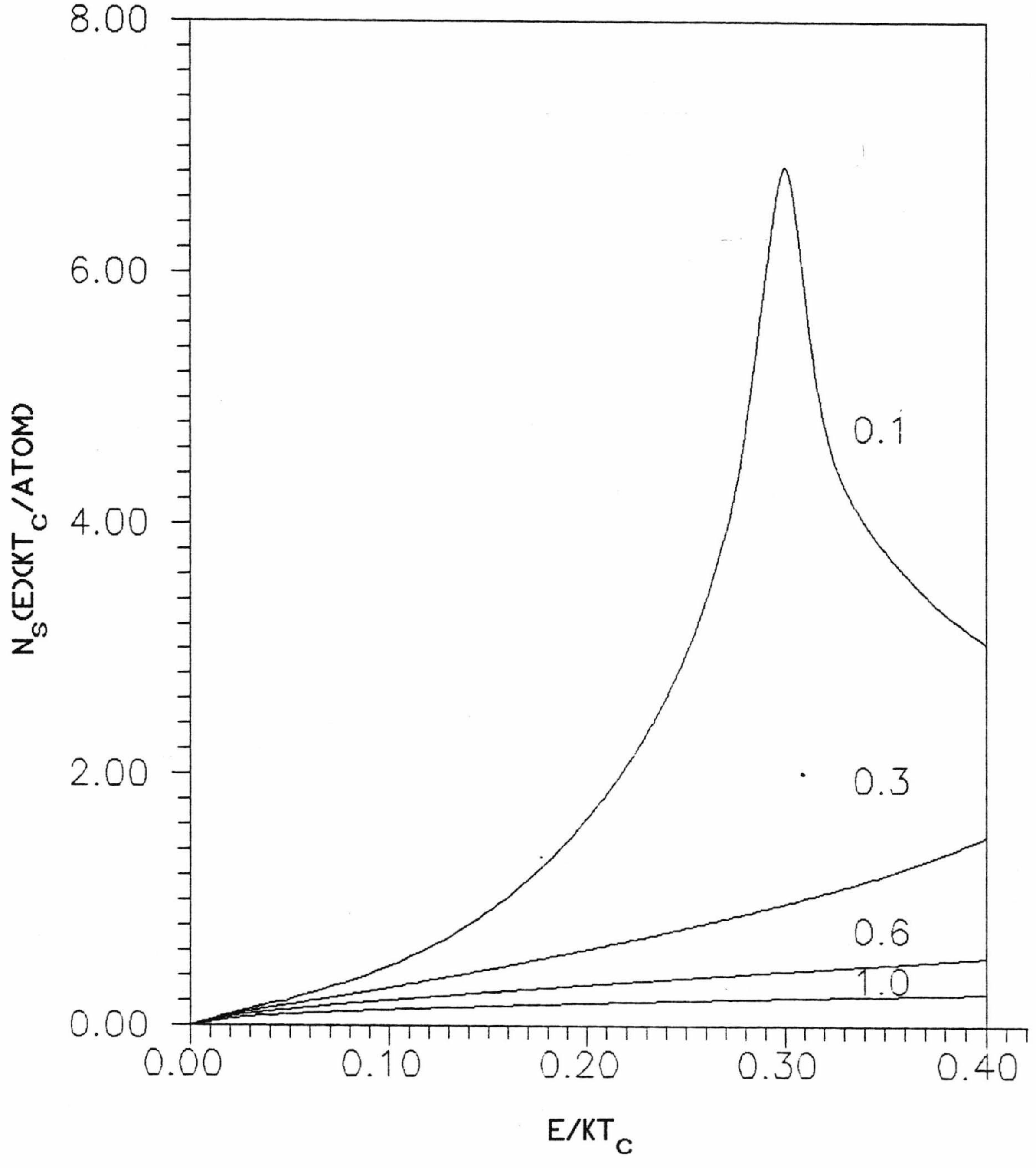

Fig.2.7 The total densities of spin waves states $N_S(E)$ in the (100) surface of a sc ferromagnet with a softened parallel exchange J_{11} within the surface of overlayer. The values of J_{11} are 0.1, 0.3, 0.6 and 1.0.

2.4.3 Special Points In The Two-Dimensional Brillouin Zone

2.4.3.1 Introduction

Calculation of the density of spin wave states at crystal surfaces involves averaging of a periodic function of wave vector parallel to the surface over two-dimensional Brillouin zone. These averages are determined by sampling the function at a discrete set of points and summing with an appropriate weight for each point.

To obtain this special wave vector points set for the two dimensional Brillouin zone which is associated with two dimensional lattice types, Cunningham (1974) developed a method, which is based on the two following important steps

i. Expanding the function $f(\vec{K})$ as

$$f(\vec{K}) = f_0 + \sum_{m=1} f_m A_m(\vec{K}), \qquad (2.4.14)$$

where

$$A_m(\vec{K}) = \sum_{|\vec{R}|=c_m} e^{i\vec{K}.\vec{R}}, \quad m=1,\ 2,\ 3,\ \ldots.., \qquad (2.4.15)$$

and where $\vec{K}$ and $\vec{R}$ are the two-dimensional wave vector and lattice vector, respectively.The sum in Eq.(2.4.15) is over all lattice vectors of equal magnitude.

ii. Obtain best set points of $\{k_i\}$ and weighting factors $\{\alpha_i\}$ such that the exact average function over two-dimensional Brillouin zone of Eq.(2.4.14) is equal to fo (See Cunningham, 1974 for details).

As an example, for square lattice, the following ten special wave vector points can be chosen in the irreducible wedge of the two-dimensional Brillouin zone (See Fig. 2.8):

i. (1/8,1/8), (3/8,3/8), (5/8,5/8) and (7/8,7/8) with weighting factor α = 1/16, and

ii. (3/8,1/8), (5/8,1/8), (7/8,1/8), (5/8,3/8), (7/8,3/8) and (7/8,5/8) with weighting factor α = 1/8.

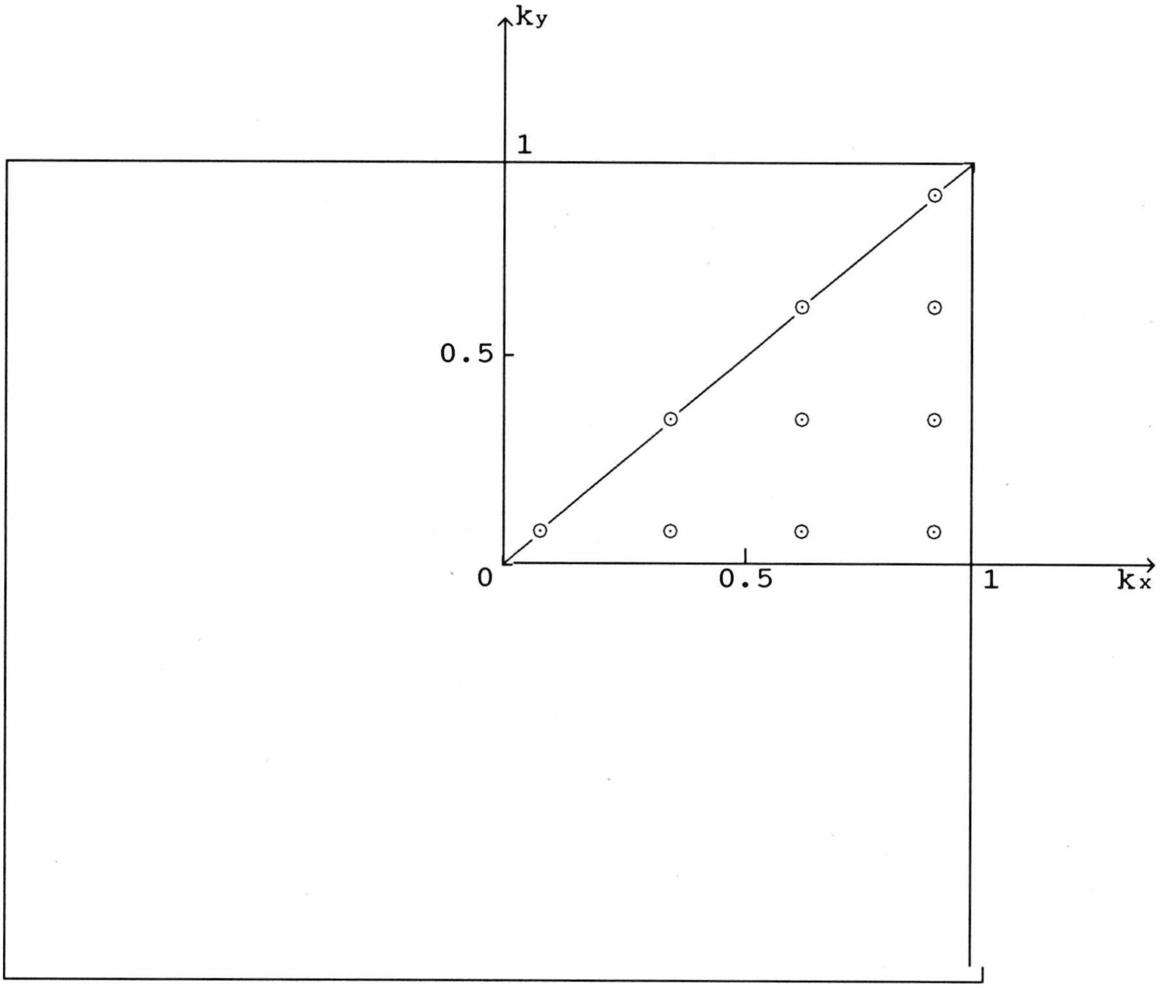

Fig. 2.8. Two-dimensional Brillouin zone for simple cubic lattice and its irreducible segment which contains a ten-point set of special wave vector points.

2.4.3.2 Brillouin Zone Summation Using Cunningham Special Wave Vector Points

We recall Eq.(1.3.14) for density of spin wave state as

$$\rho(E) = 1/\pi \sum_{k_{\parallel}} \mathrm{Im}G(m,m,k_{\parallel})$$

where

$\{k_{\parallel} = (k_x,k_y)\}$ is the set of ten special wave vector points in section 2.4.3.1 above.

We can rewrite all the wave vector points as

$$k_x = \pi - (\pi/8)(2n_1 - 1),\ n_1 = 1,\ 2,\ 3,\ 4$$

and (2.4.16)

$$k_y = \pi - (\pi/8)(2n_2 - 1),\ n_2 = 1,\ ..,\ n_1$$

Finally, in doing the summation we have to multiply each term by the respective weighting factor.

In general, the special wave vector points discussed above can be written in terms of the number of Cunningham points $nc = 2^n$ in one direction (e.g. k_x), where n is an integer. The ten special points in 1/8 of the Brillouin zone above is just a special case nc = 4. The total number of Cunningham points in 1/8 of the Brillouin zone is nc * (nc + 1)/2. Therefore, we can rewrite Eq.(2.4.16) in terms of nc as

$$k_x = \pi - (\pi/2\ nc)(2\ n_1 - 1),\ n_1 = 1,\ 2,\ \ldots.,\ nc$$

and (2.4.17)

$$k_y = \pi - (\pi/2\ nc)(2\ n_2 - 1),\ n_2 = 1,\ 2,\ \ldots.,\ n_1$$

In order to get the required degree of accuracy, the number of Cunningham points nc should be increased in the irreducible segment of the Brillouin zone until the results stabilize. To get numerically stable results, the number of Cunningham points nc should be matched to the imaginary part ε of the complex energy $ec = e + \varepsilon i$ that we use in calculating DOS. The advantages of using complex energy ec are that it removes any singularity (if present) of the function to be integrated and we can obtain the total DOS (surface spin wave DOS and bulk spin wave DOS) directly. In the next section we give the subroutine for two-dimensional Brillouin zone integration we have used in our calculation of spin wave DOS for the case $J_{11}/J < 1$, $J_{10}/J = 1$ and $S_1/S = 1$. The number of Cunningham points we used was nc = 128 and the imaginary part of the energy ec was $\varepsilon = 0.01$. These values lead to numerically stable results.

2.4.3.3 Application of the Subroutine for Two-Dimensional Brillouin Zone Integration to the Case $J_{\parallel} < J$

The subroutine below, performs the two-dimensional Brillouin zone integration using Cunningham points nc for (100) surface in a simple cubic ferromagnet. It is to be used to integrate a function gnew depending on k_1, k_2, complex energy ec, exchange integrals a and b, spin enhancement c and overlayer index n. This function is supplied as subroutine gmagov(n,k_1,k_2,ec,a,b,c,gnew) where gmagov generates a Green function gnew of an arbitrary overlayer. Here, the function dos is the integrated result.

```
       Subroutine swdos(n,ec,a,b,c,nc,dos)
       real a, b, c, k1, k2, dosk, dos
       complex ec, gnew
       dos=0
       pi = acos(-1.0)
       do 1000 nk = 1, nc
       k1 = pi*(2*nk - 1)/(2*nc) - pi
       do 1000 mk = 1, nk
       k2 = pi*(2*mk - 1)/(2*nc) - pi
       call gmagov(n,k1,k2,ec,a,b,c,gnew)
       dosk = -(1./pi)*aimag(gnew)
       dosk = 2.*dosk/(nc**2)
       if (nk.eq.mk) go to 990
       go to 991
990    dosk = 0.5*dosk
991    continue
       dos = dos + dosk
1000   continue
       return
       end
```

The results of the calculated spin wave DOS with a softened parallel exchange $J_{11} < J$ using the above subroutine are shown in Fig.2.9. It can be seen that a very good agreement is obtained with our previous results for the total DOS shown in Fig.2.7 which were obtained by treating surface and bulk spin waves separately.

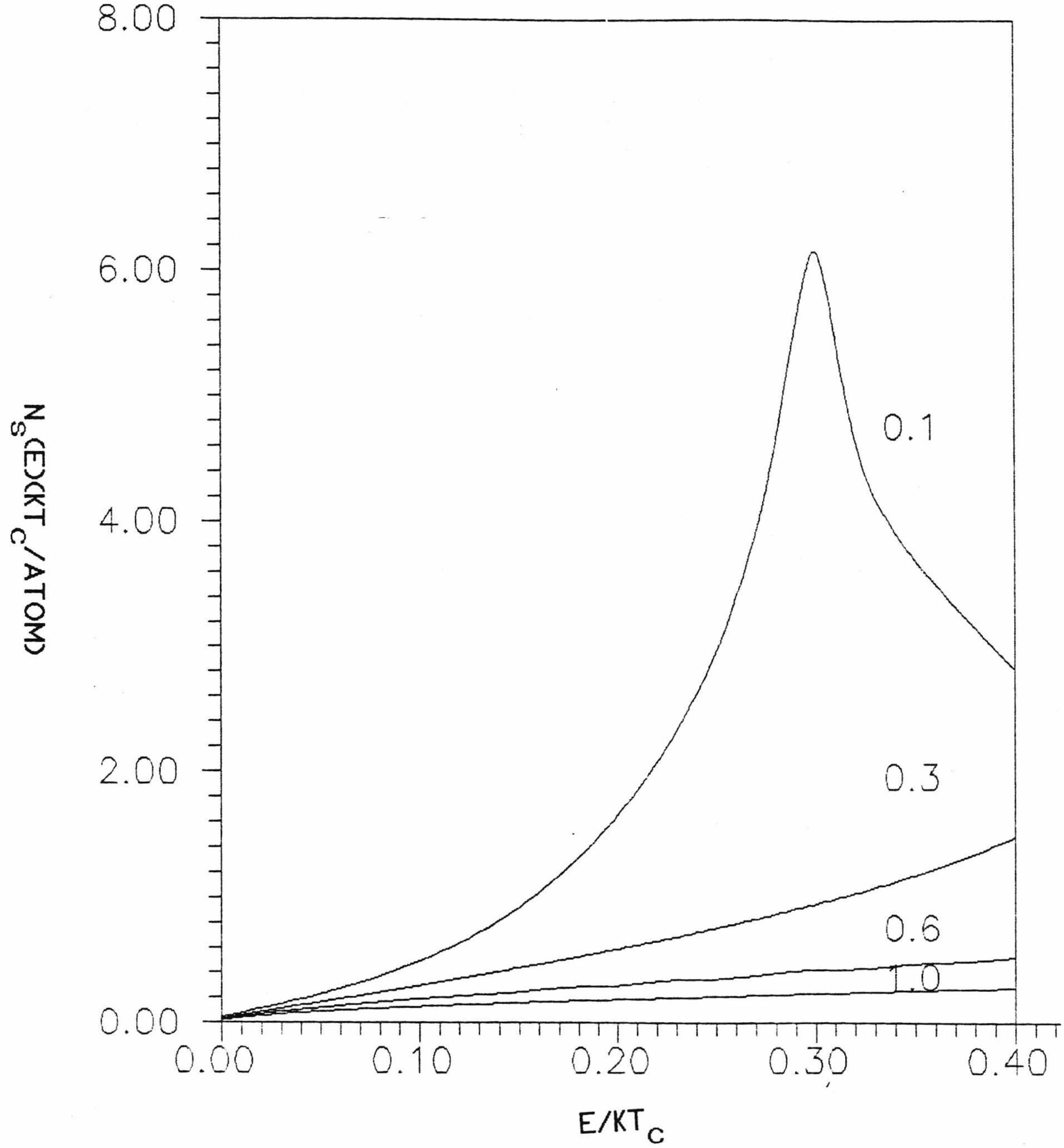

Fig.2.9 The total densities of spin waves states $N_s(E)$ for an atomic overlayer above (100) surface of sc ferromagnet with a softened parallel exchange J_{11}. The result is obtained by using Cunningham points integral in BZ: nc = 128 and eps = 0.01.

2.5. Temperature Dependence of Surface Magnetization for One Adlayer

We can now use the DOS in Fig.2.3 and Fig.2.7 to calculate the temperature dependence of the surface magnetization $M_S(T)$. Our aim is to test whether $M_S(T)$ obeys a good $T^{3/2}$ law and to investigate the effect of softening of surface exchange on $M_S(T)$. The temperature dependence of the surface magnetization $M_S(T)$ is calculated from the surface spin deviation $\Delta_s(T)$ given by Eq.(2.1.2) and from Eq.(2.3.7) or Eq.(2.3.11) for the surface DOS.

We shall first discuss briefly the $M_S(T)$ at very low temperatures when the surface DOS $N_S(E)$ is given by Eq.(2.3.13). Since $N_S(E) = 2N_B(E)$ for $E \simeq 0$, we have from Eq.(2.1.2):

$$M_s(T)/M_s(0) = 1 - 2\, B_B\, T^{3/2} \qquad (2.5.1)$$

where $B_B = 0.1174\ (k_B)^{3/2}$ is the bulk prefactor in the $T^{3/2}$ law .

We have thus proved two general results:

i. Deviations of the surface exchange integrals from the bulk J have no effect on the <u>initial</u> $T^{3/2}$ law.

ii. Deviations of the surface magnetization from its bulk value has also no effect on the initial $T^{3/2}$ law (this is because the factor S_1/S is exactly cancelled in Eq. (2.5.1)).

The first result was obtained earlier by Mills (1970) for the special case of softening of J_{11} only. We conclude that, initially, the surface magnetization always decreases twice as fast as in the bulk. This seems to contradict the experiment of Pierce et al. (1982) which gives a good $T^{3/2}$ law but with "wrong" prefactor. However, there is a natural explanation of this paradox within the spin wave theory. Although we always obtain initially the classical law , we shall show that it holds only at temperatures so low that they are of no practical interest. It is, therefore, necessary to go beyond the initial classical region.

2.5.1 Case $J_{10}/J < 1$, $J_{11}/J = 1$ and $S_1/S = 1$

From our discussion in section 2.3, we can see that there are three different regions of the spin wave density of states $N_s(E)$ depending on the energy E and on the strength of the exchange integral J_{10} with respect to bulk J. We expect that these three regions are going to lead to different behaviour of $M_S(T)$. The first region is the temperature range $T \simeq 0$, where the result of Rado and of Mills and Maradudin holds. Then comes the second (crossover) region corresponding to the upturn of the DOS curves and this is followed by an extended temperature interval where we expect with an "effective " $T^{3/2}$ law but the prefactor of this "second" $T^{3/2}$ law should depend strongly on J_{10}.

Fig.2.10 shows the temperature dependence of the surface magnetization $M_s(T)/M_s(0)$ for a range of values of J_{10}. It can be seen that a perfect fit to the experimental results of Pierce et al. (1982)(open circle) is obtained for $J_{10}/J = 0.3$. To test whether our calculated $M_S(T)$ obeys a good $T^{3/2}$ law, we plot in Fig.(2.11) the temperature dependence of the surface magnetization $M_s(T)/M_s(0)$ against the bulk dependence $M_s(T)/M_s(0)$ for $J_{10}/J = 0.3$. It can be seen from Fig.2.11 that an almost perfect straight line can be fitted to the computed points over the whole temperature range up to $T \simeq 0.4T_c$. The same straight line is also the best fit to the experimental points of Pierce et al. (1982). We recall that Pierce et al. (1982) measured $M_s(T)/M_s(0)$

between 80 and 300 K for $Ni_{40}Fe_{40}B_{20}$ with an estimated $T_c \simeq$ 700 K.

