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An Algebraic Approach to Green Functions for Surface, Interface and Overlayer Magnetism

Y. Zheng*, D. L. Lin, and Hao Che‡

Department of Physics, State University of New York at Buffalo, Buffalo, NY 14260-1500, U.S.A.

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The Gaussian elimination and back substitution formalism is employed to study magnetic lattices involving surfaces and interfaces. On the nearest neighbor interaction of Heisenberg model, it is shown that exact Green's functions for any spin layer can be found in analytical form. Surface and interface spin wave spectra as well as the surface magnetization at low temperatures are calculated for systems with variable exchange coupling strengths. The recently observed substrate-induced magnetization in over-layers is also found. The advantages and limitations of the method. in general are discussed.

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I. INTRODUCTION

There has been growing interest in the last decade in localized excitations of layered magnetic systems such as magnetic thin films, overlayers as well as interfaces in heterostructures because of the development of fabrication techniques by the molecular beam epitaxy. The experimental study of physical properties has been carried out by spin polarized low energy electron diffraction (SPLEED) [1], Mossbauer spectroscopy [2], and angle resolved photoemission [3].

On the theoretical side, the problem may be treated either by the mean field theory approach or by the Green's function approach. The former is limited to the discussion of thermodynamic properties and the latter can provide spectra of elementary excitations as well. One of the earliest works on the surface magnetism was due to Mills and Maradudin [4], who reported that the free surface magnetization deviation from the saturation value is twice as big as that in the bulk at low temperatures. In recent years, the surface magnetization

has been further investigated over the whole temperature range by Slazer and Majlis [5]. To account for the discrepancy between the theoretical prediction and experimental results of the surface magnetization, a weakened surface exchange model was proposed by Mathon [6]. In addition, there have also been a number of studies on the magnon spectrum in heterostructures of magnetic materials and magnetic superlattices. Surface spin waves (SSW) in ferromagnetic and antiferromagnetic systems were discussed by DeWames and Wolfram and by Diep, Harada and Nagai [8]. Zhengand Lin [9] calculated SSW spectra in a semi-infinite ferrimagnet. The interface spin waves (ISW) were first considered by Yaniv for a biferromagnetic system [10], by Mata and Pestana between two antiferromagnets [11] and by Che et *al.* in a bilayer of two-sublattice ferrimagnets [12]. Other related works investigating magnetic superlattices by many authors can also be found in the literature [13-17].

The central problem in such studies is of course the evaluation of the Green's function. We introduce, in this article, a new method which employs the Gaussian elimination and back substitution (GEBS) [18] formulation to obtain the exact Green's function. The method is particularly useful in dealing with systems in which the translational symmetry in the z-direction is broken, namely, systems such as slabs, heterostructures and superlattices with arbitrary exchange interactions. It can also be easily generalized to treat systems with more complicated lattice structures than simple cubic. From the Green's functions thus obtained, we can calculate spin-wave spectra and other magnetic properties for a variety of structures in a very simple manner.

In Sec. II, we first derive the equation that the Green's function satisfies on the Heisenberg model with nearest-neighbor (nn) interactions. Secondly, the equation is solved analytically for the bulk magnet. The recursive solutions are then found for an N-overlayer on a semi-infinite substrate and an interface between two semi-infinite ferromagnets of variable exchange couplings. In Sec. III, the GEBS solutions are employed to study the spectra of SSW and ISW, as well as the surface and interface magnetization. The substrate-induced magnetism in overlayers observed recently is calculated in Sec. IV and finally the advantages and limitations of the GEBS method are discussed in Sec. V.

II. GREEN'S FUNCTION AND GAUSSIAN RECURSIVE SOLUTIONS

In the absence of external magnetic fields, the Heisenberg model Hamiltonian for a ferromagnetic lattice is

$$H = -\Sigma_{\mathbf{a},\delta} J_{\mathbf{a},\mathbf{a}+\delta} \mathbf{S}_{\mathbf{a}} \cdot \mathbf{S}_{\mathbf{a}+\delta}. \tag{1}$$

For simplicity, we limit our discussion to the *nn* coupling in a simple cubic lattice with unit lattice constant. However, the treatment is general and can be extended to other lattices

without difficulty. Thus, δ stands for the relative position vector between the lattice point a and its nearest neighbors. In the energy representation, the time-retarded Zubarev Green's function [19] is found by a standard procedure [20-22] to satisfy the equation

$$\begin{aligned} \boldsymbol{E} \ll S_a^+; S_a^- \gg &= 2\langle S_a^z\rangle\delta_{\mathbf{a},\mathbf{a}'} - \Sigma_\delta J_{\mathbf{a},-\mathbf{a}+\delta} \ll S_{\mathbf{a}+\delta}^+; S_{\mathbf{a}}^- \gg \\ &+\Sigma_\delta J_{\mathbf{a},\mathbf{a}+\delta}\langle S_{\mathbf{a}+\delta}^z\rangle \ll S_{\mathbf{a}}^+; S_{\mathbf{a}}^- \gg . \end{aligned} \tag{2}$$

To accommodate the anisotropy of the interaction, we assume that the exchange coupling between any neighboring spins in the mth layer $J_{\|}(m)$ is the same and that the nn coupling between spins in mth and (m $+1$)th layers is $J_\perp(m)$. The layer magnetization or the mean spin in the mth layer is denoted by S(m).

