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Accurate Evaluation of the Cubic Lattice Green Functions Using Binomial Expansion Theorems

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Abstract A new, simple, and efficient technique for the accurate evaluation of the lattice Green functions is presented. Using binomial expansion theorems, these functions are expressed through the binomial coefficients and basic integrals. The extensive test calculations show that the proposed algorithm in this work is the most efficient method in practical computations. Finally, in order to show the practical use of analytical expressions found some computation examples and comparisons with literature are made.

Keywords Body centered cubic lattice · Anisotropic face centered cubic lattice · Lattice Green's functions · Binomial coefficients

1 Introduction

The evaluation of the lattice Green functions is fundamental to efficient numerical analysis of solid state physics, for example, statistical model of ferromagnetism such as Ising model [1, 2], Heizenberg model [3], spherical model [4], lattice dynamics [5], random walk theory [6], band structure [7], thin films [8]. In the literature, many efficient approaches have been reported for the evaluation of these functions [9–34]. Recently, in [16–25] new mathematical ideas have been introduced, and new algorithm based on the lattice Green functions provides very powerful tools to solve related solid state physics problems. It can be seen from the literature that most of the studies on lattice Green functions are based on elliptic type integral approach. In the literature generally, the formulas for the lattice Green functions have been given in terms of elliptic type integrals and related functions. In the present article we propose that 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 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.

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In this paper, a new approach to the computation of the lattice Green functions are proposed, which considerably improves its capabilities during numerical evaluations in significant cases. We note that the lattice Green functions have been expressed in terms of binomial coefficients and basic integral functions by using binomial expansion theorems for various range of parameter w. However, the series expansions obtained herein give a more accurate and efficient way to compute values for these functions over the entire permissible range of its parameters. Finally, simple examples are presented to compare the effectiveness of the described method with the established formulas for the lattice Green functions in the literature.

2 Definition and General Expressions for the Lattice Green Functions

The anisotropic face-centered and simple cubic lattices Green functions are defined as [20], respectively

$$G_1(\alpha_1, w_1) = \frac{1}{\pi^3}\int_0^\pi\int_0^\pi\int_0^\pi \frac{d\theta_1 d\theta_2 d\theta_3}{w_1 - (\cos\theta_1\cos\theta_2 + \cos\theta_2\cos\theta_3 + \alpha_1\cos\theta_3\cos\theta_1)} \quad (1)$$

$$G_2(\alpha_2, w_2) = \frac{1}{\pi^3}\int_0^\pi\int_0^\pi\int_0^\pi \frac{d\theta_1 d\theta_2 d\theta_3}{w_2 - (\cos\theta_1 + \cos\theta_2 + \alpha_2\cos\theta_3)} \quad (2)$$

where w_1, w_2, α_1 and α_2 are real parameters. In article [18], at the origin for the simple cubic (sc), body-centered cubic (bcc) and face-centered cubic (fcc) lattices a related function of the form

- for simple cubic lattices

$$G_1(w) = \frac{1}{\pi^3}\int_0^\pi\int_0^\pi\int_0^\pi \frac{d\theta_1 d\theta_2 d\theta_3}{w_1 - \frac{1}{3}(\cos\theta_1 + \cos\theta_2 + \cos\theta_3)} \quad (3)$$

- body-centered cubic lattices

$$G_2(w) = \frac{1}{\pi^3}\int_0^\pi\int_0^\pi\int_0^\pi \frac{d\theta_1 d\theta_2 d\theta_3}{w - \cos\theta_1\cos\theta_2\cos\theta_3} \quad (4)$$

- face-centered cubic lattices

$$G_3(w) = \frac{1}{\pi^3}\int_0^\pi\int_0^\pi\int_0^\pi \frac{d\theta_1 d\theta_2 d\theta_3}{w - \frac{1}{3}(\cos\theta_1\cos\theta_2 + \cos\theta_2\cos\theta_3 + \cos\theta_3\cos\theta_1)} \quad (5)$$

where w is real parameter.

