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Use of a recurrence formula in computing the lattice Green function

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Abstract. It is shown that the lattice Green function at an arbitrary lattice site of the FCC lattice can be calculated from the three values at the lattice sites (0, 0, 0), (2, 0, 0) and (2, 2, 0) with the aid of the recurrence formula presented by Inoue. The argument is extended to the BCC and SC lattices. For these lattices also, only three values are required in the corresponding calculation.

1. Introduction

The lattice Green function is a basic function in the study of solid state physics. It appears especially when impure solids are studied (see for example the introduction of the paper by Morita and Horiguchi 1972). Much effort has been focused on the value of that function at the origin, although we need also the values at various lattice sites in many problems. For the square lattice the author (Morita 1971) presented a recurrence formula which relates the values of the lattice Green function at three successive lattice sites on the diagonal. With the aid of that formula we can calculate the lattice Green function at an arbitrary lattice site, from the knowledge of the function at the origin (0, 0) and the site (1, 1).

Inoue (1974) applied the technique for deriving that recurrence formula to the FCC lattice, and obtained a recurrence formula which relates the values of the lattice Green function at 13 lattice sites within a coordinate plane. She argued that the lattice Green function at an arbitrary lattice site on this lattice can be calculated with the aid of the formula, if the values on an axis, $(2p, 0, 0)$ $(p = 0, 1, 2, \ldots)$, and the one for the lattice site (2, 2, 0) are known. In the present paper we show that the knowledge of only three values at (0, 0, 0), (2, 0, 0) and (2, 2, 0) is required in order to calculate the value of the lattice Green function at an arbitrary site of the FCC lattice if we use the recurrence formula derived by her and the difference equation defining the lattice Green function. That argument is given in the form which is applicable to the face-centred (FC) tetragonal lattice in § 2. The discussion is extended to the BCC lattice in § 3 and to the simple tetragonal and SC lattices in § 4. The results of these sections are summarized in § 5. In the appendix we derive the recurrence formula for the rectangular lattice with the nearest and next nearest neighbour interaction and show how that formula is used to give the recurrence formulae for the tetragonal and cubic lattices.

2. The FCC lattice

The lattice Green function $G(t; l, m, n)$ for the FCC lattice is defined by the difference equation:

$$\begin{aligned}\gamma[G(l+1, m+1, n) + G(l+1, m-1, n) + G(l-1, m+1, n) + G(l-1, m-1, n)] \\ + G(l+1, m, n+1) + G(l+1, m, n-1) + G(l-1, m, n+1) + G(l-1, m, n-1) \\ + G(l, m+1, n+1) + G(l, m+1, n-1) + G(l, m-1, n+1) + G(l, m-1, n-1) \\ = 4tG(l, m, n) - 4\delta_{l_0}\delta_{m_0}\delta_{n_0} \end{aligned} \tag{2.1}$$

where t is a complex number, which is described in terms of energy in solid state physics, and (l, m, n) is such a set of integers that the sum $l+m+n$ is an even number. γ is the parameter which is unity for the isotropic FCC lattice. If $\gamma \neq 1$ the lattice may be called the face-centred (FC) tetragonal lattice. The argument t showing the t dependence of the function $G(t; l, m, n)$ is often suppressed for brevity throughout the present paper. The solution of (2.1) is given by

$$G(t; l, m, n) = \frac{1}{\pi^3}\int_0^\pi \mathrm{d}x \int_0^\pi \mathrm{d}y \int_0^\pi \mathrm{d}z \frac{\cos lx \cos my \cos nz}{t - \omega(x, y, z)} \tag{2.2a}$$

where

$$\omega(x, y, z) = \gamma \cos x \cos y + \cos y \cos z + \cos z \cos x. \tag{2.2b}$$

The difference equation (2.1) connects the function $G(l, m, n)$ for three different values of each l, m and n.

The recurrence relation derived by Inoue (1974) is expressed for the FC tetragonal lattice as follows:

$$\begin{aligned}(m+1)[G(l+2, m+2, 0) - 2\gamma_2 G(l, m+2, 0) + G(l-2, m+2, 0)] \\ -4(2m+1)E_1[G(l+1, m+1, 0) + G(l-1, m+1, 0)] \\ -2m[\gamma_2 G(l+2, m, 0) - 2E_2 G(l, m, 0) + \gamma_2 G(l-2, m, 0)] \\ -4(2m-1)E_1[G(l+1, m-1, 0) + G(l-1, m-1, 0)] \\ +(m-1)[G(l+2, m-2, 0) - 2\gamma_2 G(l, m-2, 0) + G(l-2, m-2, 0)] = 0 \end{aligned} \tag{2.3}$$

where

$$E_1 \equiv (\gamma t + 1)/\gamma^2, \qquad E_2 \equiv 1 + 4(t^2 - 1)/\gamma^2, \qquad \gamma_2 \equiv (2/\gamma^2) - 1; \tag{2.4}$$

see the appendix for a derivation. For the isotropic FCC lattice, $\gamma_2 = 1$. This relation (2.3) holds for all pairs of even integers l and m or of odd integers l and m. Inoue's derivation applies except when $m = 0$. We see that (2.3) is valid also when $m = 0$ because of the symmetry property

$$G(l, -m, 0) = G(-l, m, 0) = G(l, m, 0). \tag{2.5a}$$

We shall exchange the numbers l and m in (2.3) and then use the symmetry property that

