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On the Evaluation of Lattice Green Functions and Watson-Like Integrals*

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A method is developed whereby lattice Green functions and Watson-like integrals can be readily computed by splitting them into a sum of a power series and an asymptotic series. The method is illustrated by the evaluation of an antiferromagnetic integral and a basic thermodynamic Watson's integral and followed by a treatment of the generalized problem on all the cubic lattices.

I. INTRODUCTION

Recently there has been considerable interest in the evaluation of lattice Green functions (LGF) [1, 2] and thermodynamic extensions of Watson sums (TWS) [3]; the basic Watson sum or integral being a special case of LGF. The essential ingredient of all these three-dimensional integrals is the appearance of the nearest-neighbor dispersion function in a manner which gives a singularity in the integrand. Through investigations to evaluate related integrals arising from the two-sublattice character of an antiferromagnet we have developed a technique which can also be used for the evaluation of LGF and TWS for all the cubic lattices to any desired precision.

These three-dimensional integrals arise as Brillouin zone sums of large lattices that have an essentially continuous distribution of wavevectors, while the Brillouin zone sums are themselves a direct consequence of the lattice periodicity [4]. The dispersion function considered in connection with LGF and TWS is usually restricted to problems that have only nearest-neighbor coupling, though most of the models involved in physical theories become more realistic for longer-ranged interactions.

These integrals may be written in the following manner: Starting with the general LGF,

$$W_i(\eta, l, m, n) = \frac{1}{(2\pi)^3} \iiint_{-\pi}^{\pi} dx\, dy\, dz\, \frac{\cos lx \cos my \cos nz}{\eta - \gamma_i(x, y, z)}, \tag{1}$$

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while the general TWS incorporates the Planck or Bose–Einstein distribution in the following manner:

$$T_i(\alpha, \eta, l, m, n) = \frac{1}{(2\pi)^3} \iiint_{-\pi}^{\pi} dx\, dy\, dz\, \frac{\cos lx \cos my \cos nz}{\exp\{\alpha[\eta - \gamma_i(x, y, z)]\} - 1}. \tag{2}$$

In (1) and (2) we have already converted the Brillouin zone sum to an integral, simplified the wavevector variables to x, y, and z, and arranged that they range over a cubic domain [5, 3]. Other ingredients of (1) and (2) are i, which distinguishes the lattices, $i = 1$ for sc, $i = 2$ for bcc, $i = 3$ for fcc; α physically represents an inverse temperature giving $0 < \alpha < \infty$, while $\eta \neq 1$ represents an external magnetic field (in the magnetic context) giving the range of interest as $1 < \eta < \infty$. l, m, n are integers which could be zero. The quantity $\eta - \gamma_i$ is known as the dispersion function, while γ_i is a structure factor:

$$i = 1, \quad \text{sc}, \qquad \gamma_1 = \tfrac{1}{3}(\cos x + \cos y + \cos z), \tag{3}$$

$$i = 2, \quad \text{bcc}, \qquad \gamma_2 = \cos x \cos y \cos z, \tag{4}$$

$$i = 3, \quad \text{fcc}, \qquad \gamma_3 = \tfrac{1}{3}(\cos x \cos y + \cos y \cos z + \cos x \cos z). \tag{5}$$

The singularities of the integrands of (1) and (2) occur for $\eta = 1$ at the origin $(x, y, z = 0)$ when the dispersion function vanishes. Furthermore, as $\alpha \to 0$, $T_i \to W_i/\alpha$, giving a connection between TWS and LGF.

Arising from the two-sublattice character of antiferromagnets we find the following integrals:

$$V_i(\delta, l, m, n) = \frac{1}{(2\pi)^3} \iiint_{-\pi}^{\pi} dx\, dy\, dz\, \frac{\cos lx \cos my \cos nz}{[\delta^2 - \gamma_i(x, y, z)^2]^{1/2}}, \tag{6}$$

where $\delta > 1$ represents ferrimagnetism, and physically we cannot generate the case for $i = 3$, $i = 1$ being known as the NaCl type, $i = 2$ the CsCl type. There is also some interest in the thermodynamic extension of (6).

Our method is closely related to a technique used in the evaluation of LGF by Maradudin *et al.* [6, 7] where an integral with limits from 0 to ∞ is split to permit the use of both power and asymptotic series. In the present paper we encounter the sum of an infinite number of terms which can be split in an analogous fashion.