In order to obtain the expression for lattice Green functions, (1)–(5), we use the following binomial expansion theorems for an arbitrary real or complex n and $|x| > |y|$ (see [35–37]):

$$(x \pm y)^n = \sum_{m=0}^{\infty} (\pm 1)^m F_m(n) x^{n-m} y^m \quad (6)$$

where $F_0(n) = 1$ and

$$F_m(n) = \begin{cases} n!/[m!(n-m)!] & \text{for integer } n \\ \frac{(-1)^m \Gamma(m-n)}{m!\Gamma(-n)} & \text{for noninteger } n \end{cases} \quad (7)$$

We notice that for $m < 0$ the binomial coefficient $F_m(n)$ in (7) is zero and the positive integer n terms with negative factorials do not contribute to the summation. The quantities $\Gamma(\sigma)$ in (7) are well known Gamma functions defined by [36, 38]

$$\Gamma(\sigma) = \int_0^\infty t^{\sigma-1} e^{-t} dt \tag{8}$$

Now we can move on to the evaluation of the lattice Green functions. Taking into account (6) in (1)–(5) we obtain for lattice Green functions the following relations, respectively

- for $G_1(\alpha_1, w_1)$ function

$$G_1(\alpha_1, w_1) = \frac{1}{\pi^3} \lim_{N\to\infty} \sum_{i=0}^{N} w_1^{-1-i} \sum_{j=0}^{i} \sum_{k=0}^{j} F_j(i) F_k(j) \alpha_1^k I_{i-j+k} I_{i-k} I_j \quad \text{for } w_1 \geq \alpha_1 + 2 \tag{9}$$

- for $G_2(\alpha_2, w_2)$ function

$$G_2(\alpha_2, w_2) = \frac{1}{\pi^3} \lim_{L\to\infty} \sum_{i=0}^{L} w_2^{-1-i} \sum_{j=0}^{i} \sum_{k=0}^{j} F_j(i) F_k(j) \alpha_2^k I_{i-j} I_{j-k} I_k \quad \text{for } w_2 \geq \alpha_2 + 2 \tag{10}$$

- for $G_1(w)$ function

$$G_1(w) = \frac{1}{\pi^3} \lim_{M\to\infty} \sum_{i=0}^{M} \frac{1}{(3w)^i w} \sum_{j=0}^{i} \sum_{k=0}^{j} F_j(i) F_k(j) I_{i-j} I_{j-k} I_k \quad \text{for } w \geq 1 \tag{11}$$

- for $G_2(w)$ function

$$G_2(w) = \frac{1}{\pi^3} \lim_{N'\to\infty} \sum_{i=0}^{N'} \frac{(I_i)^3}{w^{i+1}} \quad \text{for } w \geq 1 \tag{12}$$

- for $G_3(w)$ function

$$G_3(w) = \frac{1}{\pi^3} \lim_{L'\to\infty} \sum_{i=0}^{L'} \frac{1}{(3w)^i w} \sum_{j=0}^{i} \sum_{k=0}^{j} F_j(i) F_k(j) I_{i-j+k} I_{i-k} I_j \quad \text{for } w \geq 1 \tag{13}$$

In (9)–(13) the indexes N, L, M, N' and L' are the upper limits of summations, respectively. The quantities I_n occurring in (9)–(13) are determined by the relation

$$I_n = \int_0^\pi \cos^n \varphi d\varphi \tag{14}$$

In order to evaluate the integral I_n we use the formula [36, 39]

$$I_n = \begin{cases} 0, & \text{if } n \text{ odd} \\ \sqrt{\pi} \frac{\Gamma(\frac{n+1}{2})}{\Gamma(\frac{n}{2}+1)}, & \text{if } n \text{ even} \end{cases} \tag{15}$$

3 Numerical Results and Discussion

The paper has presented an efficient and reliably accurate scheme for the direct evaluation of lattice Green functions. The use of a simple numerical computation tool for modeling and simulation can be beneficial in the applications. To demonstrate the accuracy and efficiency of the methods described above we present several numerical results. On the basis of formulas obtained in this paper we constructed a program for computation of the lattice Green functions using Mathematica 5.0 international mathematical software. One can determine the accuracy of computer results obtained from the series expansion formulae by the use of well-known series and analytical formulae in the literature [18–20, 26]. The examples of computer calculation for the lattice Green functions (9)–(13) are shown in Tables 1, 2, 3, 4, 5 and 6. As can be seen from tables, the calculation results of lattice Green functions show

Table 1 The comparative values of lattice Green function $G_1(\alpha_1, w_1)$ for $N = 100$