Softening of exchange perpendicular to the surface seems, therefore, to be an explanation of the observed behaviour of $M_s(T)$ for $Ni_{40}Fe_{40}B_{20}$. However, we cannot exclude at this stage the possiblity that softening of J_{11} also plays a role. To test our theory, we need a system for which J_{10} can be varied in a controlled way. This can be achieved in magnetic layer structures and Mauri et al. (1989) designed recently an experiment which can be compared directly with our calculation for $J_{10}/J < 1$. Their experiment was done on a sandwich with Ta interlayer separating a ferromagnetic NiFe substrate from a ferromagnetic NiFe surface (See Fig.2.12). They measured, using secondary polarized electrons, the magnetization M(T) in the surface NiFe layer. By increasing of the thickness of the Ta layer, they reduced the strength of perpendicular exchange between the surface and the substrate. Therefore, the surface to bulk exchange could be weakened in a controlled way.

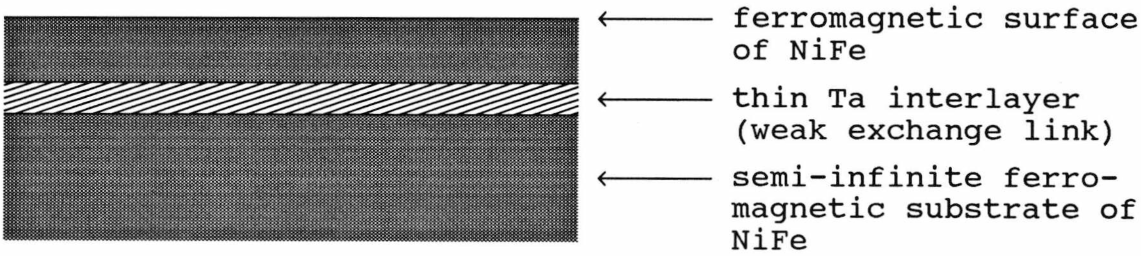

Fig.2.12 The NiFe-Ta-NiFe sandwich with thin Ta interlayer (different thicknesses) as a controller for weak exchange link.

Their experimental results for the temperature dependence $M_S(T)$ plotted against the bulk dependence $M_B(T)$ are shown in Fig.(2.13) for three thicknesses of the Ta interlayer: 0.5, 1.0, 1.5 at. layers (curves a, b, and c). The curve O is for clean parmaloy surface. This experiment shows very clearly that the surface magnetization follows a $T^{3/2}$ law at temperatures $T/T_C \leq 0.4$ with prefactors $k = 2.5$, 4.1 and 5.7 for a, b and c ferromagnetic films.

We may, therefore, conclude that

i. Good $T^{3/2}$ law is obeyed as predicted by our theory.

ii. The Prefactor in the $T^{3/2}$ law increases with decreasing J_{10}, as predicted by our theory.

It is clear that comparing the measured $M_S(T)$ with our spin wave theory, we can determine the strength of the surface to bulk exchange for this system.

For a general surface, the effect of softening of exchange in the surface plane may occur and its effect on $M_S(T)$ needs to be investigated.

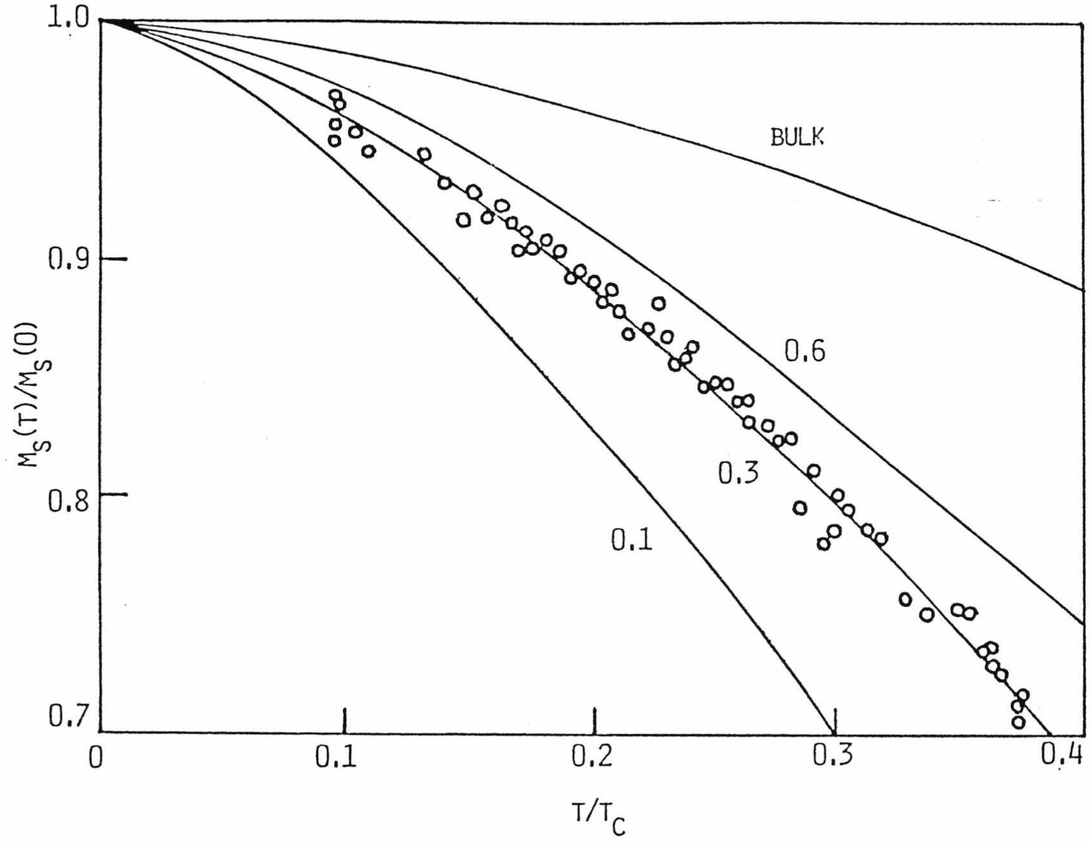

Fig.2.10 Calculated temperature dependence of the surface magnetization $M_s(T)/M_s(0)$ for an atomic overlayer with a softened J_{10} between the surface layer and the substrate. The values of J_{10}/J are 0.1, 0.3 and 0.6. Open circles are the experimental points of Pierce et al.

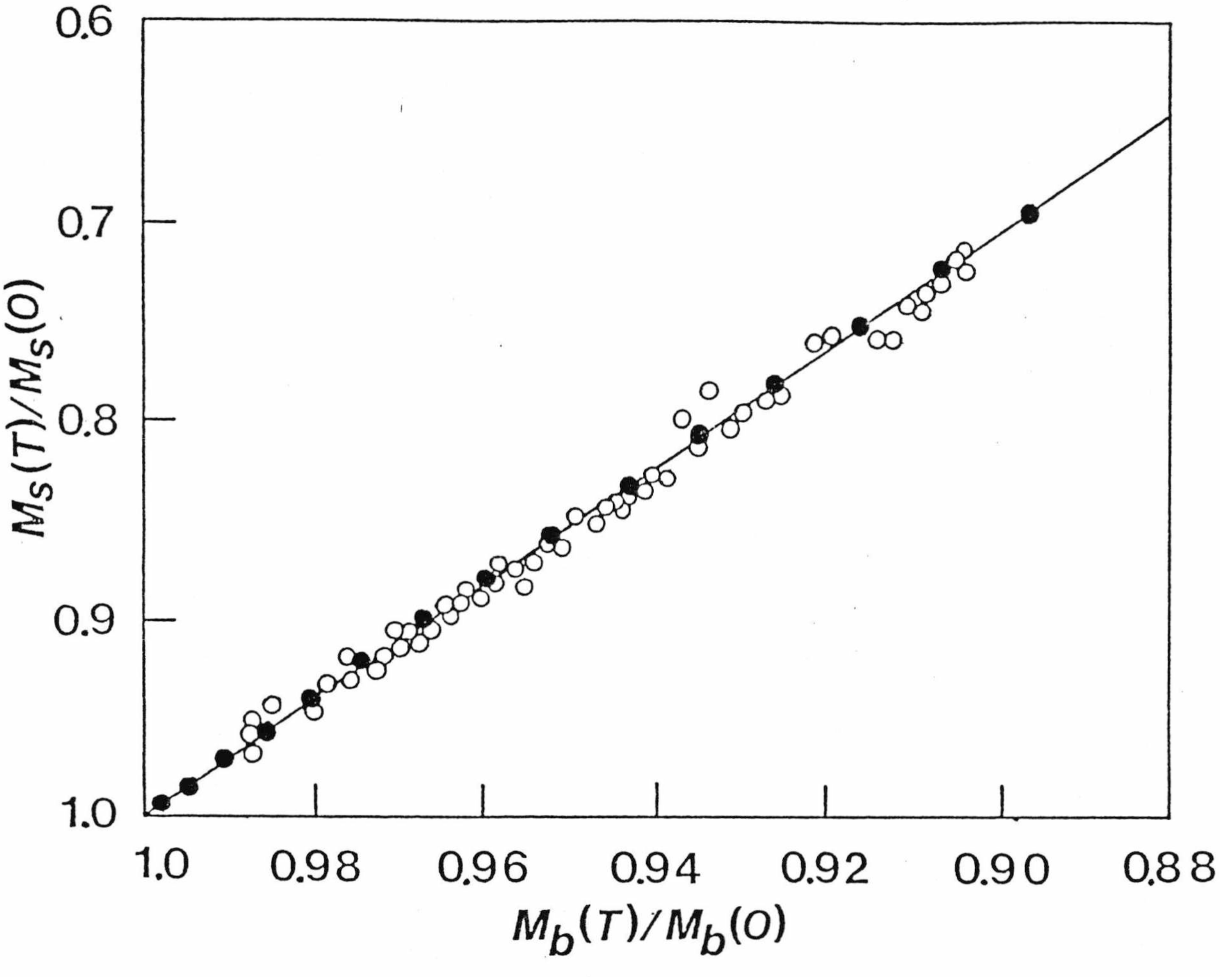

Fig.2.11 Plot of the temperature dependence of the surface magnetization $M_s(T)/M_s(0)$ against the bulk dependence $M_B(T)/M_B(0)$. Full circles are the calculated results and open circles are the SPLEEDresults of Pierce et al.. The first calculated point is for $T=0.02T_c$ and the last for $T=0.3T_c$.

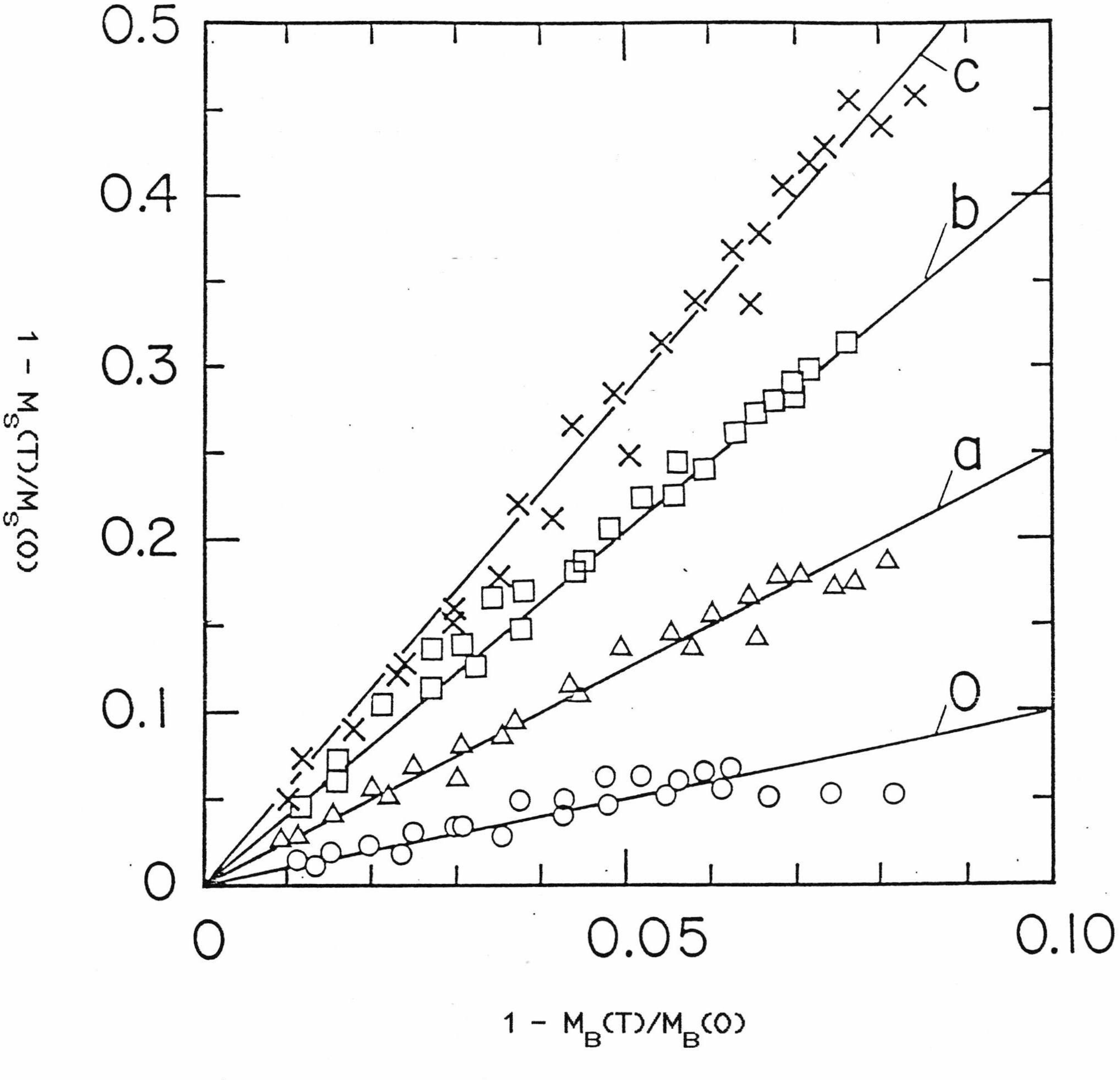

Fig.2.13 Experimental results of Mauri et al. (1989) for $M_s(T)$ in FeNi-Ta-FeNi sandwich. The surface $M_s(T)$ is plotted against the bulk $M_B(T)$ for three thicknesses of Ta interlayer: 0.5, 1.0, 1.5 at. layer (curves a, b, c; 0 is for clean permalloy surface).

2.5.2 Case $J_{11}/J < 1$, $J_{10}/J = 1$ and $S_1/S = 1$

We use the same procedure as in section 2.5.1 to calculate the surface magnetization $M_S(T)$. The computed temperature dependence $M_s(T)/M_s(0)$ against temperature T is shown in Fig.2.14 for a range of values of J_{11}/J. It can be seen that the surface magnetization decreases with temperature even faster than the surface magnetization for the case of softening J_{10} (Fig.2.10). This happens because surface spin waves are excited and they are localised in the surface plane. To test whether the calculated $M_S(T)$ curves lead to a good $T^{3/2}$ law, we have plotted in Fig.2.15 $M_s(T)$ against the true Bloch law for the bulk $M_B(T)$. It can be seen from Fig.2.15 that a very good Bloch law holds in the case $J_{11}/J = 0.6$ up to temperature $T \simeq 0.3kT_c$ with $k \simeq 5.5$. Much higher values of k are obtained for smaller J_{11} but the Bloch law is not so well obeyed over the whole temperature range shown. However, one can fit a good straight line to a curve corresponding to $J_{11}/J = 0.3$ between $T/T_c \simeq 0.1$ and 0.3. Therefore, the effect of softening of parallel exchange $J_{11}/J = 0.6$ on $M_S(T)$ is equivalent to the effect of softening of the perpendicular exchange $J_{10}/J = 0.3$.

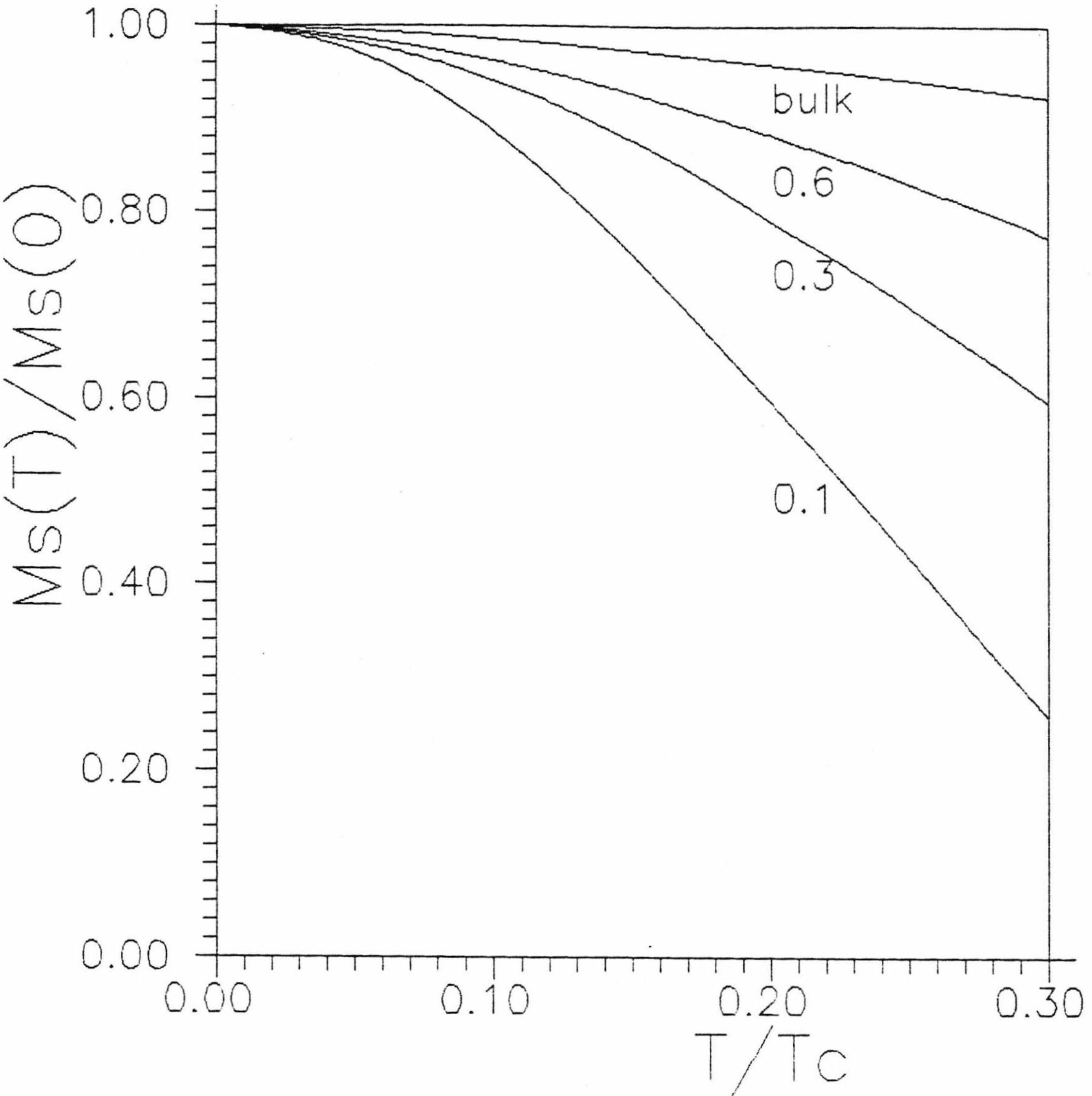

Fig.2.14 Calculated temperature dependence of the surface magnetization $M_s(T)/M_s(0)$ for an atomic overlayer with a softened J_{11} within the surface layer. The values of J_{11}/J are 0.1, 0.3 and 0.6.