Section II shows how a Fourier transform generates an infinite sum for $V_1(1, 0, 0, 0)$ and in Section III a similar result is found for $T_1(\alpha, 1, 0, 0, 0)$, albeit in a different way, and gives a method of evaluating that specific TWS in a region that was previously difficult. Finally, in Section IV, by developing general asymptotic formulas, we consider the problem of calculating the general TWS for all the cubic lattices. In doing so we also find a procedure for the general LGF (involving the split integral version) which was previously given only for the restricted cases of $W_1(\eta, 0, 0, 0)$ [6] and $W_2(\eta, 0, 0, 0)$ [8].[1]

II. Antiferromagnetic Integrals, c'

The quantity arising in antiferromagnetism is actually $V_i(1, 0, 0, 0) - 1$, known as c' [9] and for the CsCl type ($i = 2$) was definitively evaluated by Davis [10]. Davis' method was to expand the square root and integrate term by term. For the NaCl type ($i = 1$), a larger number of terms arise in the expansion, the convergence being very slow.[2] However, another type of expansion can be used profitably.

Writing $V = V_1(1, 0, 0, 0)$, we have explicitly

$$V = \frac{1}{(2\pi)^3} \iiint_{-\pi}^{\pi} \frac{dx\, dy\, dz}{[1 - (1/9)(\cos x + \cos y + \cos z)^2]^{1/2}}. \tag{7}$$

Making use of the Fourier expansion [11],

$$\frac{1}{(1 - t^2)^{1/2}} = \frac{\pi}{2} + \pi \sum_{m=1}^{\infty} J_0(m\pi) \cos(m\pi t), \; | t | < 1, \tag{8}$$

where $J_0(m\pi)$ is a Bessel function of the first kind, one finds

$$V = \frac{\pi}{2} + \pi \sum_{m=1}^{\infty} \frac{J_0(m\pi)}{(2\pi)^3} \iiint_{-\pi}^{\pi} \cos\left[\frac{m\pi}{3} (\cos x + \cos y + \cos z)\right] dx\, dy\, dx. \tag{9}$$

Expanding the cosine and using the following two identities:

$$\frac{1}{(2\pi)} \int_{-\pi}^{\pi} dx \cos(t \cos x) = J_0(t), \tag{10}$$

$$\frac{1}{(2\pi)} \int_{-\pi}^{\pi} dx \sin(t \cos x) = 0, \tag{11}$$

[1] Using a different procedure, Mannari and Kawabata [Extended Watson Integrals and their Derivatives, Research Notes of Dept. of Physics, Okayama University, No. *15* (1964)] evaluated $W_i(\eta, 0, 0, 0)$ for all the cubic lattices.

[2] This expansion can be rewritten in terms of random walk probabilities

$$V = \sum_{n=0}^{\infty} \frac{(2n)!}{n!\, n!\, 2^{2n}} p_{2n}(0, 0, 0).$$

Although this series is slowly convergent it can be accurately evaluated using the Euler–Maclaurin summation formula. [For details, see C. Domb, *Proc. Camb. Phil. Soc.* **50** (1954).]

we have

$$V = \frac{\pi}{2} + \pi \sum_{m=1}^{\infty} J_0(m\pi)\, J_0^3(m\pi/3). \tag{12}$$

This is evaluated as

$$V = \frac{\pi}{2} + \pi \sum_{m=1}^{N} J_0(m\pi)\, J_0^3(m\pi/3) + \text{asymptotic expansion}. \tag{13}$$

The asymptotic expansion is obtained from the expression [11]

$$J_0(x) \approx (2/\pi x)^{1/2} \Big\{\cos(x - \pi/4)\Big[1 - \frac{1^2 3^2}{2!\,(8x)^2} + \cdots\Big] + \sin(x - \pi/4)\Big[\frac{1^2}{1!\,(8x)} - \frac{1^2 3^2 5^2}{3!\,(8x)^3} + \cdots\Big]\Big\}. \tag{14}$$

We found that ten terms in the expansion of (13) were more than sufficient for seven-figure accuracy. Using $N = 4$ gives $c' = 0.1567154$, the same value being obtained with $N = 3, 5$. The best value previously was 0.156, given by Kubo [9] in 1952.