$$G(m, l, 0) = G(l, m, 0). \tag{2.5b}$$

As a result we have:

$$
\begin{aligned}
(l+1)[G(l+2,m+2,0)-2\gamma_2 G(l+2,m,0)+G(l+2,m-2,0)]& \\
-4(2l+1)E_1[G(l+1,m+1,0)+G(l+1,m-1,0)]& \\
-2l[\gamma_2 G(l,m+2,0)-2E_2 G(l,m,0)+\gamma_2 G(l,m-2,0)]& \\
-4(2l-1)E_1[G(l-1,m+1,0)+G(l-1,m-1,0)]& \\
+(l-1)[G(l-2,m+2,0)-2\gamma_2 G(l-2,m,0)+G(l-2,m-2,0)] = 0.& \qquad (2.6)
\end{aligned}
$$

We show that all the lattice Green functions $G(2p+1, 2q+1, 0)$ for $2p+1 \geqslant 5$ and $0 \leqslant 2q+1 \leqslant 2p+1$ are evaluated from the knowledge of $G(l, m, 0)$ for $0 \leqslant l \leqslant 2p$ and $0 \leqslant m \leqslant 4$; $G(2p+2, 2q, 0)$ for $2p+2 \geqslant 6$ and $0 \leqslant 2q \leqslant 2p+2$ if $\gamma \neq 1$, and also $G(4, 2q, 0)$ for $0 \leqslant 2q \leqslant 4$ if $\gamma = \gamma_2 = 1$, are evaluated from the knowledge of $G(l, m, 0)$ for $0 \leqslant l \leqslant 2p+1$ and $0 \leqslant m \leqslant 3$.

We first put $l = 2p \geqslant 2$ and $m = 0$ in (2.6) and write it as follows:

$$
G(2p+2,2,0)-\gamma_2 G(2p+2,0,0) = L_1, \qquad (2.7a)
$$

$$
\begin{aligned}
L_1 \equiv (2p+1)^{-1}\{&4(4p+1)E_1 G(2p+1,1,0)+4p\gamma_2 G(2p,2,0)-4pE_2 G(2p,0,0) \\
&+4(4p-1)E_1 G(2p-1,1,0)-(2p-1)[G(2p-2,2,0)-\gamma_2 G(2p-2,0,0)]\}.
\end{aligned} \qquad (2.7b)
$$

Here we collected $G(l, m, 0)$ with $l = 2p+2$ on the left-hand side, and the right-hand side L_1 involves only $G(l, m, 0)$ with $2p-2 \leqslant l \leqslant 2p+1$. In a similar fashion (2.6) and (2.3) for $l = 2p \geqslant 4$ and $m = 2$ are expressed as

$$
G(2p+2,4,0)-2\gamma_2 G(2p+2,2,0)+G(2p+2,0,0) = L_2 \qquad (2.8)
$$

and

$$
3G(2p+2,4,0)-4\gamma_2 G(2p+2,2,0)+G(2p+2,0,0) = L_3, \qquad (2.9)
$$

where L_2 and L_3 are linear combinations of $G(l, m, 0)$ with $2p-2 \leqslant l \leqslant 2p+1$ and $0 \leqslant m \leqslant 4$. We consider the set of three equations (2.7)–(2.9) for $2p+2 \geqslant 6$. *If $\gamma_2 \neq 1$ one can solve this set, obtaining three quantities $G(2p+2, 4, 0)$, $G(2p+2, 2, 0)$ and $G(2p+2, 0, 0)$ for $2p+2 \geqslant 6$, when $G(l, m, 0)$ are known for $0 \leqslant l \leqslant 2p+1$ and $0 \leqslant m \leqslant 4$.*

For the important case of the isotropic FCC lattice when $\gamma = \gamma_2 = 1$, we note that the left-hand sides of these equations (2.7)–(2.9) are not independent. The requirement that they must be consistent with each other gives a relation between the quantities on the right-hand sides: $2L_1 + 3L_2 - L_3 = 0$. Its explicit expression is given by

$$
(p-1)G(2p+1,3,0)+(7p+1)G(2p+1,1,0) = L_4, \qquad (2.10a)
$$

$$
\begin{aligned}
L_4 \equiv (1/4E_1)\{&3G(2p,4,0)+4[(p-1)E_2-p]G(2p,2,0)+(4pE_2-4p+1)G(2p,0,0) \\
&-4E_1[(p-4)G(2p-1,3,0)+(7p-4)G(2p-1,1,0)] \\
&-3G(2p-2,4,0)+4G(2p-2,2,0)-G(2p-2,0,0)\}
\end{aligned} \qquad (2.10b)
$$

for $\gamma = \gamma_2 = 1$ and $2p+1 \geqslant 5$.