We now introduce the two-dimensional (2D) Fourier transformation

$$\ll S_{\mathbf{a}}^+; S_{\mathbf{a}}^- \gg = (1/N_{\|})\Sigma_\kappa[2S(m)/JS]g(\kappa, \boldsymbol{E}; m, n)e^{i\kappa\cdot(\mathbf{a}-\mathbf{a}')} , \tag{3}$$

where $\boldsymbol{J}$ and S are bulk values of the exchange interaction and magnetization, respectively, $N_{\|}$ is the total number of unit cells in each layer and g stands for the Green's function expressed in the Bloch-Wannier representation in which Bloch function is used in the xy-plane and Wannier function is used in the z direction. The 2D wave vector κ and the factor $2S(m)$ are introduced only for conveneince. In what follows, we shall suppress $\kappa, \boldsymbol{E}$ and write from now on the Green's function $g(m,n)$ for simplicity.

Substituting Eq. (3) in Eq. (2) and rearranging the terms, we have

$$A(m)g(m,n) + B(m)g(m+1,n) + C(m)g(m-1,n) = \delta(m,n) , \tag{4}$$

Eq. (4) is valid in general for any lattice structure. For simplicity, we consider the simple cubic lattice for which the coefficients in Eq. (4) are defined by

$$A(m) = \epsilon - 4j_{\|}(m)s(m)[1-\xi(\kappa)] - B(m) - \mathrm{C(m)} , \tag{5a}$$

$$B(m) = j_\perp(m)s(m \ \mathbf{t}\ 1)) \tag{5b}$$

$$C(m) = j_\perp(m-1)s(m-1)) \tag{5c}$$

$$\xi(\kappa) = 1/2(\cos k_x + \cos k_y), \tag{5d}$$

where we have defined the dimensionless parameters

$$\boldsymbol{s(m)} = S(m)/S , \ \boldsymbol{j_{\|}(m)} = J_{\|}(m)/J , j_\perp(m) = J_\perp(m)/J . \epsilon = E/JS . \tag{6}$$

For a bulk lattice with isotropic interactions we set $j_{\|}(m) = j_\perp(m) = 1$ and s(m) $= 1$. Then Eq. (4) becomes

$$-2W(\kappa,\epsilon)g(m,n) + g(m+1,n) + g(m-1,n) = \delta(m,n) , \tag{7}$$

where

$$W(\kappa,\epsilon) = [6 - 4\xi(\kappa) - \epsilon]\,. \tag{8}$$

Eq. (7) is a second order difference equation with constant coefficient and has standard solutions. In the presnet case, we impose the boundary condition $g(m,n) = 0$ as $|m-n| \to \infty$. The solution is then

$$g(m,n) = (1/2i\sqrt{1-W^2}\,)z^{-|m-n|}\,, \tag{9}$$

where z satisfies the equation -2W + $z + 1/z = 0$, namely,

$$z = W + sgn(W)\sqrt{W^2-1}\,. \qquad |z| > 1. \tag{10}$$

With the Green's function known, we can proceed to calculate the two-particle temperature-dependent correlation function [20-22]

$$\begin{aligned}\phi(T) \;=\; & (i/2\pi JS)\int_{-\infty}^{\infty} dE(e^{\beta E}-1)^{-1}(1/2\pi)^2\int d^2\kappa \\ & \cdot[g(\kappa,E+i0^+;m,n) - g(\kappa,E-i0^+;m,n)]\,.\end{aligned} \tag{11}$$

In practical calculations, it is always more convenient to rewrite z as $z = W + i\sqrt{1-W^2} = e^{iq}$, which implies that the variable energy ϵ can be related to q via Eq. (9).

$$\begin{aligned}\phi(T) \;=\; & -2/(2\pi)^3\int d^2k\int dq\,\sin q\left[\exp\{(6JS/k_BT)[1-\delta(\kappa,q)]\}-1\right]^{-1} \\ & \cdot \mathrm{Im}\, g(\kappa,q;m,n)\,,\end{aligned} \tag{12}$$

where

$$\alpha(\kappa,q) = (1/3)(\cos k_x + \cos k_y + \cos q)\,. \tag{13}$$

With the Green's function given by (9), the correlation function becomes

$$\phi(T) = -1/(2\pi)^3\int d^2\kappa\int dq\left[\exp\{(6JS/k_BT)[1-\gamma(\kappa,q)]\}-1\right]^{-1} \tag{14}$$

which is the well-known result obtained elsewhere [19].