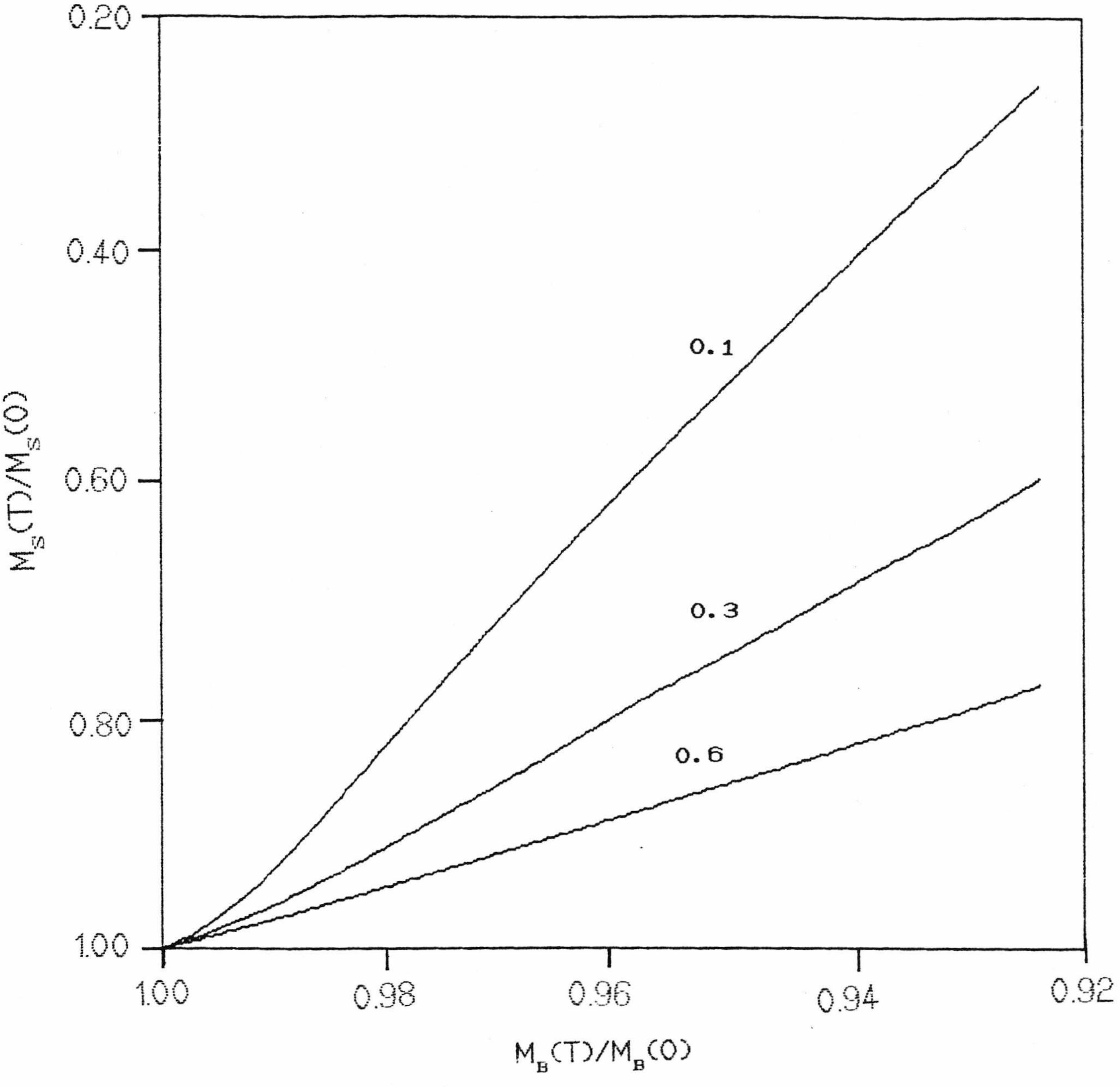

Fig.2.15 Plot of the temperature dependence of the surface magnetization $M_s(T)/M_s(0)$ against the bulk dependence $M_B(T)/M_B(0)$ for J_{11}/J: 0.1, 0.3 and 0.6.

2.6. Thick Overlayer Problem

In the section 2.3, we obtained the surface DOS for one adlayer. It is not clear what effect the thicker overlayer might have on the density of states and on $T^{3/2}$ law. To investigate this problem, we must first obtain the Green's function for an arbitrary thick overlayer using the general recursion method described in section 2.2. We will discuss in detail how to get this green's function in next section.

2.6.1 General formalism for Density of Spin Wave States in Thick ferromagnetic Overlayer

The surface Green's function for a thick overlayer can be obtained from the recursion formula Eq.(2.2.16) in section 2.2. By separating the real and imaginary parts of G_{kk} in Eq.(2.2.16), we get

$$\mathrm{Im}G_{kk} = \frac{(W_{kk})^2\,\mathrm{Im}G_{k-1k-1}}{(\omega + W_{kk} - \lambda_{k-1}\,\mathrm{Re}G_{k-1k-1})^2 + (\lambda_{k-1}\,\mathrm{Im}G_{k-1k-1})^2} \tag{2.6.1}$$

and

$$\begin{aligned}\mathrm{Re}G_{kk} = {} & \Big[(1 - W_{k-1k-1}\,\mathrm{Re}G_{k-1k-1})(\omega + W_{kk} - \lambda_{k-1}\,\mathrm{Re}G_{k-1k-1}) \\ & + \lambda_{k-1}\,W_{k-1k-1}(\mathrm{Im}G_{k-1k-1})^2\Big] \times \\ & \left[\frac{1}{(\omega + W_{kk} - \lambda_{k-1}\,\mathrm{Re}G_{k-1k-1})^2 + (\lambda_{k-1}\,\mathrm{Im}G_{k-1k-1})^2}\right]\end{aligned} \tag{2.6.2}$$

where

$$\lambda_{k-1} = \omega\, W_{k-1k-1} + W_{k-1k-1}\, W_{kk} + (W_{k-1k})^2 \qquad (2.6.3)$$

Multiplying Eq.(2.6.1) by λ_k, we obtain

$$\lambda_k\, \mathrm{ImG}_{kk} = \frac{\lambda_k\, (W_{kk})^2\, \mathrm{ImG}_{k-1k-1}}{(\omega + W_{kk} - \lambda_{k-1}\, \mathrm{ReG}_{k-1k-1})^2 + (\lambda_{k-1}\, \mathrm{ImG}_{k-1k-1})^2}$$

where $\lambda_k \mathrm{ImG}_{kk}$ is finite for $\omega \to -1$ $(E \to 0)$.

It follows that

$$I_k = \frac{\lambda_k}{\lambda_{k-1}}\, (W_{kk-1})^2\, I_{k-1}\, D_{k-1} \qquad (2.6.4)$$

where

$$\begin{aligned} I_k &= \lambda_k\, \mathrm{ImG}_{kk} \\ R_k &= \lambda_k\, \mathrm{ReG}_{kk} \end{aligned} \qquad (2.6.5)$$

and

$$D_{k-1} = \frac{1}{(\omega + W_{kk} - R_{k-1})^2 + (I_{k-1})^2} \qquad (2.6.6)$$

Multiplying Eq.(2.6.2) by λ_k, we finally obtain

$$R_k = \frac{\lambda_k}{\lambda_{k-1}} \Big[(\lambda_{k-1} - W_{k-1k-1} R_{k-1})(\omega + W_{kk} - R_{k-1}) + (W_{k-1k-1} (I_{k-1})^2 \Big] \times D_{k-1} \tag{2.6.7}$$

Applying the recursion formula (2.6.4) n times, we finally obtain the surface I_n for the overlayer as

$$I_n = \frac{\lambda n}{\lambda o} (W_{nn-1})^2 (W_{n-1n-2})^2 .. (W_{10})^2 D_{n-1} D_{n-2} \ldots D_0 I_0 \tag{2.6.8}$$

Dividing Eq.(2.6.8) by λ_n, we obtain

$$\mathrm{Im}\, G_{nn} = \prod_{k=1}^{n} (W_{kk-1})^2 D_{k-1} \mathrm{Im} G^0_{00} \tag{2.6.9}$$

The density of states in the surface plane i = n of the overlayer is then given by

$$N_s(E) = (1/N\pi) \sum_{q_\parallel} \prod_{k=1}^{n} (W_{kk-1})^2 D_{kk-1} \mathrm{Im} G^0_{00} (E, q_\parallel) \tag{2.6.10}$$

We note that only the values of R_k for $\omega^2 < 1$ are required in Eq. (2.6.10) since $\mathrm{Im}G^0_{00} = 0$ for ω outside this range. The recursion R_k starts with $R_0 = \lambda_0$. This is because $\mathrm{Re}G^0_{00} = 1$ for $\omega^2 < 1$.

We can now use the exact result (2.6.10) to discuss the analytic behaviour of density of spin wave states at the bottom of the band $E \simeq 0$.

2.6.2 The Analytic Behaviour of the Surface Spin Wave Density of States at The Bottom of the Band

By using Eq.(2.6.3), Eq.(2.6.6) and Eq.(2.2.17), we obtain

$$\lambda_{k-1} = [\rho_k(1 - \gamma_k)E + \rho_k \gamma_k(1 + \omega)] \qquad (2.6.11)$$

and

$$D_{k-1} = \{[(\omega + 1)\gamma_k + E(1 - \gamma_k) - \alpha_k \varepsilon_{k-1} - \lambda_{k-1} \operatorname{Re}G_{k-1k-1}]^2 + [\lambda_{k-1} \operatorname{Im}G_{k-1k-1}]^2\}^{-1} \qquad (2.6.12)$$

As before, to obtain the initial energy dependence $N_s(E)$, we set $\omega = -1$ and $E \simeq 0$; this leads to

$$D_{k-1} = [\tfrac{1}{2} (J_{k-1k}/J)(S_{k-1}/S)]^{-2} \qquad (2.6.13)$$

Substituting for D_{k-1} and W_{k-1k} in Eq.(2.6.10), we obtain the following exact result for $N_s(E)$ at the bottom of the band

$$\begin{aligned} N_s(E) &= (S_n/S_{n-1})(S_{n-1}/S_{n-2})\ldots(S_1/S)\ 2N_B(E) \\ &= 2N_B(E)(S_n/S) \end{aligned} \qquad (2.6.14)$$

where S_n is the surface spin and $N_B(E)$ is the bulk density of states of the substrate.

It is clear from Eq.(2.6.14) that we obtain for a thick overlayer the same result as for the single overlayer problem discussed in section 2.3.1, i.e. the density of spin wave states for a magnetic overlayer of an arbitrary thickness is independent of the exchange interactions J_{nm} and J_{nn}.

We are now in a position to generalize the result of section 2.5.1 as follows:

i. Deviations of the exchange integrals from the bulk J in an arbitrary (finite) number of surface layers have no effect on the initial $T^{3/2}$ law;

ii. a magnetization profile near the surface has also no effect on the initial $T^{3/2}$ law since the factor S_n/S in Eq.(2.6.14) is exactly canceled when the spin deviation Δ is normalized to $M_s(0)$.

This improbably looking result has a simple physical explanation. The initial behaviour of $M_s(T)$ is governed by spin waves whose wavelengths are so long that they do not feel the presence of an overlayer. On the other hand, this argument also indicates that the result (2.6.14) must break down as soon as the wavelength of thermal spin waves becomes comparable with the thickness of the overlayer. We expect, therefore, strong deviations from Eq.(2.6.14) for thick overlayer at temperatures beyond the initial region of the classical behaviour.

2.6.3 Spin Wave Density of States In the Surface With Softened Exchange

2.6.3.1 Softening of the Perpendicular Exchange $J_\perp/J$

We have calculated the density of states for an overlayer with all spins $S_n = S$ and with the bulk exchange $J_{kk} = J$ within each layer but with a softened exchange $J_{k-1k} = J_\perp < J$ between the layers. By using Eq.(2.6.10), we have calculated the density of states $N_s(E)$ for an overlayer of n atomic layers with n = 1, 2, 3, ..., 20. The $N_s(E)$ curves are shown in Fig.2.16 for $J_\perp/J = 0.3$ and n = 1, 2, 3. The asymptotic behaviour reached for $N > 20$ is indicated by broken curve.

It can be seen from Fig.2.16 that all the $N_s(E)$ curves beginning with n = 1 follow, on average, the asymptotic curve for thick overlayer. The energy range in which $N_s(E)$ obeys the "universal law" is only of the order of $0.01\text{-}0.02T_c$. It is clear that the surface density of states is determined by the exchange in the overlayer and the classical result of Rado and of Mills and Maradudin does not hold. The asymptotic curve itself corresponds to the surface density of states of a semi-infinite ferromagnet with parallel exchange $J_\parallel$ equal to the bulk J and with perpendicular exchange equal to $J_\perp$. It follows that the effect of the substrate is "forgotten" already after the first adlayer has been deposited.

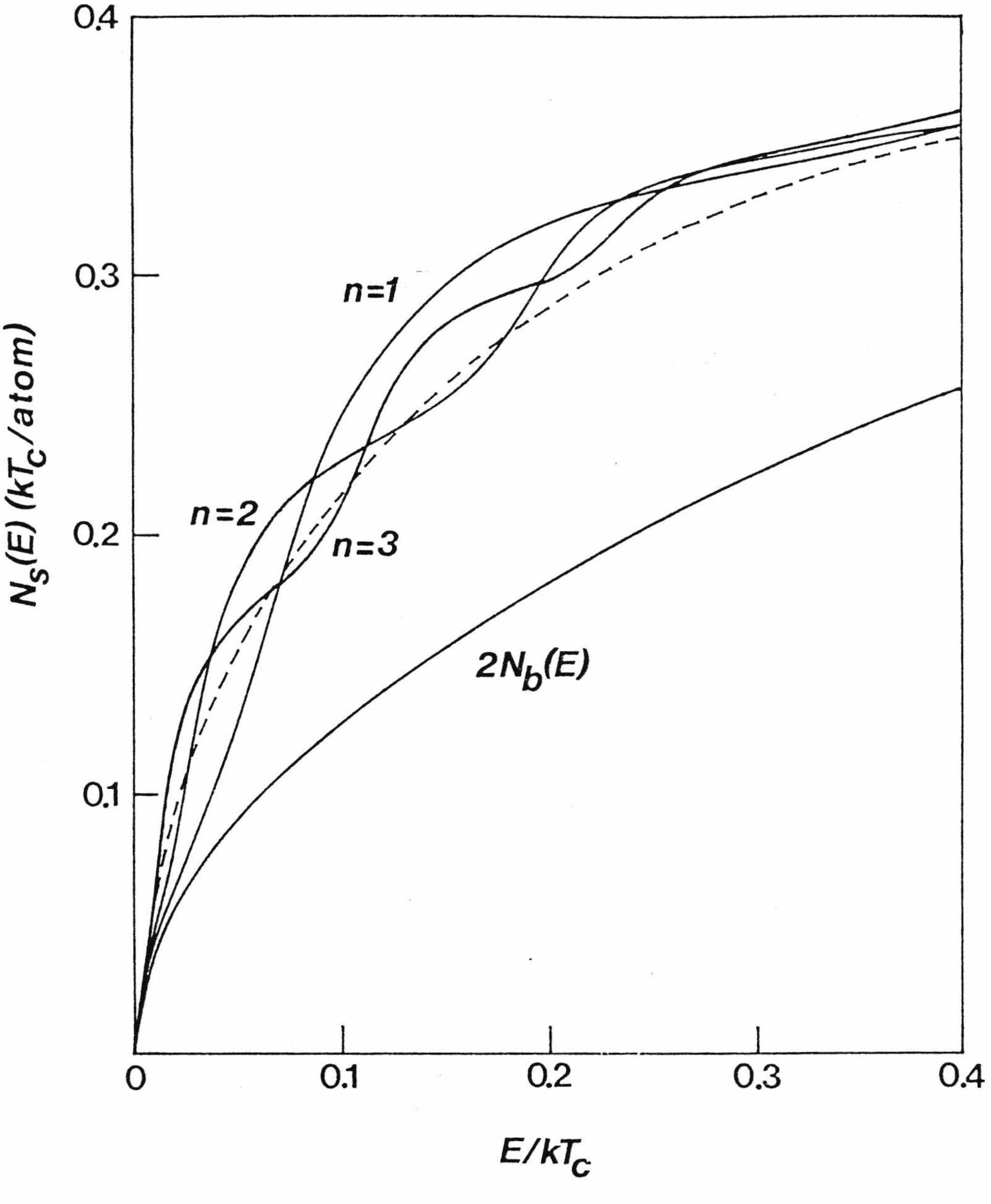

Fig. 2.16 Density of spin wave states in the surface of an overlayer of n atomic layers with a softened exchange $J_\perp/J=0.3$ between the layers. The broken curve denotes the asymptotic behaviour for n>20.

2.6.3.2 Softening of the Parallel Exchange $J_{\parallel}$

We have also calculated the density of states for an overlayer with $S_n = S$ in all layers and $J_{k-1k} = J$ but with a weaker exchange $J_{kk} = J_{\parallel} < J$. Using Eq.(2.6.10), we have obtained the density of states $N_s(E)$ for an overlayer of n atomic layers with n = 1, 2, ..20. The $N_s(E)$ curves are shown in Fig.2.17 for $J'/J = 0.3$ and n = 1, 2, 3. The asymptotic behaviour reached for $N > 20$ is indicated by broken curve. All the $N_s(E)$ curves starting with n = 1 follow again, on average, the asymptotic curve for a thick overlayer. It is interesting and unexpected that the asymptotic behaviour is reached already for an overlayer as thin as one atomic layer.

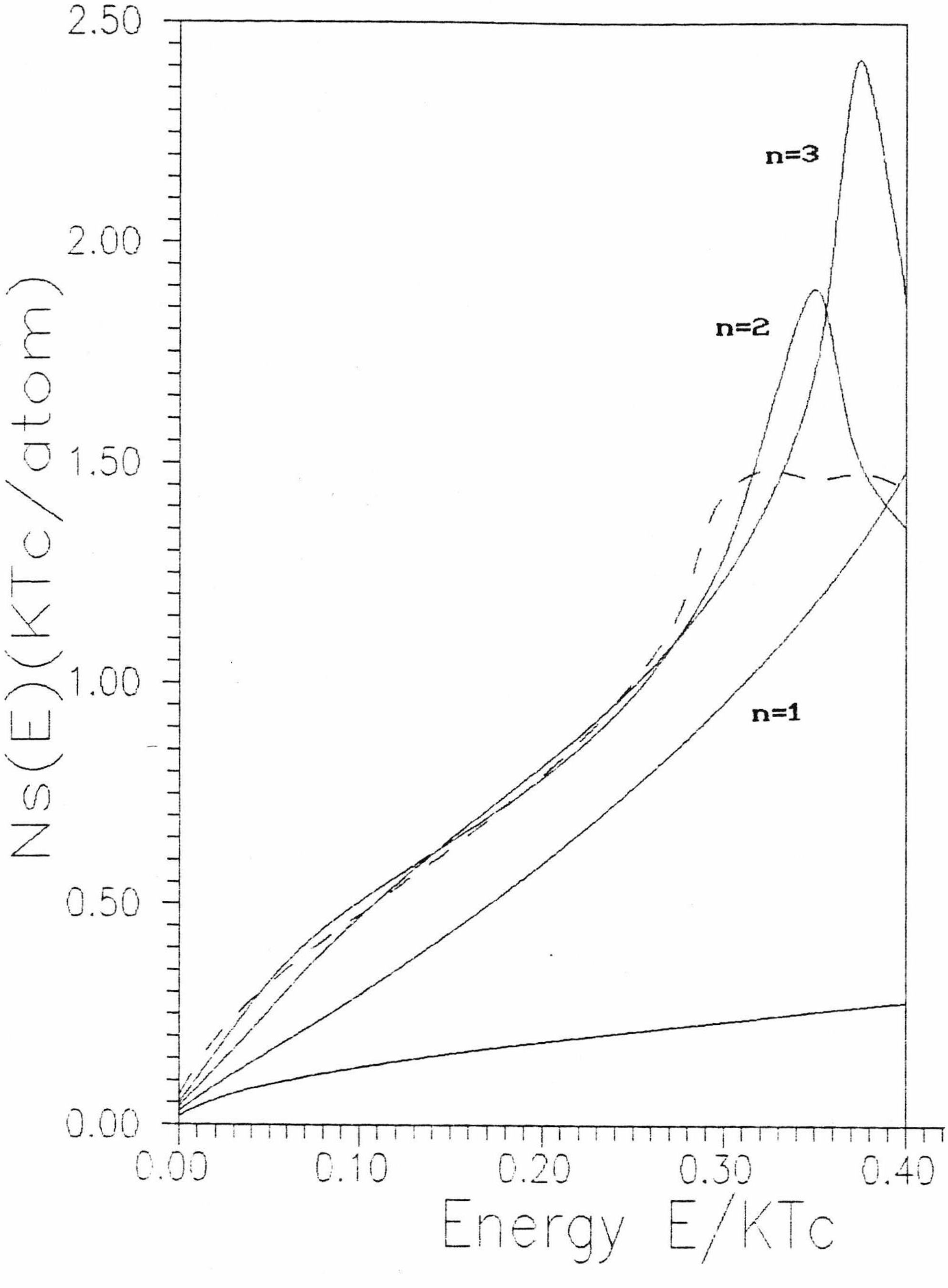

Fig. 2.17 Density of spin wave states in the surface of an overlayer of n atomic layers with a softened parallel exchange $J_{\parallel}/J=0.3$ in overlayer. The broken curve denotes the asymptotic behaviour for n>20.

2.7 Subsurface Problem

The effect of an adlayer on spin waves in the surface of an overlayer had been discussed in detail in previous sections. However, in experiments with spin polarized electrons (See Pierce et al., 1982 and Mauri et al. , 1988 and 1989), not only the surface magnetization is measured but also magnetization of several at. planes below the surface may contribute. Therefore, the magnetization of subsurface layers in a semi-infinite ferromagnetic substrate is also very important. To investigate this affect, we can again employ Green's function method to calculate the spin wave DOS and the temperature dependence of the magnetization in subsurface layers. It is clear that the problem reduces to the calculation of the Green's function for subsurface layers.

2.7.1 Green's function formalism for Subsurface layers

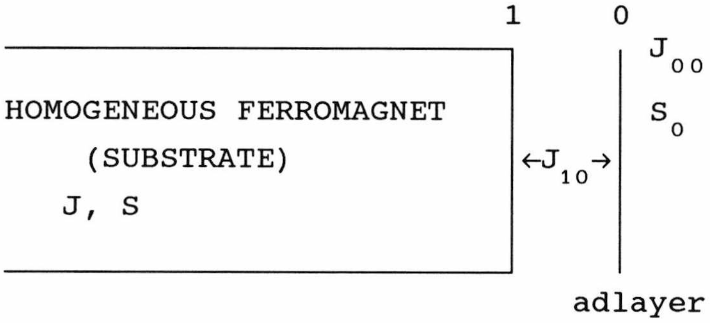

Fig.2.18 The semi-infinite homogeneous ferromagnetic substrate covered with an adlayer

To find the Green's function of subsurface layers, we have to consider again a system that consists of a magnetic overlayer of one atomic plane labeled by n=0, deposited on top of a homogeneous semi-infinite ferromagnetic substrate (see fig.2.6.1). The Green's function of the system G_{mm} can be found from Dyson's equation

$$G_{mn} = G^0_{mn} + \sum_{p,q} G^0_{mp} W_{pq} G_{qn} , \; p, q = 0, 1.$$

where

G^0 is Green's function of the system before the extra layer is added on top.