α_1	w_1	Equation (9)	Equation (2.19) in [20]
1	4	0.2694162338676949	0.2694162338676949
1.5	4.8	0.2235356974650923	0.2235356974650924
3.6	8.2	0.1311149080401095	0.1311149080401095
8.8	15.1	0.07393384726851592	0.07393384726851592
12.1	22.4	0.04874100147313111	0.04874100147313111
32.4	52.2	0.02157370800729279	0.02157370800729277
64.5	87.2	0.0138515713826008	0.0138515713826008

Table 2 The comparative values of lattice Green function $G_2(\alpha_2, w_2)$ for $L = 100$

α_2	w_2	Equation (10)	Equation (34) in [26]
1.5	5	0.2219662370202358	0.2219662370202359
4.1	8.5	0.1381536869454573	0.1381536869454574
9.3	15.4	0.0825198994943744	0.0825198994943744
19.3	25.6	0.06010979004222174	0.06010979004222174
31.9	52.5	0.02400854072769508	0.02400854072769508
43.1	75.2	0.0162350508674676	0.0162350508674676
84.3	117.5	0.01222189500170813	0.01222189500170813

Table 3 The comparative values of lattice Green function $G_1(w)$ for $M = 100$

w	Equation (11)	Equation (4.13) in [19]
2	0.523378692134745	0.523378692134745
3.8	0.2662865641363358	0.2662865641363358
24.3	0.04116388686510464	0.04116388686510463
41.3	0.02421544155071478	0.02421544155071479
54.8	0.01824918808427292	0.01824918808427292
74.3	0.01345935656575595	0.01345935656575595
174.3	0.005737266127665814	0.005737266127665817

Table 4 The comparative values of lattice Green function $G_2(w)$ for $N' = 100$

w	Equation (12)	Equation (3.3) in [18]
1.8	0.5804119188514366	0.5804119188514366
13.6	0.07357921824417764	0.07357921824417764
33.6	0.0297652012728565	0.0297652012728565
45.6	0.02193114313268718	0.02193114313268718
85.6	0.01168244229360323	0.01168244229360323
145.5	0.00687289281532574	0.00687289281532574
225.5	0.004434600701635175	0.004434600701635175

Table 5 The comparative values of lattice Green function $G_3(w)$ for $L' = 100$

w	Equation (13)	Equation (4.2) in [18]
1.4	0.7623279875448653	0.7623279875448653
5.8	0.1728699424811432	0.1728699424811432
25.8	0.03876460738828515	0.03876460738828516
41.5	0.02409756105746882	0.02409756105746883
81.5	0.01227009322524353	0.01227009322524353
174.4	0.005733960694430566	0.005733960694430564
381.1	0.002603490146674031	0.002603490146674031

Table 6 Convergence of derived expression for $G_3(w)$ as a function of summation limits L'

L'	$w = 18.1$	$w = 24.5$
10	0.05526294497056553	0.04082207323315965
15	0.05526294497056554	0.04082207323315965
20	0.05526294497056554	0.04082207323315965
25	0.05526294497056554	

good rate of convergence with literature under range of parameters [16, 18, 19, 26]. Tables 6 and 7 show that the convergence properties of the two expressions (9)–(10) considered vary widely. As can be seen from Tables 6 and 7, (9) and (10) display the most rapid convergence to the numerical result, with seventeen digits stable and correct by the fiftieth terms in the infinite summation.

The comparative computer time required for the calculation the lattice Green functions are not given in the tables due to the fact that the comparison cannot be made with the different computers used in the literature. It is seen from the algorithm presented for lattice Green functions that our CPU times are satisfactory. For instance, using (10) and (4.26) in [20] for $G_2(8.3, 17.4)$, CPU times takes about 0.05 ms and 0.07 ms, respectively. In conclusion, by means of a binomial expansion theorem, we have obtained the new simple accurate general expressions of the lattice Green functions.

Table 7 Convergence of derived expression for $G_1(\alpha_1, w_1)$ as a function of summation limits N

N	$\alpha_1 = 24.4$; $w_1 = 30.8$	$\alpha_1 = 15.2$; $w_1 = 42.3$
20	0.04132414783034567	0.02447839469388765
30	0.04135511951316856	0.02447839469474832
40	0.04135923109073288	0.02447839469474839
50	0.0413598555600943	0.02447839469474839
60	0.04135995800446002	
90	0.04135997942362581	
120	0.04135997955759622	
150	0.04135997955857419	
180	0.04135997955858199	
190	0.04135997955858204	
200	0.04135997955858204	

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