We now write (2.6) and (2.3) for $l = 2p-1 \geqslant 3$ and $m = 1$. They are

$$G(2p+1, 3, 0)-(2\gamma_2-1)G(2p+1, 1, 0) = L_5, \tag{2.11a}$$

$$\begin{aligned} L_5 \equiv (1/p)\{&2(4p-1)E_1[G(2p, 2, 0)+G(2p, 0, 0)] \\ &+(2p-1)[\gamma_2 G(2p-1, 3, 0)-(2E_2-\gamma_2)G(2p-1, 1, 0)] \\ &+2(4p-3)E_1[G(2p-2, 2, 0)+G(2p-2, 0, 0)] \\ &-(p-1)[G(2p-3, 3, 0)-(2\gamma_2-1)G(2p-3, 1, 0)] \end{aligned} \tag{2.11b}$$

and

$$G(2p+1, 3, 0)-\gamma_2 G(2p+1, 1, 0) = L_6, \tag{2.12a}$$

$$\begin{aligned} L_6 \equiv\ &2E_1[3G(2p, 2, 0)+G(2p, 0, 0)]+2\gamma_2 G(2p-1, 3, 0)-2E_2 G(2p-1, 1, 0) \\ &+2E_1[3G(2p-2, 2, 0)+G(2p-2, 0, 0)]-G(2p-3, 3, 0)+\gamma_2 G(2p-3, 1, 0) \end{aligned} \tag{2.12b}$$

respectively. *If* $\gamma_2 \neq 1$, *one can solve the set of* (2.11) *and* (2.12), *obtaining* $G(2p+1, 3, 0)$ *and* $G(2p+1, 1, 0)$ *for* $2p+1 \geqslant 5$, when $G(l, m, 0)$ are known for $0 \leqslant l \leqslant 2p$ and $0 \leqslant m \leqslant 3$.

However, *when* $\gamma = \gamma_2 = 1$ the left-hand sides of these equations are not independent of each other. For that case we already have (2.10) which is independent of these two. *We can then determine both* $G(2p+1, 3, 0)$ *and* $G(2p+1, 1, 0)$ *for* $2p+1 \geqslant 5$ *by solving either the set of* (2.10) *and* (2.11) *or the set of* (2.10) *and* (2.12), when $G(l, m, 0)$ for $0 \leqslant l \leqslant 2p$ and $0 \leqslant m \leqslant 4$ are known.

When $\gamma = \gamma_2 = 1$ consistency of equations (2.11) and (2.12) requires the relation $L_5 - L_6 = 0$ for $2p+1 \geqslant 5$. If we replace p by $p+1$ in that equation we have

$$pG(2p+2, 2, 0)+(3p+2)G(2p+2, 0, 0) = L_7, \tag{2.13a}$$

$$\begin{aligned} L_7 \equiv (1/2E_1)\{&G(2p+1, 3, 0)+(2pE_2-2p-1)G(2p+1, 1, 0) \\ &-2E_1[(p-2)G(2p, 2, 0)+3pG(2p, 0, 0)] \\ &-G(2p-1, 3, 0)+G(2p-1, 1, 0)\} \end{aligned} \tag{2.13b}$$

for $2p+2 \geqslant 4$. We note that the left-hand side of this equation is independent of that of (2.7) and that the right-hand sides of (2.7) and (2.13) involve only $G(l, m, 0)$ for $2p-2 \leqslant l \leqslant 2p+1$ and $0 \leqslant m \leqslant 3$ if $2p+2 \geqslant 4$. Hence *we can solve the set of linear equations* (2.7) *and* (2.13) *for the unknowns* $G(2p+2, 2, 0)$ *and* $G(2p+2, 0, 0)$, *if* $2p+2 \geqslant 4$ and $G(l, m, 0)$ for $0 \leqslant l \leqslant 2p+1$ and $0 \leqslant m \leqslant 3$ are known.

After $G(2p+2, 2, 0)$ and $G(2p+2, 0, 0)$ for $2p+2 \geqslant 4$ are obtained, $G(2p+2, 2q, 0)$ *for* $0 \leqslant 2q \leqslant 2p+2$ *can be calculated with the aid either of* (2.3) *or of* (2.6), if we already know $G(l, m, 0)$ for $0 \leqslant m \leqslant l \leqslant 2p+1$. Note here that when we use (2.6) the knowledge of $G(2p+2, 2, 0)$ is not required in this calculation. In particular, if we put $2p = 2$ in (2.7) we have an expression for $G(4, 2, 0)$ in terms of $G(l, m, 0)$ for $0 \leqslant m \leqslant l \leqslant 3$ and $G(4, 0, 0)$. In a similar way, when $G(2p+1, 1, 0)$ for $2p+1 \geqslant 3$ is known, $G(2p+1, 2q+1, 0)$ *for* $0 \leqslant 2q+1 \leqslant 2p+1$ *are calculated with the aid of* (2.3) *or* (2.6). For instance, if we put $l = m = 1$ in (2.3) we have an expression for $G(3, 3, 0)$ in terms of $G(l, m, 0)$ for $0 \leqslant m \leqslant l \leqslant 2$ and $G(3, 1, 0)$. We can now calculate $G(l, m, 0)$ for all l and m with the aid of two sets of equations and (2.3) or (2.6), when we initially know $G(l, m, 0)$ for $0 \leqslant m \leqslant l \leqslant 2$ and $G(3, 1, 0)$ if $\gamma = 1$, and when we know further $G(4, 0, 0)$ if $\gamma \neq 1$.

