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A simplified method of *ab initio* calculation of the electron states in relativistic magnetics: III. Helical magnetic structure

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Abstract. A technique for the calculation of electron states in a helical magnetic structure based on a derivation of the Dirac equation by the relativistic Korringa–Kohn–Rostoker method is presented. Analysis of two limiting cases has been carried out: transition from a helical magnet to a relativistic ferromagnet and to the non-relativistic variant of the theory. The main dispersive equations for a relativistic magnet with helical magnetic structure obtained in this paper makes it possible to study the dependence of the ferromagnet electronic spectrum on the spin orientation.

1. Introduction

In our previous papers [1, 2] (hereafter referred to as I and II, respectively) a simplified method of calculating the simplest collinear magnets based on the relativistic Green function (RGF) method has been presented. In this work the approach proposed is generalized to the case of the helical magnetic structure.

In recent years, rather a larger number of papers have been devoted to constructing a theoretical scheme for the calculation of the electron states in magnets based on the Dirac equation. We refer to three of these papers [3–5], allowing one to appreciate the possibilities of the commonly used technique of calculating the energy bands based on the multiple-scattering formalism. A number of recent papers [6–8] containing further development of this approach should be mentioned as well.

Consider a monatomic crystal lattice with the sites occupied by atoms whose magnetic moments form a helical structure. Choose the Oz direction along the helix axis and let a be the interatomic distance along this axis. One of the sites is referred to as the first site and the origin of the global coordinate frame is placed at this site, the axes Ox and Oy being oriented in such a way that the projection of the spin S_1 corresponding to this site onto the Oy axis is equal to zero. Denote the angle between the spin orientation and the Oz axis by β, the angle between the spin projection onto the coordinate plane (x, y) and the Ox axis by α, and let α vary by the same quantity $\Delta\alpha$ in the one-step displacement along the helix. This spin projection is also assumed to be back to the initial position in N steps, i.e. $\Delta\alpha = 2\pi/N$ or, in fact, $S_{N+1} \parallel S_1$.

Also, at each site j we introduce a local coordinate frame with its Oz_j axis along the positive spin orientation, the origin placed at the site and the direction of axes defined

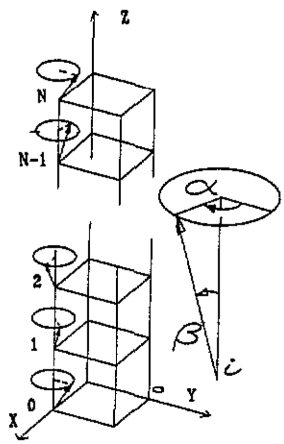

Figure 1. Unit magnetic cell.

by Euler angles $(\alpha_j, \beta_j, \gamma_j)$. It is always assumed that all $\gamma_j = 0$, for the first site $\alpha_1 = 0$ and, while passing from a site to its neighbour, the angle α varies by $\Delta\alpha$. Then for the jth site the orientation of a local coordinate frame is defined by the angles

$$\alpha_j = \Delta\alpha(j-1) \qquad \beta_j = \beta \qquad \gamma_j = 0. \tag{1}$$

Choose further the unit cell so that the vector $\boldsymbol{a}_3 = (0, 0, a)$ is one of the lattice basis vectors, and $\boldsymbol{a}_1$ and $\boldsymbol{a}_2$ are the other two vectors. The magnetic structure obtained is obviously periodic, with a period $(0, 0, Na)$; therefore, the polyhedron constructed on the vectors $\boldsymbol{a}_1, \boldsymbol{a}_2, N\boldsymbol{a}_3$ is the magnetic unit cell. Denote the vectors of the original lattice by $\boldsymbol{R}_n$, the reciprocal lattice vectors by $\boldsymbol{K}_n$, the reduced wavevector by $\boldsymbol{k}$, and the volumes of the unit cell and Brillouin zone by Ω and Ω_B, respectively. Also let $\boldsymbol{T}_n$, $\boldsymbol{Q}_n$, $\boldsymbol{q}$, Ω_M and Ω_{BM} be the corresponding quantities for the magnetic lattice.

The relations between the geometric characteristics of the crystal and magnetic lattices are obvious; we shall introduce them as required. The total geometric picture is illustrated in figure 1.

2. Mathematical formulation of the problem

The general scheme for calculating the electron energy spectrum of the helical magnetic structure described can be constructed by analogy with I and II. Again the starting point of our considerations will be the equation for the large component of the Dirac four-component spinor (see I, equation (10))

$$\hat{\Delta}\Psi + W[E - (V + \hat{\mathfrak{S}}\,\Delta V)]\Psi - (W'/W)(\boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}})(\boldsymbol{\sigma}\cdot\boldsymbol{\nabla})\Psi = 0. \tag{2}$$

Here $\sigma_i (i = x, y, z)$ are the Pauli matrices, $\hat{\boldsymbol{r}}$ is the unit vector,

$$W = 1 + (E - V)/c^2 \tag{3}$$

and c is the velocity of light.

The potential involved in (2) requires some clarifying. We assume that identical muffin-tin (MT) spheres inscribed into the crystal cell are constructed around each lattice site. In the local coordinate frame connected with a given atom the MT potential does not depend on the site number and has the usual meaning:

$$V = \tfrac{1}{2}(V_+ + V_-) \qquad \Delta V = \tfrac{1}{2}(V_+ - V_-) \tag{4}$$

where V_+ and V_- are the potentials acting on electrons with different spin orientations. The operator $\hat{\mathfrak{D}}\,\Delta V$ in the local coordinate frame also has its standard form

$$\hat{\mathfrak{D}}_j\,\Delta V = \Delta V\,\hat{\boldsymbol{\sigma}}_{z_j'} \tag{5}$$

but does depend on the site number since the Pauli matrix $\hat{\boldsymbol{\sigma}}_{z_j'}$ has the canonical form

$$\hat{\boldsymbol{\sigma}}_{z_j'} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{6}$$

only in the local coordinate frame connected with the site j.