For the overlayer problem, we consider a system of N spin monolayers on the top of a semi-infinite ferromagnet as shown in Fig. 1. The exchange coupling is assumed to be layer dependent and different from the bulk. With only the nn coupling, Eq. (4) is a tridiagonal linear equation. Following the GEBS procedure [18], we assume that the Green's function satisfies the backward recursive relation

$$g(m-1,n) = \alpha(m)g(m,n) + \beta(m,n) \tag{15}$$

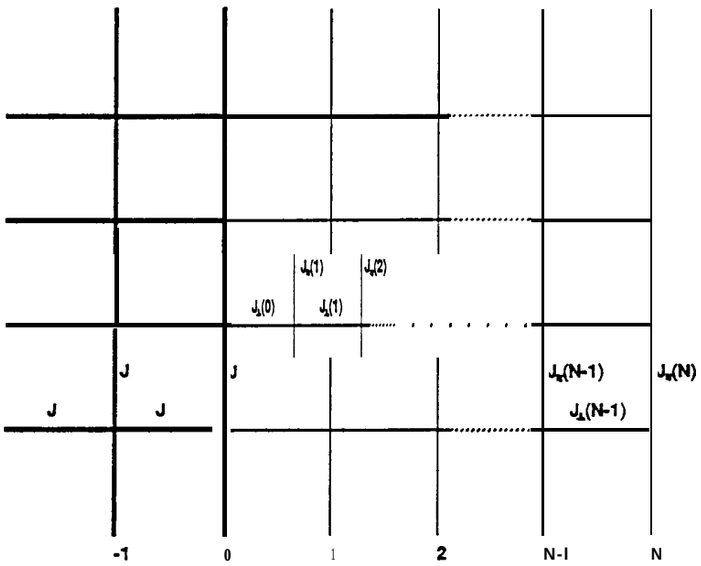

FIG. 1. The overlayer model. N overlayers are grown on top of a semi-infinite ferromagnetic substrate.

which is possible for any $g(m,n)$ because the functions $\alpha(m)$ and $\beta(m,n)$ are not specified. Substituting Eq. (15) in (4), we obtain

$$g(m,n) = -B(m)g(m+1,n)/[A(m)+C(m)\alpha(m)] + [\delta(m,n)-C(m)\beta(m,n)]/[A(m)+C(m)\alpha(m)]. \tag{16}$$

By comparing Eqs. (15) and (16), we can identify the forward recursion relations

$$\alpha(m+1) = -B(m)\Gamma(m), \tag{17a}$$

$$\beta(m+1,n) = [\delta(m,n)-C(m)\beta(m,n)]\Gamma(m), \tag{17b}$$

$$\Gamma(m) = 1/[A(m) \text{ t } C(m)+)]. \tag{17c}$$

To start the recursion, we note once again the bulk solution which applies to $m \leq 0$ in the present case. It is clear from Eq. (9) that for $n > 0$,

$$g(m-1,n) = g(m,n)/z. \tag{18}$$

A comparison with Eq. (15) yields for $n > 0$,

$$a(0) = 1/z, \qquad \beta(0,n) = 0. \tag{19}$$

Inserting Eq. (19) in the forward recursion formulas (17), we can determine the coefficients successively from $\alpha(1), \beta(1,n)$ to $\alpha(N+1), \beta(N+1,n)$. The backward recursion formula (15) then generates the Green's function layer after layer from the top-layer function

$$g(N,n) = \beta(N+1,n) \tag{20}$$

which follows from the boundary condition $\alpha(N+1) = 0$. On the other hand, recursion relations for a fixed m can also be obtained from Eq. (15). The procedure is outlined in the Appendix and the results are for all n > 0,

$$g(m, n-1) = -C(n)\Gamma(n-1)g(m, n) \tag{21a}$$

$$g(n-1, n-1) = \Gamma(n-1)[1-C(n)\alpha(n)g(n,n)]. \tag{21b}$$

Since most physical quantities of interest involve only diagonal elements of the Green's function, Eq. (21b) is very useful in practical calculations such as the magnon spectra and monolayer magnetization.

