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Analytical Treatment of the Isotropic and Tetragonal Lattice Green Functions for the Face-centered Cubic, Body-centered Cubic and Simple Cubic Lattices

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Abstract: In this paper, we propose an efficient method to calculate the isotropic and tetragonal lattice Green functions for the face-centered cubic (FCC), body-centered cubic (BCC) and simple cubic (SC) lattices. The method is based on binomial expansion theorems, which provide us with analytical formulae through basic integrals. The resulting series present better convergence rates. Several acceleration techniques are combined to further improve the efficiency of the established formulas. The obtained results for the lattice Green functions are in good agreement with the known numerical calculation results.

Keywords: Isotropic lattice Green functions, tetragonal lattice Green functions, face-centered cubic lattice, body-centered cubic lattice, simple cubic lattice.

1 Introduction

The lattice Green functions plays a decisive role in the theory of solid state physics [Economou (1983); Morita and Horiguchi (1972)]. These functions arise not only in their own right, but are also central to the calculation of the lattice statistical problems [Berlin and Kac (1952); Economou (1983); Kobelev, Kolomeisky and Fisher (2002); Montroll and Weiss (1965); Tewary and Read (2004); Tewary and Vaudin (2011); Yakhno and Ozdek (2012)]. In the literature, various efficient methods have been proposed for improving the evaluation of the lattice Green functions [Economou (1983); Berlin and Kac (1952); Kobelev, Kolomeisky and Fisher (2002); Montroll and Weiss (1965); Tewary and Read (2004); Tewary and Vaudin (2011); Yakhno and Ozdek (2012)]. In literature, most of the studies on lattice functions are based on elliptic integral and recurrence relations [Borwein, Glasser, McPhedran, Wan and Zucker (2013); Inoue (1974); Iwata (1969); Morita and Horiguchi (1971); Morita (1975)]. Unfortunately, for most of these purely

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elliptic integrals and recurrence relations, there are some limitations in their applicability despite the huge development in the computational methods. The reproduce properties of the recurrence relation schemes can lead to a decrease in the accuracy of calculation results. Therefore, it is desirable to use the binomial expansion theorems from which the problems of evaluation of lattice Green functions do not arise. Simple yet accurate analytical formulae have proposed to compute anisotropic lattice Green functions for FCC, BCC and SC lattices [Guseinov and Mamedov (2007); Mamedov and Askerov (2008)]. Notice that, the obtained simple analytical formulas for the lattice Green functions are completely general for $t \geq 3$.

In the present article we propose the series expression formulas occur as one infinite sum and in terms of I_n basic integral, which make possible the fast and accurate evaluation of the isotropic and tetragonal lattice Green functions. This simplification and the use of the computer memory for calculation of binomial coefficients may extend the limits of large arguments to the calculators and result in speedier calculation, should such limits be reached in practice. The new analytical approach for evaluating the isotropic and tetragonal lattice Green functions for FCC, BCC and SC lattices is conceptually simpler than existing methods in the literature.

2 Definition and basic formulas

The isotropic and tetragonal lattice Green functions are defined as

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

where t is a complex number, which is described in terms of energy in solid state physics, and (l,m,n) is a set of integers such that the sum $l+m+n$ is an even number [Morita (1975)]. γ is the parameter which is unity for the isotropic lattice. If $\gamma \neq 1$ lattice may be called tetragonal lattice [Morita (1975)]. The parameters $\omega(x,y,z)$ are defined as follows:

for FCC lattice

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

for BCC lattice

$$\omega(x,y,z) = \cos x \cos y \cos z \tag{3}$$

for SC lattice

$$\omega(x,y,z) = \cos x + \cos y + \gamma \cos z \tag{4}$$

$$\omega(x,y,z) = 2\cos x \cos y + \gamma \cos z \tag{5}$$

In order to establish expressions for the lattice Green functions we shall first consider well known binomial expansion theorems for an arbitrary real or complex n and $|x| > |y|$ [Gradshteyn and Ryzhik (1980)],

$$(x \pm y)^n = \lim_{N' \to \infty} \sum_{m=0}^{N'} (\pm 1)^m F_m(n) x^{n-m} y^m. \tag{6}$$