By virtue of the above discussion the general solution inside the jth MT sphere will be written in the proper coordinate frame in exactly the same way as before (see II, equation (7))

$$\Psi_{\rm I}^{(j)}(\boldsymbol{\rho}_j) = \sum_{l\mu,\nu} \mathrm{i}^l C_{l\mu,\nu}^{(j)} \begin{pmatrix} g_{l\mu,\nu+}(\rho_j) Y_{lm}(\hat{\rho}_j) \\ g_{l\mu,\nu-}(\rho_j) Y_{lm'}(\hat{\rho}_j) \end{pmatrix}. \tag{7}$$

Here $\boldsymbol{\rho}_j$ is the radius vector measured from the jth site in the local coordinate frame; l is the orbital quantum number; μ is the projection of the total angular momentum onto the axis Oz_j'; $m = \mu - \tfrac{1}{2}$ and $m' = \mu + \tfrac{1}{2}$. The index $\nu = 1, 2$ labels two linearly independent solutions of the set of radial equations (see I, equation (13))

$$\begin{aligned} &g''_{l\mu+} + (2/\rho)g'_{l\mu+} + [W(E - V_+) - l(l+1)/\rho^2]g_{l\mu+} \\ &\quad = (W'/W)[\![\{g'_{l\mu+} - [(\mu - \tfrac{1}{2})/\rho]g_{l\mu+}\} + S_\mu\sqrt{(l+\mu+\tfrac{1}{2})(l-\mu+\tfrac{1}{2})}(1/\rho)g_{l\mu-}]\!] \\ &g''_{l\mu-} + (2/\rho)g'_{l\mu-} + [W(E - V_-) - l(l+1)/\rho^2]g_{l\mu-} \\ &\quad = (W'/W)[\![\{g'_{l\mu-} - [(\mu + \tfrac{1}{2})/\rho]g_{l\mu-}\} + S_\mu\sqrt{(l+\mu+\tfrac{1}{2})(l-\mu+\tfrac{1}{2})}(1/\rho)g_{l\mu+}]\!] \end{aligned} \tag{8}$$

($S_\mu = \mu/|\mu|$, and the index j labelling ρ is omitted).

The empty-lattice Green function of a structure with base will be written in the form [9, 10]

$$G^{jj'}(\boldsymbol{q}, E'; \boldsymbol{r}_j, \boldsymbol{r}'_{j'}) = -\frac{1}{\Omega_{\rm M}} \sum_t \frac{\exp[\mathrm{i}(\boldsymbol{q} + \boldsymbol{Q}_t)\cdot(\boldsymbol{r}_j + \boldsymbol{h}_j - \boldsymbol{r}'_{j'} - \boldsymbol{h}_{j'})]}{|\boldsymbol{q} + \boldsymbol{Q}_t|^2 - E'} \tag{9}$$

where $E' = E(1 + E/c^2)$, $\boldsymbol{h}_j = \boldsymbol{a}_3(j-1)$, and $\boldsymbol{r}_j$ and $\boldsymbol{r}'_{j'}$ are the coordinates measured from the corresponding sites of the magnetic cell in the global coordinate frame. Using the expansion of the Green function in terms of spherical harmonics, one can write the solution of equation (2) outside the MT spheres as follows (see II, equation (12)):

$$\Psi_{\rm II}(\boldsymbol{r}_j) = \sum_{j'} \sum_{\substack{lm,\\ l'm'}} \mathrm{i}^l [B_{lm,l'm'}^{jj'}(\boldsymbol{q}, E') j_l(\eta r_j) + \eta\delta_{jj'}\delta_{lm,l'm'} n_l(\eta r_j)] Y_{lm}(\hat{r}_j) \begin{cases} b_{l'm'+}^{(j)} \\ b_{l'm'-}^{(j)} \end{cases}. \tag{10}$$

Here $\eta = (E')^{1/2}$, j_l and n_l are the spherical Bessel and Neumann functions, respectively,

$B^{jj'}_{lm,l'm'}$ are the structure constants of the lattice with a base and $b^{(j)}_{lm\pm}$ are unknown expansion coefficients.

The main dispersive equation is obtained from the condition of smooth joining of the solutions $\Psi^{(j)}_{\mathrm{I}}$ and Ψ_{II} through the MT spheres of the magnetic cell:

$$\Psi^{(j)}_{\mathrm{I}}(\boldsymbol{\rho}_j) = \Psi_{\mathrm{II}}(\boldsymbol{r}_j) \qquad (\partial/\partial r_j)\Psi^{(j)}_{\mathrm{I}}(\boldsymbol{\rho}_j) = (\partial/\partial r_j)\Psi_{\mathrm{II}}(\boldsymbol{r}_j) \tag{11}$$

with $|\boldsymbol{r}_j| = |\boldsymbol{\rho}_j| = r_s$.

3. General formalism

To make use of conditions (11), one should express the solution $\Psi^{(j)}_{\mathrm{I}}$ inside the MT spheres and the solution Ψ_{II} outside the MT spheres in the same coordinate frame. So we rewrite solutions (7) in the global coordinate frame. According to [11] the spherical harmonics are transformed in this case to the following form:

$$Y_{lm}(\hat{\boldsymbol{\rho}}_j) = \sum_{m'} R^{(l)}_{m'm}(\alpha_j, \beta_j, \gamma_j) Y_{lm'}(\hat{\boldsymbol{r}}_j) \tag{12}$$

where, taking account of (1),

$$R^{(l)}_{m'm}(\alpha_j, \beta, 0) = \exp(-\mathrm{i}m'\alpha_j) \sum_t (-1)^t \frac{\sqrt{(l+m')!(l-m')!(l+m)!(l-m)!}}{(l+m'-t)!(l-m-t)!t!(t-m'+m)!}$$
$$\times [\cos(\beta/2)]^{2l+m'-m-2t}[\sin(\beta/2)]^{2t-m'+m}. \tag{13}$$

Also, it must be taken into consideration that the spinors themselves are transformed too, this transformation being defined by the matrix

$$\mathbf{R}^{(1/2)}(j) = \begin{pmatrix} u_j & v_j \\ -v_j^* & u_j^* \end{pmatrix} \tag{14}$$

where

$$u_j = \exp(-\mathrm{i}\alpha_j/2)\cos(\beta/2) \qquad v_j = -\exp(-\mathrm{i}\alpha_j/2)\sin(\beta/2). \tag{15}$$

Thus, expansion (7) is transformed to the following:

$$\Psi^{(j)}_{\mathrm{I}}(\boldsymbol{r}_j) = \sum_{l\mu,\nu} \mathrm{i}^l C^{(j)}_{l\mu,\nu} \mathbf{R}^{(1/2)}(j) \begin{pmatrix} g_{l\mu,\nu+}(r_j) \sum_{m_1} R^{(l)}_{m_1 m}(j) Y_{lm_1}(\hat{\boldsymbol{r}}_j) \\ g_{l\mu,\nu-}(r_j) \sum_{m_1} R^{(l)}_{m_1 m'}(j) Y_{lm_1}(\hat{\boldsymbol{r}}_j) \end{pmatrix}. \tag{16}$$