We now turn our attention to the interface between two semi-infinite ferromtignets as shown in Fig. 2. For convenience, we assume the backward recursive solutions on the left-hand side and forward recursive solutions on the right. Thus,

$$g(m+1,n) = \alpha_R(m)g(m,n) + \beta_R(m,n), \qquad m > 1, \tag{22a}$$

$$g(m-1,n) = \alpha_L(m)g(m,n) + \beta_L(m,n), \qquad m < 0, \tag{22b}$$

where the subscripts ***L*** and ***R*** indicate quantities for the left and right half-spaces, respectively. Substituting these equations in Eq. (4), we can express $g(m,n)$ in terms of g(m + 1, n). A comparison of the results with Eq. (22) then leads to recursion relations

$$\alpha_R(m-1) = -C(m)\Gamma_R(m), \tag{23a}$$

$$\beta_R(m-1,n) = [\delta(m,n) - B(m)\beta_R(m,n)]\Gamma_R(m), \tag{23b}$$

$$\Gamma_R(m) = [A(m) + B(m)\alpha_R(m)]^{-1}, \tag{23c}$$

$$\alpha_L(m+1) = -B(m)\Gamma_L(m), \tag{23d}$$

$$\beta_L(m+1,n) = [\delta(m,n) - C(m)\beta_L(m,n)]\Gamma_L(m), \tag{23e}$$

$$\Gamma_L(m) = [A(m) + C(m)\alpha_L(m)]^{-1}. \tag{23f}$$

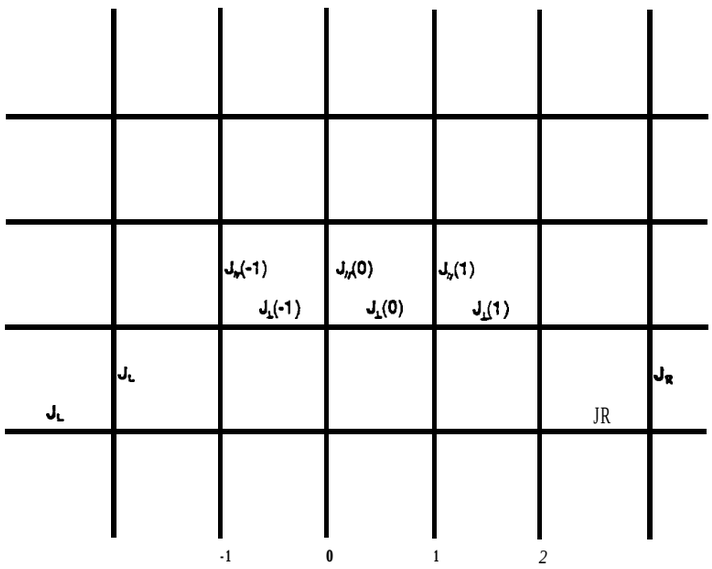

FIG. 2. The interface model. Two semi-infinite lattices are coupled by the interface exchange interaction $J_\perp(0)$.

Once more, we set the boundary conditions by considering the deep bulk regions where

$$\alpha_L(-\infty) = z_L^{-1}, \qquad \beta_L(-\infty, n) = 0, \tag{24a}$$

$$\alpha_R(+\infty) = z_R^{-1}, \qquad \beta_R(+\infty, n) = 0. \tag{24b}$$

Repeated applications of the recursion relations (23) then yield $\alpha_L(1), \beta_L(1,n), \alpha_R(0)$ and $\beta_R(0,n)$. In all the existing calculations to our knowledge, only the interface is taken to be different. The present method can easily be extended to cases in which more spin layers near the interface may differ from the bulk. The Green's function for the interface can be obtained from either of Eq. (22) but must be the same because of the continuity. Hence, it is determined by the coupled equations

$$g(0,n) = \alpha_L(1) g(1,n) + \beta_L(1,n), \tag{25a}$$

$$g(1,n) = \alpha_R(0) g(0,n) + \beta_R(0,n). \tag{25b}$$

Upon solving Eq. (25) we find $g(0,n)$ and $g(1,n)$ which are then employed to start the recursion relations (22). A similar procedure that leads to Eq. (21) gives the following relations for the interface Green's function:

$$g(m,n-1) = -C(n)\Gamma_L(n-1)g(m,n)\,, \qquad n<0\,,\ m\neq n-1\,, \tag{26a}$$

$$g(n-1,n-1) = [1-C(n)\alpha_L(n)g(n,n)]\Gamma_L(n-1)\,, \qquad n\leq 0\,, \tag{26b}$$

$$g(m,n+1) = -B(n)\Gamma_R(n+1)g(m,n)\,, \qquad n\geq 1\,,\ m\neq n+1\,, \tag{26c}$$

$$g(n+1,n+1) = [1-C(n)\alpha_R(n)g(n,n)]\Gamma_R(n+1)) \qquad n\geq 1. \tag{26d}$$

As usual, the relations between the diagonal matrix elements are more useful in practical calculations.

