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Ferrimagnets and antiferromagnets

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## A simplified method of *ab initio* calculation of electron states in relativistic magnetics: II. Ferrimagnets and antiferromagnets

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**Abstract.** A technique of electron states calculation in a collinear two-sublattice ferrimagnet and antiferromagnet based on a derivation of the Dirac equation by the relativistic Korringa-Kohn-Rostoker method, is presented. The scheme suggested can be easily generalized to systems with several atoms in the crystalline and magnetic cell.

### 1. Introduction

In our previous paper [1] a simplified technique of calculation for collinear ferromagnets based on the relativistic Green function (RGF) method was presented. The approach suggested can be easily applied to the collinear two-sublattice ferrimagnet and antiferromagnet.

Consider a crystal lattice at the sites of which atoms with different magnitudes and spin moments which are opposite in direction are located, so that the structure has two atoms (with different spins) in the unit cell of the new lattice. Denote the vectors of the original lattice by  $R_n$ , those of the reciprocal lattice by  $K_n$  and the reduced wavevector by  $k$ . Let  $T_p$ ,  $Q_p$  and  $q$  be the corresponding quantities for the new extended lattice,  $h_1$  and  $h_2$  being the vectors of its base. (This lattice will be called the magnetic lattice.) Denoting the volumes of the unit cell and Brillouin zone of the crystal lattice by  $\Omega$  and  $\Omega_B$  and the corresponding quantities for the magnetic lattice by  $\Omega_M$  and  $\Omega_{BM}$ , we obviously have in this case  $\Omega_M = 2\Omega$  and  $\Omega_B = 2\Omega_{BM}$ .

Choose further the origin of coordinates so that  $h_1 = 0$ . Then  $h_2 = h$  is one of the vectors  $R_n$  and, consequently, the joining of all the vectors  $T_p$  and  $h + T_p$  coincides with the set of vectors  $R_n$ . Similarly, in reciprocal space the lattice defined by vectors  $Q_p$  can be divided into two sublattices whose sites are specified by vectors  $K_n$  and  $\kappa + K_n$ .

The lattice of CsCl type can be an example of the above structure, if atoms with different spins are located at the points of its unit cell  $h_1 = 0$  and  $h_2 = (1, 1, 1)a/2 = h$  ( $a$  is the lattice constant). Then  $R_n$  are the vectors of the BCC lattice,  $K_n$  forms the reciprocal FCC lattice and  $k$  varies within the first Brillouin zone of the BCC lattice. In turn,  $T_p$  and  $Q_p$  form simple cubic lattices,  $q$  varies within its own Brillouin zone (half as large) and  $\kappa$  can be set equal to  $2\pi(0, 1, 0)/a$ , for example. Note, by the way, that antiferromagnetic chromium has such a structure when its small non-collinearity is neglected.

## 2. General formalism

The technique for calculating the electronic structure of the above simplest ferrimagnets and antiferromagnets within the RGF formalism can be developed quite by analogy with [1]. The main points of our approach are identical with the statements presented in [2-4]. The distinctions between these techniques have been discussed in detail in [1].

Again, instead of the Dirac equation we shall consider the equivalent equation for the large component  $\Psi$  of the Dirac four-component spinor (see equation (10) in [1]):

$$\hat{\Delta}\Psi + W[E - (V + \Delta V \sigma_z)]\Psi - (W'/W)(\sigma \times \hat{r}) \cdot (\sigma \times \nabla)\Psi = 0. \quad (1)$$

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

$$W = 1 + (E - V)/c^2 \quad (2)$$

and  $c$  is the velocity of light.

The potential  $V + \Delta V \sigma_z$  involved in (1) is to be described in more detail. Since the magnetic lattice under consideration is a lattice with a base, then inside the magnetic cell there are two muffin-tin (MT) spheres centred at the points  $\mathbf{h}_j$ . Within these spheres the potentials are spherically symmetric. Let the Oz axis be oriented along the spin direction so that the positive semi-axis coincides with the positive spin orientation on the first atom of the base. Then for the first site the quantities  $V$  and  $\Delta V$  have the same meaning as before, i.e.

$$V_1 = \frac{1}{2}(V_{1+} + V_{1-}) \quad \Delta V = \frac{1}{2}(V_{1+} - V_{1-}) \quad (3)$$

where  $V_{1+}$  and  $V_{1-}$  are the potentials acting on the electrons with different spin orientations. For the other site we also introduce an average potential and an additional term caused by the spin polarization:  $V_2$  and  $\Delta V_2$ . We put further formally

$$V_{2+} = V_2 + \Delta V_2 \quad V_{2-} = V_2 - \Delta V_2 \quad (4)$$

although it is clear that the meaning of these quantities will differ for ferrimagnets and antiferromagnets.

