Magnetic elementary excitations effects on a Co super-lattice properties

A. Fahmi and A. Qachaou

Laboratoire de Physique de la matière condensée, Faculté des sciences, KENITRA

The magnetization and the spin wave spectra are studied for a cobalt super-lattice, using the localized spins Heisenberg hamiltonian with nearest neighbors and next nearest neighbors exchange interactions. The added magnetic dipolar and anisotropy effects are discussed also.The calculation of the spin waves dispersion curves and the magnetization are carried out in the framework of Green's functions. As experimentally expected, our results show that the surface magnetization is smaller than the inner one.

Key words: Spin waves, super-lattices, Green's functions, dispersions curves, magnetization.

I-INTRODUCTION

In the last few years, several attentions have been given to the development and the research on magnetic ultrathin films and the multi-layer one. This is due to both the interest towards the comprehension of magnetic properties in quasi-two-dimensional systems and their various potential technical applications. Theoretically, the treatment of these systems as being quasi-twodimensional(by taking account the break of symmetry) gives results generally rather coherent with experiment [1,2].

In order to understand the magnetic properties of this systems, it is necessary to determine the importance of the magnetic elementary excitations contribution. In this work we present a preliminary study of a cobalt super-lattice in the framework of linear spin wave theory. The first Brillowin light scattering (BLS) investigation on a two-dimensional systems performed by Kerkmann and al[14] has showed that spin waves exist in a cobalt monolayer film on Cu(001) layer.

The corresponding Hamiltonian which describes the various interactions can be represented by the intra-plane Heisenberg ferromagnet with nearest neighbors (NN) and next nearest neighbors (NNN) exchange interaction and the inter-plane Heisenberg ferromagnet with nearest neighbors (NN) exchange interaction including magnetic dipolar interactions. Between planes only the Heisenberg exchange with (NN) interactions are taking account. The others are negligible.

We also treated the particular monolayer case in order to show the main role of the anisotropy in this systems as it is done in precedent works, and as expected by experience[4,5,6].

I- ANALYTICAL FORMULATION

We consider the bcc cobalt structure of mesh a, each Co layer is represented by a ferromagnetic plane. We assume that the film is parallel to the (xz) plane and it is perpendicular to the y axis.

The hamiltonian describing this system can be expressed as:

$$H = H_{//}^{ex} + H_{//}^{dip} + H_{\perp}^{ex} \qquad (1)$$

where the three terms are defined as follows:

i- $H_{//}^{ex}$ is the Heisenberg exchange interactions between NN and NNN in the film plane. These interactions are represented respectively by the integrals J_1 and J_2:

$$H_{//}^{ex} = -J_1 \sum_{\langle ij \rangle} (S_i^x S_j^x + S_i^y S_j^y + \alpha S_i^z S_j^z) - J_2 \sum_{\langle ij' \rangle} S_i S_{j'} \qquad (2)$$

where α is the magnetocrystalline anisotropy.

ii- $H_{//}^{dip}$ represents the magnetic dipolar interactions between NN in the film plane such as:

$$H_{//}^{dip} = \frac{1}{2}\sum_{\langle ij\rangle}\frac{(g\mu_B)^2}{|r_i - r_j|^3}\left[S_i S_j - 3\frac{(S_i r_{ij})(S_i r_{ij})}{r_{ij}^2}\right] \quad (4)$$

$r_{ij}=r_j-r_i$, r_i and r_j are the position atoms *i* and *j* respectively.

iii- $H_{\perp}^{ex}$ is associated to the exchange interaction represented by the integral $J_\perp$ and active between NN which are not belonging to the same layer:

$$H_{\perp}^{ex} = -J_\perp \sum_{\langle ij_\perp\rangle} S_i S_{j_\perp} \quad (5)$$

(i,j) and (i,j') are respectively the intraplane NN and NNN pairs, while (i,$j_\perp$) are the interplane NN pairs.

The linear spin waves theory consists in transforming from spin to boson operators by the linear Holstein-Primakoff (H-P) transformation[7]

$$\begin{cases} S_i^+ = \sqrt{2S}\,a_i \\ S_i^- = \sqrt{2S}\,a_i^+ \\ S_i^z = S - a_i^+ a_i \end{cases} \quad (6)$$

Considering that the symmetry translation along y axis is broken, the Fourier transform of the creation a_i^+ and the annihilation a_i operators is introduced as follows:

$$\begin{aligned} a_i^+ &= \frac{1}{\sqrt{L}}\sum_k a_{k_{//},l}^+ e^{ik_{//}.i_{//}} \\ a_i &= \frac{1}{\sqrt{L}}\sum_k a_{k_{//},l} e^{-ik_{//}.i_{//}} \end{aligned} \quad (7)$$

where L is the atoms number per film layer; $k_{//}$ is the wave vector whose direction is parallel to the film surface, while *l* and r_i describe the lattice site, i.e., *l* is the atomic plane index and r_i is the position vector of a lattice site *l*.