Here N is the upper limit of summations and$F_m(n)$ are binomial coefficients defined by

$$F_m(n) = \begin{cases} \frac{n(n-1)...(n-m+1)}{m!} & \text{for integer } n \\ \frac{(-1)^m \Gamma(m-n)}{m!\Gamma(-n)} & \text{for noninteger } n \end{cases} \tag{7}$$

We notice that for $m < 0$ the binomial coefficient $F_m(n)$ in Eq. (7) is zero and the positive integer n terms with negative factorials do not contribute to the summation. Taking into account Eq. (6) we obtain for the function $(t - \omega)^{-1}$ occurring in Eq. (1) the following series expansion relations:

$$(t-\omega)^{-1} = \sum_{i=0}^{\infty} F_i(-1) \times \begin{cases} (-1)^i t^{-1-i} \omega^i & \text{for } \omega \le t \le \infty \\ (-1)^{i+1} \omega^{-1-i} t^i & \text{for } 0 \le t \le \omega \end{cases} \tag{8}$$

Thus, substituting Eq. (8) into Eq. (1), we obtain the series expansion formulas for the isotropic and tetragonal lattice Green functions in terms of binomial coefficients and basic integrals, respectively

for FCC lattice

$$\begin{aligned} G(t,l,m,n) = & \frac{1}{\pi^3} \lim_{N \to \infty} \sum_{i=0}^{N} (-1)^i F_i(-1) t^{-1-i} \times \sum_{j=0}^{i} F_j(i) \gamma^{i-j} \sum_{k=0}^{j} F_k(j) \\ & \times J_{i-j+k}(l) J_{i-k}(m) J_j(n) \quad \text{for } t \ge 3, \end{aligned} \tag{9}$$

for BCC lattice

$$G(t,l,m,n) = \frac{1}{\pi^3} \lim_{N' \to \infty} \sum_{i=0}^{N'} (-1)^i F_i(-1) t^{-1-i} \times J_i(l) J_i(m) J_i(n) \quad \text{for} \quad t \ge 1, \tag{10}$$

for SC lattice

$$\begin{aligned} G(t,l,m,n) = & \frac{1}{\pi^3} \lim_{M' \to \infty} \sum_{i=0}^{M'} (-1)^i F_i(-1) t^{-1-i} \times \sum_{j=0}^{i} F_j(i) 2^{i-j} \gamma^j J_{i-j}(l) \\ & \times J_{i-j}(m) J_j(n) \ for \ t \ge 3, \end{aligned} \tag{11}$$

$$G(t,l,m,n) = \frac{1}{\pi^3} \lim_{M\to\infty} \sum_{i=0}^{M} (-1)^i F_i(-1) t^{-1-i} \times \sum_{j=0}^{i} F_j(i) \sum_{k=0}^{j} F_k(j) \gamma^k J_{i-j}(l) \times J_{j-k}(m) J_k(n) \; for \;\; t \geq 3 \tag{12}$$

By using the proposed method, we can obtain alternative series formulas for lattice Green functions, respectively:

for FCC lattice

$$G(t,l,m,n) = \frac{1}{\pi^3} \lim_{\substack{N\to\infty \\ L\to\infty}} \sum_{i=0}^{N} (-1)^i F_i(-1) t^{-1-i} \times \sum_{j=0}^{L} (-1)^j F_j(-1-i) \gamma^j t^{-j} \sum_{k=0}^{i} F_k(i) \times J_{j+k}(l) J_{j+i-k}(m) J_i(n) \text{ for t} \geq 3 \tag{13}$$

for SC lattice

$$G(t,l,m,n) = \frac{1}{\pi^3} \lim_{\substack{N\to\infty \\ L\to\infty}} \sum_{i=0}^{N} (-1)^i F_i(-1) t^{-1-i} \times \sum_{j=0}^{L} (-1)^j F_j(-1-i) t^{-j} \sum_{k=0}^{i} F_k(i) \times J_j(l) J_{i-k}(m) J_k(n) \; for \;\; t \geq 3 \tag{14}$$

$$G(t,l,m,n) = \frac{1}{\pi^3} \lim_{\substack{N\to\infty \\ L\to\infty}} \sum_{i=0}^{N} (-1)^i F_i(-1) \gamma^i t^{-1-i} \times \sum_{j=0}^{L} (-1)^j F_j(-1-i) 2^j t^{-j} J_j(l) \times J_j(m) J_i(n) \;\; for \; t \geq 3 \tag{15}$$