The method of solution developed above is easy to use and greatly simplifies the calculation in practice. To demonstrate the powerfulness of the GEBS solutions, we first work out surface and interface magnon spectra and the surface mangetization. The method is then applied to study numerically the substrate-induced magnetization in overlayers observed recently [23,24].

III. SURFACE AND INTERFACE SPIN WAVE SPECTRA

For the surface spin wave, we consider a simple model of two-overlayer with magnetization the same as that in the bulk. The Green's function for the overlayer can be written down directly following Eqs. (20), (17a) and (17b) by noting that $\beta(2,2) = 0$. The result is

$$g(2,2) = \beta(3,2) = 1/[A(2) + C(2)\alpha(2)]\,. \tag{27}$$

We now label the top two layers of the semi-infinite system by 1 and 2 and treat them as an overlayer on the substrate surface. The exchange coupling J is assumed to be unity throughout the bulk except for the first two layers. Thus we have $j_\perp(1) = j_\perp, j_{||}(1) = j_1$, $j_{||}(2) = j_2$ and $j_\perp(m) = j_{||}(m) = 1$ for all m $\leq$ 0. From Eq. (6), we find by setting s(m) = 1 for any m

$$B(1) = j_\perp\,, \tag{28a}$$

$$C(1) = 1, \tag{28b}$$

$$\mathbf{A(1)} = \epsilon - 4j_1(1-\xi) + j_\perp - 1\,, \tag{28c}$$

$$\mathbf{B(2) = 0}\,, \tag{29a}$$

$$C(2) = j_\perp\,, \tag{29b}$$

$$A(2) = \epsilon - 4j_2(1-\xi) - j_\perp = -(z + 1/z) + 2 + 4(1-\xi)(1-j_2) - j_\perp\,, \tag{29c}$$

where we have made use of Eqs. (9) and (10) in the last step of (29a). From the condition in Eq. (19) and relations in Eq. (17), we obtain easily the recursion formula for a

$$\begin{aligned}\alpha(2) &= -B(1)/[A(1) + C(1)\alpha(1)] \\ &= j_\perp/[z + 4(j_1-1)(1-\xi) + j_\perp - 1]\,.\end{aligned} \tag{30}$$

The SSW spectrum is determined by the singularity of $g(2,2)$ or, according to Eq. (27), by the equation

$$A(2) + C(2)\alpha(2) = 0. \tag{31}$$

Inserting (29b,c) and (30) in Eq. (31), we have

$$\begin{aligned}&(z + 1/z) - 2 - 4[1-\xi(\kappa)](1-j_2) + j_\perp \\ &\quad - j_\perp^2\left\{z + 4(j_1-1)[(1-\xi(\kappa)] + j_\perp - 1\right\}^{-1} = 0\,.\end{aligned} \tag{32}$$

It is noted that (32) is cubic in z and the solution is physical only if $|z| > 1$ as z is related to the energy by Eq. (10).

We emphasize that the method is quite general and can handle magnetic slabs of arbritary thickness with layer-dependent $j_{\|}(n)$ and $j_\perp(m)$. In fact, it is rather simple to program the recursion relations into a symbolic calculation software, and let the computer generate expressions for all the Green's functions automatically.

If we assume, like the general practice in the literature, that all the exchange interactions are the same except for those related to the surface spin, then we just set $j_1 = 1$. Eq. (32) becomes, after the rearrangement of terms,

$$z^3 + bz^2 + Cz + d = 0\,, \tag{33a}$$

$$b = -(3-2j_\perp) - 4[1-\xi(\kappa)](1-j_1)\,, \tag{33b}$$

$$c = (1-j_\perp)\left\{3 - 4[1-\xi(\kappa)](1-j_2)\right\}, \tag{33c}$$

$$d = j_\perp - 1. \tag{33d}$$

Eq. *(33)* is exactly what is given in the first paper of Ref. [7] as expected.

The energy spectrum of the ISW is determined by the determinant equation of Eq. (25), namely

$$\begin{vmatrix} 1 & -\alpha_L(0) \\ -\alpha_R(0) & 1 \end{vmatrix} = 0\,. \tag{34}$$

The simplest model is two identical semi-infinite ferromagnets connected by the exchange integral J_{12} as has been considered by Yaniv [10]. The Green's function is found in Ref. [10] by solving the Dyson equation of perturbation.

We consider the interface of two different semi-infinite ferromagnets, one with the nn exchange $j_L = 1$ and the other $j_R =$ j in the bulk as shown in Fig. 2. On the interface, $j_{\|}(0) = j_0, j_{\|}(1) = j_1$ and $j_\perp(0) = j_\perp$.