Now substituting (16) and (10) into the first of conditions (11) and multiplying the result on the left by $[\mathbf{R}^{(1/2)}(j)]^{-1}$ yields

$$\sum_{l\mu,\nu} \mathrm{i}^l C^{(j)}_{l\mu,\nu} \begin{pmatrix} g_{l\mu,\nu+}(r_s) \sum_{m_1} R^{(l)}_{m_1 m}(j) Y_{lm_1}(\hat{\boldsymbol{r}}_j) \\ g_{l\mu,\nu-}(r_s) \sum_{m_1} R^{(l)}_{m_1 m'}(j) Y_{lm_1}(\hat{\boldsymbol{r}}_j) \end{pmatrix}$$
$$= \sum_{j} \sum_{\substack{lm \\ l''m''}} \mathrm{i}^l [B^{jj'}_{lm,l''m''}(\boldsymbol{q}, E') j_l(\eta r_s) + \eta \delta_{jj'} \delta_{lm,l''m''} n_l(\eta r_s)] Y_{lm}(\hat{\boldsymbol{r}}_j) \begin{pmatrix} a^{jj'}_{l''m''+} \\ a^{jj'}_{l''m''-} \end{pmatrix} \tag{17}$$

where the following notation is introduced:

$$a^{jj'}_{lm+} = u^*_j b^{(j')}_{lm+} - v_j b^{(j')}_{lm-} \tag{18a}$$

$$a^{jj'}_{lm-} = v^*_j b^{(j')}_{lm+} + u_j b^{(j')}_{lm-}. \tag{18b}$$

Multiplying (17) further by $Y^*_{l'_1 m'_1}(\hat{r}_j)$ and using the orthogonality of spherical functions we get

$$\sum_{\mu,\nu} C^{(j)}_{l\mu,\nu} \begin{pmatrix} R^{(l)}_{m_1 m}(j) & g_{l\mu,\nu+} \\ R^{(l)}_{m_1 m}(j) & g_{l\mu,\nu-} \end{pmatrix} = \sum_{\substack{j' \\ l''m''}} (B^{jj'}_{lm_1,l''m''} j_l + \eta \delta_{jj'} \delta_{lm_1,l''m''} n_l) \begin{pmatrix} a^{jj'}_{l''m''+} \\ a^{jj'}_{l''m''-} \end{pmatrix}. \tag{19}$$

(In writing (19) we have replaced l_1 by l and m_1 by m.) Finally, we multiply the first equality in (19) by $R^{(l)*}_{m_1 \tilde{m}}(j)$ and the second by $R^{(l)*}_{m_1 \tilde{m}'}(j)$ $(\tilde{m}' = \tilde{m} + 1)$ and sum over m_1. Then, by virtue of the unitarity

$$\sum_m R^{(l)}_{mm'}(j) R^{(l)*}_{mm''}(j) = \delta_{m'm''} \tag{20}$$

equations (19) are transformed to expressions analogous to those obtained in our previous papers:

$$\begin{aligned} C^{(j)}_{l\tilde{\mu},1} g_{l\tilde{\mu},1+} + C^{(j)}_{l\tilde{\mu},2} g_{l\tilde{\mu},2+} &= \sum_{j'l''m''} \sum_{m_1} [R^{(j)*}_{m_1 \tilde{m}}(j)(B^{jj'}_{lm_1,l''m''} j_1 + \eta \delta_{jj'} \delta_{lm_1 l''m''} n_l)] a^{jj'}_{l''m''+} \\ C^{(j)}_{l\tilde{\mu},1} g_{l\tilde{\mu},1-} + C^{(j)}_{l\tilde{\mu},2} g_{l\tilde{\mu},2-} &= \sum_{j'l''m''} \sum_{m_1} [R^{(j)*}_{m_1 \tilde{m}}(j)(B^{jj'}_{lm_1,l''m''} j_l + \eta \delta_{jj} \delta_{lm_1 l''m''} n_l)] a^{jj'}_{l''m''-}. \end{aligned} \tag{21}$$

Further, as before, one has to write the equations for the radial derivatives and group in pairs the equations in the unknown $C^{(j)}_{l\mu,\nu}$ with the same spin orientation; then one should express $C^{(j)}_{l\mu,\nu}$ from each pair of equations and equate the relations obtained, etc. The main steps of the algebraic manipulations are presented in appendix 1.

4. Dispersive equation and its analysis

The algebra in appendix 1 results in a system of algebraic equations in the unknown $b^{(j)}_{lm\pm}$ whose solvability condition gives the main dispersive equation

$$\begin{vmatrix} \mathbf{B}^{jj'} + \delta_{jj'} \mathbf{T}^+_j & \delta_{jj'} \mathbf{T}_j \exp(-\mathrm{i}\alpha_j) \\ \delta_{jj'} \mathbf{T}^+_j \exp(\mathrm{i}\alpha_j) & \mathbf{B}^{jj'} + \delta_{jj'} \mathbf{T}^-_j \end{vmatrix} = 0. \tag{22}$$

Here $\mathbf{B}^{jj'} = B^{jj'}_{lm,l'm'}(\boldsymbol{q}, E')$ are the matrices of the structure constants, and the matrices $\mathbf{T}_j$ are related to certain auxiliary matrices $\mathbf{S}_j$ by the following expressions:

$$\begin{aligned} 2\mathbf{T}^+_j &= (\mathbf{S}^+_j + \mathbf{S}^-_j) + (\mathbf{S}^+_j - \mathbf{S}^-_j)\cos\beta - (\mathbf{S}_j + \mathbf{S}^+_j)\sin\beta \\ 2\mathbf{T}^-_j &= (\mathbf{S}^+_j + \mathbf{S}^-_j) - (\mathbf{S}^+_j - \mathbf{S}^-_j)\cos\beta + (\mathbf{S}_j + \mathbf{S}^+_j)\sin\beta \\ 2\mathbf{T}_j &= (\mathbf{S}_j - \mathbf{S}^+_j) - (\mathbf{S}_j + \mathbf{S}^+_j)\cos\beta + (\mathbf{S}^+_j - \mathbf{S}^-_j)\sin\beta. \end{aligned} \tag{23}$$

The matrices $\mathbf{S}_j$, in turn, are expressed in terms of the scattering-phase cotangents:

$$\mathbf{S}^\pm_j = \left(\sum_{\tilde{m}} R^{(l)}_{m\tilde{m}}(j) R^{(l)*}_{m'\tilde{m}}(j) W^{\pm\pm}_{l\tilde{\mu}} \right) \tag{24a}$$

$$\mathbf{S}_j = \left(\sum_{\tilde{m}} R^{(l)}_{m\tilde{m}}(j) R^{(l)*}_{m'\tilde{m}+1}(j) W^{+-}_{l\tilde{\mu}} \right) \tag{24b}$$

where, in the notation of appendix 1,

$$W^{\pm\pm}_{l\mu} = \eta(\Delta^{\pm\pm}_{l\mu}/\Delta_{l\mu}) \qquad (25a)$$

$$W^{+-}_{l\mu} = \eta(\Delta^{+-}_{l\mu}/\Delta_{l\mu}). \qquad (25b)$$

The general structure of the matrices $\mathbf{S}_j$ and the explicit expression for $l = 1$ are presented in appendix 2.