The quantities $J_n(k)$ occurring in Eqs. (9)-(15) are determined by the relation

$$J_n(k) = \begin{cases} I_n & \text{for} \quad k = 0 \\ L_n(k) & \text{for} \quad k > 1 \\ I_{n+1} & \text{for} \quad k = 1 \\ 0 & \text{for } k > n \text{ or } k+n \text{ odd} \end{cases} \tag{16}$$

The basic integrals $L_n(k)$ and I_n occurring in Eq. (16) are determined from the following relations, respectively

$$L_n(k) = \int_0^{\pi} \cos kx \cos^n x dx = 2^{k-1} I_{k+n} + k \sum_{i=1}^{E[k/2]} \frac{(-1)^i 2^{k-2i-1} F_{i-1}(k-i-1) I_{k+n-2i}}{i} \tag{17}$$

and

$$I_n = \int_0^{\pi} \cos^n \varphi \, d\varphi = \begin{cases} 0, & \text{if } n \text{ odd} \\ \sqrt{\pi}\frac{\Gamma\left(\frac{n+1}{2}\right)}{\Gamma\left(\frac{n}{2}+1\right)}, & \text{if } n \text{ even} \end{cases} \tag{18}$$

In Eq. (17) the index $E[k/2]$ is the upper limit of summation defined by

$$E(n/2) = \frac{n}{2} - \frac{1}{4}[1-(-1)^n]. \tag{19}$$

In Eqs. (9)-(15) the indexes $N, N', M \, and \, M'$ are the upper limits of summations. In the present work, we propose an alternative accurate method for the analytical evaluation of the lattice Green functions for FCC, BCC and SC lattices. The obtained formulas are practically simple and they offer some advantages over currently available methods.

3 Numerical results and discussion

We have presented a new approach to the calculations of isotropic and tetragonal lattice Green functions using binomial expansion theorems. The analytical results are validated by the numerical calculations for each lattice Green function. The numerical computation of the lattice Green functions has been performed by using the scientific software Mathematica 7.0. Comparisons of the numerical and analytical results are presented in Tables 1, 2 and 3. It is clear from these tables that the results from the literature and Mathematica numerical integration and the analytical method proposed in this article are satisfactory for all sets of the parameters. The computer time required for the calculation of lattice Green functions is not given in tables due to the fact that the comparison cannot be made as computer times are different because different computers have been used in various studies reported in literature. It is seen from the algorithm presented for lattice Green functions that our CPU times are satisfactory. For instance, for lattice Green functions with sets $t = 2.7; l = 4; m = 2; n = 0; \gamma = 1; N' = 80$ the CPU times taken are about 0.015 s and 0.038 s by using formulas Eq. (10) and Eq. (3.2) in [Morita (1975)], respectively. The calculations have been made on a Pentium 4 PC at 800MHz with 128

Table 1: The comparative values of FCC isotropic lattice Green function for $N = 120$.

t	l	m	n	Eq. (9)	Mathematica numerical integration results
4	2	1	1	5.3062307621299137683455E-03	5.306230761691927860157E-03
3.5	6	0	0	3.6079167865531488070641E-04	3.607916588543670594077E-04
3.8	4	3	3	1.6110394471151018383981E-04	1.611038325096119013263E-04
4.3	3	3	6	6.5403200327858619784236E-06	6.540340964471339796059E-06
7.5	6	0	0	1.8199237462528864261211E-07	1.8199237733671659348793E-07
3.2	8	0	0	5.3955876002755865605106E-04	5.3977039895542549565637E-04
5	7	4	3	1.9477065970304899504571E-07	
4	5	5	6	2.1683762666557503630379E-06	
8	8	8	8	4.0649237534969050228644E-14	
9.4	10	9	9	2.47159951774980913243029E-17	
5.4	12	10	10	3.60265033981501958314341E-14	
6.2	4	4	4	2.85696417818323232226771E-07	
16.2	6	5	5	2.20926265243354104623488E-13	