In each of the MT spheres the two-component spinor is represented as a product of the radial functions  $g_{\mu,\pm}^{(j)}$  by the spherical harmonics

$$\Psi(\mathbf{r}_j) = \begin{pmatrix} g_{\mu,+}^{(j)} Y_{lm} \\ g_{\mu,-}^{(j)} Y_{l'm'} \end{pmatrix} \quad (5)$$

where  $\mathbf{r}_j$  is the radius vector measured from the  $j$ th point of the magnetic cell,  $l$  is the orbital quantum number and  $\mu$  is the projection of the total angular momentum onto the Oz axis. Substituting (4) into (1) yields, by analogy with [1], the two following sets of radial equations (see equation (13) in [1]):

$$g_{\mu,+}^{(j)'} + (2/r)g_{\mu,+}^{(j)} + [W_j(E - V_{j+}) - l(l+1)/r^2]g_{\mu,+}^{(j)} \\ = (W_j'/W_j)[\{g_{\mu,+}^{(j)'} - [(\mu - \frac{1}{2})/r]g_{\mu,+}^{(j)}\} + S_\mu \sqrt{(l + \frac{1}{2})^2 - \mu^2} (1/r)g_{\mu,-}^{(j)}] \quad (6a)$$

$$g_{\mu,-}^{(j)'} + (2/r)g_{\mu,-}^{(j)} + [W_j(E - V_{j-}) - l(l+1)/r^2]g_{\mu,-}^{(j)} \\ = (W_j'/W_j)[\{g_{\mu,-}^{(j)'} + [(\mu + \frac{1}{2})/r]g_{\mu,-}^{(j)}\} + S_\mu \sqrt{(l + \frac{1}{2})^2 - \mu^2} (1/r)g_{\mu,+}^{(j)}] \quad (6b)$$

( $S_\mu = \mu/|\mu|$ ; the index  $j$  labelling  $r$  is omitted, although of course  $r = |\mathbf{r}_j|$ .) Each set of

equations has two linearly independent solutions regular at zero; therefore, the general solution of (1) inside the MT spheres can be given in the form

$$\Psi_I^{(j)}(\mathbf{r}) = \sum_{\mu, \nu} i^l C_{\mu, \nu}^{(j)} \begin{pmatrix} g_{\mu, \nu+}^{(j)} Y_{lm} \\ g_{\mu, \nu-}^{(j)} Y_{lm+1} \end{pmatrix} \quad (7)$$

( $\nu = 1, 2; j = 1, 2; \mu = m + \frac{1}{2}$ ) with arbitrary coefficients  $C_{\mu, \nu}^{(j)}$ .

It is convenient to write the empty-lattice Green function for a structure with a base as follows [5]:

$$G^{jj'}(\mathbf{q}, E'; \mathbf{r}_j, \mathbf{r}_{j'}) = -\frac{1}{\Omega_M} \sum_p \frac{\exp[i(\mathbf{q} + \mathbf{Q}_p) \cdot (\mathbf{r}_j + \mathbf{h}_j - \mathbf{r}_{j'} - \mathbf{h}_{j'})]}{|\mathbf{q} + \mathbf{Q}_p|^2 - E'} \quad (8)$$

where  $E' = E(1 + E/c^2)$ , and  $\mathbf{r}_j$  and  $\mathbf{r}_{j'}$  are the radius vectors measured from the corresponding base sites. Making use of this Green function, one can represent the general solution of (1) outside the MT spheres (for zero potential) in the following way:

$$\Psi_{II}(\mathbf{r}_j) = \sum_{j'} \int_{\Omega_{MT}^{(j')}} d\mathbf{r}_{j'} G^{jj'}(\mathbf{q}, E'; \mathbf{r}_j, \mathbf{r}_{j'}) \begin{pmatrix} \Phi_+^{(j')}(\mathbf{r}_{j'}) \\ \Phi_-^{(j')}(\mathbf{r}_{j'}) \end{pmatrix} \quad (9)$$

where  $\Phi_{\pm}^{(j)}$  are arbitrary functions,  $\Omega_{MT}^{(j)}$  is the volume of the  $j$ th MT sphere, and  $\mathbf{r}_j$  is a vector measured from its (this sphere) centre and terminating beyond the MT spheres.

With such an approach the dispersive equation is obtained from the standard condition of smooth joining of the solutions  $\Psi_I^{(j)}$  and  $\Psi_{II}$  through the MT spheres:

$$\begin{aligned} \Psi_I^{(j)}(\mathbf{r}_j) &= \Psi_{II}(\mathbf{r}_j) \\ (\partial/\partial r)[\Psi_I^{(j)}(\mathbf{r}_j)] &= (\partial/\partial r)[\Psi_{II}(\mathbf{r}_j)] \end{aligned} \quad (10)$$

with  $|\mathbf{r}_j| = r_{Sj}$ , where  $r_{Sj}$  is the radius of the  $j$ th sphere. It is natural for our problem to consider the radii of the MT spheres as being equal; so the index  $j$  labelling  $r_S$  and  $\Omega_{MT}$  will be omitted hereafter.

Depending on the origin of  $r$  and  $r'$ , one can construct four expansions of the Green function (8) in terms of spherical harmonics [6]:

$$\begin{aligned} G^{jj'}(\mathbf{q}, E'; \mathbf{r}_j, \mathbf{r}_{j'}) &= \sum_{\substack{lm, \\ l'm'}} i^{l-l'} [B_{lm, l'm'}^{jj'}(\mathbf{q}, E') j_l(\eta r_j) j_{l'}(\eta r_{j'}) \\ &+ \eta \delta_{jj'} \delta_{lm, l'm'} \eta_l(\eta r_j) j_{l'}(\eta r_{j'})] Y_{lm}(\hat{r}_j) Y_{l'm'}^*(\hat{r}_{j'}) \end{aligned} \quad (11)$$

where  $\eta = \sqrt{E'}$ ,  $j_l$  and  $n_l$  are the spherical Bessel and Neumann functions, respectively, and  $B_{lm, l'm'}^{jj'}$  are the structure constants of the lattice with base. Substituting expansion (11) into (9) and integrating over  $\mathbf{r}_{j'}$ , yields the following representation for the solution (1) outside the MT spheres:

$$\begin{aligned} \Psi_{II}(\mathbf{r}_j) &= \sum_{j'} \sum_{\substack{lm, \\ l'm'}} i^l [B_{lm, l'm'}^{jj'}(\mathbf{q}, E') j_l(\eta r_j) \\ &+ \eta \delta_{jj'} \delta_{lm, l'm'} n_l(\eta r_j)] Y_{lm}(\hat{r}_j) \begin{cases} b_{l'm'+}^{(j)} \\ b_{l'm'-}^{(j)} \end{cases} \end{aligned} \quad (12)$$

where  $b_{lm\pm}^{(j)}$ , because of the arbitrariness of  $\Phi_{\pm}^{(j)}$ , are arbitrary constants themselves.

Further it is necessary to substitute expansions (7) and (12) into relations (10), to use the orthogonality of the spherical harmonics  $Y_{lm}(\hat{r}_j)$ , and to obtain a system of algebraic

equations in the unknown  $C_{\mu,\nu}^{(j)}$  and  $b_{lm\pm}^{(j)}$ , the condition of the solvability of which results in the main dispersive equation. The necessary calculations are presented in appendix 1. It also seems useful to compare formulae (7) and (12) with equations (15) and (19) of [1] to ensure close analogy of the general formalism.