In fact, equation (22) itself can be used to perform calculations. However, the form of the equation in which the structure constants $\mathbf{B}^{jj'}$ of the magnetic lattice are expressed in terms of the structure constants $\mathbf{A}$ of the original lattice seems to be more convenient. It is shown in appendix 3 that

$$B^{jj'}_{lm,l'm'}(\boldsymbol{q}, E') = \exp[\mathrm{i}\boldsymbol{q}\cdot(\boldsymbol{h}_j - \boldsymbol{h}_{j'})\frac{1}{N}\sum_p \exp[\mathrm{i}\boldsymbol{\kappa}_p\cdot(h_j - h_{j'})]\,A_{lm,l'm'}(\boldsymbol{k}_p, E') \qquad (26)$$

where $\boldsymbol{k}_p = \boldsymbol{q} + \boldsymbol{\kappa}_p$,

$$\boldsymbol{\kappa}_p = (p/N)\boldsymbol{b}_3 \qquad \boldsymbol{h}_j = j\boldsymbol{a}_3 \qquad j, p = 0, 1, \ldots, N-1. \qquad (27)$$

Denote the Nth root $\exp(\mathrm{i}2\pi/N)$ of unity by ω, the matrix of the structure constants at the point $\boldsymbol{k}_p$ by $\mathbf{A}_p$, and the scalar matrix $\boldsymbol{\omega}^{pj}$ of the same size as $\mathbf{A}_p$ by $1/N^{1/2}\Omega_{pj}$. In this notation, equation (22) becomes

$$\begin{vmatrix} \sum_{\tilde{p}} \Omega_{\tilde{p}j}\Omega^*_{\tilde{p}j'}\mathbf{A}_p + \delta_{jj'}\mathbf{T}^+_j & \delta_{jj'}\mathbf{T}_j\exp(-\mathrm{i}\alpha_j) \\ \delta_{jj'}\mathbf{T}^+_j\exp(\mathrm{i}\alpha_j) & \sum_{\tilde{p}} \Omega_{\tilde{p}j}\Omega^*_{\tilde{p}j'}\mathbf{A}_p + \delta_{jj'}\mathbf{T}^-_j \end{vmatrix} = 0. \qquad (28)$$

Form, next, the matrices

$$\boldsymbol{\Omega}_1 = \begin{pmatrix} \Omega^*_{pj} & 0 \\ 0 & \Omega^*_{pj} \end{pmatrix} \qquad \boldsymbol{\Omega}_2 = \begin{pmatrix} \Omega_{p'j'} & 0 \\ 0 & \Omega_{p'j'} \end{pmatrix} \qquad (29)$$

whose elements are the blocks Ω_{pj} $(p, j = 0, 1, \ldots, N-1)$ and multiply equation (28) on the left by $\boldsymbol{\Omega}_1$ and on the right by Ω_2.

Taking into account the orthogonality

$$\sum_j \Omega_{p'j}\Omega^*_{p''j} = \delta_{p'p''}\hat{\mathbf{I}} \qquad (30)$$

we get

$$\begin{vmatrix} \mathbf{A}'_p\delta_{pp'} + \sum_j \Omega^*_{pj}\Omega_{p'j}\mathbf{T}^+_j & \sum_j \Omega^*_{pj}\Omega_{p'j}\mathbf{T}_j\exp(-\mathrm{i}\alpha_j) \\ \sum_j \Omega^*_{pj}\Omega_{p'j}\mathbf{T}^+_j\exp(\mathrm{i}\alpha_j) & \mathbf{A}_p\delta_{pp'} + \sum_j \Omega^*_{pj}\Omega_{p'j}\mathbf{T}^-_j \end{vmatrix} = 0 \qquad (31)$$

or in the explicit form.

$$\begin{vmatrix} \mathbf{A}_p\delta_{pp'} + \sum_j \mathbf{T}_j^+ \exp[-\mathrm{i}(\boldsymbol{\kappa}_p - \boldsymbol{\kappa}_{p'})\cdot \boldsymbol{h}_j] & \sum_j \exp[-\mathrm{i}(\boldsymbol{\kappa}_p - \boldsymbol{\kappa}_{p'})\cdot \boldsymbol{h}_j]\,\mathbf{T}_j \exp(-\mathrm{i}\alpha_j) \\ \sum_j \exp[-\mathrm{i}(\boldsymbol{\kappa}_p - \boldsymbol{\kappa}_{p'})\cdot \boldsymbol{h}_j]\,\mathbf{T}_j^+ + \exp(\mathrm{i}\alpha_j) & \mathbf{A}_p\delta_{pp'} + \sum_j \mathbf{T}_j^- \exp[-\mathrm{i}(\boldsymbol{\kappa}_p - \boldsymbol{\kappa}_{p'})\cdot \boldsymbol{h}_j] \end{vmatrix} = 0. \tag{32}$$

Since equation (32) is obtained from (22) by unitary transformation, these equations are sure to be entirely equivalent to each other. The transition from the site representation (22) to the quasi-momentum representation (32) performed in the dispersive equation was used by us earlier for another problem [12].

Two limiting cases are interesting to analyse: a ferromagnet and the non-relativistic version of theory.

In the first case, $\beta = 0$ and, according to (23) and (24) (see also appendix 2),

$$\mathbf{T}_j^{\pm} = \mathbf{S}_j^{\pm} = \mathbf{W}^{\pm\pm} \qquad \mathbf{T}_j = \mathbf{S}_j = \mathbf{W}^{+-}\exp(\mathrm{i}\alpha_j) \tag{33}$$

i.e. the matrices $\mathbf{T}_j^{\pm}$ and $\mathbf{T}_j\exp(-\mathrm{i}\alpha_j)$ do not actually depend on j. Then, in (31),

$$\Big(\sum_j \Omega_{pj}^*\Omega_{p'j}\Big)\mathbf{T}^{\pm} = \delta_{pp'}\mathbf{W}^{\pm\pm} \qquad \Big(\sum_j \Omega_{pj}^*\Omega_{p'j'}\Big)\mathbf{T}_j\exp(-\mathrm{i}\alpha_j) = \delta_{pp'}\mathbf{W}^{+-} \tag{34}$$

and the dispersive equation becomes divided into N independent blocks of the form

$$\begin{vmatrix} \mathbf{A}_p + \mathbf{W}^{++} & \mathbf{W}^{+-} \\ \mathbf{W}^{-+} & \mathbf{A}_p + \mathbf{W}^{--} \end{vmatrix} = 0. \tag{35}$$

Since with $\boldsymbol{q}$ varying in the first Brillouin zone of the magnetic lattice, the set of vectors $\boldsymbol{k}_p$ does fill the whole Brillouin zone of the crystal lattice, the system of equations (35) is obviously equivalent to the dispersive equation for a ferromagnet (see I, equation (22)).