Starting with the boundary conditions

$$\alpha_L(0) = 1/z = \mathrm{w} - sgn(W)\sqrt{W^2 - 1}\,, \tag{35a}$$

$$\alpha_R(1) = 1/z_R = W_R - sgn(W_R)\sqrt{W_R^2 - 1}\,, \tag{35b}$$

where W is given by Eq. (8) and W_R is defined by

$$W_R = [6j - 4j\xi(\kappa) - \epsilon]\,. \tag{36}$$

Since the left half is identical to the substrate we discussed above, $\alpha_L(1)$ is the same as Eq. (30). To find $\alpha_R(0)$, we note from Eq. (6) that

$$\mathrm{A}(1) = \epsilon - 4j_1(1-\xi) - j_\perp - j\,, \tag{37a}$$

$$B(1) = j\,, \tag{37b}$$

$$\mathrm{C}(1) = j_\perp\,. \tag{37c}$$

By substituting Eqs. (37) in Eqs. (23a), (23c) and making use of (35b) and (36), we find

$$\begin{aligned}\alpha_R(0) &= -C(1)/[A(1) + B(1)\alpha_R(0)] \\ &= j_\perp/[z_R + 4(j_1 - j)(1-\xi) + j_\perp - j]\,.\end{aligned} \tag{38}$$

The ISW spectrum is then determined by inserting (33) and (30) in Eq. (34), that is, by

$$j_\perp^2 = [z + 4(j_0 - 1)(1-\xi) + j_\perp - 1][z_R + 4(j_1 - j)(1-\xi) + j_\perp - j]\,. \tag{39}$$

Once more, we emphasize that for the physically acceptable solution we must take $|z| > 1$.

If the two ferromagnets are the same, we have j = 1 and $j_1 = j_0$. Eq. (39) can then be solved analytically and the solutions are

$$z_1 = 1 - 4(j_0 - 1)(1-\xi), \tag{40a}$$

$$z_2 = -2(j_\perp - 1) - 1 - 4(j_0 - 1)(1-\xi)\,. \tag{40b}$$

When the interface effect is neglected by setting $j_0 = 1$, (40b) becomes

$$z = 1 - 2j_{\perp} \tag{41}$$

which is just the result of Yaniv [10] as it should be. Thus the GEBS method is far more powerful and effective than the usual Dyson's perturbation in dealing with spin waves in systems in which many exchange coupling parameters may deviate from the bulk value.

We now turn our attention to the layer magnetization. In general, the layer magnetization must be calculated from the correlation function which is defined via the imaginary part of the Green's function. But the Green's function itself depends on the layer magnetization. Therefore an exact calculation of the magnetication can only be made by solving a set of coupled transcendental equations. At low temperatures, however, the correlation is generally small and the zero-temperature magnetization may be assumed in the Green's function. In this approximation, all the quantities A, B, C, Γ and a become layer-independent, and as a consequence, Eq. (21b) reduces to

$$g(n-1, n-1) = \Gamma[1 - \alpha C g(n, n)]. \tag{42}$$

This is a first-order difference equation and can be solved analytically with the initial condition (20). The standard solution can be put in to the form

$$g(\kappa, q; n, n) = 1/(2i \sin q) + i(1 - e^{iq})e^{i2q(1-n)}/[2 \sin q + i(1 - e^{-i2q})], \tag{43}$$

where we have made use of Eq. (17c) with $\alpha = 1/z = e^{-iq}$. The first term represents the bulk Green's function whereas the second term results from the perturbation of the surface.

To find the correlation (12), we note that at low temperatures the contribution to the integral comes mainly from the region where $\gamma(\kappa, q) \approx 1$, that is, $q \approx 0$ and $\kappa \approx 0$. In this limit, Eq. (23) yields $\mathrm{Im} g(\kappa, q; 1, 1) \approx -1/q$. As a consequence, we have

$$\begin{aligned} \Phi_s(T) &= [2/(2\pi)^3] \int d^2\kappa \int q \exp 6\{(6\ k/3T)[1 - \gamma(\kappa - q)]\} - 1\Big)^{-1} \\ &\approx 2\Phi_{\mathrm{bulk}}(T). \end{aligned} \tag{44}$$

This is of course well known. If we look deep into the bulk where $n \gg 1$, the second term of Eq. (43) oscillates rapidly. Thus,

$$\begin{aligned} \phi_n &\approx \phi_{\mathrm{buik}} - (k_B T/JS)(1/2\pi)^3 \int d^2\kappa \int dq e^{-i2qn}/(\kappa^2 \ t \ q^2) \\ &= \phi_{\mathrm{bulk}} + 0(T/n) \end{aligned} \tag{45}$$

The magnetization on the interface can be worked out in a similar fashion. In the zero-temperature limit, we find

$$g(n, n) = 1/(2i \sin q_L) + a_L \exp(-2inq_L), \qquad n \leq 0, \tag{46a}$$

$$g(n, n) = 1/(2i \sin q_R) + a_R \exp[-2i(1 - n)q_R], \qquad n \geq 1, \tag{46b}$$

where the constants a_L and a_R are determined by the initial condition $g(0,0)$ from Eq. (25). Detailed discussions are already available in Ref. [10] and is not repeated here.