### 3. The dispersive equation and its analysis

#### 3.1. Two forms of writing the dispersive equation

The resulting dispersive equation (see appendix 1) has a structure peculiar to lattices with a base

$$\left| \begin{array}{cc|cc} B^{11} + W^{++}(1) & W^{+-}(1) & B^{12} & 0 \\ W^{-+}(1) & B^{11} + W^{--}(1) & 0 & B^{12} \\ \hline B^{12} & 0 & B^{22} + W^{++}(2) & W^{+-}(2) \\ 0 & B^{12} & W^{-+}(2) & B^{22} + W^{--}(2) \end{array} \right| = 0. \quad (13)$$

Here  $B^{ij} = B_{lm,l'm'}^{ij}(\mathbf{q}, E')$  are the structure constant matrices.  $W^{SS'}(j)$  are the scattering-phase cotangent matrices. In the notation of appendix 1,

$$W^{\pm\pm}(j) = \eta[\Delta_{\mu}^{\pm\pm}(j)/\Delta_{l\mu}(j)]\delta_{lm,l'm'} \quad (14a)$$

$$W^{\pm\mp}(j) = \eta[\Delta_{\mu}^{\pm\mp}(j)/\Delta_{l\mu}(j)]\delta_{lm\pm 1,l'm'} \quad (14b)$$

( $\mu = m \pm \frac{1}{2}$ ). The picture of the spectrum formation can be lucidly represented in the following way. Under the effect of the MT potential, spin-polarized states form on each site; the states with opposite spins are not 'pure' but mix owing to the spin-orbit interaction at their site; the interconnection of the sites is purely structural.

The presented form of dispersive equation (13) is obviously suitable for describing any relativistic problem with two atoms in the unit cell. In our case of a two-sublattice magnet the magnetic structure has been constructed on the basis of an original crystal lattice consisting of identical atoms. This allows us to simplify the consideration greatly.

It is shown in appendix 2 that in this case

$$B_{lm,l'm'}^{11}(\mathbf{q}, E') = B_{lm,l'm'}^{22}(\mathbf{q}, E') = \frac{1}{2}[A_{lm,l'm'}(\mathbf{k}_1, E') + A_{lm,l'm'}(\mathbf{k}_2, E')]$$

$$B_{lm,l'm'}^{12}(\mathbf{q}, E') = B_{lm,l'm'}^{21}(\mathbf{q}, E') = \frac{1}{2}[A_{lm,l'm'}(\mathbf{k}_1, E') - A_{lm,l'm'}(\mathbf{k}_2, E')] \exp(\mp i \mathbf{q} \cdot \mathbf{h}) \quad (15)$$

where  $A_{lm,l'm'}(\mathbf{k}, E')$  are the structure constants of the original crystal lattice;  $\mathbf{k}_1 = \mathbf{q}$ ,  $\mathbf{k}_2 = \mathbf{q} + \boldsymbol{\kappa}$ . Substitute (15) into matrix (13) and transform the resulting expression with the help of the unitary transformation of the form

$$\frac{1}{\sqrt{2}} \left[ \begin{array}{cc|cc} \mathbf{1} & 0 & \mathbf{1} & 0 \\ 0 & \mathbf{1} & 0 & \mathbf{1} \\ \hline -\mathbf{1} & 0 & \mathbf{1} & 0 \\ 0 & -\mathbf{1} & 0 & \mathbf{1} \end{array} \right] \quad (16)$$

where  $\hat{\mathbf{1}}$  is the unit matrix of the same size as the blocks in (13). As a result, the dispersive equation (13) becomes

$$\begin{vmatrix} A_1 + W^{++} & W^{+-} \\ W^{-+} & A_1 + W^{--} \\ \hline \Delta W^{++} & \Delta W^{+-} \\ \Delta W^{-+} & \Delta W^{--} \end{vmatrix} \begin{vmatrix} \Delta W^{++} & \Delta W^{+-} \\ \Delta W^{-+} & \Delta W^{--} \\ \hline A_2 + W^{++} & W^{+-} \\ W^{-+} & A_2 + W^{--} \end{vmatrix} = 0. \tag{17}$$

Here  $A_j = A_{lm,l'm'}(k_j, E')$  are the structure constant matrices at the points  $k_1$  and  $k_2$  of the original-lattice Brillouin zone and

$$W^{SS'} = \frac{1}{2}[W^{SS'}(1) + W^{SS'}(2)] \tag{18a}$$

$$\Delta W^{SS'} = \frac{1}{2}[W^{SS'}(2) - W^{SS'}(1)]. \tag{18b}$$

With such a form for the dispersive equation the process of spectrum formation can be described in another way. The spin-polarized states are formed at two conjugate points of the  $k$ -space by a site-averaged potential. These states are mixed at each point  $k_j$  owing to the average spin-orbit interaction, while intermixing of the states at different points  $k_j$  occurs because the potentials are different.