According to I, equation (39), in the non-relativistic limit the matrices $\mathbf{W}^{\pm\mp}$ are equal to zero and $\mathbf{W}^{\pm\pm}$ are diagonal (their matrix elements do not depend on μ). Taking this into account gives

$$\mathbf{S}_j^{\pm} = \mathbf{W}^{\pm\pm}(N - \mathbf{R}) \qquad \mathbf{S}_j = 0 \tag{36a}$$

$$2\mathbf{T}_j^{\pm} = (\mathbf{S}_j^+ + \mathbf{S}_j^-) \pm (\mathbf{S}_j^+ - \mathbf{S}_j^-)\cos\beta \qquad 2\mathbf{T}_j = (\mathbf{S}_j^+ - \mathbf{S}_j^-)\sin\beta \tag{36b}$$

i.e. $\mathbf{T}_j^{\pm}$ and $\mathbf{T}_j$ do not depend on j and are diagonal. Substituting (36*b*) in the sums (31) yields

$$\Big(\sum_j \Omega_{pj}^*\Omega_{p'j}\Big)\mathbf{T}^{\pm} = \delta_{pp'}(\bar{W} \pm \Delta W\cos\beta) \tag{37}$$

where

$$\bar{W} = \tfrac{1}{2}(\mathbf{W}^{++} + \mathbf{W}^{--}) \qquad \Delta W = \tfrac{1}{2}(\mathbf{W}^{++} - \mathbf{W}^{--}). \tag{38}$$

Taking into account that $\exp(\mathrm{i}\alpha_j) = \Omega_{1j}$, we get for the two other sums

$$\begin{aligned} \Big(\sum_j \Omega_{pj}^*\Omega_{p'j}\Omega_{1j}^*\Big)\mathbf{T} &= \delta_{p',p+1}\,\Delta W\sin\beta \\ \Big(\sum_j \Omega_{pj}^*\Omega_{p'j}\Omega_{1j}\Big)\mathbf{T}^+ &= \delta_{p,p'+1}\,\Delta W\sin\beta. \end{aligned} \tag{39}$$

Thus in the non-relativistic limit for a helical structure the equation is again divided into N blocks, although of more complicated form than for a ferromagnet:

$$\begin{vmatrix} \mathbf{A}_p + \bar{W} + \Delta W \cos\beta & \Delta W \sin\beta \\ \Delta W \sin\beta & \mathbf{A}_p + \bar{W} + \Delta W \cos\beta \end{vmatrix} = 0. \tag{40}$$

One can see that, in the non-relativistic case in a helical structure, two neighbouring points k_p and k_{p+1} are interconnected, the 'positive' spin orientation at the point p interacting with the 'negative' spin orientation at the point $p+1$. Detailed consideration of theory can be found in [13–15].

5. Conclusion

To conclude, it should be mentioned that equation (22) enables us to study the dependence of the electron spectrum of a ferromagnet on the spin orientation. For that it is sufficient to replace in (22) the structure constants $B^{jj'}(q, E')$ by $A(k, E')$, with k assumed to vary in the Brillouin zone of the crystal lattice, and to omit the site index j in all other quantities.

Note also that the formal generalization of the above scheme to the case of the crystal cell with a larger number of atoms and to the case of more complicated magnetic structures is not difficult to carry out. In fact, the possibility of conducting calculations is limited by the computers available. It must be realized, of course, that the antiferromagnetic state as well as the states with inverted spin in general cannot be obtained within the framework of the technique presented, since the spin inversion is connected with time inversion rather than with rotations and reflections and requires special consideration. However, the generalization to such a case can be performed, if necessary, using the results of [2].

Appendix 1

The first pair of equations for the spin 'up' is written in the following way:

$$C^{(j)}_{l\bar{\mu},1} g_{l\bar{\mu},1+} + C^{(j)}_{l\bar{\mu},2} g_{l\bar{\mu},2+} = \sum_{j'} \sum_{l''m''} \sum_{m_1} R^{(l)*}_{m_1\bar{m}}(j)(B^{jj'}_{lm_1,l''m''} j_{l'} + \eta\delta_{jj'}\delta_{lm_1,l''m''} n_l) a^{(j')}_{l''m''+} \tag{A1.1}$$

$$C^{(j)}_{l,\bar{\mu},1} g'_{l,\bar{\mu},1+} + C^{(j)}_{l\bar{\mu},2} g'_{l\bar{\mu},2+} = \sum_{j'} \sum_{l''m''} \sum_{m_1} R^{(l)*}_{m_1\bar{m}}(j)(B^{jj'}_{lm_1,l''m''} \tilde{j}'_l + \eta\delta_{jj'}\delta_{lm_1,l''m''} n'_l) a^{(j')}_{l''m''+}.$$

Hence

$$C^{(j)}_{l\bar{\mu},1} = \frac{1}{g_{l\bar{\mu},1+}, g_{l\bar{\mu},2+}} \Bigg[\sum_{j'} \sum_{l''m''} \left(\sum_{m_1} R^{(l)*}_{m_1\bar{m}}(j) B^{jj'}_{lm_1,l''m''} a^{jj'}_{l''m''+} \right) \times [j_l, g_{l,\bar{\mu},2+}] + \eta \sum_{m_1} R^{(l)}_{m_1\bar{m}}(j) a^{jj'}_{lm_1+} [n_l, g_{l\bar{\mu},2+}] \Bigg] \tag{A1.2a}$$

$$C^{(j)}_{l\bar{\mu},2}=\frac{1}{g_{l\bar{\mu},2+},g_{l\bar{\mu},1+}}\left[\sum_{j'}\sum_{l''m''}\left(\sum_{m_1}R^{(l)*}_{m_1\bar{m}}(j)B^{jj'}_{lm_1,l''m''}a^{jj'}_{l''m''+}\right)\right.$$
$$\left.\times[j_l,g_{l\bar{\mu},1+}]+\eta\sum_{m_1}R^{(l)}_{m_1\bar{m}}(j)a^{jj'}_{lm_1+}[n_l,g_{l\bar{\mu},1+}]\right] \qquad (A1.2b)$$