Therefore, substituting equations (6) and (7) into H and retaining only quadratic terms in bosons operators, we have a non-diagonal hamiltonians:

$$H_{//}^{ex} = \sum_{k_{//}}\sum_{l=1}^{L} A_{k_{//}}^{ex} a_{k_{//},l}^+ a_{k_{//},l} \quad (8\text{-a})$$

$$H_{//}^{dip} = \sum_{k_{//}}\sum_{l=1}^{L} A_{k_{//}}^{dip} a_{k_{//},l}^+ a_{k_{//},l} + \frac{1}{2}\sum_{k_{//}}\sum_{l=1}^{L} B_{k_{//}}^{dip}(a_{k_{//},l}^+ a_{-k_{//},l}^+ + a_{k_{//},l} a_{-k_{//},l}) \quad (8\text{-b})$$

$$H_{\perp}^{ex} = \sum_{k_{//}}\sum_{l=1}^{L} W_{k_{//},l}^{ex} a_{k_{//},l}^+ a_{k_{//},l} + \sum_{k_{//}}\sum_{l=1}^{L-1} D_{k_{//}}^{ex}(a_{k_{//},l}^+ a_{k_{//},l+1} + a_{k_{//},l} a_{k_{//},l+1}^+) \quad (8\text{-c})$$

In order to calculate the excitation spectra E(k) and the magnetization, we have used the Green's function method[9] where the following Fourier-transformed retarded Green's functions $G_{l,m}$ and $G'_{l,m}$ are defined as:

$$\begin{aligned} G_{l,m} &= \ll a_{k_{//},l}, a_{k_{//},l}^+ \gg \\ G'_{l,m} &= \ll a_{k_{//},l}^+, a_{k_{//},l}^+ \gg \end{aligned} \quad (9)$$

Otherwise, the motion equations associated with these Green's functions lead to the following equations system which we represented in matrix form as:

$$\underline{M}\begin{pmatrix} \underline{G} & 0 \\ \underline{G'} & 0 \end{pmatrix} = \frac{-1}{2\pi}\begin{pmatrix} \underline{1} & \underline{0} \\ \underline{0} & \underline{0} \end{pmatrix} \quad (10)$$

where

$$\underline{M} = \begin{pmatrix} \underline{A} - E & \underline{B} \\ -\underline{B} & -\underline{A} - E \end{pmatrix}$$

and $\underline{A}$, $\underline{B}$, $\underline{G}$ and $\underline{G}$' are an N order matrices, their expressions are given in the appendix.

Then, the resolution of the system (10) makes it possible to obtain the magnons dispersion curves E(k).

Likewise, the super-lattice n^{th} plane magnetization per site can be obtained according to the magnons occupation number average value, it's expressed as :

$$\frac{< S_n^Z >}{S} = 1 - \frac{1}{S}\frac{v}{(2\pi)^2}\int_{BZ} < a_{k_{//},n}^+, a_{k_{//},n} > dk_x dk_z \quad (11)$$

where *v* is the 2D elementary cell surface.

The average value $< a_{k_{//},n}^+, a_{k_{//},n} >$ calculation is carried out using the well known spectral theorem :

$$< a^{+}_{k_{//}}, a_{k_{//}} >= -2 \int \frac{Im << a^{+}_{k_{//}}, a_{k_{//}} >>}{e^{\beta E_k} - 1}$$

(12)

Furthermore, this average value can be expressed in terms of the real matrices P and its inverse P^{-1} which diagonalise the matrix M as follows :

$$< a^{+}_{k_{//},n}, a_{k_{//},n} >= \sum_{j=1}^{N} \left[\frac{P_{nj} P^{-1}_{jn} - P_{nj'} P^{-1}_{j'n}}{e^{\beta E_k} - 1} - P_{nj'} P^{-1}_{j'n} \right] \qquad \text{avec } j' = N+j$$

(13)

Finally, we obtain the n^{th} layer magnetization per site expression :

$$\frac{< S^{Z}_{n} >}{S} = 1 - \frac{1}{S} \frac{v}{(2\pi)^2} \sum_{j=1}^{N} \int_{BZ} \left[\frac{P_{nj} P^{-1}_{jn} - P_{nj'} P^{-1}_{j'n}}{e^{\beta E_k} - 1} - P_{nj'} P^{-1}_{j'n} \right] dk_x dk_z$$

(14)

The analytical resolution of the equations (10) and (14) is rather difficult to realize for more than one monolayer. Thus, in a first stage, we calculate the analytical expressions of the excitation spectra and the magnetization corresponding to one monolayer. Whereas for N>1, the resolution is carried out numerically.