For the isotropic FCC lattice where $\gamma = 1$ we show that $G(1,1,0)$ and $G(3,1,0)$ are calculated from $G(0,0,0)$, $G(2,0,0)$ and $G(2,2,0)$. By putting $\gamma = 1$ and $(l, m, n) = (0,0,0)$ in the difference equation (2.1) defining the lattice Green function, we have

$$G(1,1,0) = \tfrac{1}{3}(tG(0,0,0)-1). \tag{2.14}$$

If we write the equation (2.1) for $\gamma = 1$ and $(l, m, n) = (2,0,0)$ and $(1,1,0)$ and then eliminate $G(2,1,1)$ from the two equations, we have

$$G(3,1,0) = \tfrac{1}{4}G(2,2,0)+(t+\tfrac{1}{2})G(2,0,0)-(\tfrac{1}{3}t^2-\tfrac{1}{4})G(0,0,0)+\tfrac{1}{3}t. \tag{2.15}$$

For the isotropic FCC lattice we can now calculate the lattice Green function $G(l, m, 0)$ for all l and m by starting from the values of $G(0,0,0)$, $G(2,0,0)$ and $G(2,2,0)$. The expressions of these in terms of the complete elliptic integrals of the first and second kind have been provided by Iwata (1969) and Inoue (1974). A numerical procedure of computing these functions was discussed by Morita and Horiguchi (1971, 1973).

After $G(l, m, n)$ for $n = 0$ are calculated, we can use (2.1) *in order to calculate the values for nonzero n.*

3. The BCC lattice

The lattice Green function $G(t; l, m, n)$ for the BCC lattice is given by (2.2*a*) with

$$\omega(x, y, z) = \cos x \cos y \cos z, \tag{3.1}$$

where l, m and n are either all even or all odd integers. The recurrence relation corresponding to (2.3), for this lattice, is given by

$$\begin{aligned}(m+1)[G(l+2, m+2, 0)+2G(l, m+2, 0)+G(l-2, m+2, 0)]\\ +2m[G(l+2, m, 0)-2E_2G(l, m, 0)+G(l-2, m, 0)]\\ +(m-1)[G(l+2, m-2, 0)+2G(l, m-2, 0)+G(l-2, m-2, 0)] = 0\end{aligned} \tag{3.2}$$

where l and m are both even numbers and

$$E_2 \equiv 4t^2-1;$$

see the appendix for a derivation of (3.2). Exchanging l and m and using a symmetry property, we have

$$\begin{aligned}(l+1)[G(l+2, m+2, 0)+2G(l+2, m, 0)+G(l+2, m-2, 0)]\\ +2l[G(l, m+2, 0)-2E_2G(l, m, 0)+G(l, m-2, 0)]\\ +(l-1)[G(l-2, m+2, 0)+2G(l-2, m, 0)+G(l-2, m-2, 0)] = 0.\end{aligned} \tag{3.3}$$

We put $l = 2p \geqslant 2$ and $m = 0$ in (3.3) and obtain

$$G(2p+2, 2, 0)+G(2p+2, 0, 0) = M_1, \tag{3.4a}$$

$$\begin{aligned}M_1 \equiv (2p+1)^{-1}\{-4p[G(2p, 2, 0)-E_2G(2p, 0, 0)]\\ -(2p-1)[G(2p-2, 2, 0)+G(2p-2, 0, 0)]\}.\end{aligned} \tag{3.4b}$$

We write (3.2) and (3.3) for $l = 2p \geqslant 4$ and $m = 2$:

$$3G(2p+2,4,0)+4G(2p+2,2,0)+G(2p+2,0,0) = M_2, \tag{3.5a}$$

$$M_2 \equiv -6G(2p,4,0)+8E_2G(2p,2,0)-2G(2p,0,0)$$
$$-3G(2p-2,4,0)-4G(2p-2,2,0)-G(2p-2,0,0) \tag{3.5b}$$

and

$$G(2p+2,4,0)+2G(2p+2,2,0)+G(2p+2,0,0) = M_3, \tag{3.6a}$$

$$M_3 \equiv (2p+1)^{-1}\{-4p[G(2p,4,0)-2E_2G(2p,2,0)+G(2p,0,0)]$$
$$-(2p-1)[G(2p-2,4,0)+2G(2p-2,2,0)+G(2p-2,0,0)]\}. \tag{3.6b}$$

The left-hand sides of (3.4)–(3.6) are not independent of each other. Their consistency requires the relation $2M_1+M_2-3M_3 = 0$ for $2p \geqslant 4$. By writing this equation and replacing p by $p+1$ we have

$$3G(2p+2,4,0)+4(p+1+pE_2)G(2p+2,2,0)$$
$$-[4(p+1)E_2+4p+3]G(2p+2,0,0) = M_4, \tag{3.7a}$$

$$M_4 \equiv -3G(2p,4,0)-4G(2p,2,0)-G(2p,0,0) \tag{3.7b}$$

for $2p+2 \geqslant 4$. The left-hand side of this equation is independent of those of (3.4)–(3.6). Hence *we can determine* $G(2p+2,4,0)$, $G(2p+2,2,0)$ *and* $G(2p+2,0,0)$ *for* $2p+2 \geqslant 6$ *by solving the set of* (3.7) *and two of* (3.4)–(3.6). The solution for $2p+2 \geqslant 6$ is obtained when $G(l,m,0)$ are known for $2p-2 \leqslant l \leqslant 2p$ and $0 \leqslant m \leqslant 4$.

Here we put $2p = 2$ in (3.4), (3.5) and (3.7). If $G(l,m,0)$ for $0 \leqslant m \leqslant l \leqslant 2$ are known *this set of linear equations can be solved for the unknowns* $G(4,0,0)$, $G(4,2,0)$ *and* $G(4,4,0)$.