The perturbation W due to an adlayer is given by Eq.(2.2.5) and Eq.(2.2.15').

To obtain G_{mm}, we write the Dyson's equation as

$$G_{mn} = G^0_{mn} + G^0_{m0} W_{01} G_{1n} + G^0_{m1} W_{10} G_{0n} + G^0_{m1} W_{11} G_{1n} \qquad (2.7.1)$$

and find the elements G_{0n} and G_{1n} by setting m=0 and m=1 in Eq.(2.7.1).

We obtain

$$G_{1n} = \frac{G^0_{1n} + W_{10}G^0_{0n}G^0_{11}}{1 - W_{11}G^0_{11} - W_{01}W_{10}G^0_{00}G^0_{11}} \qquad (2.7.2)$$

and

$$G_{0n} = \frac{G^0_{0n}(1 - G^0_{11}W_{11}) + W_{01}G^0_{00}G^0_{1n}}{1 - G^0_{11}W_{11} - W_{01}W_{10}G^0_{00}G^0_{11}} \qquad (2.7.3)$$

Substituting Eq.(2.7.2) and Eq.(2.7.3) into Eq.(2.7.1) and setting n = m, we find that the Green's function of the system is given by

$$\begin{aligned} G_{mm} = G^0_{mm} &+ \chi\, W_{01}(G^0_{0m})^2 + (\xi\, W_{10} + \zeta\, W_{11})(G^0_{1m})^2 \\ &+ (\varphi\, W_{10} + \chi\, W_{11} + \xi\, W_{01})\, G^0_{0m}G^0_{1m} \end{aligned}$$

for m = 0, 1, 2, ... (2.7.4)

where

$$\Delta = 1 - W_{11}G^0_{11} - W_{01}W_{10}G^0_{00}G^0_{11}$$

$$\chi = \frac{W_{10}\ G^0_{11}}{\Delta}$$

$$\zeta = 1/\Delta$$

$$\varphi = \frac{1 - W_{11}\ G^0_{11}}{\Delta} \qquad (2.7.5)$$

and

$$\xi = \frac{W_{01}\ G^{0}_{00}}{\Delta}$$

Since the fourth term in Eq.(2.7.4) is always zero, the equation reduces to

$$G_{mm} = \begin{cases} G^{0}_{mm} + \chi\ W_{01}\ (G^{0}_{0m})^{2} & \text{for } m = 0 \\ G^{0}_{mm} + (\xi\ W_{01} + \zeta\ W_{11})(G^{0}_{1m})^{2} & \text{for } m = 1, 2, 3, \ldots \end{cases}$$

(2.7.6)

In this section we consider only the second part of Eq.(2.7.6) because we want to investigate the behaviour of subsurface layers after adding one extra layer on top of the substrate.

We can rewrite Eq.(2.7.6) as

$$G_{mm} = G^{0}_{mm} + \frac{\lambda\ (G^{0}_{1m})^{2}}{\omega + W_{00} - \lambda G_{11}} \quad \text{for } m = 1, 2, 3, \ldots . \qquad (2.7.7)$$

where λ is given by Eq.(2.3.3), G^{0}_{mm} is given by Eq.(1.6.27) and W_{00} is given by Eq.(2.2.5).

Equation (2.7.7) is the Green's function for the subsurface layers and we will use it to calculate the DOS of spin waves in subsurface layers in the next section.

2.7.2 Density of Spin Wave States for Subsurface Layers

The imaginary part of G_{mm} can be obtained from Eq.(2.7.7). Substituting it into Eq.(1.3.14), we find that the spin wave DOS in a subsurface layer m is given by

$$N^{m}_{ss}(E) = (1/\pi N) \sum_{q_{\parallel}} \quad \mathrm{Im} \left\{ G^{0}_{mm} + \left\{ \frac{\lambda \, (G^{0}_{1m})^{2}}{\omega + W_{00} - \lambda \, G^{0}_{11}} \right\} \right\} \tag{2.7.8}$$

We can simply write G^{0}_{mm} and G^{0}_{1m} as

$$G^{0}_{mm} = G^{0}_{11} + 2 \sum_{m=1}^{m-1} \gamma^{2m} \tag{2.7.9}$$

and

$$G^{0}_{1m} = \gamma^{m-1} \, G^{0}_{11} \tag{2.7.10}$$

where $\gamma = \omega + i\mu$

Substituting Eq.(2.7.9) and Eq.(2.7.10) into Eq.(2.7.8), we finally obtain

$$N^{m}_{ss}(E) = (1/\pi N) \sum_{q_{\parallel}} \quad \left(I + 2 \sum_{m=1}^{m-1} \sin(2m \tan^{-1}(\frac{(1 - \omega^{2})^{1/2}}{\omega})) + \frac{\lambda(UQ + VP)}{(\omega + W_{00} - \lambda R)^{2} + (\lambda I)^{2}} \right) \tag{2.7.11}$$

where

$$P = (\omega + W_{oo} - \lambda R)(R^2 - I^2) - 2\lambda I^2 R,$$

$$Q = I\ [2R(\omega + W_{oo} - \lambda R) + \lambda(R^2 - I^2),$$

$$U = \cos(2(m-1)\ \tan^{-1}(\frac{(\ 1 - \omega^2)^{1/2}}{\omega}))$$

and

$$V = \sin(2(m-1)\ \tan^{-1}(\frac{(\ 1 - \omega^2)^{1/2}}{\omega}))$$

The density of spin wave states at the bottom of the band is dominated by the singularity of I at $\omega = -1$. We already know from Eq.(2.3.8) that $\omega + W_{oo} - \lambda R \simeq -\alpha$ and $\lambda \simeq 0$ at the bottom of the band $E \simeq 0$. Therefore, we get again the simple result

$$N^m_{ss}(E) = 2\ N_B(E) \tag{2.7.12}$$

It follows that the initial spin wave DOS for subsurface layers is independent of surface exchange J_{10} and J_{11} and surface spin S_0. It also independent of the position of the subsurface layer m, i.e. each subsurface layer behaves just like the surface layer. This behaviour is obtained because at the bottom of the band, spin waves have wavelengths so long that the spin wave amplitude does not change significantly over the first m layers.

However, from our experience with the surface DOS, we expect that this initial result breaks down almost immediately and the subsurface DOS at higher energies must depend on the location of the subsurface layer and also on the distribution of exchange and spin in the surface region. In the next section, we shall investigate the effect of softening of the perpendicular exchange J_{10} while keeping $J_{11} = J$ and $S_0 = S$.

2.7.3 Subsurface Density of States With Softened Exchange

The spin wave DOS in subsurface layers for a range of values of $J_{10}/J \leq 1$ with $J_{11}/J = 1$ and $S_0/S = 1$ was calculated from Eq.(2.7.8) and the results are shown in Fig.2.19, Fig.2.20, Fig.2.21, Fig.2.22 and Fig.2.23. The Brillouin zone summation in Eq.(2.7.8) was performed using Cunningham points (See section 2.4). It can be seen from Fig.2.19 for subsurface layer n = 1 that all the DOS curves follow the universal curve $2N_B(E)$ and then start to deviate at energies $\simeq 0.01kT_c$ depending on the value of J_{10}/J. In the energy range $0.01\text{-}0.08kT_c$ DOS deviations from universal curve are very small but they become much bigger at higher energies. For deeper layers with n=2, 5 and 10 we can see very clearly that all the DOS curves approach the bulk $N_B(E)$ curve (broken curve) (See Fig.2.22). To illustrate how the DOS curves deviate from the universal curve $2N_B(E)$ and approach the curve $N_B(E)$, we plot in Fig.(2.23) the DOS for a specific value $J_{10}/J=0.3$ and for a range of layer indices n = 1, 2, 5 and 10 against the energy E measured in units of kT_c.

To see how this DOS influences the $T^{3/2}$ law, we have to calculate the corresponding subsurface magnetization. This is the subject of the next section.

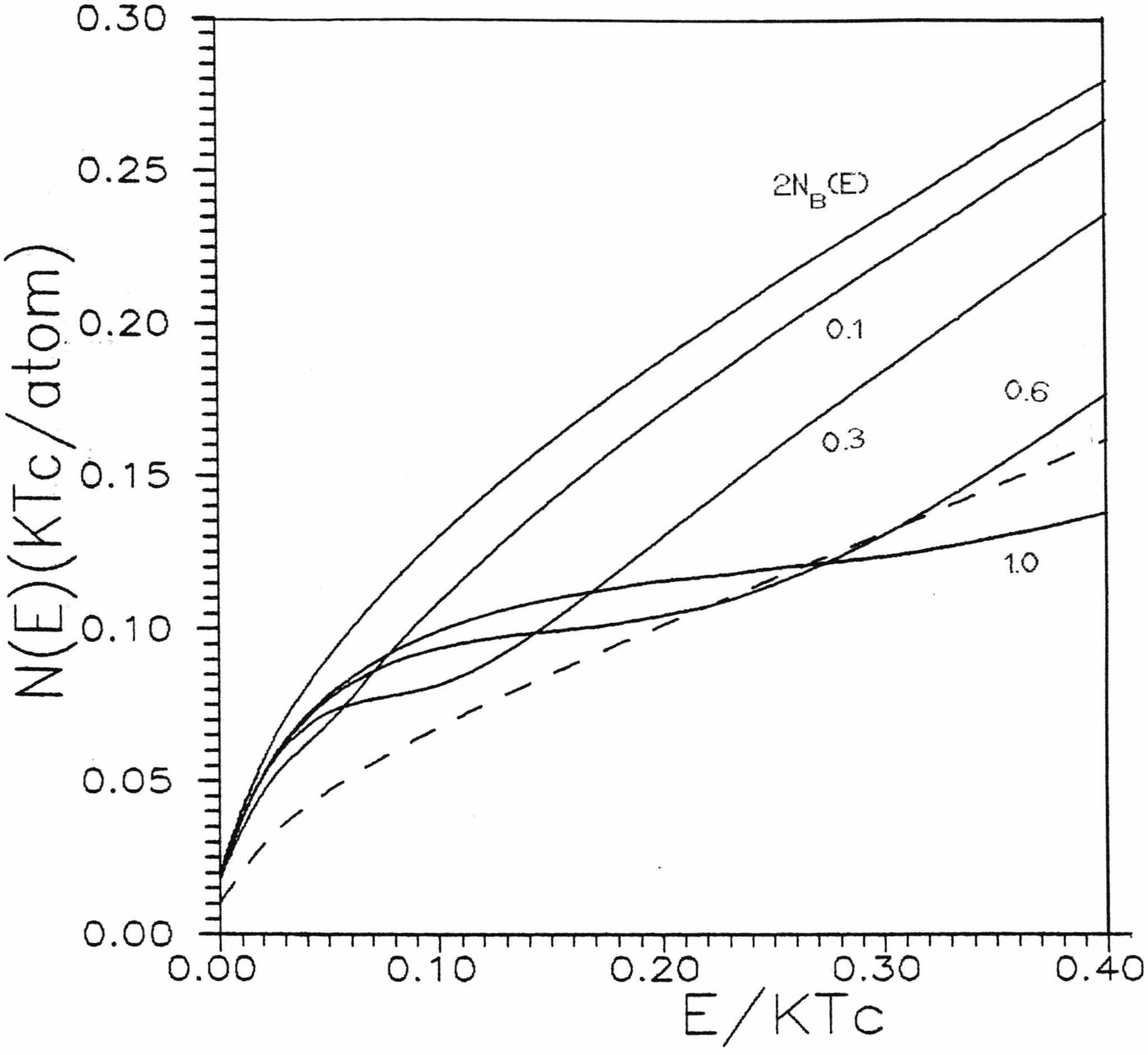

Fig. 2.19 The density of spin wave states in the subsurface layer n=1 for an overlayer with softened surface-bulk exchange $J_{10}/J=0.1$, 0.3, 0.6 and 1.0. The broken curve denotes the DOS of the bulk $N_B(E)$ and the curve 2N (E) denotes the DOS of a geometric surface.

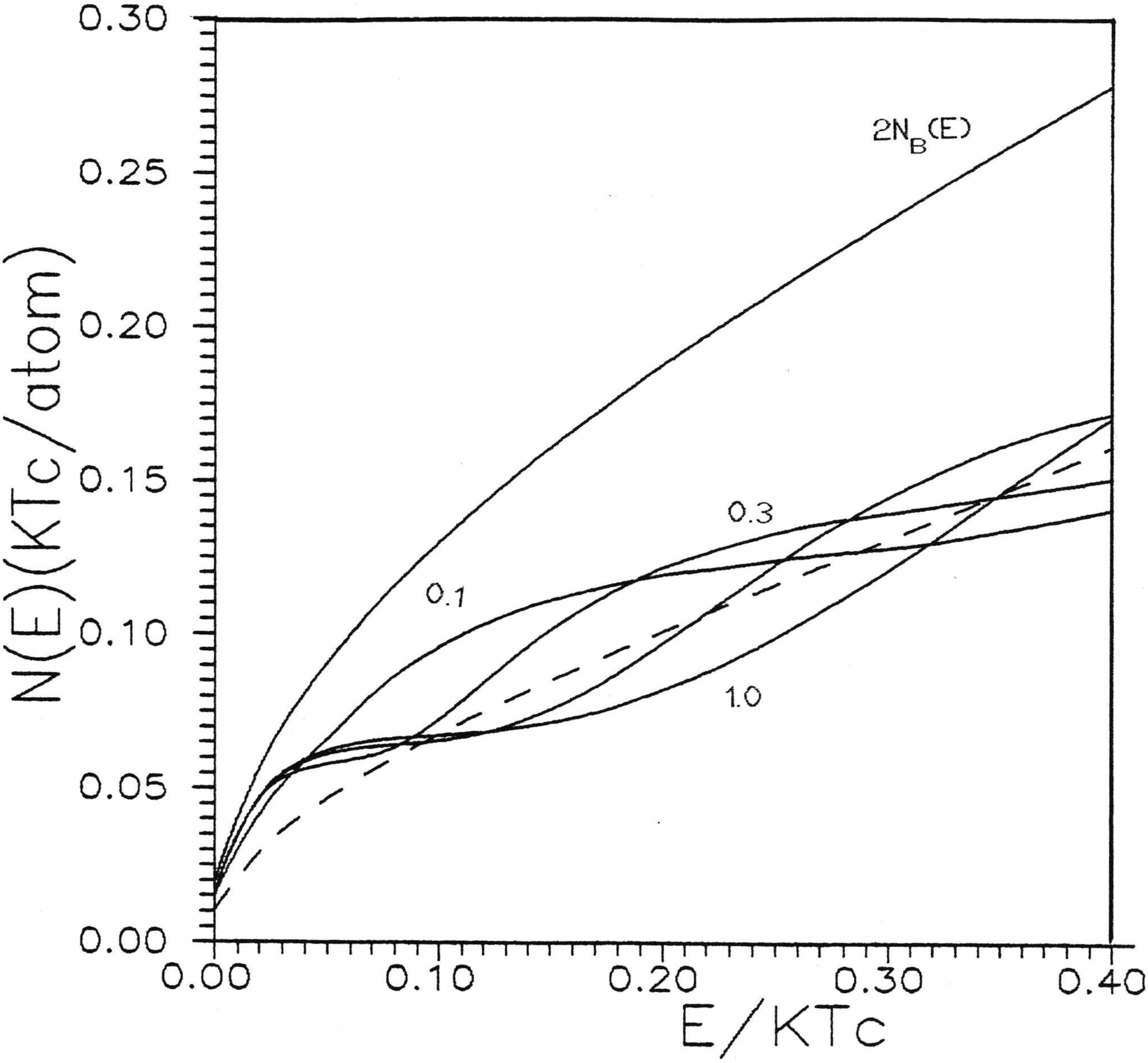

Fig.2.20 The density of spin wave states in the subsurface layer n=2 for an overlayer with softened surface-bulk exchange J_{10}/J=0.1, 0.3, 0.6 and 1.0. The broken curve denotes the DOS of the bulk N_B(E) and the curve $2N_B$(E) denotes the DOS of a geometric surface.

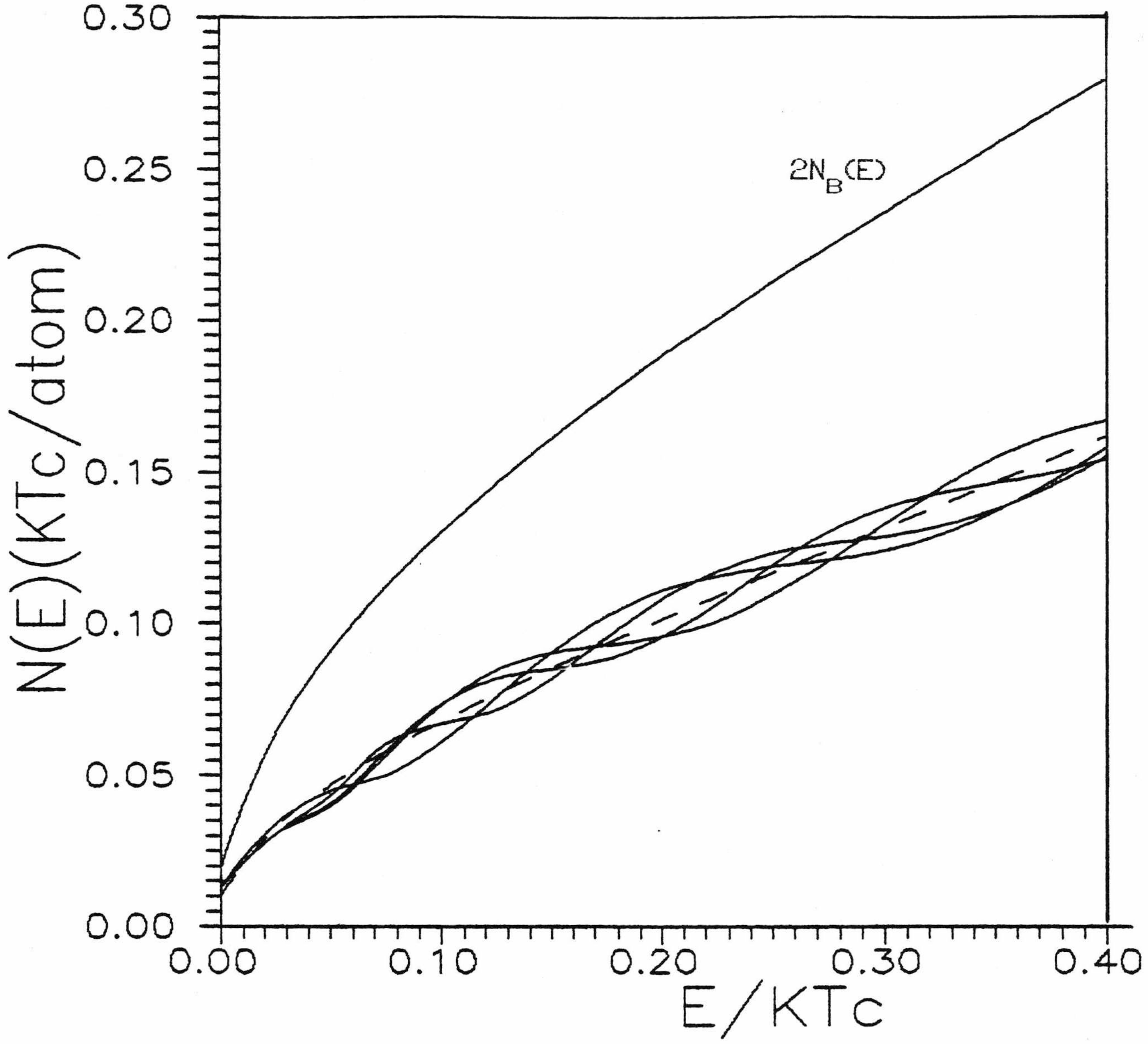

Fig.2.21 The density of spin wave states in the subsurface layer n=5 for an overlayer with softened surface-bulk exchange $J_{10}/J=0.1$, 0.3, 0.6 and 1.0. The broken curve denotes the DOS of the bulk $N_B(E)$ and the curve $2N_B(E)$ denotes the DOS of a geometric surface.