III- RESULTS AND DISCUSSIONS :

1.1- Monolayer Case:

For the case N=1, there is no coupling between planes($J_{\perp}$=0); thus the matrix representing the Hamiltonian is reduced to a second order square matrix. Its resolution can be carried out analytically. So the obtained expression of the dispersion relation is written as follows:

$$E_k = \left[(A_k - B_k)(A_k + B_k) \right]^{1/2} \qquad (14)$$

where

$$A_{k_{//}} = 4J_1 S(\alpha - \cos\frac{k_x a}{2}\cos\frac{k_z a}{2}) + 2J_2 S(2 - \cos k_x a - \cos k_z a) + DS(2 + \cos\frac{k_x a}{2}\cos\frac{k_z a}{2})$$

(15-a)

$$B_{k_{//}} = -3DSc\,\mathrm{os}\frac{k_x a}{2}\cos\frac{k_z a}{2} \qquad (15\text{-b})$$

1.1.1- Excitation spectra:

On the figure1, we represent the reduced spin waves excitation spectra E(k)/J_1 in both the anisotropy presence ($\alpha \neq 0$) and absence ($\alpha = 0$).

We notice that in the last case (dotted line) the spectra does not present any gap, and consequently two-dimensional Co is not stable; it may be does not have any more privileged direction of the spin moments. Whereas, in the presence of the anisotropy (solid line) there is an opening of the gap which directly depends on the exchange interaction strength :

$E_g = S[(-4J_1\alpha+3D)^2 - (3D)^2]^{1/2} = 0.167SJ_1$. This favours the magnetic properties stabilization of the system and consequently, it has well an easy magnetization direction which is parallel to the z axis.

Such a results are rather well consistent with what is previously obtained. Indeed, fundamentally the Mermin and Wagner theorem[13] indicates that the magnetic order cannot exist in a two-dimensional isotropic Heisenberg ferromagnet. Experimentally, the Brillowin light scattering investigation on a cobalt monolayer on Cu(001) [14] shows that the presence of a stable ferromagnetic phase is due to the strong uniaxial anisotropy presence.

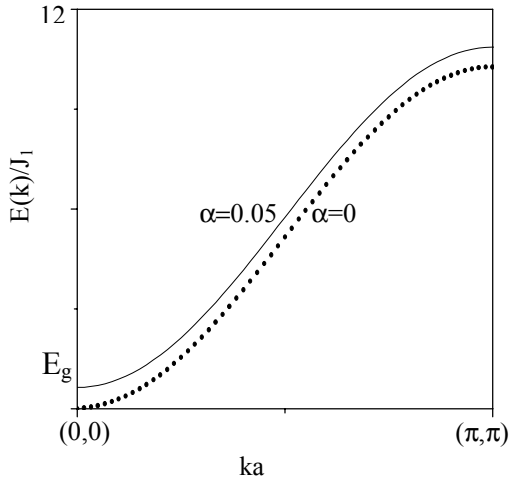

FIG.1

Spin waves dispersion curves in a Co monolayer along (11) direction. The parameters are: $J_2 = J_1/2.83$, $D = 0.01J_1$[10]. Dotted line : without anisotropy, solid line: in presence of anisotropy $\alpha = 0.05$[11].