$[f_1,f_2]=f_1f'_2-f'_1f_2.$

The second pair of equations for the spin 'down' differs from (A1.1) only in the fact that we have the index $-$ instead of $+$ and $\bar{m}'=\bar{m}+1$ instead of $\bar{m}$. Again we find $C^{(j)}_{l\bar{\mu},1}$ and $C^{(j)}_{l\bar{\mu},2}$ and equate the expressions obtained to those in (A1.2). Taking into account

$$[g_{l\mu,1+},g_{l\mu,2+}]=-[g_{l\mu,1-},g_{l\mu,2-}] \qquad (A1.3)$$

yields

$$\sum_{j'}\sum_{l''m''}\sum_{m_1}\{R^{(l)*}_{m_1\bar{m}}(j)B^{jj'}_{lm_1,l''m''}a^{jj'}_{l''m''+}[j_l,g_{l\bar{\mu},2+}]+R^{(l)*}_{m_1\bar{m}'}(j)B^{jj'}_{lm_1,l''m''}a^{jj'}_{l''m''-}[j_l,g_{l\bar{\mu},2-}]\}$$
$$+\eta\sum_{m_1}\{R^{(l)*}_{m_1\bar{m}}(j)a^{jj'}_{lm_1+}[n_l,g_{l\bar{\mu},2+}]+R^{(l)*}_{m_1\bar{m}'}(j)a^{jj'}_{lm_1-}[n_l,g_{l\bar{\mu},2-}]\}=0 \qquad (A1.4a)$$

$$\sum_{j'}\sum_{l''m''}\sum_{m_1}\{R^{(l)*}_{m_1\bar{m}}(j)B^{jj'}_{lm_1,l''m''}a^{jj'}_{l''m''+}[j_l,g_{l\bar{\mu},1+}]+R^{(l)*}_{m_1\bar{m}'}(j)B^{jj'}_{lm_1,l''m''}a^{jj'}_{l''m''-}[j_l,g_{l\bar{\mu},1-}]\}$$
$$+\eta\sum_{m_1}\{R^{(l)*}_{m_1\bar{m}}(j)a^{jj'}_{lm_1+}[n_l,g_{l\bar{\mu},1+}]+R^{(l)*}_{m_1\bar{m}'}(j)a^{jj'}_{lm_1-}[n_l,g_{l\bar{\mu},1-}]\}=0. \qquad (A1.4b)$$

Perform one more transformation in (A1.4). Let us multiply the first equation by $[j_l,g_{l\bar{\mu},1-}]$, the second by $[j_l,g_{l\bar{\mu},2-}]$ and subtract the second from the first. The equation obtained is written as follows:

$$\sum_{j'}\sum_{l''m''}\sum_{m_1}[R^{(l)*}_{m_1\bar{m}}(j)B^{jj'}_{lm_1,l''m''}a^{jj'}_{l''m''+}\Delta_{l\bar{\mu}}]+\eta\sum_{m_1}[R^{(l)*}_{m_1\bar{m}}(j)a^{jj}_{lm_1+}\Delta^{++}_{l\bar{\mu}}]$$
$$+\eta\sum_{m_1}[R^{(l)*}_{m_1\bar{m}'}(j)a^{jj}_{lm_1-}\Delta^{+-}_{l\bar{\mu}}]=0. \qquad (A1.5)$$

Similarly, multiplying equations in (A1.4) by $[j_l,g_{l\bar{\mu},1+}]$ and $[j_l,g_{l\bar{\mu},2+}]$ and subtracting one from the other gives

$$\sum_{j'}\sum_{l''m''}\sum_{m_1}[R^{(l)*}_{m_1\bar{m}'}(j)B^{jj'}_{lm_1,l''m''}a^{jj'}_{l''m''-}\Delta_{l\bar{\mu}}]+\eta\sum_{m_1}[R^{(l)*}_{m_1\bar{m}'}(j)a^{jj}_{lm_1-}\Delta^{--}_{l\bar{\mu}}]$$
$$+\eta\sum_{m_1}[R^{(l)*}_{m_1\bar{m}}(j)a^{jj}_{lm_1+}\Delta^{-+}_{l\bar{\mu}}]=0. \qquad (A1.6)$$

Here, as before (II, appendix 1, equation (A1.3)), the following notation is used:

$$\Delta_{l\bar{\mu}}=[j_l,g_{l\bar{\mu},1+}][j_l,g_{l\bar{\mu},2-}]-[j_l,g_{l\bar{\mu},1-}][j_l,g_{l\bar{\mu},2+}] \qquad (A1.7a)$$

$$\Delta^{++}_{l\bar{\mu}}=[n_l,g_{l\bar{\mu},1+}][j_l,g_{l\bar{\mu},2-}]-[j_l,g_{l\bar{\mu},1-}][n_l,g_{l\bar{\mu},2+}]$$
$$\Delta^{--}_{l\bar{\mu}}=[j_l,g_{l\bar{\mu},1+}][n_l,g_{l\bar{\mu},2-}]-[n_l,g_{l\bar{\mu},1-}][j_l,g_{l\bar{\mu},2+}] \qquad (A1.7b)$$

$$\Delta_{l\bar{\mu}}^{+-} = [n_l g_{l\bar{\mu},1-}][j_l g_{l\bar{\mu},2-}] - [j_l g_{l\bar{\mu},1-}][n_l g_{l\bar{\mu},2-}] = [n_l j_l][g_{l\bar{\mu},1-} g_{l\bar{\mu},2-}]$$
$$\Delta_{l\bar{\mu}}^{-+} = [j_l g_{l\bar{\mu},1+}][n_l g_{l\bar{\mu},2+}] - [n_l g_{l\bar{\mu},1+}][j_l g_{l\bar{\mu},2+}] = -[n_l j_l][g_{l\bar{\mu},1+} g_{l\bar{\mu},2+}]. \qquad \text{(A1.7}c\text{)}$$