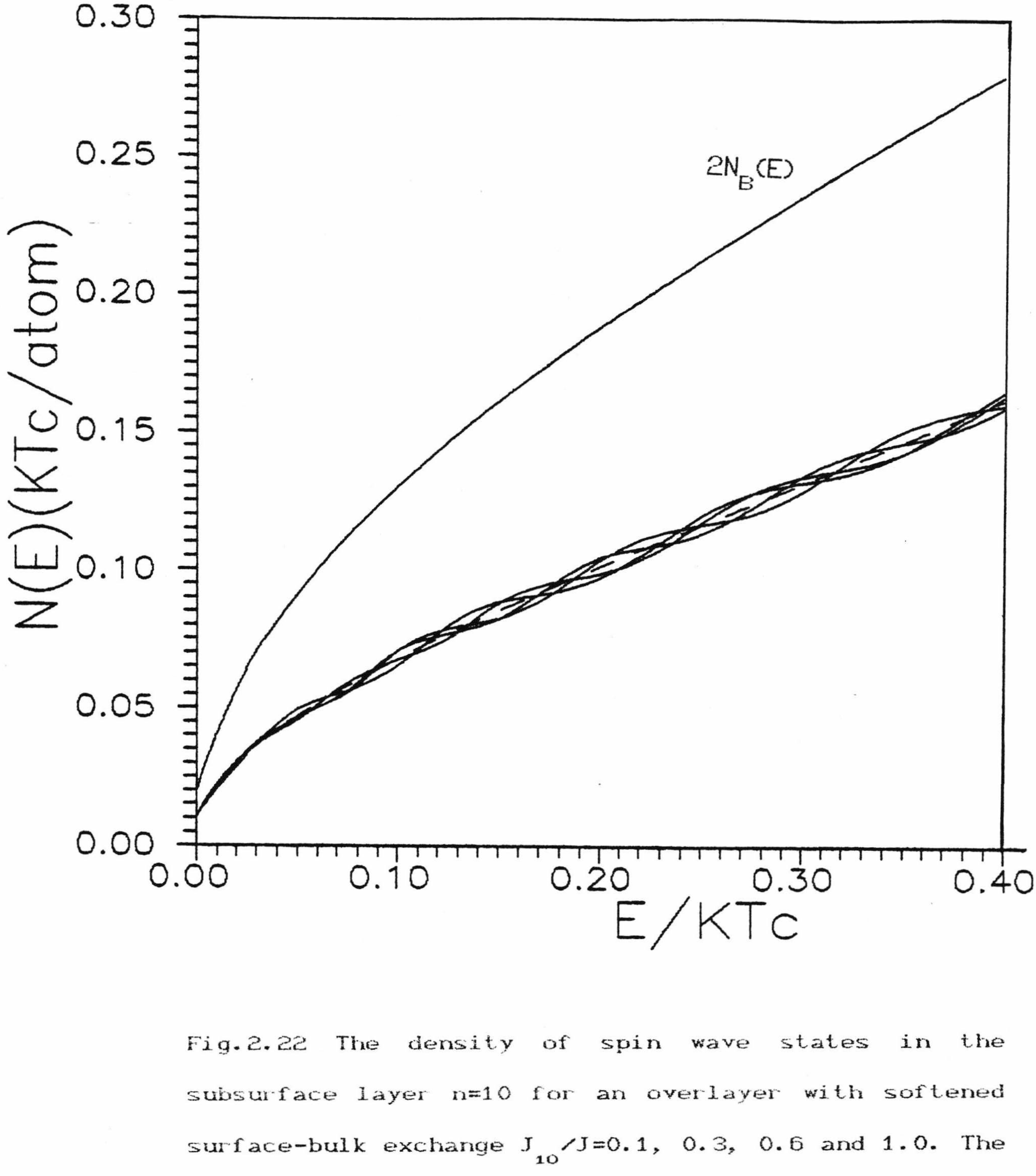

Fig.2.22 The density of spin wave states in the subsurface layer n=10 for an overlayer with softened surface-bulk exchange $J_{10}/J=0.1$, 0.3, 0.6 and 1.0. The broken curve denotes the DOS of the bulk $N_B(E)$ and the curve $2N_B(E)$ denotes the DOS of a geometric surface.

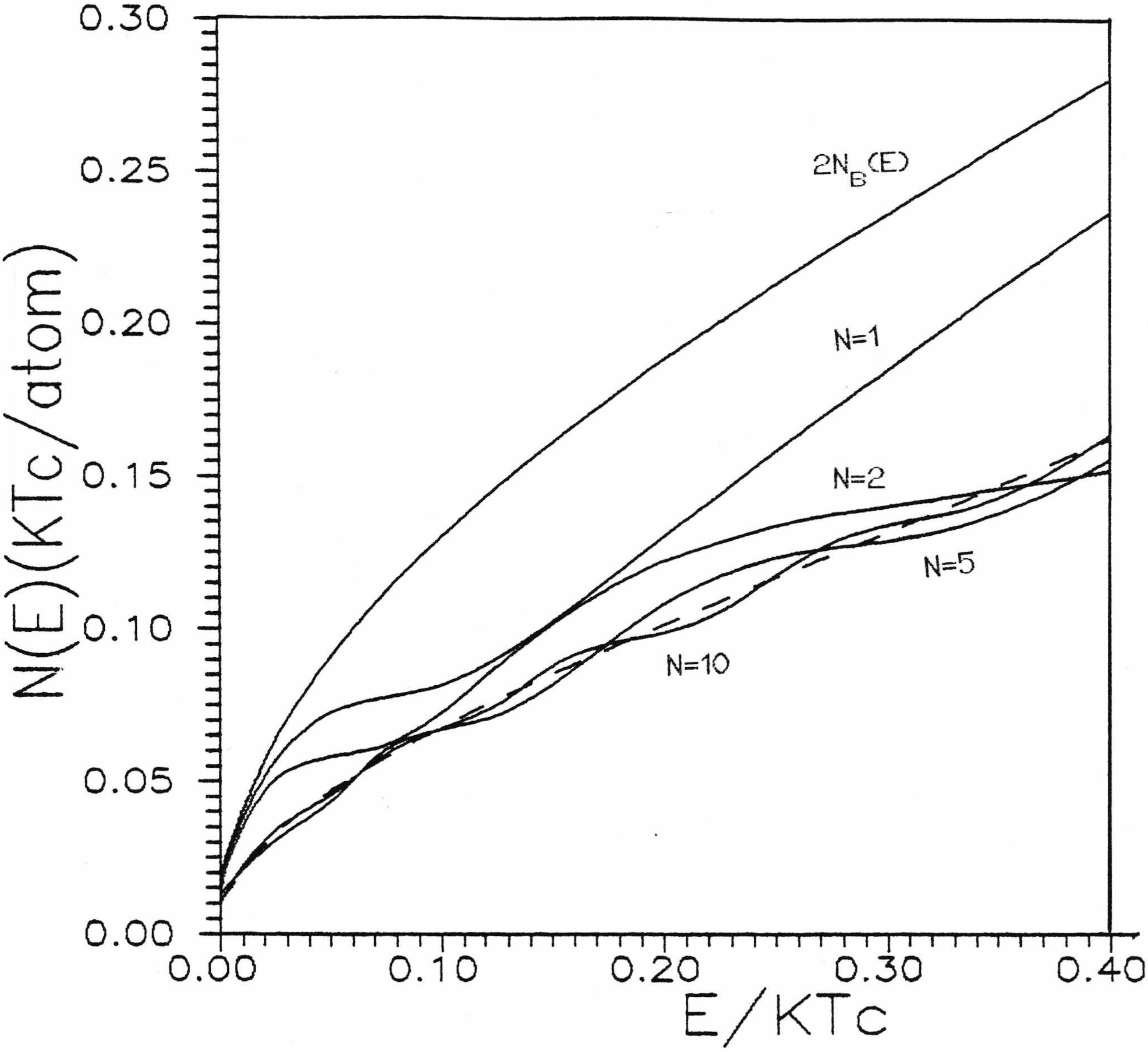

Fig.2.23 The density of spin wave states in the subsurface layer n=1, 2, 5 and 10 for an overlayer with softened surface-bulk exchange $J_{10}/J=0.3$. The broken curve denotes the DOS of the bulk $N_B(E)$ and the curve $2N_B(E)$ denotes the DOS of a geometric surface.

2.7.4 Temperature Dependence of Subsurface Magnetization

In section 2.7.2 we have discussed the spin wave density of states in subsurface layers of ferromagnet but our discussion is not complete without investigating their temperature dependence of the subsurface magnetization M(T). To calculate the temperature dependence $M_i(T)$, we can use Eq.(3.1.2) to obtain first the corresponding spin deviation. We expect that $M_i(T)$ will decrease with temperature faster than $M_B(T)$ for the bulk and obey a $T^{3/2}$ law. To check this, we have plotted in Fig.2.24 the curves $M_1(T)$ against temperature T up to $0.4T_C$ for the layer i = 1 below the surface for different surface to bulk exchange J_{10}, i.e., 0.1J, 0.3J, 0.6J and 1.0J but with the same surface exchange $J_{00} = J$ and the same surface spin $S_0 = S$ Obviously, the deviation from the saturation magnetization $1 - M_1(T)/M_1(0)$, is larger for the subsurface layer than the bulk deviation. It is not clear from Fig.2.24 that the temperature dependence $M_1(T)$ varies with T according the same power law as in the bulk. Therefore, we plot in Fig.2.25 the temperature dependence for the subsurface layer $M_1(T)/M_1(0)$ against the bulk dependence $M_B(T)/M_B(0)$ for various values of J_{10} but with fixed value of $J_{00} = J$ and $S_0 = S$. It can be seen from Fig.2.25 that a very good $T^{3/2}$ law holds in the case $J_{10}/J = 0.1$ with prefactor k = 1.6. However, for $J_{10}/J = 0.3$, 0.6 and 1.0, the $M_S(T)$ curves are no longer good straight lines. This behaviour occurs because, for $J_{10} \simeq 0$, the layer n=1 becomes essentially surface and we know that surface has good $T^{3/2}$

law with $B_S = 2B_B$. But for J_{10} not weak, the second layer changes from "surface" layer at very low temperatures (see the initial DOS) to essentially bulk layer at higher temperatures. Therefore, there is a change of slope from layer n = 2 to n = 1. We have not computed $M_i(T)$ for deeper layers because it can be seen from Fig.2.23 for the density of states that they behave essentially as bulk layers.

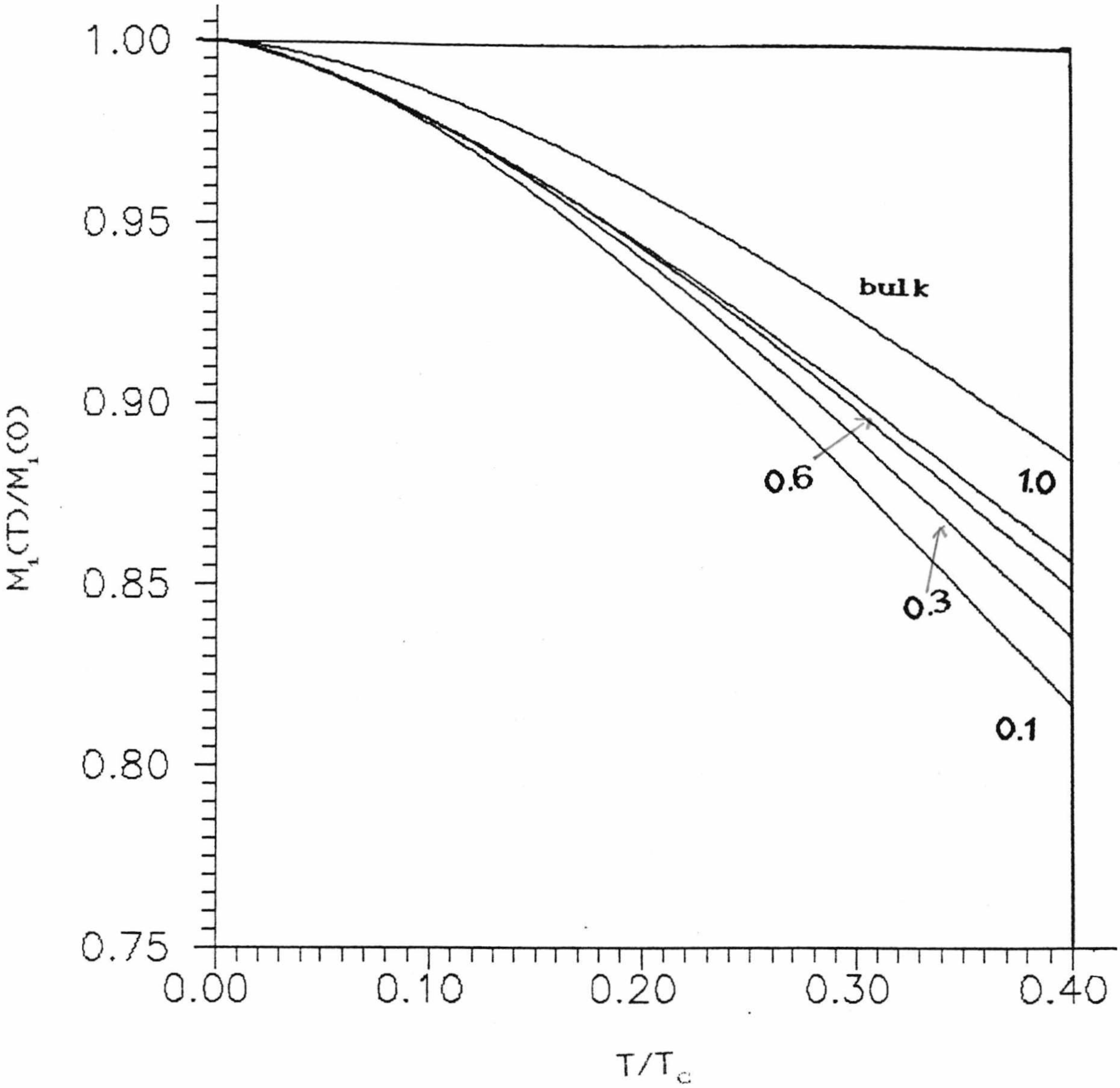

Fig. 2.24 Calculated temperature dependence of the subsurface magnetization $M_1(T)/M_1(O)$ for the subsurface layer n=1 with softened exchange J_{10}. The values of J_{10}/J are 0.1, 0.3, 0.6 and 1.0.

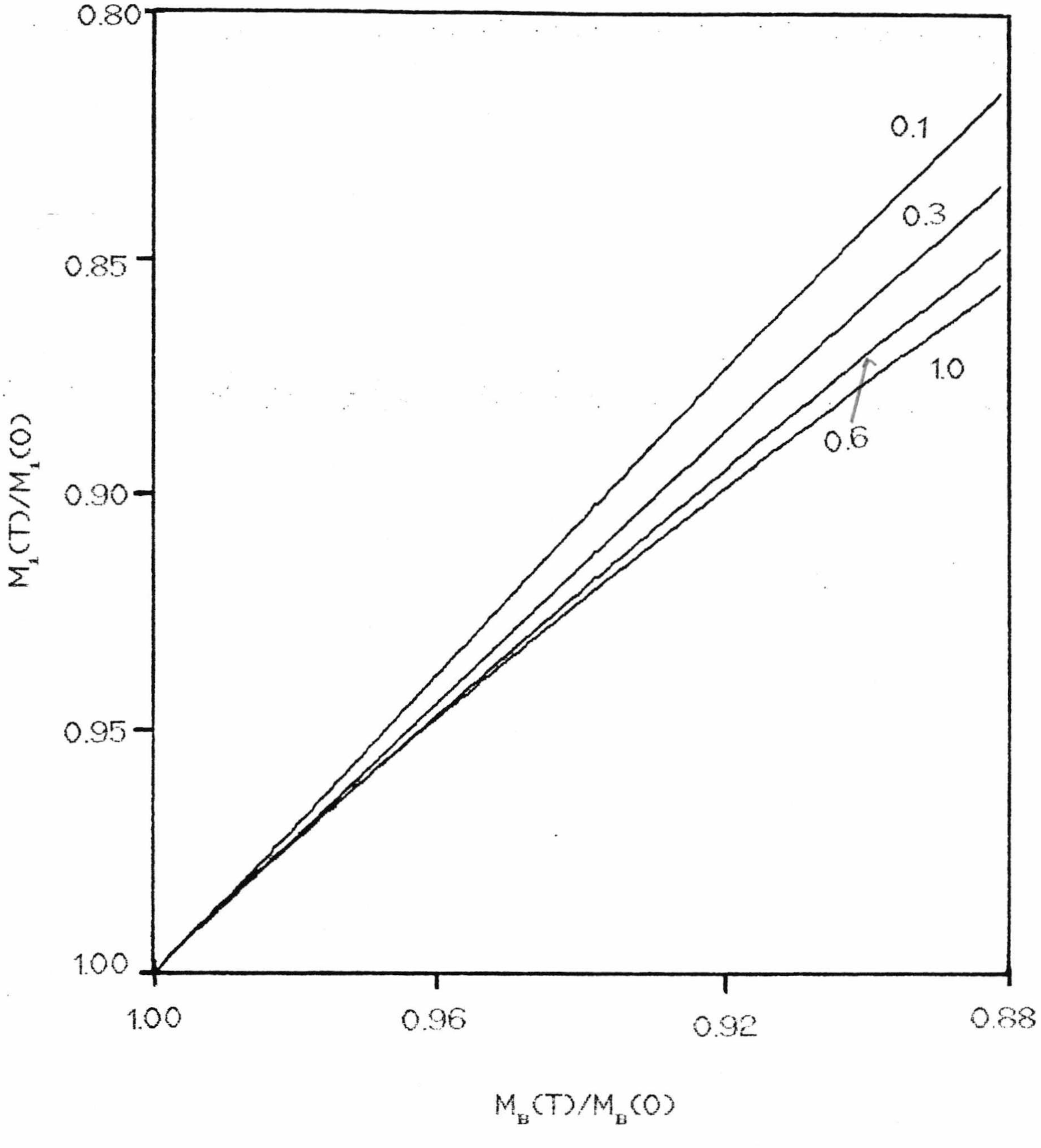

Fig.2.25 Plot of the temperature dependence of the subsurface magnetization $M_1(T)/M_1(0)$ for the subsurface layer n=1 against the bulk dependence $M_B(T)/M_B(0)$ for J_{10}/J are 0.1, 0.3, 0.6 and 1.0.

CHAPTER 3.Application of The Adlayers Method to Interfaces

3.1. Introduction

The study of localized excitation modes at the planar interface formed between two crystals is relatively new branch of the surface physics. Like many other studies in this field, it is stimulated by the progress in experimental techniques. In particular, the method of molecular-beam epitaxy enables one to obtain well-defined interfaced bicrystals (See e.g. Massies et al., 1980). The existence of such interfaces lead, under certain circumstances, to the existance of interface states. In single particle excitations, interface electronic states were considered by several workers, including Yaniv (1978 and 1980) and Lawy and Madhukar (1978). The collective excitations of such interfaces were also studied actively. For example, the vibrational properties and the existence of interface phonons were discussed by authors like Djafari-Rouhani et al. (1977) and Masri (1981).

Spin waves at interfaces in cubic Heisenberg systems were investigated by Yaniv (1983), Bu Xing Xu et al. (1985) and Selzer and Majlis (1986). All these authors applied Green's function method to the simplest model of an interface consisting of two semi-infinite Heisenberg ferromagnets coupled via a nearest-neighbour interface exchange. The present work is a generalization of the Green's function method to an arbitrary interface model reported by us recently (See Ahmad et al.,1988 and Mathon, 1989). We shall study the behaviour of the interface spin wave density of states and also the temperature dependence of the interface magnetization using the method of adlayers.

3.2 General Formulation of the Interface Problem

The interface we consider consists of n atomic planes seperating two magnetically homogeneous semi-infinite ferromagnets (Fig.3.1). The exchange integrals between neighbouring atomic planes and within atomic planes of the interface are arbitrary. It is, therefore of fundamental importance to know how to define and calculate the Green's function associated with such a system. We will show that it is easy to calculate the Green's function for every layer of an interfaces using our method of adlayers.

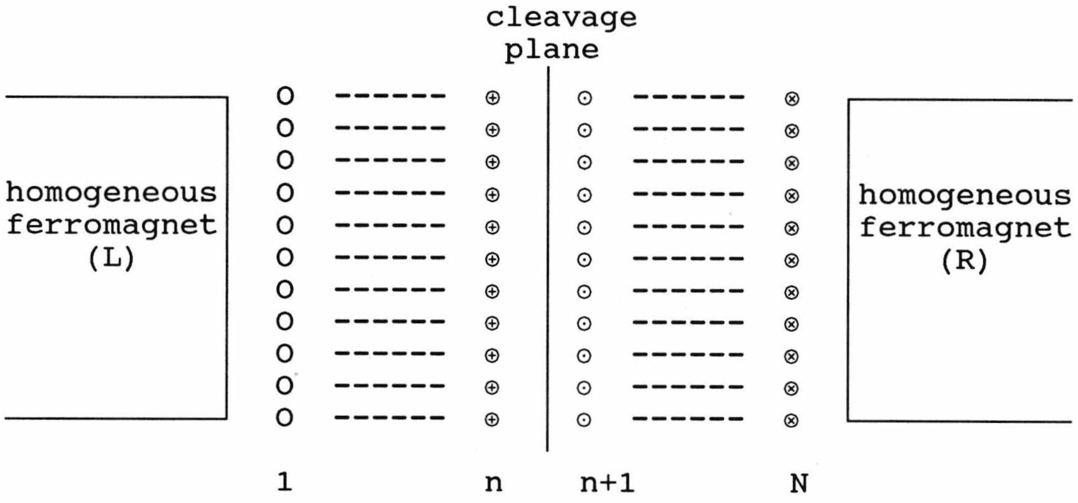

FIG. 3.1. Schematic representation of the ferromagnetic interface.