1.1.1- Magnetization:

The obtained expression of the matrix P which diagonalises the hamiltonian is written in this simple case as:

$$P = \begin{pmatrix} ch\theta_k & -sh\theta_k \\ -sh\theta_k & ch\theta_k \end{pmatrix} \qquad with \qquad th2\theta_k = \frac{A_k}{B_k}$$

(16)

Then, the magnetization per site expression can be written as follows

$$\frac{<S_n^Z>}{S} = 1 - \frac{1}{S}\frac{v}{(2\pi)^2}\int_{BZ}\left[\frac{A_k}{E_k(e^{\beta E_k}-1)} + \frac{A_k - E_k}{2E_k}\right]dk_x dk_z \quad (17)$$

In absence of dipolar interaction, we can explicit the last magnetization expression for low wave vector spin waves. So, we can carry out a development for low k_x and k_z. Thus, we put

$$\xi = \frac{k_x a}{2} \quad \text{and} \quad \eta = \frac{k_z a}{2} \quad \text{then,} \quad \cos\left(\frac{k_x a}{2}\right) = 1 - \xi^2$$

and $$\cos\left(\frac{k_z a}{2}\right) = 1 - \eta^2$$

Furthermore, the spin wave energy is then reduced in this simple case to :

$$E(k) = 4J_1 S\left(\alpha - \cos\frac{k_x a}{2}\cos\frac{k_z a}{2}\right) + 2J_2 S(2 - \cos(k_x a)\cos(k_z a)) \quad (18)$$

So, it can be expressed for low wave vector as follows,

$$E(k) = 4J_1 S\,\square' + 4S(J_1 + 2J_2)\,\square^2 \quad \text{with} \quad \square^2 = \square^2 + \square^2 \quad \text{and} \quad \square' = \square - 1 \quad (19)$$

Substituting expression (19) in equation (17) and performing the integration with a help of a transformation to a polar coordinates, we find the magnetization expression for low wave vector as follows,

$$\frac{\langle S^z \rangle}{S} = 1 + \frac{1}{S}\frac{1}{2\pi}\frac{k_B T}{4S(J_1 + 2J_2)} Ln\left[1 - \exp(-4SJ_1\alpha'/k_B T)\right] \quad (20)$$

On the figure 2, we represented the magnetization thermal variation deduced from the analytical expression (20) (dotted line) and numerical calculation (solid line).
We notice that more than the temperature increases more than the difference between the two curves becomes significant. This is due to the fact that for very low temperature, only the spin waves having low frequencies are excited, the development which we proceeded remains valid. While, more than the temperature increases more than the effect of excitations having high frequencies becomes more significant, they cannot be neglected and the last simple development is rather unsuitable.
Moreover, we have examined the effects of the dipolar term presence. So the obtained results (circles) are not practically distinguishable from the values corresponding to the case where these effects are absent (triangles) suggesting that for a monolayer with a small NN number, the dipolar interaction contribution can be neglected.

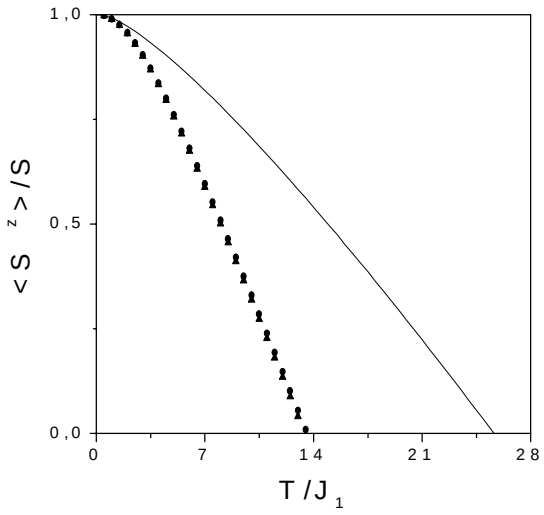

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FIG.2
Thermal variation of 1 ML magnetization, solid line: analytical expression (17), circles: numerical calculation in presence of dipolar term, triangles: numerical calculation in absence of dipolar term.

1.1- Super-lattice case (N >1) :

For a super-lattice (N>1), the resolution of the equations system (10) is carried out numerically by trigonalising the matrix M, and then by seeking the energy values corresponding to a null determinant.
On the figure 3a (resp. fig. 3b) we represented the spin waves dispersion curves in a super-lattice of N=3 (resp. N=4) layers. We highlighted well the existence of N different modes of which one is transverse, the others are longitudinals. The existence of these modes is due mainly to the break of symmetry along the film growth axis.