Table 2: The comparative values of BCC isotropic lattice Green function for $N = 80$.

t	l	m	n	Eq.(10)	Mathematica numerical integration results
1.3	2	2	2	0.015328185311883785799202	0.0153281966390183833347492
3.1	4	2	2	1.57355130627778862489406E-05	1.573711806736570394474906E-05
4.5	4	2	2	2.26195771005028166150425E-06	2.261960562366932080302652E-06
5.6	6	4	4	8.67874138669806066405194E-10	
8.5	2	6	2	2.7430637413164117682923E-10	
2.1	10	10	10	8.5712939506842540919149E-12	
12	8	8	8	1.28450509931113334829599E-17	
1.1	12	12	12	3.15175393922039510877721E-06	

Table 3: The comparative values of SC isotropic lattice Green function for $N = 80$.

t	l	m	n	Eq. (11)	Borwein, Glasser, McPhedran, Wan and Zucker (2013)
4.8	2	1	1	4.92502989502253462788641E-04	4.92502989502253462788641E-04
5.5	4	2	2	7.40028930038766807138731E-07	7.4002893003876680717664E-07
4.1	6	3	3	4.63923075405655182523850E-07	4.6392307669113602187456E-7
3.5	8	4	4	9.55401135846749948703423E-07	9.55942586475958801483921E-07
8.3	10	5	5	4.69853135335122975660583E-18	4.69853135335122975660583E-18
12.6	12	6	6	6.73673151065469189786922E-26	6.73673151065469189786922E-26
18.6	14	12	12	9.58228756482614247423874E-35	9.58228756482614247423874E-35

Table 4: Convergence of derived expression for FCC lattice (Eq.(9)) as a function of summation limit N for $l = 4$; $m = 5$; $n = 5$; $\gamma = 1$.

N	$t = 3.6$	$t = 7.3$
50	4.00398211097867414956991692E-05	7.11326487186323909822468636E-09
60	4.00698936760028318721439499E-05	7.11326487186324022662787621E-09
70	4.00742317957675876305810460E-05	7.11326487186324022676650383E-09
80	4.00748569241555778559327183E-05	7.11326487186324022676652082E-09
90	4.00749472845982961016203988E-05	7.11326487186324022676652082E-09
100	4.00749604069890322643812232E-05	
110	4.00749623224744173196273600E-05	
120	4.0074962603515980801043828E-05	

Table 5: Convergence of derived expression for BCC lattice (Eq.(10)) as a function of summation limit N for $l = 6$; $m = 6$; $n = 6$.

N	$t = 2.3$	$t = 6.7$
20	4.1251372055755555759088E-08	7.488251696692016617660855E-12
30	4.12540274336981408265343E-08	7.488251696737438699096846E-12
40	4.12540281884603820487692E-08	7.488251696737438699393929E-12
50	4.12540281886387878008419E-08	7.488251696737438699393929E-12
60	4.12540281886388275748139E-08	
70	4.12540281886388275835067E-08	
80	4.12540281886388275835087E-08	

MB of RAM. The results show that the three methods almost have the satisfactory precision, but the CPU time of the presented method is less than those of the other methods. In the Tables 4 and 5 list partial summations, corresponding to progressively increasing upper summations limits of equations (9) and (10). Using the new decomposition, the obtained results are presented in Tables 4 and 5 to demonstrate the improvements in convergence rates. The reason for empty columns in Tables 1 and 2 is that the indicated equations (Eqs. (9) and (10)) are not valid for the value of the lattice Green functions parameters. We expect that our new formulae for the FCC, BCC and SC lattice Green functions will be useful, in particular, in the calculations of various lattice structures of solids.

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