Equations of the form (13) or (17) do actually describe the simplest ferrimagnet when the MT potentials at sites of the magnetic cell base are different, i.e. the magnetic moments of the base atoms differ in magnitude and are anticollinear. These equations cannot be simplified without further approximations. The more interesting case of an antiferromagnet gives more concrete expression to our formalism.

### 3.2. Antiferromagnets

The feature peculiar to a two-sublattice antiferromagnet is that the mean values of the potentials at the magnetic-cell base sites are equal and the 'polarizing' additional terms  $\Delta V \sigma_z$  are opposite in sign. The latter can be taken into account by merely changing the sign before  $\Delta V$ . So

$$V_{j\pm} = \begin{cases} V \pm \Delta V & j = 1 \\ V \mp \Delta V & j = 2. \end{cases} \tag{19}$$

Then, after writing explicit expressions for sets (5) at the first and the second sites and comparing them, it is clear that we can always put

$$g_{\mu+}^{(2)} = g_{\bar{\mu}-}^{(1)} \quad g_{\mu-}^{(2)} = -g_{\bar{\mu}+}^{(1)}. \tag{20}$$

These relations actually resulting from the symmetry of Hamiltonian (1) are here accepted as a formal mathematical fact.

By direct substitution of (20) into equation (A1.3) of appendix 1 one can see that

$$\begin{aligned} \Delta_{l\mu}(2) &= \Delta_{l\bar{\mu}}(1) \\ \Delta_{l\mu}^{\pm\pm}(2) &= \Delta_{l\bar{\mu}}^{\mp\mp}(1) \\ \Delta_{l\mu}^{\pm\mp}(2) &= -\Delta_{l\bar{\mu}}^{\mp\pm}(1) \end{aligned} \tag{21}$$

and, hence,

$$\begin{aligned} W_{lm,l'm'}^{\pm\pm}(2) &= W_{l\bar{m},l'\bar{m}'}^{\mp\mp}(1) \\ W_{lm,l'm'}^{\pm\mp}(2) &= -W_{l\bar{m},l'\bar{m}'}^{\mp\pm}(1). \end{aligned} \tag{22}$$

So the spectrum of the simplest antiferromagnet can be calculated by finding the

scattering-phase cotangents and constructing the dispersive equation (17) with the use of relations (22).

### 3.3. Limiting cases

One can most easily proceed to ferromagnetic order. In a ferromagnet the base sites are obviously equivalent; therefore  $W^{SS'}(1) = W^{SS'}(2)$ . Then, in the dispersive equation (17), all  $\Delta W^{SS'}$  are equal to zero and it is divided into two equations of lower order:

$$\begin{vmatrix} A_j + W^{++} & W^{+-} \\ W^{-+} & A_j + W^{--} \end{vmatrix} = 0. \quad (23)$$

With the assumption that the reduced wavevector  $k$  does vary within the Brillouin zone of the original lattice the index  $j$  can be omitted and the resulting dispersive equation is quite identical with equation (22) of [1].

Proceeding to the non-relativistic version of the theory according to equation (39) of [1] consists in neglecting the blocks which are non-diagonal in spin in equation (13) or (17). This leads to partition with respect to the spin of each of the dispersive equations into two:

$$\begin{vmatrix} B^{11} + W^{SS}(1) & B^{12} \\ B^{12} & B^{11} + W^{SS}(2) \end{vmatrix} = 0 \quad (24a)$$

or

$$\begin{vmatrix} A_1 + W^{SS} & \Delta W^{SS} \\ \Delta W^{SS} & A_2 + W^{SS} \end{vmatrix} = 0. \quad (24b)$$

That is, for each spin orientation a separate branch of the spectrum is forming. Hybridization of states on various sites (at different points  $k_j$ ) occurs owing to the structure factor  $B^{12}$  (the potential difference  $\Delta W^{SS}$ ). The number of spectrum branches will remain the same with different potentials at the base sites.