Let us assume that we require the local Green function G_{nn} in the n-th layer of the interface. To obtain G_{nn}, we first pass an imaginary cleavage plane between the layer n and n+1, separating the whole structure into two independent semi-infinite systems (i.e. there are no exchange bonds between the right-hand and left-hand halves). We can then define a Green function G^c for the cleaved system by

$$G^c_{nm} = \begin{cases} G^L_{nm} & ;\ n,m \in L \\ 0 & ;\ n \in L,\ m \in R \text{ (or vice versa)} \\ G^R_{nm} & ;\ n,m \in R \end{cases} \qquad (3.2.1)$$

where G^L and G^R are the Green functions for the left-hand and right-hand halves of the cleaved interface. Since each half is just a magnetic overlayer on a homogeneous substrate, the matrix elements G^c_{nn} and $G^c_{n+1\,n+1}$ can be calculated by the recursion method for overlayers described in chapter 2.

To determine the exact G_{nn} in the interface, we need only switch on the exchange J_{nn+1} between the layers n and n+1 and then reconnect the two halves using the Dyson's equation (2.2.4). When the two halves are being reconnected, both the diagonal elements G^c_{nn} and $G^c_{n+1\,n+1}$ are perturbed. Since we consider nearest-neighbour exchange only, the perturbation to the diagonal elements is equivalent to the perturbation caused by the deposition of a single atomic layer (the surface layer of the other half of the cleaved structure), i.e. is again described by the matrix W defined in Eq.(2.2.5). It is, therefore, useful first to "prepare" two auxilliary Green function G^D_{nn} and $G^D_{n+1\,n+1}$ which include this diagonal perturbation. There are given by

$$G^D_{nn} = G^L_{nn}\,(1 - W_{nn}\,G^L_{nn})^{-1}$$

and (3.2.2)

$$G^D_{n+1\,n+1} = G^R_{n+1\,n+1}\,(1 - W_{n+1n+1}\,G^R_{n+1\,n+1})^{-1}$$

where W_{nn} and W_{n+1n+1} are given by Eq.(2.2.5). When these two auxilliary Green functions are finally reconnected, only the off-diagonal element W_{nn+1} defined by Eq.(2.2.5) needs to be considered in the Dyson's equation (2.2.4). We can easily show that the required green's function G_{nn} is given by

$$G_{nn} = G^D_{nn}\,(1 - G^D_{nn}\,W^2_{nn+1}\,G^D_{n+1n+1})^{-1} \qquad (3.2.3)$$

By passing the cleavage plane between any two atomic planes of the interface, we can determine from equations (2.2.16), (2.2.17), (3.2.1), (3.2.2) and(3.2.3) all the diagonal elements G_{nn}, n = 1, 2, ..., N, of the exact interface Green's function.

For example, to compute by this method the local density of spin wave states (DOS) in every layer of the interface, all G^L_{nn} and G^R_{mm} for n, m = 1, 2, ..., N, are required. The computational effort needed to evaluate the local DOS in every layer of the interface is, therefore, equivalent to the effort required to calculate the surface DOS for two overlayers (left and right) by using the adlayer method of chapter 2.

3.3 Spin Wave DOS for an Interface

We shall now discuss briefly the structure of magnetic exitations in an interface. To this end we shall apply the Green's function derived in the preceeding section to obtain Im G_{nn}. Writing $G^D_{nn} = R + iI$ and $G^D_{n+1n+1} = R' + iI'$, we can express ImG_{nn} from Eq.(3.2.3) as follows:

$$\mathrm{Im}G_{nn} = \frac{I + W^2_{nn+1}(R^2 + I^2)I'}{[1 - W^2_{nn+1}(RR' - II')]^2 + [W^2_{nn+1}(RI' + IR')]^2} \qquad (3.2.4)$$

It is clear from the explicit expression Eq.(3.2.4) that for a fixed $\underline{k}_{\parallel}$ the diagonal matrix element of the interface Green's function G_{nn} has nonvanishing continuous imaginary part for energies which are inside the bulk spin wave band of either the first or the second overlayer forming the interface. Since this imaginary part is proportional to the local spin wave DOS, it follow that the spin wave bandwidth of an interface is at least the union of the spin wave bands of two separate overlayers. However, it also follows from Eq.(3.2.4), that there may be additional excitations outside the bulk spin wave bands. These correspond to isolated poles, i.e, to zeroes of the denominator in Eq.(3.2.3). All spin wave excitations can, therefore, be classified into three groups according to their localization properties with respect to the interface.

To facilitate our further analysis we define two $\underline{q}_{\parallel}$ subbands of the two overlayers considered. These subbands span the energy range over which the corresponding bulk spin wave energy varies for the fixed $\underline{k}_{\parallel}$. These subbands are described by the intersection of the bulk spin wave spectra $E_1(\underline{q})$ and $E_2(\underline{q})$, Eq.(1.6.15), where the plane $\underline{q}_{\parallel}$ equals a constant.

The various spin waves of the interface can be labeled by their $\underline{k}_{\parallel}$ values. The first type of spin wave extends throughout the entire interface. This kind of behaviour is associated with states whose energy lies inside the $\underline{k}_{\parallel}$ subbands of both overlayers, i.e., with those energies satisfying

$$\begin{aligned} &|E - 6S_1J_1 - 2S_1J_1(\cos(q_xa) + \cos(q_ya))| < 2S_1J_1, \\ &|E - 6S_2J_2 - 2S_2J_2(\cos(q_xa) + \cos(q_ya))| < 2S_2J_2. \end{aligned} \tag{3.2.5}$$

The second type of spin wave extend to infinity on one side of the interface only, and decay exponentially with the distance from the interface on the other side. Such kind of behaviour occurs for energies which are inside the $\underline{k}_{\parallel}$ subband of one of the overlayer, but outside the corresponding subband of the other, i.e.

$$\begin{aligned} &|E - 6S_1J_1 - 2S_1J_1(\cos(q_xa) + \cos(q_ya))| < 2S_1J_1, \\ &|E - 6S_2J_2 - 2S_2J_2(\cos(q_xa) + \cos(q_ya))| > 2S_2J_2. \end{aligned} \tag{3.2.6}$$

or

$$|E - 6S_1J_1 - 2S_1J_1(\cos(q_xa) + \cos(q_ya))| > 2S_1J_1,$$
$$|E - 6S_2J_2 - 2S_2J_2(\cos(q_xa) + \cos(q_ya))| < 2S_2J_2. \tag{3.2.7}$$

The third, and most interesting, are interface spin waves. These are magnetic excitations whose wave function is exponentially localized on both sides of the interface. This situation occurs for energies satisfying

$$|E - 6S_1J_1 - 2S_1J_1(\cos(q_xa) + \cos(q_ya))| > 2S_1J_1,$$
$$|E - 6S_2J_2 - 2S_2J_2(\cos(q_xa) + \cos(q_ya))| > 2S_2J_2. \tag{3.2.8}$$

A complete discussion of the three cases was given by Yaniv (1983) for a simple model of an interface. However, as for the surface problem, it becomes very difficult to separate localized spin wave states from bulk states for an interface with exchange that varies over many atomic planes. Fortunately, such a separation is not necessary here since we are only interested in the total local density of spin wave states that can be determined directly from Eq.(3.2.3). We shall again add a small imaginary part to the energy in the spin wave Green's function and this ensures automatically that both bulk and localized modes are included.

As an example, we shall make specific calculation for symmetric interfaces where the exchange interactions in the two overlayers are mirror images of one another. We shall also restrict ourselves to the situation where the exchange integrals in all interface planes have the same values but different from the values for the left and right semi-infinite ferromagnets. The notation for the exchange interactions in Fig.3.1 can be then simplified as $J_{nm}/J = \alpha$, $J_{nn}/J = \beta$ and $S_n/S = 1$.

We shall first consider $\alpha < 1$ corresponding to the most interesting case of a weak ferromagnetic link separating two ferromagnets with bulk exchange J. The simplest case is when two homogeneous semi-infinite ferromagnets are separated by a single weak link α. The corresponding interface density of states are shown in Fig.3.2 for a range of values of α. All the DOS curves start following the universal curve $N_B(E) \propto E^{1/2}$ for a bulk ferromagnet and then begin to deviate depending on the exchange coupling J_{10} between the two semi-infinite ferromagnets forming the interface. This initial behaviour is obtained because long-wavelength spin waves do not feel the weak link and behave as bulk spin waves.

Another interesting problem is when the exchange in the interface is weakened in the direction parallel to the interface. As an illustration, we have computed the interface DOS for an interface consisting of two at. planes with $J_{\parallel}/J = \beta < 1$ and with all perpendicular exchange integrals $J_{\perp}/J = \alpha = 1$. The results are shown in Fig.3.3

for a range of β. The graphs show that the density of states for this model has behaviour similar to the behaviour we obtained for one overlayer problem but with a magnitude of DOS which is only about half of the value found for the overlayers. This clearly indicates the presence of interface spin waves. In fact, it is obvious that if one starts from two overlayer subsystems each having a surface state below the corresponding bulk subband and couple them via an exchange coupling J_{12} then the interface system will have an interface spin wave branch below the bulk subband provided J_{12} is weak enough.

To study how the local DOS varies in the profile of the interface separating the two semi-infinite substrates, we first considered an interface consisting of ten layers with $\alpha = 0.3$ and $\beta = 1$. Because of symmetry , it is only necessary to compute DOS at layers 0, 1, 2, 3, 4 and 5. Fig.3.4 shows the corresponding densities of states. Initially they all start following the same curve. This initial behaviour is obtained because long-wavelength spin waves do not feel the weak link and behave as bulk spin wave. The DOS curves for layers 2, 3, 4 and 5 remain very close together especially in the range $\simeq 0.0\text{-}0.4kT_C$. Having obtained the profile of DOS across an interface, we shall now discuss the dependence of the local DOS in the middle of the interface on its thicknesses. We again consider a homogeneous interface with $\alpha = 0.3$ and $\beta = 1.0$ but the number of at. planes in the interface varies from N = 2 to N = 50. The results for N = 2 to N = 10 are shown in

Fig.3.5. It can be seen that the DOS curves approach very quickly an asymptotic behaviour for $N > 10$. This asymptotic behaviour corresponds to the DOS for a ferromagnet with $J_{\parallel} = J$ and $J_{\perp} = 0.3J$. The approqch to the asymptotic DOS is faster than for an overlayer.

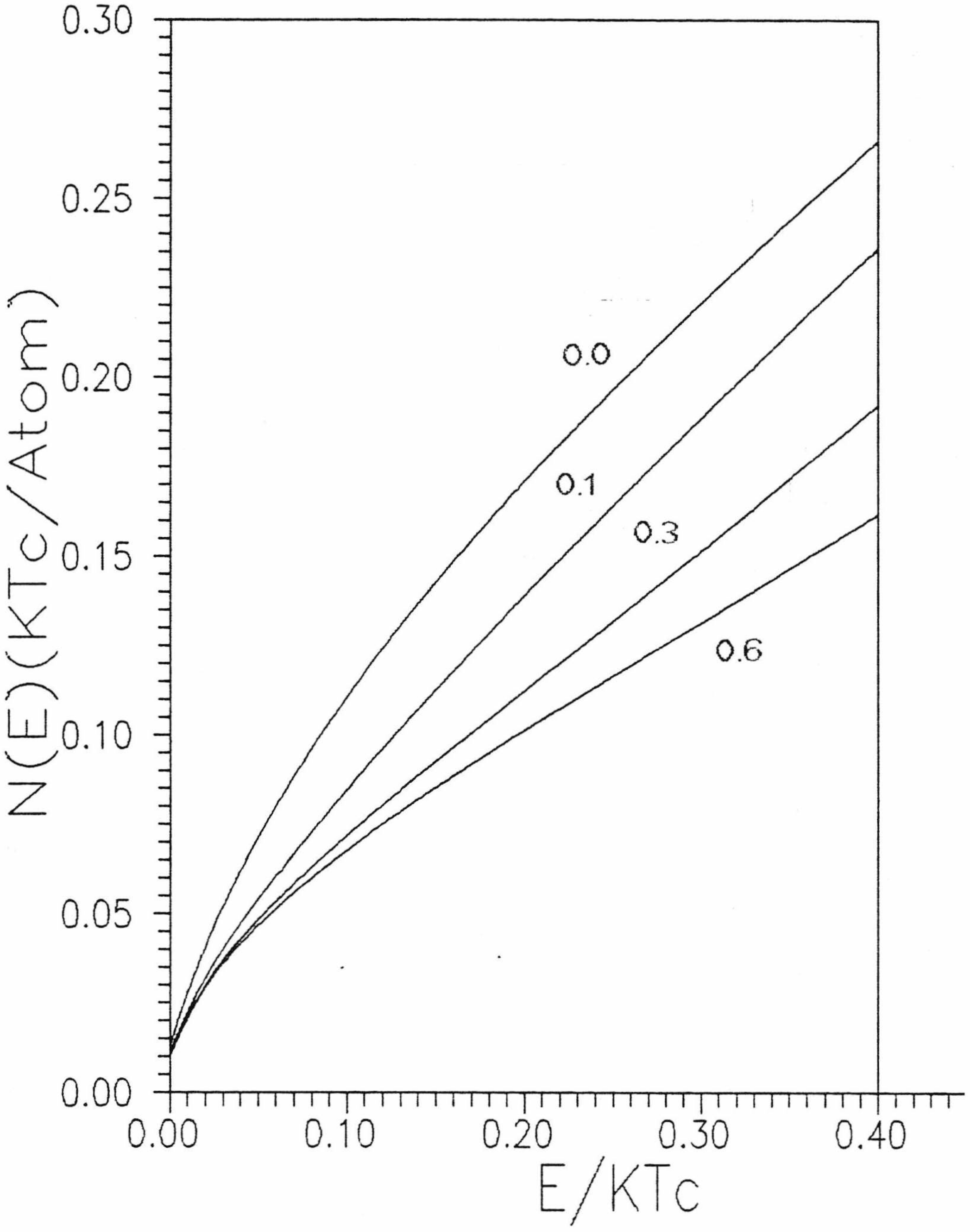

Fig. 3.2 Calculated density of spin wave states N(E) in the (100) interface separating two identical semi-infinite Heisenberg ferromagnets. Only the exchange integral J_{10} perpendicular to the interfaces is softened. The values of J_{10}/J are 0.0, 0.1, 0.3 and 0.6.

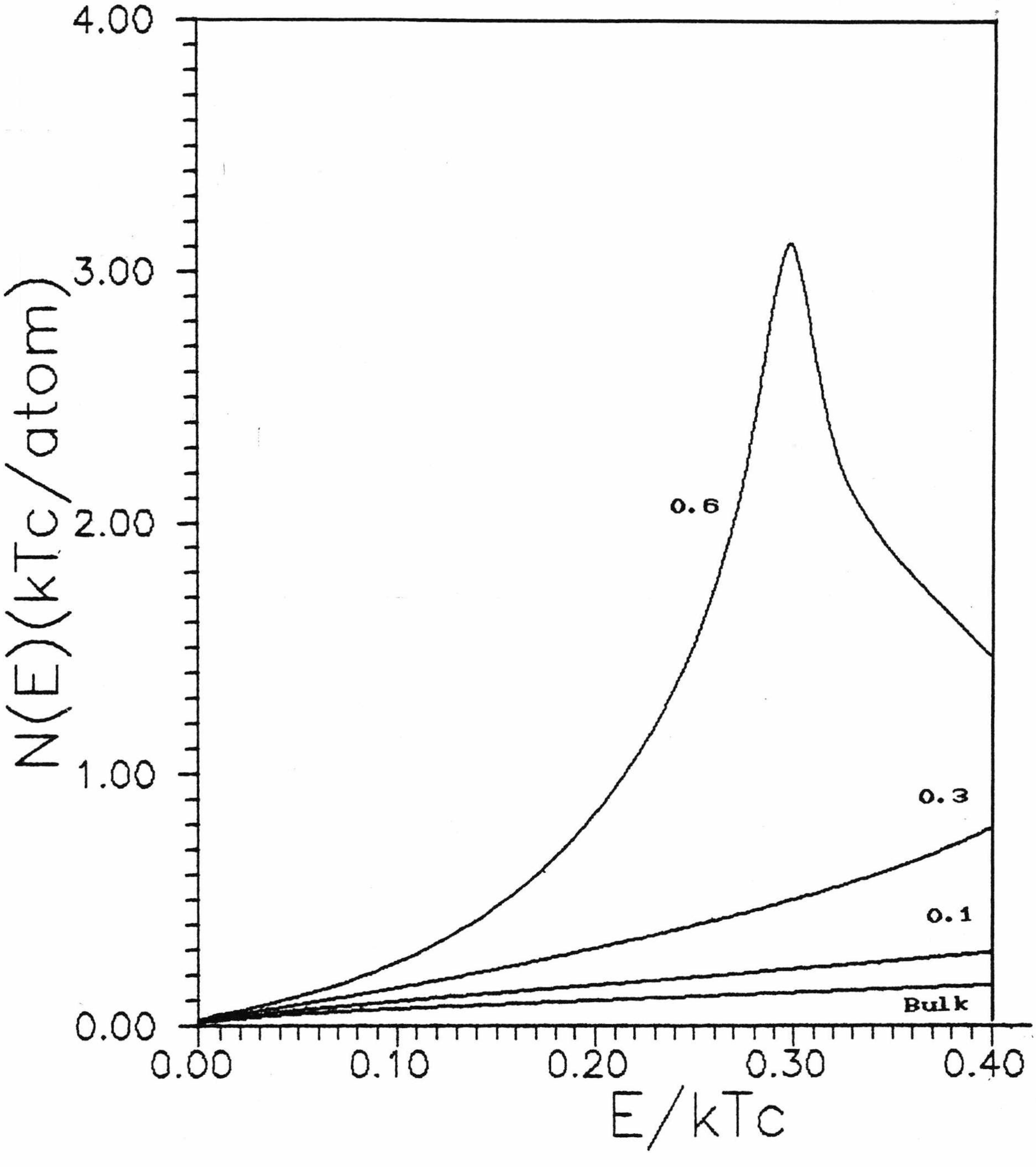

Fig.3.3 Calculated density of spin wave states N(E) in the (100) interface separating two identical semi-infinite Heisenberg ferromagnets. Only the parallel exchange $J_{\parallel}$ within the interface layer is softened. The values of $J_{\parallel}/J$ are 0.1, 0.3 and 0.6.

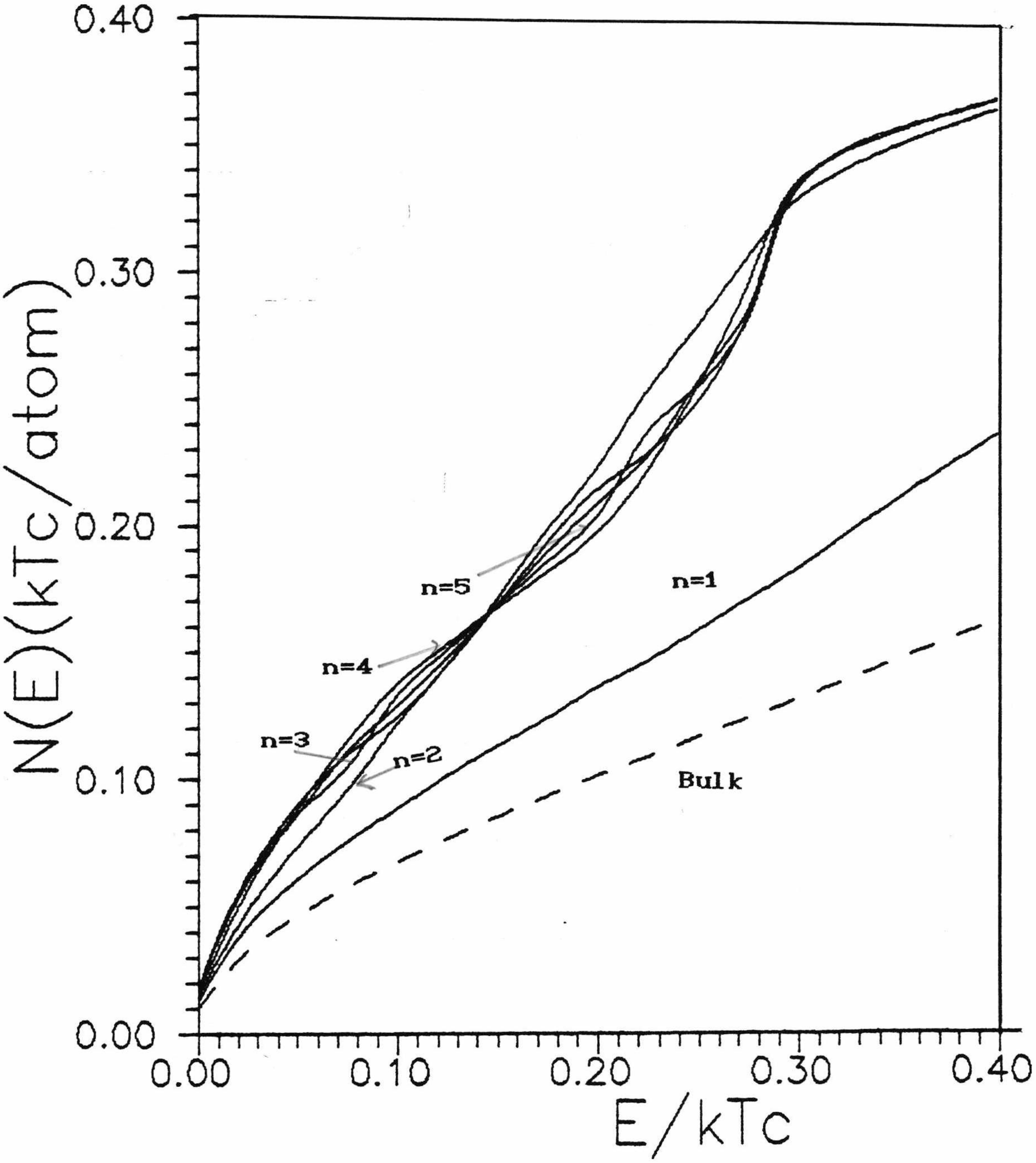

Fig. 3.4 Calculated density of spin wave states N(E) in interface layers n=1, 2, 3, 4 and 5 for an interface consisting of 10 at. layers with the perpendicular exchange integral $J_\perp/J=0.3$.