We can now calculate $G(l,m,0)$ for all l and m with the aid of (3.2) or (3.3), and of the set of (3.7) and two of (3.4)–(3.6), if the values of $G(0,0,0)$, $G(2,0,0)$ and $G(2,2,0)$ are known. The expression of these functions in terms of the complete elliptic integrals of the first and second kind has been provided (Joyce 1971). The numerical calculation of these complete elliptic integrals was discussed by Morita and Horiguchi (1971, 1973).

The values of $G(l,m,n)$ for nonzero n are calculated from those for $n = 0$, with the aid of the difference equation defining the lattice Green function.

4. The SC lattice

In the SC lattice each lattice site corresponds to a set of three integral numbers (l, m, n), and *vice versa*, in the ordinary way of introducing the coordinate axes. If we write the coordinate plane for $n = 0$, we have figure 1(a). We note that we can also take the axes along the diagonal directions of the plane as in figure 1(b). In the case of the square lattice on this plane the recurrence formula along the l' axis was found simpler than the one along the l axis; the former relates the values of lattice Green function at three lattice sites (Morita 1971) but the latter relates those at five lattice sites (see the appendix). We shall now use the set of (l', m', n) in specifying the lattice site, where l' and m' are both even or both odd integers and n is an arbitrary integer. The lattice Green function is

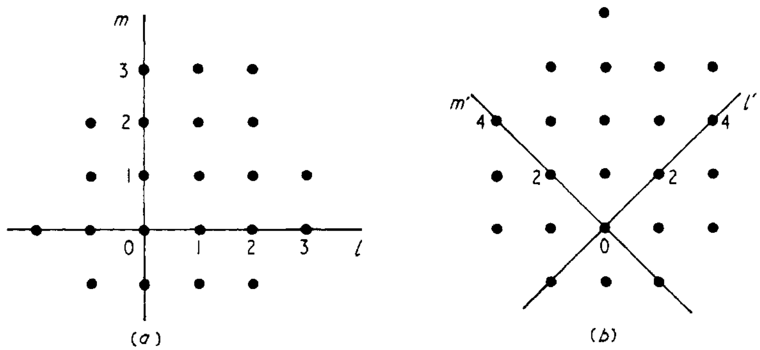

Figure 1. Two natural ways of introducing the coordinate axes in the square lattice. (*a*) The ordinary way. (*b*) An alternative way (reproduced from Morita 1971).

then given by

$$G'(t; l', m', n) = \frac{1}{\pi^3}\int_0^\pi dx' \int_0^\pi dy' \int_0^\pi dz \frac{\cos l'x' \cos m'y' \cos nz}{t-\omega'(x', y', z)} \tag{4.1a}$$

$$\omega'(x', y', z) = 2\cos x' \cos y' + \gamma \cos z. \tag{4.1b}$$

In the ordinary definition the lattice Green function $G(t; l, m, n)$ is given by (2.2*a*) with

$$\omega(x, y, z) = \cos x + \cos y + \gamma \cos z. \tag{4.2}$$

Here γ is the parameter which is unity for the isotropic SC lattice. When $\gamma \neq 1$ the lattice is called the simple tetragonal lattice. The Green functions $G'(t; l', m', n)$ and $G(t; l, m, n)$ are related by

$$\begin{aligned} G'(t; l', m', n) &= G(t; (l'+m')/2, (l'-m')/2, n), \\ G'(t; l+m, l-m, n) &= G(t; l, m, n). \end{aligned} \tag{4.3}$$

By the procedure described in the appendix we obtain the following recurrence formula for $G'(l', m', n)$:

$$\begin{aligned} (m'+1)&[G'(l'+2, m'+2, 0) + 2G'(l', m'+2, 0) + G(l'-2, m'+2, 0)] \\ &- 2(2m'+1)t[G'(l'+1, m'+1, 0) + G'(l'-1, m'+1, 0)] \\ &+ 2m'[G'(l'+2, m', 0) + 2E_2 G'(l', m', 0) + G'(l'-2, m', 0)] \\ &- 2(2m'-1)t[G'(l'+1, m'-1, 0) + G'(l'-1, m'-1, 0)] \\ &+ (m'-1)[G'(l'+2, m'-2, 0) + 2G'(l', m'-2, 0) + G'(l'-2, m'-2, 0)] = 0 \end{aligned} \tag{4.4}$$

where

$$E_2 \equiv t^2 + 1 - \gamma^2. \tag{4.5}$$

By exchanging l' and m' and using the symmetry property

$$G'(m', l', 0) = G'(l', m', 0),$$

we have

$$(l'+1)[G'(l'+2,m'+2,0)+2G'(l'+2,m',0)+G'(l'+2,m'-2,0)]$$
$$-2(2l'+1)t[G'(l'+1,m'+1,0)+G'(l'+1,m'-1,0)]$$
$$+2l'[G'(l',m'+2,0)+2E_2G'(l',m',0)+G'(l',m'-2,0)]$$
$$-2(2l'-1)t[G'(l'-1,m'+1,0)+G'(l'-1,m'-1,0)]$$
$$+(l'-1)[G'(l'-2,m'+2,0)+2G'(l'-2,m',0)+G'(l'-2,m'-2,0)] = 0. \quad (4.6)$$