On the figure 4 we represented the temperature dependence of the cobalt super-lattice magnetization for three (fig.3a) and four cobalt layers (fig.3b) deduced from a numerical resolution of the expression (14). As is shown, the reduced magnetization follows an usual spin waves magnetization behavior. It vanishes at a critical temperature $T_c(J_1)$. This characteristic temperature depends on a multilayer parameters. Indeed, T_c increases when the layers number increases. It passes from $T_c=16J_1$ for 3 layers to $T_c=17J_1$ for 4 layers. This is may be du to the variation in the cobalt atoms neighborhood where the NN pairs number increases with increasing a cobalt layer

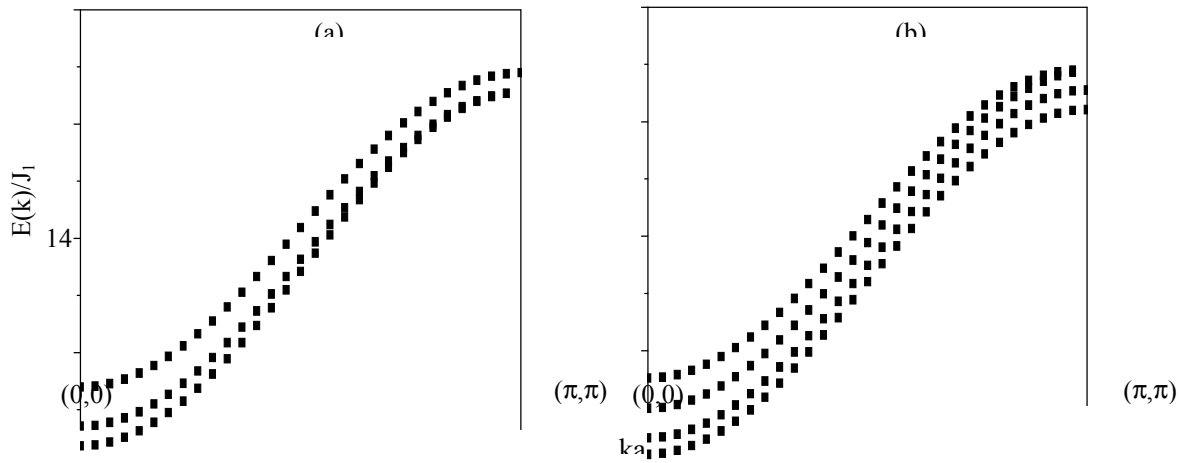

FIG.3

Spin waves dispersion curves. a :corresponding to 3 ferromagnetic monolayers. b : corresponding to 4 ferromagnetic monolayers. the parameters are the same as in fig.1, $J_{\perp}=0.1J_1$.

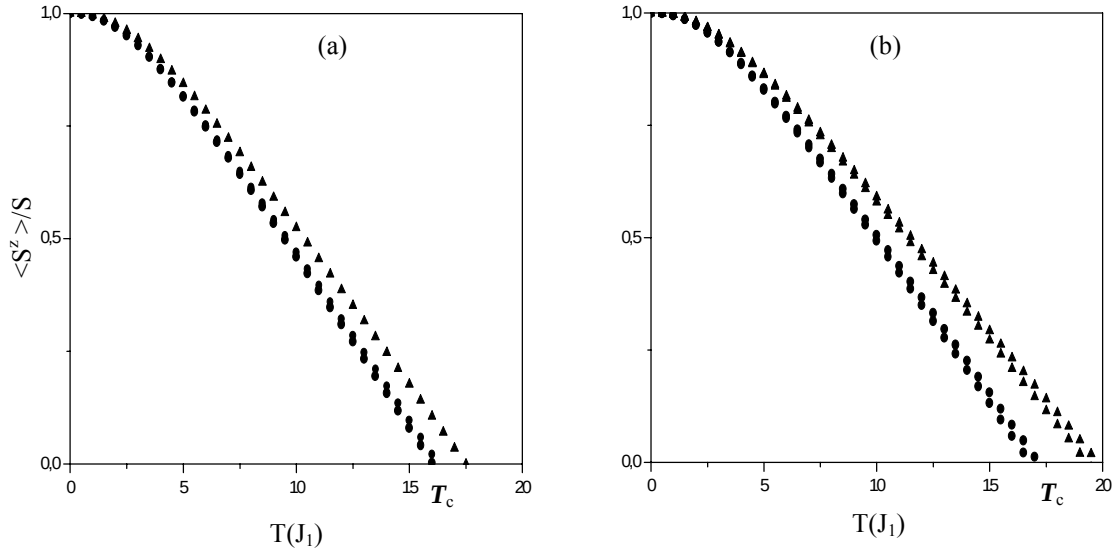

FIG. 4

Temperature dependence of the super-lattice magnetization in the cases: a. three layers, b. four layers. Circles : surface plane, triangles : bulk planes. the parameters are the same as in fig.2.

thickness leading to an exchange interaction (J_1) strengthening.