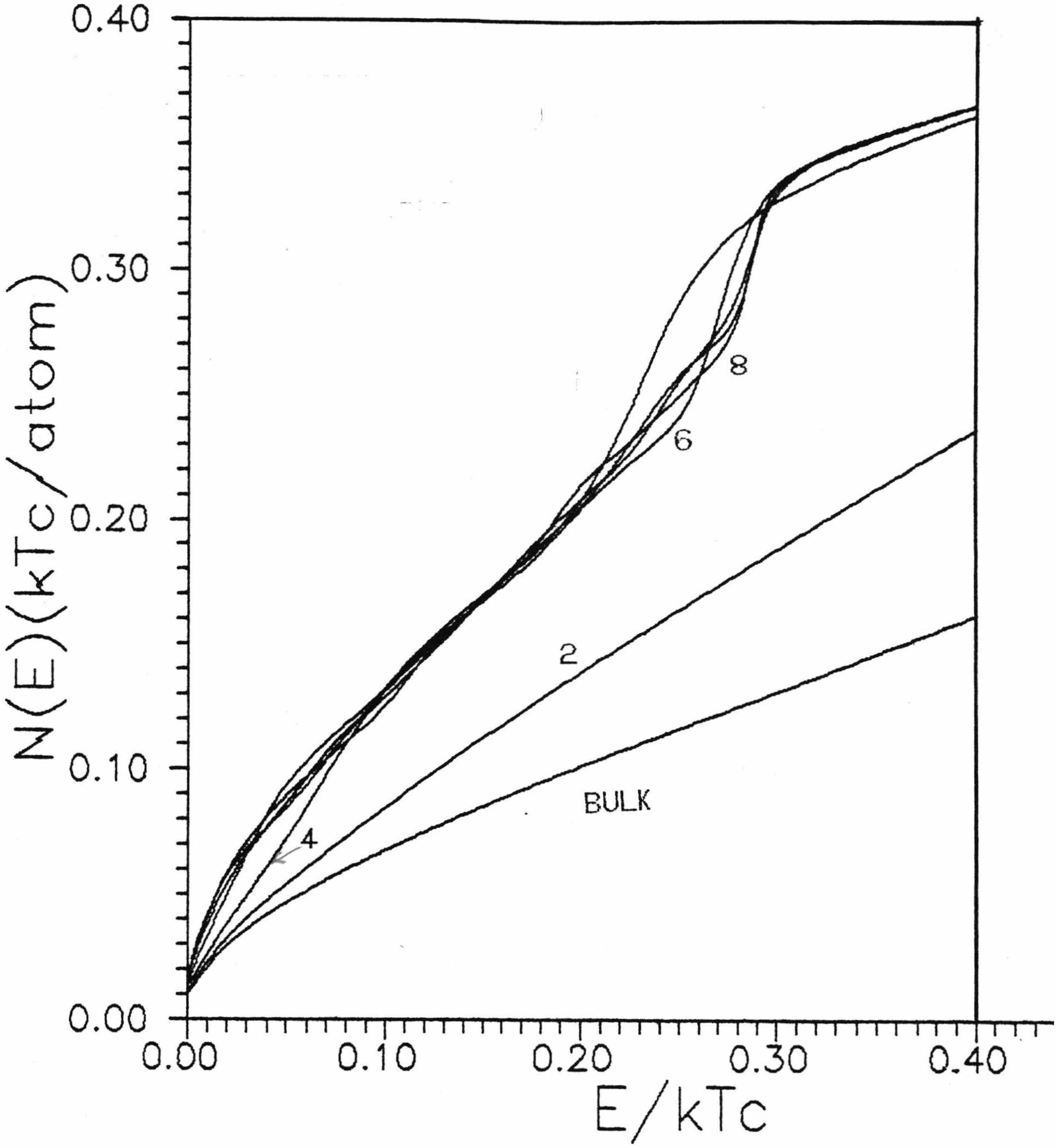

Fig. 3.5 Calculated density of spin wave states N(E) in the middle of an interface for various thicknesses of interface N: 2, 4, 6, 8 and 10. The perpendicular exchange integral is J /J=0.3. Asymptotic behaviour is attained for $N\geq 10$.

3.4 The Temperature Dependence of Interface Magnetization

As interface temperature is raised from absolute zero, the local magnetization starts to deviate from its saturation value. This deviation is given by the thermal average in Eq.(2.3.2). At low temperatures the only spin waves that contribute to the Eq.(2.3.2) are those having a small excitation energy of the order k_BT. These are spin waves near the bottom of the band. As discussed by Yaniv (See section 3.3), no interface spin waves exist below the bulk subbands for $J_{10}/J < 1$. Therefore, the low temperature contribution to the local magnetization comes from bulk spin waves in the interface. To illustrate this, we consider the simplest interface consisting of two homogeneous semi-infinite ferromagnets connected by a single weak link $J_{10} < J$. We show in Fig.3.6 the temperature dependence M(T)/M(0) for such an interface with J_{10}/J: 0.0, 0.1, 0.3 and 0.6. To check whether M(T) obeys good $T^{3/2}$ law, we plot in Fig.3.7 $M_i(T)$ against the bulk $M_B(T)$. It is clear that the interface M(T) varies with T according to the same power law as in the bulk but with different prefactors depending on J_{10}.The corresponding prefactors for the different interface exchanges considered are 1.8, 1.5, 1.3 and 1.1.

It is also very important to investigate the contribution of interface spin waves to local magnetization. As discussed in section 3.3, interface spin wave exists below the bulk band when parallel exchange of interface is softened. To illustrate this, we consider the interface consisting of two at. planes with $J_{\parallel} < J$ and $J_{\perp} = J$. The contribution to local magnetization now comes from the both bulk spin wave and interface spin wave. The computed results of the temperature dependence of interface magnetization are shown in Fig.3.8 for range of $J_{\parallel}/J$: 0.1, 0.3 and 0.6. To see whether they give good $T^{3/2}$ law or not, we plot temperature dependence of the interface $M(T)/M(0)$ against bulk dependence $M_B(T)/M_B(0)$ in Fig.3.9. There are good straight lines for $J_{11}/J = 0.6$ with prefactor $k = 1.1$ but for $J_{11}/J = 0.3$ we obtain the good straight line at temperature bigger than $\simeq 0.02T_C$. Therefore, temperature dependence of interface magnetization follow $T^{3/2}$ law with prefactor depends on interface exchange interaction.

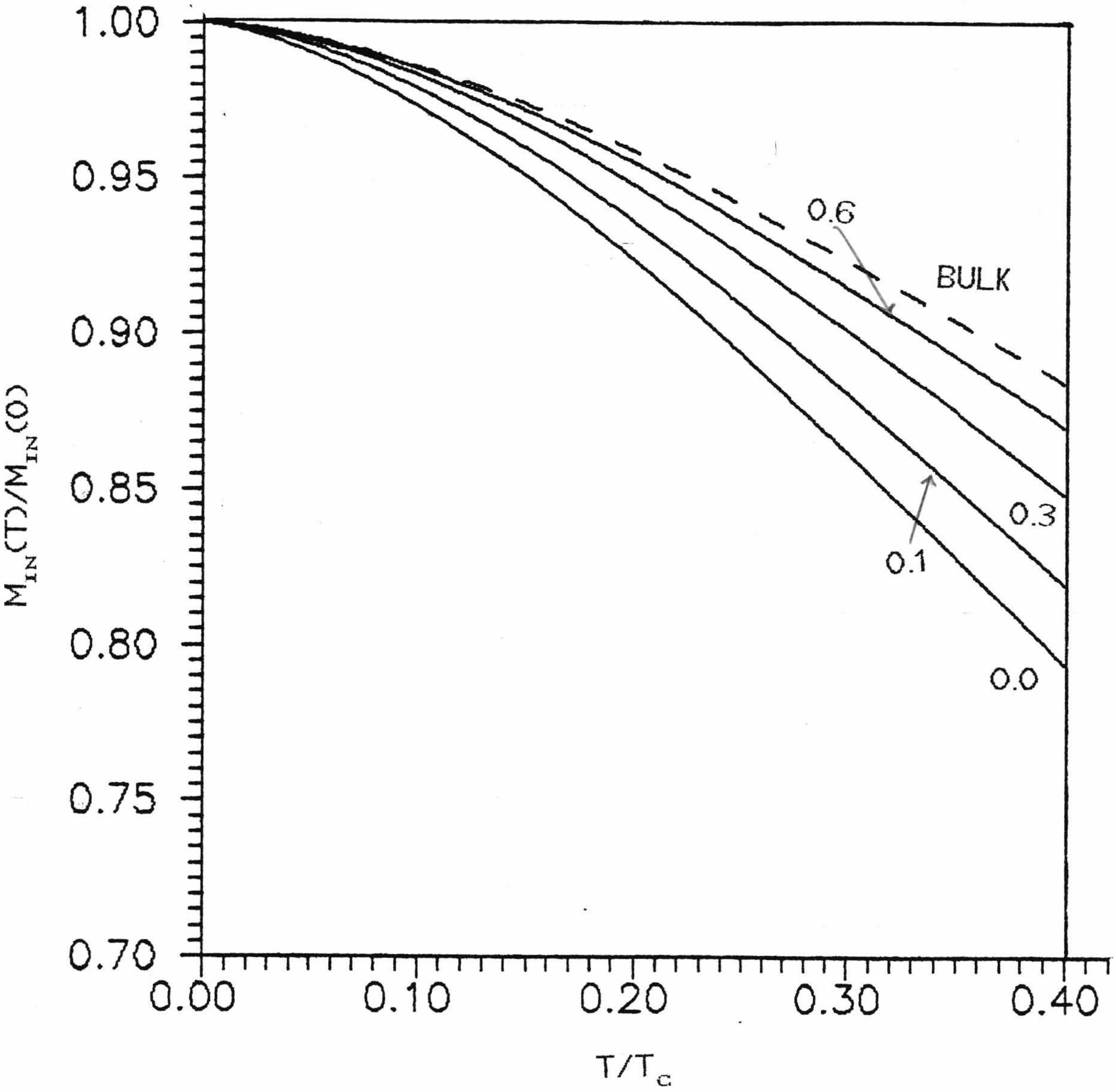

Fig. 3.6 Calculated temperature dependence of the interface magnetization $M_{IN}(T)/M_{IN}(0)$ for an interface separating two identical semi-infinite Heisenberg ferromagnets with a softened perpendicular exchange J_{10}/J. The values of J_{10}/J are 0.0, 0.1, 0.3 and 0.6.

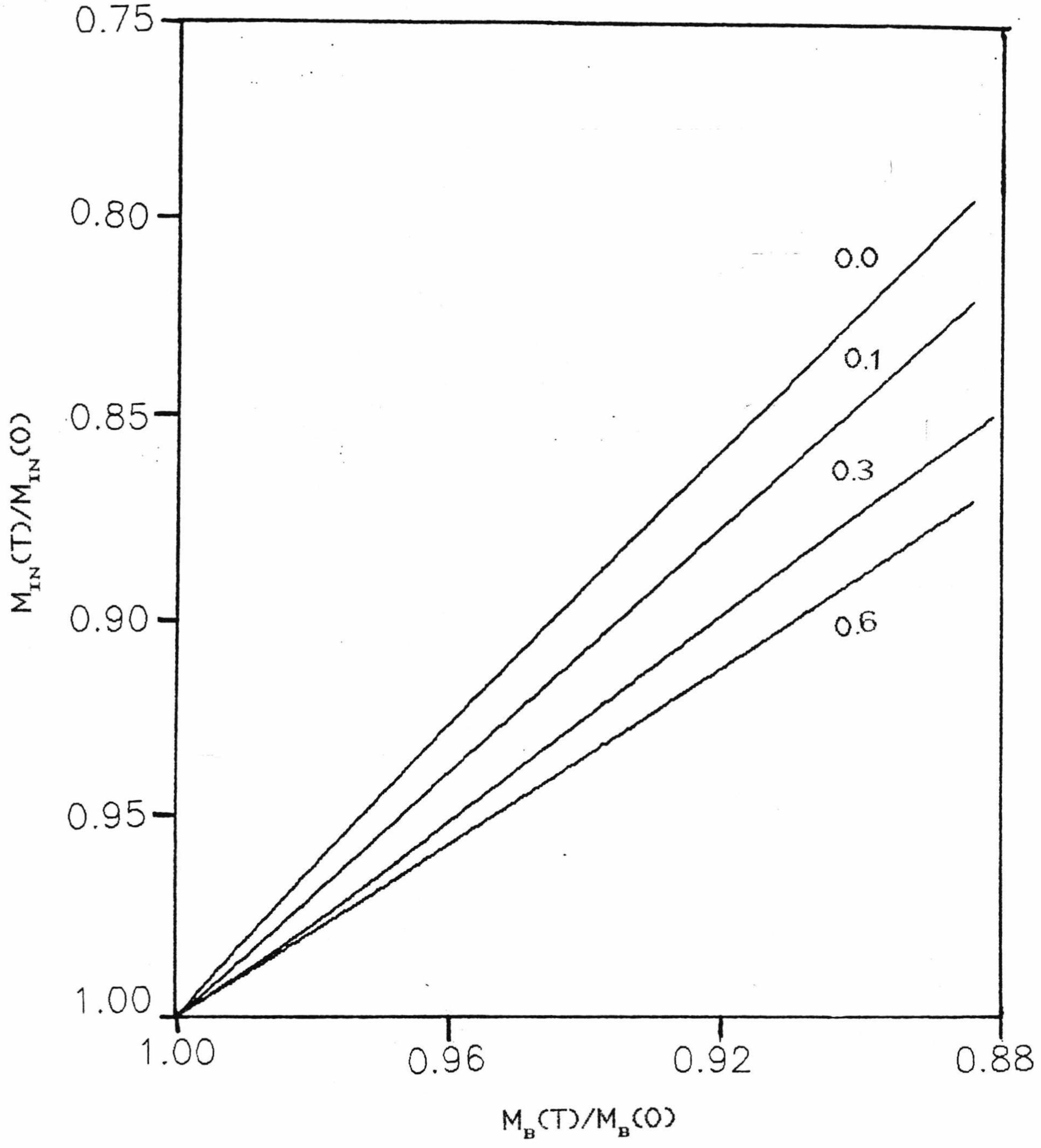

Fig. 3.7 Plot of the temperature dependence of interface magnetization $M_{IN}(T)/M_{IN}(0)$ against the bulk dependence $M_B(T)/M_B(0)$ for an interface separating two identical semi-infinite Heisenberg ferromagnets. The values of J_{10}/J are 0.0, 0.1, 0.3 and 0.6.

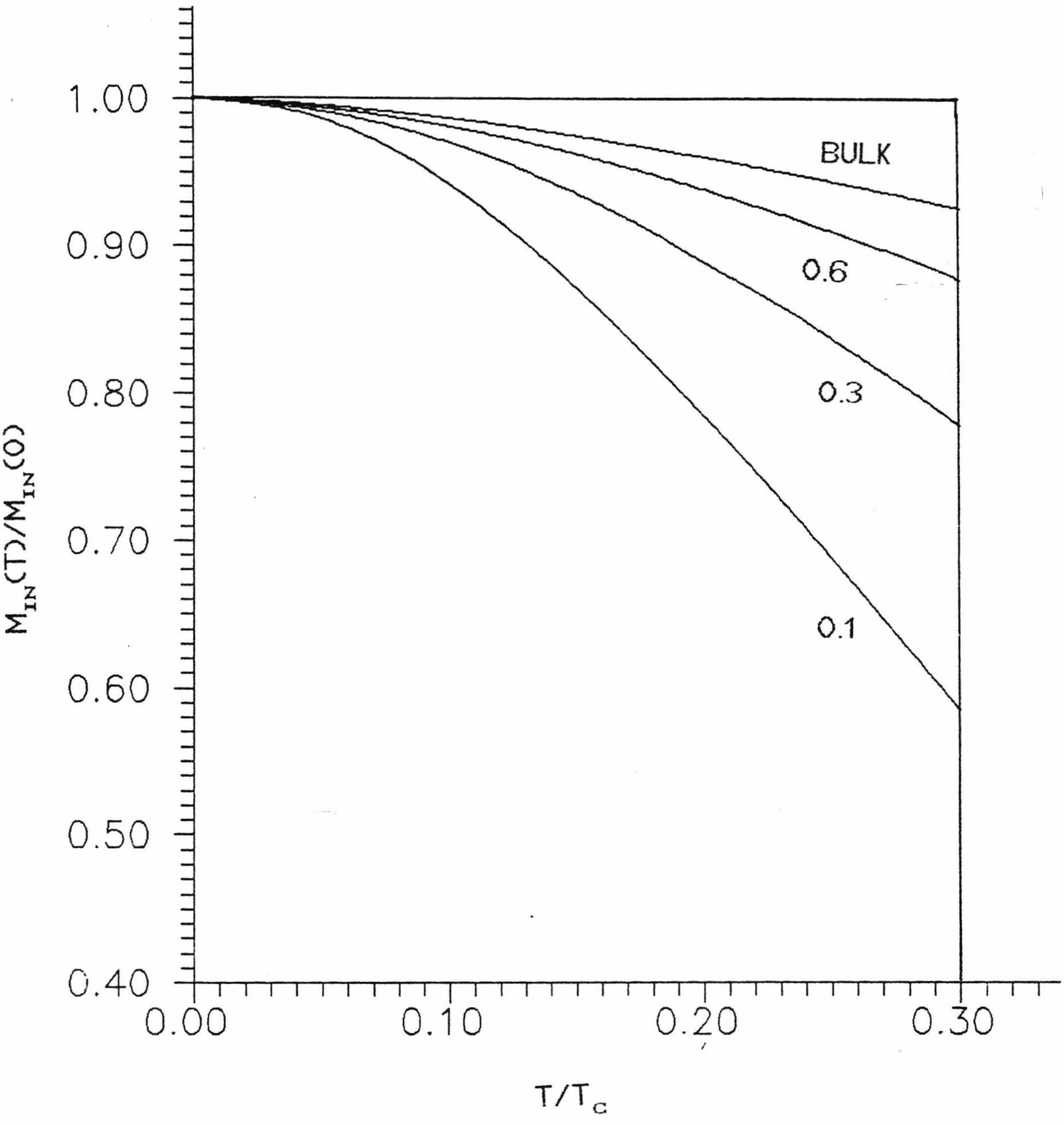

Fig. 3.8 Calculated temperature dependence of interface magnetization $M_{IN}(T)/M_{IN}(0)$ in the middle of an interface consisting of two at. atomic layers with a softened parallel exchange $J_{\parallel}$. The values of $J_{\parallel}/J$ are 0.1, 0.3 and 0.6.