Since in the non-relativistic limit the  $m(\mu)$ -dependence of the diagonal matrix elements  $W_{lm, l'm'}^{SS}$  disappears (see equation (39) of [1]) we have for an antiferromagnet

$$W^{SS}(2) = W^{\bar{S}\bar{S}}(1) \quad (25)$$

and, therefore,

$$W^{++} = W^{--} = \frac{1}{2}[W^{++}(1) + W^{--}(1)] = W \quad (26a)$$

$$\Delta W^{--} = -\Delta W^{++} = \frac{1}{2}[W^{++}(1) - W^{--}(1)] = \Delta W. \quad (26b)$$

Then the form of the non-relativistic dispersive equations for antiferromagnets becomes much simpler:

$$\begin{vmatrix} B^{11} + W^{SS} & B^{12} \\ B^{12} & B^{11} + W^{\bar{S}\bar{S}} \end{vmatrix} = 0 \quad (27a)$$

$$\begin{vmatrix} A_1 + W & \Delta W \\ \Delta W & A_2 + W \end{vmatrix} = 0. \quad (27b)$$

It is seen from the formulae presented (especially (27b)) that the four spectrum branches in an antiferromagnet are joined in pairs.

The non-relativistic dispersive equations discussed in this section are worth comparing with those obtained in [7] where the non-relativistic variant was used from the very beginning.

4. Conclusions

To conclude we would like to point out some possibilities of the above approach in discussing the electron structure of systems with spin order.

(i) Uniformity of the scheme for calculating the electron structure of crystals with different magnetic order (paramagnets, ferromagnets, antiferromagnets and ferrimagnets) enables one to treat within the common theoretical model the change in electronic structure with change in the magnetic state of a material. It seems possible to estimate which of the magnetic states is energetically most advantageous.

(ii) The scheme suggested can be easily generalized to systems with several atoms in the crystalline and/or magnetic cell.

Appendix 1

The system of equations in the unknown coefficients  $C_{l\mu,\nu}^{(j)}$   $b_{lm,\pm}^{(j)}$  is as follows (the indices  $l, \mu$  on the left-hand side are omitted):

$$\begin{aligned}
 C_1^{(j)} g_{1+}^{(j)} + C_2^{(j)} g_{2+}^{(j)} &= \sum_{j',l'm'} (B_{lm,l'm'}^{jj'} j_l + \eta \delta_{jj'} \delta_{lm,l'm'} n_l) b_{l'm'}^{(j')} \\
 C_1^{(j)} g_{1+}^{(j')} + C_2^{(j)} g_{2+}^{(j')} &= \sum_{j',l'm'} (B_{lm,l'm'}^{jj'} j_l' + \eta \delta_{jj'} \delta_{lm,l'm'} n_l') b_{l'm'}^{(j')}
 \end{aligned}
 \tag{A1.1a}$$

and

$$\begin{aligned}
 C_1^{(j)} g_{1-}^{(j)} + C_2^{(j)} g_{2-}^{(j)} &= \sum_{j',l'm'} (B_{lm,l'm'}^{jj'} j_l + \eta \delta_{jj'} \delta_{lm,l'm'} n_l) \\
 C_1^{(j)} g_{1-}^{(j')} + C_2^{(j)} g_{2-}^{(j')} &= \sum_{j',l'm'} (B_{lm,l'm'}^{jj'} j_l' + \eta \delta_{jj'} \delta_{lm,l'm'} n_l') b_{l'm'}^{(j')}
 \end{aligned}
 \tag{A1.1b}$$