Let us further multiply equation (A1.5) by $R^{(l)}_{\bar{m}\bar{m}}(j)$, (A1.6) by $R^{(l)}_{m\bar{m}'}(j)$ and sum over $\bar{m}$ and $\bar{m}'$, respectively. Because of the unitarity of the rotation matrices we have

$$\sum_{\substack{j' \\ l'm'}} \left[\left(B^{jj'}_{lm,l'm'} + \eta\delta_{jj'}\delta_{ll'} \sum_{\bar{m}} R^{(l)}_{m\bar{m}}(j) R^{(l)*}_{m'\bar{m}}(j) W^{++}_{l\bar{\mu}}(j) \right) a^{jj'}_{l'm'+} + \left(\eta\delta_{jj'}\delta_{ll'} \sum R^{(l)}_{m\bar{m}}(j) R^{(l)*}_{m'\bar{m}}(j) W^{+-}_{l\bar{\mu}}(j) \right) a^{jj'}_{l'm'-} \right] = 0 \qquad \text{(A1.8}a\text{)}$$

$$\sum_{\substack{j' \\ l'm'}} \left[\left(B^{jj'}_{lm,l'm'} + \eta\delta_{jj'}\delta_{ll'} \sum_{\bar{m}'} R^{(l)}_{m\bar{m}'}(j) R^{(l)*}_{m'\bar{m}'}(j) W^{--}_{l\bar{\mu}}(j) \right) a^{jj'}_{l'm'-} + \left(\eta\delta_{jj'}\delta_{ll'} \sum_{\bar{m}'} R^{(l)}_{m\bar{m}'}(j) R^{(l)*}_{m'\bar{m}}(j) W^{-+}_{l\bar{\mu}}(j) \right) a^{jj'}_{l'm'+} \right] = 0. \qquad \text{(A1.8}b\text{)}$$

Here all the terms were joined in one sum, division by $\Delta_{l\bar{\mu}}$ was performed and summation over $l''m''$ in the first term and over m_1 in the second and third terms was replaced by that over $l'm'$.

Finally, it is necessary to come back to the unknown $a^{jj}_{lm\pm} b^{j}_{lm\pm}$. For that let us rewrite (A1.8) in the block matrix form.

$$\begin{pmatrix} \mathbf{B}^{jj'} + \delta_{jj'}\mathbf{S}^{+}_{j} & \delta_{jj'}\mathbf{S}_{j} \\ \delta_{jj'}\mathbf{S}^{+}_{j} & \mathbf{B}^{jj'} + \delta_{jj'}\mathbf{S}^{-}_{j} \end{pmatrix} \begin{pmatrix} a^{jj'}_{+} \\ a^{jj'}_{-} \end{pmatrix} = 0 \qquad \text{(A1.9)}$$

where $\mathbf{B}^{jj'} = (\mathbf{B}^{jj'}_{lm,l'm'})$ are the structure constant matrices (26) and $a^{jj'}_{\pm} = (a^{jj'}_{lm\pm})$ are the vector columns. Pass from the vector $a^{jj}_{\pm}$ to $b^{(j)}_{\pm} = (b^{(j)}_{lm\pm})$ and multiply (A1.9) by the matrix of inverse transformation:

$$\begin{pmatrix} u_j I & v_j I \\ -v^*_j I & u^*_j I \end{pmatrix} \begin{pmatrix} \mathbf{B}^{jj'} + \delta_{jj'}\mathbf{S}^{+}_{j} & \delta_{jj'}\mathbf{S}_{j} \\ \delta_{jj'}\mathbf{S}^{+}_{j} & \mathbf{B}^{jj'} + \delta_{jj'}\mathbf{S}^{-}_{j} \end{pmatrix} \begin{pmatrix} u^*_j I & -v_j I \\ v^*_j I & u_j I \end{pmatrix} \begin{pmatrix} b^{j}_{+} \\ b^{j}_{-} \end{pmatrix} = 0. \qquad \text{(A1.10)}$$

This is the main system of equations.

Appendix 2

According to (24) the matrices $\mathbf{S}^{\mp}_{j}$ and $\mathbf{S}_j$ are expressed in terms of the rotation matrices $\mathbf{R}^{(l)}(j)$ and scattering phase cotangents matrices $\mathbf{W}^{ss'}$. Since, in the latter, only the diagonal in the l blocks $W^{ss}(l)$ are different from zero, the matrices $\mathbf{S}$ as seen from (24) retain the same structure, i.e. consist of non-zero blocks diagonal in l: $S^{\mp}_{j}(l)$, $S_j(l)$. (The fact that, in blocks $W^{ss'}(l)$, only the elements belonging to one of the diagonals are non-zero does not generally result in any peculiar feature of $S(l)$, i.e. all their elements are other than zero.) The diagonals in spin blocks $S^{\mp}_{j}(l)$ are obviously Hermitian, the blocks $S_j(l)$ having no additional properties. For example, at $l = 1$ the matrix $\mathbf{R}^{(1)}(j)$ according to (13) has the following form:

$$\begin{vmatrix} \exp(\mathrm{i}\alpha_j)\,\xi^2 & -2^{1/2}\xi\eta & \exp(-\mathrm{i}\alpha_j)\,\eta^2 \\ \exp(\mathrm{i}\alpha_j)\,2^{1/2}\xi\eta & \xi^2 - \eta^2 & -\exp(-\mathrm{i}\alpha_j)\,2^{1/2}\xi\eta \\ \exp(\mathrm{i}\alpha_j)\,\eta^2 & 2^{1/2}\xi\eta & \exp(-\mathrm{i}\alpha_j)\,\xi^2 \end{vmatrix} \qquad \text{(A2.1)}$$

where

$$\xi = \cos(\beta/2) \qquad \eta = \sin(\beta/2) \tag{A2.2}$$

and directly from (24) we have for the matrices $\mathbf{S}_j^+(1)$ and $\mathbf{S}_j$

$$\begin{aligned}
(\bar{1}\,\bar{1}) &= \xi^4 W_{\bar{1}\bar{1}}^{++} + 2\xi^2\eta^2 W_{10}^{++} + \eta^4 W_{11}^{++} \\
(\bar{1}\,0) &= 2^{1/2}\xi\eta[-\xi^2 W_{\bar{1}\bar{1}}^{++} + (\xi^2 - \eta^2)W_{10}^{++} + \eta^2 W_{11}^{++}]\exp(\mathrm{i}\alpha_j) \\
(\bar{1}\,1) &= \xi^2\eta^2(W_{\bar{1}\bar{1}}^{++} - 2W_{10}^{++} + W_{11}^{++})\exp(2\mathrm{i}\alpha_j) \\
(0\,0) &= 2\xi^2\eta^2 W_{\bar{1}\bar{1}}^{++} + (\xi^2 - \eta^2)^2 W_{10}^{++} + 2\xi^2\eta^2 W_{11}^{++} \\
(0\,1) &= -2^{1/2}\xi\eta(\eta^2 W_{\bar{1}\bar{1}}^{++} + (\xi^2 - \eta^2)W_{10}^{++} - \xi^2 W_{11}^{++})\exp(\mathrm{i}\alpha_j) \\
(1\,1) &= \eta^4 W_{\bar{1}\bar{1}}^{++} + 2\xi^2\eta^2 W_{10}^{++} + \xi^4 W_{11}^{++}
\end{aligned} \tag{A2.3}$$