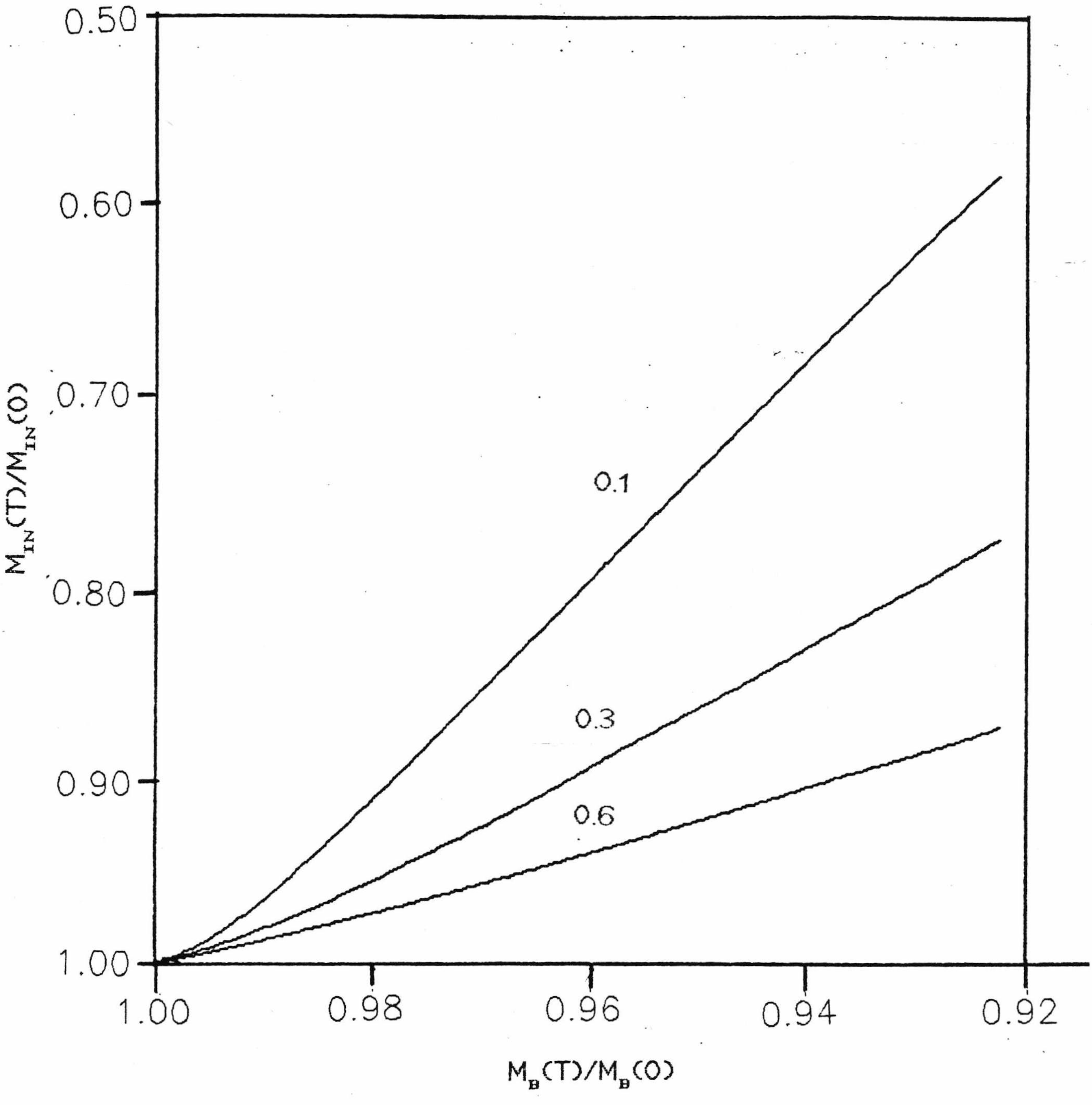

Fig.3.9 Plot of the interface $M_{IN}(T)/M_{IN}(0)$ against the bulk dependence $M_B(T)/M_B(0)$ for an interface consisting of two at. layers with parallel exchange $J_{\parallel}/J=0.1$, 0.3 and 0.6

CONCLUSIONS

In sections 1.1 - 1.6, we reviewed all the concepts necessary for chapter 2. In particular, the main results for the spin wave Green's function and for the bulk spin waves in a Heisenberg ferromagnet are summarized. The classical Bloch law for the temperature dependence of the magnetization is also briefly discussed.

In section 1.6, a brief preliminary account was given of the effect of surface on spin waves in a Heisenberg ferromagnet. It has been shown that in the simplest model the effect of surface can be treated by setting the bulk exchange equal to zero across the surface. This is the geometric effect of surface which leads to the classical result that the initial surface density of spin wave states is twice as large as the bulk density of states. This implies that the surface magnetization should decrease with increasing temperature twice as fast as in the bulk.

In section 2.1, the experimental results on the temperature dependence of the surface magnetization M(T) were reviewed. All these measurements show that $M_S(T)$ decreases following a Bloch $T^{3/2}$ law but with a prefactor B_S which is different for different surfaces and usually greater than $2B_B$. These results, therefore, contradict the classical spin wave theory which predicts for a geometric surface that the surface prefactor in the $T^{3/2}$ law is given by $B_S = 2B_B$. The main objective of chapter 2 was to resolve this discrepancy between the spin wave theory and experiment using a model which assumes softening of surface exchange. To this purpose, a new adlayer method for calculating the Green's function of an arbitrary ferromagnetic surface or an arbitrary overlayer was developed. It provides an exact expression for the surface density of spin wave states in terms of the known substrate Green's function.

The method of adlayers was used in Secs. 2.3 and 2.6 to derive an exact result for the initial spin wave density of states in the surface of an arbitrary magnetic overlayer. It states that the initial surface density of states is independent of the exchange in the overlayer. This would seem to imply that the surface magnetization should always decrease twice as fast as in the bulk, which contradicts the experiment. However, our further investigations in Secs. 2.3 - 2.6 showed that this initial behaviour is valid only at energies so low that they are of no practical interest. We were able to show that at higher energies the surface density of states depends very strongly on the exchange in the overlayer (surface region) and it increases rapidly when the surface exchange is weakened. We investigated both the cases of weakening of exchange perpendicular and parallel to the surface. In the case of weakening of the parallel exchange, we had to consider in Sec. 2.4 the contribution of surface spin waves to the density of states.

Our results for the spin wave density of states were used in Sec. 2.5 to calculate the temperature dependence of the surface magnetization $M_s(T)$. Our principal finding is that beyond the very narrow initial region of the classical $T^{3/2}$ law, there is another extended region of temperatures in which a very good $T^{3/2}$ law holds but the prefactor in this "second" $T^{3/2}$ law now depends very strongly on the surface exchange. This "second" $T^{3/2}$ law can not only explain very well the existing experimental results on $M_s(T)$ but was confirmed recently by new experiments designed specifically to test the effect of softening of the perpendicular exchange on $M_s(T)$.

In section 2.6, we investigated the effect of surface weakening of exchange in a thick overlayer. The most interesting an unexpected result is that an overlayer of one at. layer of a material with different exchange has already the surface density of states which is qualitatively the same as for a very thick overlayer of the same material.

In section 2.7, we have determined the local density of states and the local M(T) below the surface of a ferromagnet with a softened surface to bulk exchange. We found that the local M(T) becomes essentially bulk and independent of the surface exchange already in the third at. plane below the surface. However, M(T) in the second at. layer does not obey a good $T^{3/2}$ law. This is because at low temperature the wave length of thermal spin waves is long and the second layer behaves as the surface. At higher temperatures it becomes more bulk-like and that means that the prefactor in the $T^{3/2}$ law for the second layer becomes temperature dependent.

Finally, in chapter 3 we have shown that the calculation of the local density of states and of the local M(T) in an arbitrary ferromagnetic interface reduces to the problem of two overlayers which can be again treated by our method of adlayers. As an illustration, we have made specific calculations for model interfaces with a weaker exchange in the interfaces. We studied both the dependence of the local density of states on the thickness of the interface and the strength of the exchange in the interface. There is clear connection between the results for the interface and the results for an overlayer. This is discussed in Secs. 3.3 - 3.4.

APPENDIX A

A.1 Evaluating Spin Wave Green's function for a Bulk ferromagnet

From Eq.(1.5.18), rewrite the spin wave green's function $G^0(n)$ for finite ferromagnetic crystal as

$$G^0(n) = 1/2\pi \int_{-\pi}^{\pi} e^{int} [\omega - i\delta - \{ 2SJ \cos(t)\}]^{-1} dt \qquad (A.1.1)$$

where $\omega = E' - W$, $E' = E - 6SJ$, $W = 2SJ\Lambda(\underline{q}_{\parallel})$ and $\Lambda(\underline{q}_{\parallel}) = \cos(q_x a) + \cos(q_y a)$.

To evaluate the integral in (A.1.1), we first consider the case $n > 0$.

Setting $Z = e^{it}$, then G^0 becomes

$$G^0(n) = -1/(2SJ\pi i) \oint_c \frac{Z^n}{Z^2 - (\omega - i\delta)Z + 1} dz, \qquad (A.1.2)$$

where c is a unit circle centred at origin.

The poles of the integrand are given by

$$Z = \frac{(\omega - i\delta) \pm \{(\omega - i\delta)^2 - 4S^2J^2\}^{1/2}}{2SJ} \qquad (A.1.3)$$

We set first $\delta = 0$ to determine the position of the poles. Then the poles are

$$Z = \frac{\omega \pm (\omega^2 - 4S^2J^2)^{1/2}}{2SJ} \ .$$

For $\omega^2 - 4S^2J^2 < 0$, then

$$Z = \frac{\omega \pm i(\omega^2 - 4S^2J^2)^{1/2}}{2SJ}$$

and

$$|Z_{1,2}|^2 = \frac{\omega^2}{4S^2J^2} + \frac{4S^2J^2 - \omega^2}{4S^2J^2} = \frac{\omega^2 + 4SJ - \omega^2}{4S^2J^2} = 1.$$

Since the poles lie on the boundary $Z = 1$, it is necessary to keep $\delta \neq 0$ and take the limit $\delta \rightarrow 0$ only after integration. We can expand in powers of δ and keep only linear term in δ. We first evaluate the square root,

$$[(\omega - i\delta)^2 - 4S^2J^2]^{1/2} = [\omega^2 - \delta^2 - 4S^2J^2 + i2\omega(-\delta)]^{1/2}$$

$$= (x + iy)^{1/2} \equiv \pm (a + ib)$$

where x, y, a and b are real numbers defined by

$$x + iy \equiv (a + ib)^2 = a^2 - b^2 + i2ab.$$

Here $x = a^2 - b^2 = \omega^2 - \delta^2 - 4S^2J^2$

and $y = 2ab = 2\omega(-\delta)$.

It follows that

$$\frac{dx}{d\delta} = -2\delta = 2a\frac{da}{d\delta} - 2b\frac{db}{d\delta}$$

$$\frac{dy}{d\delta} = -2\omega = 2b\frac{da}{d\delta} + 2a\frac{db}{d\delta} .$$

Therefore

$$a = \frac{\omega(-\delta)}{(4S^2J^2 - \omega^2)^{1/2}} + O(\delta^2)$$

and

$$b = (4S^2J^2 - \omega^2)^{1/2} + O(\delta^2).$$

Hence

$$Z \simeq \frac{\omega + i(-\delta) \pm \dfrac{\omega(-\delta)}{(4S^2J^2 - \omega^2)^{1/2}} \pm i(4S^2J^2 - \omega^2)^{1/2}}{2SJ}$$

which can be written as

$$Z \simeq \frac{\omega+i(-\delta)\pm \dfrac{\omega(-\delta)}{i\ \mathrm{sign}(\omega)(\omega^2-4S^2J^2)^{1/2}} \pm i\ \mathrm{sign}(\omega)(4S^2J^2-\omega^2)^{1/2}}{2SJ} \tag{A.1.4}$$

where

$$(4S^2J^2 - \omega^2) = i\ \mathrm{sign}(\omega)\ (\omega^2 - 4S^2J^2)^{1/2},\ \text{for}\ \omega^2 > 4S^2J^2$$

and

$$\mathrm{sign}(\omega) = \begin{cases} 1; & \omega > 0 \\ -1; & \omega < 0 \end{cases} . \tag{A.1.5}$$

For $4S^2J^2 > \omega^2$, we obtain

$$2SJ\ Z_{1,2} \simeq \omega + i(-\delta) \pm \frac{\omega(-\delta)}{(4S^2J^2 - \omega^2)^{1/2}} \pm i(4S^2J^2 - \omega^2)^{1/2}$$

Then

$$4S^2J^2|Z_{1,2}|^2 \simeq 4S^2J^2 \pm \frac{8S^2J^2(-\delta)}{(4S^2J^2 - \omega^2)^{1/2}} .$$

Therefore

$$|Z_{1,2}|^2 \simeq 1 \pm \frac{2(-\delta)}{(4S^2J^2 - \omega^2)^{1/2}} \tag{A.1.6}$$

If we take (+), one of the poles lies inside the unit circle, i.e.

$$Z \simeq \frac{\omega + i(-\delta) + \dfrac{\omega(-\delta)}{(4S^2J^2 - \omega^2)^{1/2}} - i(4S^2J^2 - \omega^2)^{1/2}}{2SJ} \tag{A.1.7}$$

or

$$Z = \frac{(\omega - i\delta) + i\{4S^2J^2 - (\omega - i\delta)^2\}^{1/2}}{2SJ} \qquad (A.1.8)$$

We now subsitute (A.1.8) into (A.1.2) to evaluate $G^0(n)$.

$$G^0(n) = -1/(2\pi iSJ) \oint_c \frac{\frac{Z^n}{Z - Z_2}}{Z - Z_1}\, dz \qquad (A.1.9)$$

where

$$Z_1 = \frac{(\omega - i\delta) + [(\omega - i\delta)^2 - 4S^2J^2]^{1/2}}{2SJ}$$

and

$$Z_2 = \frac{(\omega - i\delta) - [(\omega - i\delta)^2 - 4S^2J^2]^{1/2}}{2SJ}$$

By Cauchy's integral formula, we obtain

$$G^0(n) = [(\omega-i\delta)^2-4S^2J^2]^{-1/2}\ [\{\frac{(\omega-i\delta)+\{(\omega-i\delta)^2-4S^2J^2\}^{1/2}}{2SJ}\}]^n.$$

Taking limit $\delta \to 0$ for $4S^2J^2 > \omega^2$, the final formula for $G^0(n)$ becomes

$$G^0(n) = i(4S^2J^2 - \omega^2)^{-1/2}\ [\ \frac{\omega + i(4S^2J^2 - \omega^2)^{1/2}}{2SJ}\ ]^n,$$

for n>0. (A.1.10)

Now we consider the case $n<0$.

For $n<0$, (A.1.1) becomes

$$G^0(n) = 1/2\pi \int_{-\pi}^{\pi} e^{-int} [\omega - i\delta - \{2SJ\cos(t)\}]^{-1} dt \qquad (A.1.11)$$

where

$\underline{q}_\perp d = -t$.

Setting $z = e^{it}$, we can transform (A.1.11) to

$$G^0(n) = -1/(2SJ\pi i) \oint_c \frac{\underline{Z}^{-n}}{Z^2 - (\omega - i\delta)Z + 1} dz, \qquad (A.1.12)$$

The poles of (A.1.12) are

$$Z = \frac{(\omega - i\delta) \pm \{(\omega - i\delta)^2 - 4S^2J^2\}^{1/2}}{2SJ}$$

are the same as the poles defined by (A.1.3).

The pole

$$Z = \frac{(\omega - i\delta) + \{(\omega - i\delta)^2 - 4S^2J^2\}^{1/2}}{2SJ}$$

lies inside the unit circle.

Evaluating the integral for $4S^2J^2 > \omega^2$ and taking the limit $\delta \to 0$, we find that (A.1.12) becomes

$$G^0(n) = i(4S^2J^2 - \omega^2)^{-1/2} \left[\frac{\omega + i(4S^2J^2 - \omega^2)^{1/2}}{2SJ} \right]^{-n} . \tag{A.1.13}$$

Both result (A.1.10) and (A.1.13) can be combined into one formula

$$G^0(n) = i(4S^2J^2 - \omega^2)^{-1/2} \left[\frac{\omega + i(4S^2J^2 - \omega^2)^{1/2}}{2SJ} \right]^{|n|},$$

$$\text{for } \omega^2 - 4S^2J^2 \text{ and } n = \pm 1, \pm 2, \pm 3, \ldots. \tag{A.1.14}$$

where (A.1.14) is the Green's function for semi-infinite Heisenberg ferromagnet.

APPENDIX B

The Approximation of Density of Spin Wave States for The Simple Cubic lattice at Surface

The matrix element G_{00}^{0} in the surface plane of the spin wave Green's function G^{0} for simple geometric effect of the surface is given by

$$G_{00}^{0}(E,\ \underline{q}_{\parallel}) = 1 + [(1 - \omega)/(1 + \omega)]^{1/2},\ \text{for}\ \omega^{2} < 1 \qquad \text{(B1)}$$

where $\omega = E - 3 - [\cos(q_x a) + \cos(q_y a)]$, a is the lattice constant and all energies are measured in unit of 2SJ.

The density of spin wave states $N_0(E)$ is given by Eq.(1.3.14), i.e.

$$N_S(E) = \frac{1}{\pi N_{\parallel}} \sum_{\underline{q}_{\parallel}} \mathrm{Im}G_{00}^{0}(E,\ \underline{q}_{\parallel}) \qquad \text{(B2)}$$

Using Eq.(B1) and transforming the sum over $\underline{q}_{\parallel}$ to an integral over the first Brillouin zone,

$$\sum_{\underline{q}_{\parallel}} \rightarrow N_{\parallel}\ (a/2\pi)^{2} \int_{-\pi/a}^{+\pi/a} \int_{-\pi/a}^{+\pi/a} dq_x\ dq_y\ , \qquad \text{(B3)}$$

then Eq.(B2) becomes

$$N_S(E) = \frac{a^{2}}{4\pi^{3}} \int\int_{-\pi/a}^{+\pi/a} [(1 - \omega)/(1 + \omega)]^{1/2}\ dq_x\ dq_y \qquad \text{(B4)}$$

Setting $q_x a = x - \pi$, $q_y a = y - \pi$ and the symmetry property of integrand then Eq.(B4) becomes

$$N_S(E) = 1/\pi^3 \int_0^{\pi}\int [(1 - \omega)/(1 + \omega)]^{1/2}\, dx\, dy. \qquad (B5)$$

Now we consider

$$\omega = E - 3 - [\cos(q_x a) + \cos(q_y a)]$$

We can write ω in term of variables x and y as

$$\omega = E - 3 + [\cos(x) + \cos(y)] \qquad (B6)$$

Expanding cos(x) and cos(y) in power of x and y respectively, we obtain

$$\cos(x) = 1 - \frac{x^2}{2} + \ldots\ldots.$$

and (B7)

$$\cos(y) = 1 - \frac{y^2}{2} + \ldots\ldots.$$

Substituting Eq.(B7) into Eq.(B6), therefore

$$\begin{aligned}\omega &\simeq (E - 3) + 2 - 1/2\ (x^2 + y^2)\\ &= E - 1 - 1/2\ (x^2 + y^2) \qquad (B8)\end{aligned}$$

Substituting $x = r\cos(\theta)$ and $y = r\sin(\theta)$ into Eq.(B8), it follows that

$$\omega \simeq E - 1 - r^2/2 \qquad \text{(B9)}$$

Combining Eqs.(B5), (B7) and (B9), then

$$N_S(E) = 1/\pi^3 \int_{\theta=0}^{\theta=\pi/2} \int_{r=0}^{r} [2 - (E - r^2/2)/(E - r^2/2)]^{1/2}\, r\, dr\, d\theta$$

with the restriction $E - r^2/2 > 0$.

It follows that

$$N_S(E) = 1/2\pi^2 \int_{r=0}^{r=\sqrt{2E}} [2 - (E - r^2/2)/(E - r^2/2)]^{1/2}\, r\, dr \qquad \text{(B10)}$$

We set $t = E - r^2/2$ and Eq.(B10) becomes

$$N_S(E) = 1/\pi^2 \int_{r=0}^{r=E} [(2 - t)/t]^{1/2}\, dt \qquad \text{(B11)}$$

We expand the term $(2 - t)/t$ in Eq.(B11) as

$$(2 - t)/t = (2/t)^{1/2}\, (1 - t/4 - t^2/32 - \ldots\ldots)$$

and substituting into Eq.(B11), then Eq.(B11) reduces to

$$N_S(E) = 1/\pi^2\, (2E)^{1/2} + O(E^{3/2}) \qquad \text{(B12)}$$

Equation B(12) is the approximation of density of spin wave states at the surface of simple cubic semi-infinite Heisenberg ferromagnet near the bottom of spin wave band.

APPENDIX_C

Relation Between Surface Density of Spin Wave States and Bulk Density of Spin Wave States

The Imaginary part of Green's function for the bulk of Heisenberg ferromagnet is given by well-known expression as

$$\mathrm{Im}G^{b} = [(1 - \omega)(1 + \omega)]^{-1/2} \text{ for } \omega^{2} < 1$$

and recall Eq.(2.3.4) for imaginary part of Green's function for spin wave at the surface of semi-infinite Heisenberg ferromagnet

$$\mathrm{Im}G^{0}_{00} = \begin{cases} [(1 - \omega)/(1 + \omega)]^{1/2}, & \omega^{2} < 1 \\ 0, & \omega^{2} > 1 \end{cases}$$

then writes $\mathrm{Im}G^{0}_{00}$ in term of $\mathrm{Im}G^{b}$ as

$$[(1 - \omega)/(1 + \omega)]^{1/2} = (1 - \omega)[(1 - \omega)(1 + \omega)]^{-1/2}.$$

Therefore,

$$\mathrm{Im}G^{0}_{00}(E,\underline{q}_{\parallel}) = (1 - \omega)\ \mathrm{Im}G^{b}(E,\underline{q}_{\parallel}) \text{ for } \omega^{2} < 1 \qquad \text{(C1)}$$

The behaviour of the density of spin wave states at the bottom of the spin wave band is determined by a weak singularity of $\mathrm{Im}G^{0}_{00}(E,\underline{q}_{\parallel})$ and $\mathrm{Im}G^{b}(E,\underline{q}_{\parallel})$ at $\omega = -1$. Replace $\omega = -1$ in Eq.(C1), this leads to the result

$$\mathrm{Im}G^{0}{}_{00}(E,\underline{q}_{\parallel}) = 2\ \mathrm{Im}G^{b}(E,\underline{q}_{\parallel}) \text{ for } \omega^{2} < 1 \qquad \text{(C2)}$$

To obtain the density of spin wave states, substitutes Eq.(C2) into Eq.(B4).

Therefore, density of spin wave states at the surface at the bottom of spin wave band in term of density of states in the bulk is given by

$$N_S(E) = 2\ N_B(E) \tag{C3}$$

Finally, from Eq.(B12) and Eq.(C3), the density of spin wave states in the bulk at the bottom of the band is given by

$$N_B(E) = 1/2\pi^2\ (2E)^{1/2} \tag{C4}$$

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