( $m = \mu - \frac{1}{2}, m' = \mu + \frac{1}{2}$ ) and only the presence of the  $j$ th site index distinguishes it from that previously obtained (equation (A1.1) of appendix 1 in [1]). Consequently, having repeated the same calculations as before, one can get

$$\begin{aligned}
 \sum_{j',l'm'} \{ [B_{lm,l'm'}^{jj'} \Delta_{l\mu}^{(j)} + \eta \delta_{jj'} \delta_{lm,l'm'} \Delta_{l\mu}^{j+}(j)] b_{l'm'}^{(j')} \\
 + \eta \delta_{jj'} \delta_{lm+1,l'm'} \Delta_{l\mu}^{j-}(j) b_{l'm'}^{(j')} \} = 0
 \end{aligned}
 \tag{A1.2a}$$



$$\sum \{ [B_{lm, l'm'}^{jj'} \Delta_{l\mu}(j) + \eta \delta_{jj'} \delta_{lm, l'm'} \Delta_{l\mu}^{\bar{-}}(j)] b_{l'm'}^{(j')} + \eta \delta_{jj'} \delta_{lm-1, l'm'} \Delta_{l\mu}^{\bar{+}}(j) b_{l'm'+}^{(j')} \} = 0 \quad (\text{A1.2b})$$

where

$$\Delta_{l\mu}(j) = [j_l g_{1+}^{(j)}][j_l g_{2-}^{(j)}] - [j_l g_{1-}^{(j)}][j_l g_{2+}^{(j)}] \quad (\text{A1.3a})$$

$$\Delta_{l\mu}^{\bar{+}}(j) = [n_l g_{1+}^{(j)}][j_l g_{2-}^{(j)}] - [j_l g_{1-}^{(j)}][n_l g_{2+}^{(j)}] \quad (\text{A1.3b})$$

$$\Delta_{l\mu}^{\bar{-}}(j) = [j_l g_{1+}^{(j)}][n_l g_{2-}^{(j)}] - [n_l g_{1-}^{(j)}][j_l g_{2+}^{(j)}]$$

and

$$\Delta_{l\mu}^{\bar{-}}(j) = [n_l g_{1-}^{(j)}][j_l g_{2-}^{(j)}] - [j_l g_{1-}^{(j)}][n_l g_{2-}^{(j)}] = [n_l j_l][g_{1-}^{(j)} g_{2-}^{(j)}] \quad (\text{A1.3c})$$

$$\Delta_{l\mu}^{\bar{+}}(j) = [j_l g_{1+}^{(j)}][n_l g_{2+}^{(j)}] - [n_l g_{1+}^{(j)}][j_l g_{2+}^{(j)}] = -[n_l j_l][g_{1+}^{(j)} g_{2+}^{(j)}]$$

In these equations,  $[f_1 f_2] = f_1 f_2^* - f_1^* f_2$ .

Naturally, the Hermiticity in the dispersive equation remains, i.e. the matrix  $\Delta^{\bar{-}}(j)$  is equal to the transposed and complex conjugate to  $\Delta^{\bar{+}}(j)$  matrix.

## Appendix 2

Let us separate the sum over  $Q_p$  in (8) into two parts over  $K_n$  and to take outside the factors not depending on the summation index:

$$\begin{aligned} G^{jj'}(q, E'; r_j, r_{j'}) &= \frac{1}{2} \left( -\frac{1}{\Omega} \sum_n \frac{\exp[i(q + K_n) \cdot (r_j + h_j - r_{j'} - h_{j'})]}{(q + K_n)^2 - E'} \right. \\ &\quad \left. - \frac{1}{\Omega} \sum_n \frac{\exp[i(q + \kappa + K_n) \cdot (r_j + h_j - r_{j'} - h_{j'})]}{|\mathbf{q} + \boldsymbol{\kappa} + \mathbf{K}_n|^2 - E'} \right) \\ &= \frac{1}{2} \left[ \exp[iq \cdot (h_j - h_{j'})] \left( -\frac{1}{\Omega} \sum_n \frac{\exp[i(q + K_n) \cdot (r_j - r_{j'})]}{(q + K_n)^2 - E'} \right) \right. \\ &\quad \left. + \exp[i(q + \kappa) \cdot (h_j - h_{j'})] \right. \\ &\quad \left. \times \left( -\frac{1}{\Omega} \sum_n \frac{\exp[i(q + \kappa + K_n) \cdot (r_j - r_{j'})]}{(q + \kappa + K_n)^2 - E'} \right) \right]. \quad (\text{A2.1}) \end{aligned}$$