We first write (4.4) and (4.6) for $l' = 2p-1 \geqslant 3$ and $m' = 1$. They are

$$G'(2p+1,3,0)+G'(2p+1,1,0)$$
$$= 3tG'(2p,2,0)+tG'(2p,0,0)-2G'(2p-1,3,0)-2E_2G'(2p-1,1,0)$$
$$+3tG'(2p-2,2,0)+tG'(2p-2,0,0)-G'(2p-3,3,0)-G'(2p-3,1,0) \quad (4.7)$$

and

$$G'(2p+1,3,0)+3G'(2p+1,1,0)$$
$$= (1/p)\{(4p-1)t[G'(2p,2,0)+G'(2p,0,0)]$$
$$-(2p-1)[G'(2p-1,3,0)+(2E_2+1)G'(2p-1,1,0)]$$
$$+(4p-3)t[G'(2p-2,2,0)+G'(2p-2,0,0)]$$
$$-(p-1)[G'(2p-3,3,0)+3G'(2p-3,1,0)]\}. \quad (4.8)$$

From these we can calculate both $G(2p+1,3,0)$ *and* $G(2p+1,1,0)$ *for* $2p+1 \geqslant 5$, from the knowledge of $G'(l',m',0)$ for $0 \leqslant l' \leqslant 2p$ and $0 \leqslant m' \leqslant 3$.

We put $l' = 2p \geqslant 2$ and $m' = 0$ in (4.6) and obtain

$$G'(2p+2,2,0)+G'(2p+2,0,0) = N_1, \quad (4.9a)$$

$$N_1 \equiv (2p+1)^{-1}\{2(4p+1)tG'(2p+1,1,0)-4p[G'(2p,2,0)+E_2G'(2p,0,0)]$$
$$+2(4p-1)tG'(2p-1,1,0)-(2p-1)[G'(2p-2,2,0)$$
$$+G'(2p-2,0,0)]\}. \quad (4.9b)$$

We write (4.4) and (4.6) for $l' = 2p \geqslant 4$ and $m' = 2$:

$$3G'(2p+2,4,0)+4G'(2p+2,2,0)+G'(2p+2,0,0) = N_2, \quad (4.10a)$$

$$N_2 \equiv 2t[5G'(2p+1,3,0)+3G'(2p+1,1,0)]-6G'(2p,4,0)-8E_2G'(2p,2,0)$$
$$-2G'(2p,0,0)+2t[5G'(2p-1,3,0)+3G'(2p-1,1,0)]$$
$$-3G'(2p-2,4,0)-4G'(2p-2,2,0)-G'(2p-2,0,0) \quad (4.10b)$$

and

$$G'(2p+2,4,0)+2G'(2p+2,2,0)+G'(2p+2,0,0) = N_3, \quad (4.11a)$$

$$N_3 \equiv (2p+1)^{-1}\{2(4p+1)t[G'(2p+1,3,0)+G'(2p+1,1,0)]-4p[G'(2p,4,0)$$
$$+2E_2G'(2p,2,0)+G'(2p,0,0)]+2(4p-1)t[G'(2p-1,3,0)+G'(2p-1,1,0)]$$
$$-(2p-1)[G'(2p-2,4,0)+2G'(2p-2,2,0)+G'(2p-2,0,0)]\}. \quad (4.11b)$$

The left-hand sides of (4.9)–(4.11) are not independent of each other. Their consistency requires the relation $2N_1+N_2-3N_3 = 0$ for $2p \geqslant 4$. By writing this equation explicitly and eliminating $G'(2p+1, 3, 0)$ and $G'(2p+1, 1, 0)$ with the aid of (4.7) and (4.8), we have a formula of the form:

$$3G'(2p, 4, 0)-4[(p-1)\gamma^2-1]G'(2p, 2, 0)+(4p\gamma^2+1)G'(2p, 0, 0) = N_4.$$

If we replace p by $p+1$ in this equation we have

$$3G'(2p+2, 4, 0)-4(p\gamma^2-1)G'(2p+2, 2, 0)+[4(p+1)\gamma^2+1]G'(2p+2, 0, 0) = N'_4, \quad (4.12a)$$

$$\begin{aligned} N'_4 \equiv & -2[p-3+(2p+3)t-2t^2]G'(2p+1, 3, 0)+2[p+3-4(p+1)E_2+t]G'(2p+1, 1, 0) \\ & -3G'(2p, 4, 0)-4[1+(p+1)t^2]G'(2p, 2, 0)-(1-4pt^2)G'(2p, 0, 0) \\ & +2(p+1)tG'(2p-1, 3, 0)-2(p-1)tG'(2p-1, 1, 0) \qquad (4.12b) \end{aligned}$$

for $2p+2 \geqslant 4$. We note that the left-hand side of (4.12) is independent of those of (4.9)–(4.11). *We can now determine* $G'(2p+2, 4, 0)$, $G'(2p+2, 2, 0)$ *and* $G'(2p+2, 0, 0)$ *for* $2p+2 \geqslant 6$ *by solving the set of* (4.12) *and two of* (4.9)–(4.11), if $G'(l', m', 0)$ for $0 \leqslant l' \leqslant 2p+1$ and $0 \leqslant m' \leqslant 4$ are known.