IV. SUBSTRATE-INDUCED MAGNETIZATION IN OVERLAYERS

There has been great interest in magnetic properties of rare-earth over-layers on other metal substrates in recent years [5]. Theoretical studies, however, have thus far been limited to the Ginzburg-Landau model [24]. In an attempt to understand the phenomenon microscopically, we calculate the substrate-induced magnetization in five overlayers on top of a ferromagnet with spin $1/2$ by means of the GEBS method.

Although the GEBS approach provides us with the exact analytical expression of Green's function for any individual layer in principle, it is often rather complicated to analyze the Green's function which may be very bulky even for a reasonably simple system. But the GEBS method is quite effective and practical in computational implementation, and can be handled by a computer in a software language for symbolic calculations.

The procedure can be outlined as follows. We start with a set of reasonable magnetization values for various layers by guessing, and implement GEBS algorithm to evaluate the Green's functions as in Sec. II. The correlation functions are then computed on the imaginary part of the Green's function to obtain a new set of magnetization values, which are inserted back to GEBS to repeat the cycle. The procedure keeps on until self-consistency is achieved. It is possible in some cases that the system may converge to different final values of magnetization if different initial values are assigned. This only means that the system of magnetic lattice has relaxed into a local stability near the configuration specified by the initial condition.

The mean magnetization for spin $1/2$ system is related to the correlation function by

$$\langle S\rangle = 1/2[1+\phi(T)] \tag{47a}$$

and for general spin [21,22] by

$$\langle S\rangle = \left\{[S-\phi(T)][1+\phi(T)]^{2S+1} + [S+1+\phi(T)][\phi(T)]^{2S+1}\right\}\Big/ \left\{[1+\phi(T)]^{2S+1} - [\phi(T)]^{2S+1}\right\}. \tag{47b}$$

For simplicity, we consider a substrate of exchange coupling strength $j = 1$, and five overlayers of variable coupling strengths $j_\perp$ and $j_{||}$. The critical temperature of the substrate is denoted by T_{c1} and that of the bulk material of the overlayers is $T_{c2} = 0.3T_{c1}$ if $j_{||}(m) = j_1(m-1) = 0.3$. It is well known that in general T_c decreases with decreasing thickness of a slab of any magnetic material.

The overlayer magnetization is computed for $T = 0.4T_{c1}$, and numerical results obtained for various exchange parameters are listed in Table I. The overlayer magnetization

TABLE I. Substrate-induced overlayer magnetization at $T = 0.4T_{C1}$.

exchange \ layer #	1	2	3	4	5
$j_\perp(0) = 0.1, j_\perp = j_\parallel = 0.3$	0.8501	0.8444	0.8311	0.8195	0.7959
$j_\perp(0) = -0.5, j_\perp = 0.3, j_\parallel = 0.1$	0.8372	0.8356	0.8307	0.8251	0.8168
$j_\perp(0) = -10.0, j_\perp = 0.3, j_\parallel = 0.1$	0.8322	0.8258	0.8148	0.8013	0.7799
$j_\perp(0) = -1.0, j_\perp = j_\parallel = 0.2$	0.8112	0.8102	0.8065	0.8010	0.7888

must have been induced by the ferromagnetic substrate because the overlayer is supposed to be paramagnetic at this temperature. The critical temperature of the overlayer is much lower than T_{c2}. The size of the magnetization generally decreases with increasing distance from the interface, but the rate is not large enough to account for the experiments [23]. Since our calculation is based on the isotropic Heisenberg Hamiltonian (1), an anisotropic interaction is expected to describe the overlayer more realistically. In fact, as has been noted in Ref. [23], the panisotropy seems to be a major cause for the substrate-induced magnetization in overlayers. Furthermore, the long range force such as the next nearest neighbor coupling may also change the results appreciably. More careful investigation is necessary and results will be reported elsewhere.

To check the validity of our calculation, we have also examined a semi-infinite ferromagnet at various temperatures by setting s(m) = 1, $j_\perp(5) = 0$, and $j_\parallel(m) = j_\perp(m-1) = 1$ for m $= 1, 2, 3, 4, 5$. Results are tabulated in Table II. It is observed that the 5th layer magnetizations are in agreement with those found in Ref. [5].

TABLE II. Surface layer magnetizations of semi-infinite ferromagnet.