and

$$\begin{aligned}
(\bar{1}\,\bar{1}) &= 2^{1/2}\xi\eta(\xi^2 W_{\bar{1}\bar{1}}^{+-} + \eta^2 W_{10}^{+-}) \\
(\bar{1}\,0) &= \xi^2[(\xi^2 - \eta^2)W_{\bar{1}\bar{1}}^{+-} + 2\eta^2 W_{10}^{+-}]\exp(\mathrm{i}\alpha_j) \\
(\bar{1}\,1) &= -2^{1/2}\xi^3\eta(W_{\bar{1}\bar{1}}^{+-} - W_{10}^{+-})\exp(2\mathrm{i}\alpha_j) \\
(0\,\bar{1}) &= \eta^2[-2\xi^2 W_{\bar{1}\bar{1}}^{+-} + (\xi^2 - \eta^2)W_{10}^{+-}]\exp(-\mathrm{i}\alpha_j) \\
(0\,0) &= -2^{1/2}\xi\eta(\xi^2 - \eta^2)(W_{\bar{1}\bar{1}}^{+-} - W_{10}^{+-}) \\
(0\,1) &= \xi^2[2\eta^2 W_{\bar{1}\bar{1}}^{+-} + (\xi^2 - \eta^2)W_{10}^{+-}]\exp(\mathrm{i}\alpha_j) \\
(1\,\bar{1}) &= 2^{1/2}\xi\eta^3(W_{\bar{1}\bar{1}}^{+-} - W_{10}^{+-})\exp(-2\mathrm{i}\alpha_j) \\
(1\,0) &= \eta^2[(\xi^2 - \eta^2)W_{\bar{1}\bar{1}}^{+-} - 2\xi^2 W_{10}^{+-}]\exp(-\mathrm{i}\alpha_j) \\
(1\,1) &= -2^{1/2}\xi\eta(\eta^2 W_{\bar{1}\bar{1}}^{+-} + \xi^2 W_{10}^{+-}).
\end{aligned} \tag{A2.4}$$

Appendix 3

Let $\boldsymbol{b}_1, \boldsymbol{b}_2, \boldsymbol{b}_3$ be the main vectors of the reciprocal lattice. Then the main vectors of the lattice reciprocal to the magnetic lattice will be $\boldsymbol{b}_1, \boldsymbol{b}_2, \boldsymbol{b}_3/N$. Denote by $\boldsymbol{\kappa}_p$ N vectors of the form

$$\boldsymbol{\kappa}_p = (p/N)\boldsymbol{b}_3 \qquad p = 0, 1, 2, \ldots, N-1. \tag{A3.1}$$

Obviously, the vectors $\boldsymbol{\kappa}_p$ coincide with N vectors $\boldsymbol{Q}_p$ located inside the cell constructed on the vectors $\boldsymbol{b}_1, \boldsymbol{b}_2, \boldsymbol{b}_3$. All the other vectors $\boldsymbol{Q}_n$ can be obtained from them by adding the vectors $\boldsymbol{K}_n$. Therefore in sum (9) the summation over $\boldsymbol{Q}_t$ can be replaced by that over $\boldsymbol{K}_n$ and $\boldsymbol{\kappa}_p$. Then in analogy with II, appendix 2, equation (A2.1), we have

$$\begin{aligned}
G^{jj'}(\boldsymbol{q}, E'; \boldsymbol{r}_j, \boldsymbol{r}'_{j'}) &= \exp[\mathrm{i}\boldsymbol{q}\cdot(\boldsymbol{h}_j - \boldsymbol{h}_{j'})]\frac{1}{N}\sum_{p=0}^{N-1}\exp[\boldsymbol{\kappa}_{p}\cdot(\boldsymbol{h}_j - \boldsymbol{h}_{j'})] \\
&\times\left(-\frac{1}{\Omega}\sum_n \frac{\exp[\mathrm{i}(\boldsymbol{k}_p + \boldsymbol{K}_n)\cdot(\boldsymbol{r}_j - \boldsymbol{r}_{j'})]}{|\boldsymbol{k}_p + \boldsymbol{K}_n|^2 - E'}\right)
\end{aligned} \tag{A3.2}$$

where $\boldsymbol{k}_p = \boldsymbol{q} + \boldsymbol{\kappa}_p$. The expression in large parentheses is the Green function of the original crystal lattice, i.e.

$$G^{jj'}(\boldsymbol{q}, E'; \boldsymbol{r}_j, \boldsymbol{r}'_{j'}) = \exp[\mathrm{i}\boldsymbol{q} \cdot (\boldsymbol{h}_j - \boldsymbol{j}_{j'})] \times \frac{1}{N}\sum_{p=0}^{N-1} \exp[\boldsymbol{\kappa}_p \cdot (\boldsymbol{h}_j - \boldsymbol{h}_{j'})]\, G(\boldsymbol{k}_p, E', \boldsymbol{r}_j, \boldsymbol{r}_{j'}). \tag{A3.3}$$

Writing the lattice Green functions on the left- and right-hand sides of (A3.3) as the expansions in spherical harmonics and equating the corresponding terms of the expansions, one easily gets

$$B^{jj'}_{lm,l'm'}(\boldsymbol{q}, E')\exp[\mathrm{i}\boldsymbol{q}\cdot(\boldsymbol{h}_j - \boldsymbol{h}_{j'})]\frac{1}{N}\sum_{p=0}^{N-1} \exp[\boldsymbol{\kappa}_p \cdot(\boldsymbol{h}_j - \boldsymbol{h}_{j'})]A_{lm,l'm'}(\boldsymbol{k}_p, E') \tag{A3.4}$$

where $B^{jj'}_{lm,l'm'}$ and $A_{lm,l'm'}$ are the structure constants of the magnetic and original lattices, respectively. Note also that by definition

$$\boldsymbol{\kappa}_p \cdot \boldsymbol{h}_j = (pj/N)\boldsymbol{b}_3 \cdot \boldsymbol{a}_3 = 2\pi(pj/N) \tag{A3.5}$$

and hence $\exp[\mathrm{i}\boldsymbol{\kappa}_p \cdot (\boldsymbol{h}_j - \boldsymbol{h}_{j'})]$ is one of the values of the Nth root of unity.

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