Here we consider (4.9), (4.10) and (4.12) for $2p = 2$. If $G'(l', m', 0)$ for $0 \leqslant m' \leqslant l' \leqslant 3$ are known, *this set of linear equations is solved for the unknowns* $G'(4, 4, 0)$, $G'(4, 2, 0)$ *and* $G'(4, 0, 0)$. $G'(3, 3, 0)$ *is calculated by* (4.7) *for* $2p = 2$, if $G'(3, 1, 0)$ and $G'(l', m', 0)$ for $0 \leqslant m' \leqslant l' \leqslant 2$ are known. The rest are

$G'(0, 0, 0) = G(0, 0, 0)$, $\quad G'(1, 1, 0) = G(1, 0, 0)$,

$G'(2, 0, 0) = G(1, 1, 0)$, $\quad G'(2, 2, 0) = G(2, 0, 0)$ and $G'(3, 1, 0) = G(2, 1, 0)$.

We may use $G'(3, 3, 0) = G(3, 0, 0)$ in place of $G'(3, 1, 0) = G(2, 1, 0)$, because we can calculate each from the other of the pair by the above-mentioned equation for $G'(3, 3, 0)$. For the isotropic SC lattice we note that this equation is equivalent to some of the relations which were given by Horiguchi (1971b) in order to express the lattice Green functions $G(l, m, n)$ for $l+m+n \leqslant 5$ in terms of $G'(l', 0, 0)$ for $0 \leqslant l' \leqslant 5$.

For the isotropic SC lattice $G(1, 0, 0)$ and $G(1, 1, 0)$ are expressed in terms of the others, and hence we need the values $G(0, 0, 0)$, $G(2, 0, 0)$ and $G(3, 0, 0)$. $G(0, 0, 0)$ have been expressed in terms of the complete elliptic integrals of the first and second kind (Joyce 1973). It is hoped that such an expression will be found also for $G(2, 0, 0)$ and $G(3, 0, 0)$ in the near future.

$G(l, m, n)$ for nonzero n are calculated from those for $n = 0$ with the aid of the difference equation defining the lattice Green function (see for example Morita 1971).

5. Summary and remarks

The results of the preceding §§ 2–4 are summarized in table 1. The second row lists the functions which are required in obtaining the lattice Green function at an arbitrary lattice site. The third row gives the set S_1 of equations which are used in calculating $G(2p+1, 1, 0)$ and $G(2p+1, 3, 0)$ for $2p+1 \geqslant 5$, when $G(l, m, 0)$ for $0 \leqslant l \leqslant 2p$ and $0 \leqslant m \leqslant 3$ or 4 are known. The fourth row gives the set S_2 which is used in obtaining $G(2p+2, 2q, 0)$ for $2p+2 \geqslant 4$ or 6 and $0 \leqslant q \leqslant 1$ or 2, when $G(l, m, 0)$ for $0 \leqslant l \leqslant 2p+1$ and $0 \leqslant m \leqslant 3$ or 4 are known. The last row lists the equation E which gives $G(l, m+2, 0)$

Table 1. List of the necessary lattice Green functions and the equations to be used in obtaining the lattice Green function at an arbitrary site $(l, m, 0)$ on a coordinate plane from them. For the SC lattice the same equations are used as for the simple tetragonal lattice.

	FC tetragonal ($\gamma \neq 1$, $\gamma_2 \neq 1$)	FCC ($\gamma = \gamma_2 = 1$)	BCC	simple tetragonal	SC ($\gamma = 1$)
Necessary data	$G(0,0,0)$ $G(1,1,0)$ $G(2,0,0)$ $G(2,2,0)$ $G(3,1,0)$ $G(4,0,0)$	$G(0,0,0)$ $G(2,0,0)$ $G(2,2,0)$	$G(0,0,0)$ $G(2,0,0)$ $G(2,2,0)$	$G(0,0,0)$ $G(1,0,0)$ $G(1,1,0)$ $G(2,0,0)$ $G(3,0,0)$	$G(0,0,0)$ $G(2,0,0)$ $G(3,0,0)$
S_1	(2.11) (2.12)	(2.10) (2.11) or (2.10) (2.12)		(4.7) (4.8)	
S_2	(2.7) (2.8) (2.9)	(2.7) (2.13)	(3.7) and two from (3.4), (3.5) and (3.6)	(4.12) and two from (4.9), (4.10) and (4.11)	
E	(2.3) or (2.6)	(2.3) or (2.6)	(3.2) or (3.3)	(4.4) or (4.6)	

for $l \geqslant 3$ and $l \geqslant m+2 \geqslant 2$ when $G(l, m', 0)$ for $0 \leqslant m' \leqslant m$ and $G(l', m', 0)$ for $0 \leqslant m' \leqslant l' \leqslant l-1$ are known.

In all the cases, after the values $G(l, m, 0)$ on a coordinate plane are determined, the values $G(l, m, n)$ for nonzero n are calculated with the aid of the difference equation defining the lattice Green function.

In the present paper we considered the tetragonal and cubic lattices with the nearest neighbour interaction. We note that the generalization of the discussion to the simple tetragonal and the SC lattice with an interaction up to third neighbours is straightforward.

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Appendix. Derivation of the recurrence formulae

In this appendix we first derive the recurrence formula along an axis for the rectangular lattice with the nearest and next nearest neighbour interaction, and then give a sketch of how it is used in deriving the recurrence formulae (2.3), (3.2) and (4.4) for the tetragonal and cubic lattices.