It is easy to see that the expressions in large parentheses in the last two lines are none other than the Green functions of the initial crystalline lattice at the points  $q$  and  $q + \kappa$ . Taking into account that  $\kappa \cdot h = \pi$ , we have

$$\begin{aligned} G^{jj'}(q, E'; r_j, r_{j'}) &= \frac{1}{2} \exp[iq \cdot (h_j - h_{j'})] [G(q, E'; r_j, r_{j'}) \\ &\quad \pm G(q + \kappa, E'; r_j, r_{j'})] \quad (\text{A2.2}) \end{aligned}$$

and hence

$$\begin{aligned} B_{lm, l'm'}^{jj'}(q, E') &= \frac{1}{2} \exp[iq \cdot (h_j - h_{j'})] [A_{lm, l'm'}(q, E') \\ &\quad \pm A_{lm, l'm'}(q + \kappa, E')]. \quad (\text{A2.3}) \end{aligned}$$

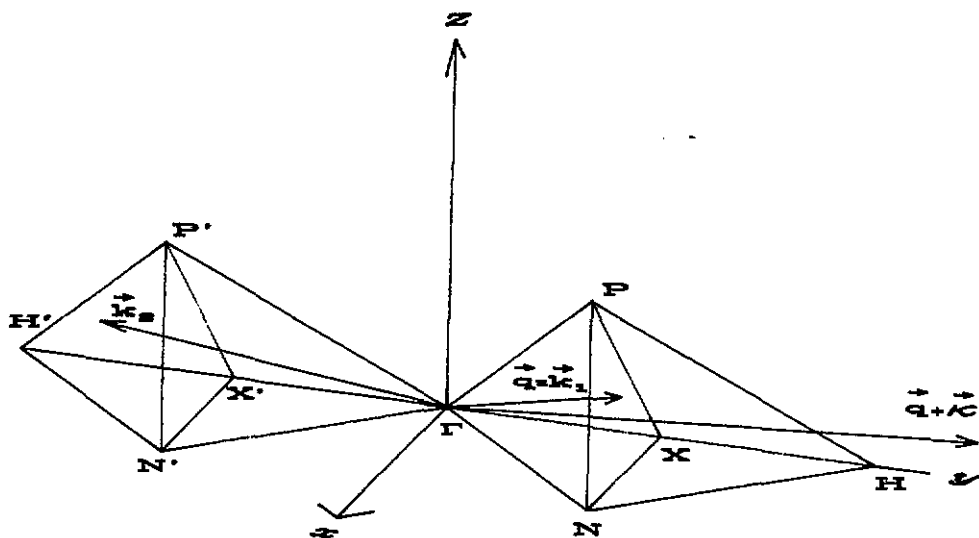


Figure 1. One forty-eighth of the Brillouin zone of a BCC lattice  $\Gamma\text{NHP}$  and its regular reflection  $\Gamma\text{N}'\text{H}'\text{P}'$ .

Note that the vector  $q + \kappa$  can go beyond the Brillouin zone of the original lattice; so in the general case we get  $k_2 = q + \kappa + K$ , where  $K$  is one of the reciprocal lattice vectors. Since the addition of the reciprocal lattice vector  $K$  to  $q + \kappa$  results only in renumbering the terms of the second sum (A2.1), we shall not revert to this any longer.

For illustration consider the example given in section 1. One forty-eighth of the Brillouin zone of a BCC lattice  $\Gamma\text{NHP}$  and its regular reflection  $\Gamma\text{N}'\text{H}'\text{P}'$  are shown in figure 1. The polyhedron  $\Gamma\text{NXP}$  represents one forty-eighth of the Brillouin zone of the magnetic lattice of CsCl. Let  $q$  lie in  $\Gamma\text{NXP}$ . Then  $q + \kappa$  ( $\kappa = 2\pi(0, 1, 0)/a$ ) falls outside the limits of the Brillouin zone of the BCC lattice. Putting  $K = 2\pi(0, \bar{2}, 0)/a$  we get  $k_2 = q + \kappa + K$  in the polyhedron  $\Gamma\text{N}'\text{H}'\text{P}'$ .

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