T \ layer #	1	2	3	4	5
$0.1T_c$	0.9965	0.9955	0.9940	0.9917	0.9899
$0.2T_c$	0.9971	0.9952	0.9913	0.9842	0.9750
$0.3T_c$	0.9969	0.9944	0.9894	0.9773	0.9561
$0.4T_c$	0.9993	0.9960	0.9911	0.9751	0.9379
$0.5T_c$	1.001	1.013	0.9938	0.9753	0.9208

V. DISCUSSION

We have applied the GEBS formalism to derive the exact Green's function for spin lattices involving surfaces and interfaces. It is demonstrated that the energy spectra of the surface or interface excitations can be found easily without the explicit evaluation of the Green's function. The method can be applied to systems in which the nn coupling strength may be strongly altered near the surface and interfaces. As a matter of fact, it is rather easy to program the recursion in a symbolic calculation software language and let the computer generate the Green's function. Furthermore, the technique can be generalized without difficulty to include external magnetic fields to treat magnetic lattices with anisotropic exchange interactions or to handle systems with different lattice structures. The formulation can be modified to a matrix version for the study of antiferromagnetic and ferrimagnetic lattices as is discussed in Ref. [22].

There are, on the other kand, limitations in the application of GEBS technique to investigate magnetic problems. As the GEBS formalism is designed especially to invert tri-diagonal matrices, it may encounter substantial difficulty in dealing with longer range interactions such as the next-nearest-coupling, in which case the equation of motion can never be written as tri-diagonal. Although analytical Green's functions of a large number of layers can be found exactly, it is usually very difficult to extract useful information regarding properties of physical quantities from such expressions, leaving the numerical study the only alternative.

APPENDIX

We start with the relations (15) and (17)a1ong with the boundary conditions (19) and (20). For m < n, we have $\delta(m,n)$ = 0. Equation (17b) implies that $\beta(m+1,n)=0$ if $\beta(m,n)=$ 0. We now apply the method of mathematical induction for all positive integer n. From the condition (19) together with the above conditions we find $\beta(0,n)=\beta(1,n)=\cdots=\beta(n,$ n) = 0.

When $m=n$, Eq. (17b) becomes

$$\beta(n+1,n)=[1-C(n)\beta(n,n)]\Gamma(n) = \Gamma(n), \tag{A1}$$

or, after replacing n by $(n-1)$,

$$\beta(n,n-1) = \Gamma(n-1). \tag{A2}$$

After making the replacements $m \to n$ and n $\to n-$ 1, Eq. (17b) takes the form

$$\begin{aligned}\beta(n+1,n-1) &= -C(n)\beta(n,n-1)\Gamma(n)\\ &= -C(n)\Gamma(n-1)\beta(n+1,n),\end{aligned} \tag{A3}$$

where we have made use of Eqs. (Al) and (A2).

Next, we consider $m > n$. Equation (17b) can now be rewritten as

$$\beta(m+1, n) = -C(m)\Gamma(m)\beta(m, n), \qquad m > n . \tag{A4}$$

Replacing n by $n-1$ in (A4) and setting $m = n+1$ in Eq. (A3), we have

$$\begin{aligned} \beta(m+1, n-1) &= -C(m)\Gamma(m)\beta(m, n-1) \\ &= -C(m)\Gamma(m)[-C(n)\Gamma(n-1)]\beta(m, n) \\ &= -C(n)\Gamma(n-1)\beta(m+1, n) . \end{aligned} \tag{A5}$$

From the boundary condition (20) we find

$$\begin{aligned} g(N, n-1) &= \beta(N+1, n-1) \\ &= -C(n)\Gamma(n-1)\beta(N+1, n) \\ &= -C(n)\Gamma(n-1)g(N, n) . \end{aligned} \tag{A6}$$

Now, we replace n by $n-1$ in the recursion relation (15) and use Eqs. (A5) and (A6),

$$\begin{aligned} g(m-1, n-1) &= \alpha(m)g(m, n-1) + \beta(m, n-1) \\ &= \alpha(m)[-C(n)\Gamma(n-1)]g(m, n) - C(n)\Gamma(n-1)\beta(m, n) \\ &= -C(n)\Gamma(n-1)g(m-1, n), \qquad m \geq n . \end{aligned} \tag{A7}$$

On the other hand, we can also write

$$\begin{aligned} g(n-1, n-1) &= \alpha(n)g(n, n-1) + \beta(n, n-1) \\ &= \alpha(n)[-C(n)\Gamma(n-1)g(n, n)] + \Gamma(n-1) \\ &= [1 - C(n)\alpha(n)g(n, n)]\Gamma(n-1). \end{aligned} \tag{A8}$$

It is clear that Eqs. (A7) and (A8) are identical to (21a) and (21b).

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* Present address: Department of Electrical & Computer Engineering, Purdue University, West Lafayette, IN 47907, U.S.A.

‡ Present address: Department of Electrical and Computer Engineering, University of Texas, Austin, TX 28712, U.S.A.

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