Also, we find that the surface plane magnetization is lower than that of the inner ones. We notice that the surface magnetization is obtained by replacing the index n in the magnetization expression given by formula (14) by 1 or N; indices representing the two extreme layers of the super-lattice. The difference between the values of the two magnetizations is due to the difference in the matrix M diagonal elements according to whether it is a surface layer or an inner one. Indeed, for the first one, the term which represents the inter-plane interaction is $W_k=4J_{\perp}S$, whereas for the last, this same term is given by $W_k=8J_{\perp}S$. This difference is due to the fact that the surface cobalt atoms have a number of inter-plane NN lower than that of the bulk cobalt atoms. This is consistent with the results obtained by the previous measurements[12].

4- CONCLUSION

We calculated within the framework of Green's function method the excitation spectrum E(k) and the magnetization for a cobalt super-lattice.
In the case of monolayer, we showed that the main role of the anisotropy is to open a gap in its excitation spectra E(k) and to favour a magnetic state stability.
The extension to the general case of magnetic super-lattice (N>1) allowed to highlight a number of excitation modes equal to the number of magnetic layers. Our results show that the surface planes have a magnetization lower than that of the inner one. What is in agreement with the measurement results carried out on the super-lattices.

Appendix

By introduction of the Fourier transform, the different terms of the transformed hamiltonian becomes:

$$H_{//}^{ex} = \sum_{k_{//}} \sum_{l=1}^{N} A_{k_{//}}^{ex} a_{k_{//},l}^{+} a_{k_{//},l}$$

$$H_{//}^{dip} = \sum_{k_{//}} \sum_{l=1}^{N} A_{k_{//}}^{dip} a_{k_{//},l}^{+} a_{k_{//},l} + \frac{1}{2} \sum_{k_{//}} \sum_{l=1}^{N} B_{k_{//}}^{dip} (a_{k_{//},l}^{+} a_{-k_{//},l}^{+} + a_{k_{//},l} a_{-k_{//},l})$$

$$H_{\perp}^{ex} = \sum_{k_{//}} \sum_{l=1}^{N} W_{k_{//},l}^{ex} a_{k_{//},l}^{+} a_{k_{//},l} + \sum_{k_{//}} \sum_{l=1}^{N-1} D_{k_{//}}^{ex} (a_{k_{//},l}^{+} a_{k_{//},l+1} + a_{k_{//},l} a_{k_{//},l+1}^{+})$$

with

$$A_{k_{//}}^{ex} = 4J_1 S(\alpha - \cos\frac{k_x a}{2}\cos\frac{k_z a}{2}) + 2J_2 S(2 - \cos k_x a - \cos k_z a)$$

$$A_{k_{//}}^{dip} = DS(2 + \cos\frac{k_x a}{2}\cos\frac{k_z a}{2})$$

$$D_{k_{//}}^{ex} = -2J_{\perp} S(\cos\frac{k_x a}{2} + \cos\frac{k_z a}{2})$$

$$B_{k_{//}} = -3DSc\,\mathrm{os}\frac{k_x a}{2}\cos\frac{k_z a}{2}$$

for the $W_{k_{//},j}^{ex}$ term, it depends on the plane according to whether it is a surface plane or a bulk one, its expression is given by:

$W_{k_{//},j}^{ex} = 4J_{\perp} S$ for j=1and N

$W_{k_{//},j}^{ex} = 8J_{\perp} S$ for j=2,N-1

The final forms of the matrix elements A, B and D are:

$$A_{1,1} = A_{N,N} = A_{k_{//}}^{ex} + A_{k_{//}}^{dip} + W_{k_{//},1}^{ex}$$

$$A_{j,j} = A_{k_{//}}^{ex} + A_{k_{//}}^{dip} + W_{k_{//},j}^{ex}, \quad j=2,N-1$$

$$A_{j,j+1} = A_{j+1,j} = D_{k_{//}}, \quad j=1,N-1$$

$$B_{j,j+N} = B_{k_{//}}, \quad j=1,N$$

The expressions of G and G' are given by:

$$\underline{G}_{i,j} = G_{i,j}(k_{//},E) = \langle\langle a_{k_{//},i}, a_{k_{//},j}^{+} \rangle\rangle_E$$

$$\underline{G}'_{i,j} = G'_{i,j}(k_{//},E) = \langle\langle a_{-k_{//},i}^{+}, a_{k_{//},j}^{+} \rangle\rangle_E$$

i and j=1,N

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