The lattice Green function for the rectangular lattice with the nearest and next nearest neighbour interaction is given by

$$G_2(t; m, n; \alpha_1, \alpha_2, 2\beta) \equiv \frac{1}{\pi^2} \int_0^\pi \mathrm{d}y \int_0^\pi \mathrm{d}z \frac{\cos my \cos nz}{t - \omega_2(y, z)}, \tag{A.1}$$

$$\omega_2(y, z) = \alpha_1 \cos y + \alpha_2 \cos z + 2\beta \cos y \cos z. \tag{A.2}$$

When $n = 0$,

$$G_2(t; m, 0; \alpha_1, \alpha_2, 2\beta) = \frac{1}{\pi}\int_0^\pi \mathrm{d}y \frac{1}{D}\cos my, \tag{A.3}$$

where

$$D = [(t-\alpha_1 \cos y)^2 - (\alpha_2 + 2\beta \cos y)^2]^{1/2}. \tag{A.4}$$

We consider the integral

$$\frac{1}{\pi}\int_0^\pi \mathrm{d}y\, D\cos my = \frac{1}{\pi}\int_0^\pi \mathrm{d}y \frac{1}{D} D^2 \cos my. \tag{A.5}$$

Substituting (A.4) for D^2 in the numerator of the expression on the right-hand side, we have

$$\begin{aligned}\frac{1}{\pi}\int_0^\pi \mathrm{d}y \frac{1}{D}\cos my[(t^2-\alpha_2^2) - 2(\alpha_1 t + 2\alpha_2\beta)\cos y + (\alpha_1^2 - 4\beta^2)\cos^2 y] \\ = (t^2-\alpha_2^2)G_2(m,0) - (\alpha_1 t + 2\alpha_2\beta)[G_2(m+1,0) + G_2(m-1,0)] \\ + \tfrac{1}{4}(\alpha_1^2 - 4\beta^2)[G_2(m+2,0) + 2G_2(m,0) + G_2(m-2,0)],\end{aligned} \tag{A.6}$$

where the parameters t, α_1, α_2 and 2β are suppressed for brevity. On the other hand, by a partial integration of the expression on the left-hand side of (A.5), we have

$$\begin{aligned}-\frac{1}{m\pi}\int_0^\pi \mathrm{d}y \sin my \frac{\alpha_1(t-\alpha_1\cos y) + 2\beta(\alpha_2 + 2\beta\cos y)}{D}\sin y \\ = \frac{1}{2m}(\alpha_1 t + 2\alpha_2\beta)[G_2(m+1,0) - G_2(m-1,0)] \\ - \frac{1}{4m}(\alpha_1^2 - 4\beta^2)[G_2(m+2,0) - G_2(m-2,0)].\end{aligned} \tag{A.7}$$

By equating (A.6) and (A.7) we have

$$\begin{aligned}(\alpha_1^2 - 4\beta^2)[(m+1)G_2(m+2,0) + (m-1)G_2(m-2,0)] \\ - 2(\alpha_1 t + 2\alpha_2\beta)[(2m+1)G_2(m+1,0) + (2m-1)G_2(m-1,0)] \\ + 2m(2t^2 - 2\alpha_2^2 + \alpha_1^2 - 4\beta^2)G_2(m,0) = 0.\end{aligned} \tag{A.8}$$

This recurrence formula for $G_2(t; m, 0; \alpha_1, \alpha_2, 2\beta)$ was derived by Morita and Horiguchi (unpublished, see Horiguchi 1971a).

The lattice Green function $G(t; l, m, n)$ defined by (2.2*a*) with (2.2*b*) for the face-centred tetragonal and the FCC lattice is expressed in terms of $G_2(t; m, n; \alpha_1, \alpha_2, 2\beta)$ as follows:

$$G(t; l, m, n) = \frac{1}{\pi}\int_0^\pi \mathrm{d}x \cos lx\, G_2(t; m, n; \gamma\cos x, \cos x, 1). \tag{A.9}$$

We substitute $\alpha_1 = \gamma\cos x$, $\alpha_2 = \cos x$ and $2\beta = 1$ into (A.8) and then multiply both sides of (A.8) by $(\cos lx)/\pi$. The integral with respect to x of the expression obtained gives, with the aid of the relation (A.9), the recurrence formula (2.3) in the text.

For the BCC lattice we express the lattice Green function (2.2*a*) with (3.1) as follows:

$$G(t\,;l,m,n)=\frac{1}{\pi}\int_0^{\pi}\mathrm{d}x\cos lx\,G_2(t\,;m,n\,;0,0,\cos x). \qquad \text{(A.10)}$$

We now put $\alpha_1=\alpha_2=0$ and $2\beta=\cos x$ in (A.8), multiply by $(\cos x)/\pi$ and then integrate with respect to x. With the aid of (A.10) we then obtain (3.2).

The lattice Green function defined by (4.1) for the simple tetragonal and SC lattice is written as

$$G'(t\,;l',m',n)=\frac{1}{\pi}\int_0^{\pi}\mathrm{d}x'\cos l'x'G_2(t\,;m',n\,;2\cos x',\gamma,0). \qquad \text{(A.11)}$$

We put $\alpha_1=2\cos x', \alpha_2=\gamma$ and $2\beta=0$ in (A.8), multiply by $(\cos x)/\pi$ and then integrate with respect to x. We then obtain (4.4).

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