III. Thermodynamic Integral $T_1(\alpha, 1, 0, 0, 0)$

Letting $T(\alpha) \equiv T_1(\alpha, 1, 0, 0, 0)$, we have explicitly that

$$T(\alpha) = \frac{1}{(2\pi)^3} \iiint_{-\pi}^{\pi} \frac{dx\, dy\, dz}{\exp \alpha[1 - (1/3)(\cos x + \cos y + \cos z)] - 1}. \tag{15}$$

For small α (high temperature) we can expand the integrand in a power series about $\alpha = 0$ and integrate term by term with the result

$$T(\alpha) = \frac{W}{\alpha} - \frac{1}{2} + \sum_{m=1}^{\infty} A_m \alpha^{2m-1}, \qquad \alpha < \pi, \tag{16}$$

where W is Watson's integral [5] ($= 1.516386...$) and

$$A_m = \frac{(-1)^{m-1}}{2m} B_m \sum_{k=0}^{m-1} \frac{1}{(2m - 2k - 1)!\, 6^{2k}} \sum_{l=0}^{k} \frac{(2k)!}{[(l)!]^4](k - l)!]^2}, \tag{17}$$

B_m being Bernoulli's numbers. The first few terms of this series have been given before [12].

For large α it is possible to find an asymptotic low temperature expansion [13]. A brief review is appropriate because our method involves a modification of this expansion. Rewriting (15) as a geometrical series and interchanging the order of summation and integration, we get

$$T(\alpha) = \frac{1}{(2\pi)^3} \sum_{m=1}^{\infty} \iiint_{-\pi}^{\pi} dx\, dy\, dz \exp[-m\alpha\{1 - (1/3)(\cos x + \cos y + \cos z)\}]. \tag{18}$$

This can be expressed as a product of modified Bessel functions by using the integral representation [11]

$$I_k(u) = \frac{1}{(2\pi)} \int_{-\pi}^{\pi} \cos kx\, e^{u \cos x}\, dx \tag{19}$$

to obtain[3]

$$T(\alpha) = \sum_{m=1}^{\infty} e^{-m\alpha} I_0^3(m\alpha/3), \qquad 0 < \alpha < \infty. \tag{20}$$

Using the following asymptotic form [11] of $I_0(u)$,

$$I_0(u) \approx [e^u/(2\pi u)^{1/2}][1 + (1/8u) + (9/128u^2) + \cdots] \tag{21}$$

(for u large), (20) may be expressed as

$$T(\alpha) \approx \sum_{m=1}^{\infty} \frac{1}{(2\pi m\alpha/3)^{3/2}} \left[1 + \frac{3}{8(m\alpha/3)} + \cdots\right] \tag{22}$$

$$= \left(\frac{3}{2\pi\alpha}\right)^{3/2} \left[\zeta(3/2) + \frac{9}{8\alpha}\, \zeta(5/2) + \cdots\right] \tag{23}$$

where

$$\zeta(p) = \sum_{m=1}^{\infty} 1/m^p \tag{24}$$

is the Riemann zeta function. This is an asymptotic series so that the results are useful only for large values of α.

[3] This expression appears to have been first developed by Tanaka and Glass (unpublished work) cited in S. H. Charap and E. L. Boyd, *Phys. Rev.* *A*133 (1966), 811.

In order to get definitive results for smaller α, consider the following splitting procedure for (20):

$$T(\alpha) = \sum_{m=1}^{N-1} e^{-m\alpha} I_0^3(m\alpha/3) + (3/2\pi\alpha)^{3/2} [\zeta_N(3/2) + (9/8\alpha)\, \zeta_N(5/2) + \cdots], \qquad 0 < \alpha < \infty, \quad (25)$$

where $\zeta_N(p)$ is a truncated Riemann zeta function

$$\zeta_N(p) = \sum_{m=N}^{\infty} 1/m^p. \quad (26)$$

Due to the fact that

$$\zeta_N(p) \approx \zeta(p)/N^p, \quad (27)$$

for any α we can always find N large enough so that (25) converges in the same manner as (23) does when α is large. By trial and error we find that for six place accuracy N must satisfy the condition

$$N \gtrsim 24/\alpha. \quad (28)$$

With this method one can calculate $T(\alpha)$ for arbitrary α, though for $\alpha \leqslant 1$ it will be more efficient to use the high temperature series (16). For α from 1 to 20

TABLE I

Comparison of three methods for calculating $T(\alpha)$. Ten terms of high temperature series and ten terms of low temperature expansion were used.

α	Low temp. expansion (23)	Extended low temp. expansion (25)	High temp. expansion (16)
0.05		2.98319×10^{1}	2.98319×10^{1}
0.1		1.46722×10^{1}	1.46722×10^{1}
0.5		2.57418	2.57418
1.0		1.09773	1.09773
3.0		2.15227×10^{-1}	2.14803×10^{-1}
5.0		9.13117×10^{-2}	
10.0		2.92608×10^{-2}	
15.0		1.54934×10^{-2}	
20.0	9.94334×10^{-3}	9.94337×10^{-3}	
25.0	7.06705×10^{-3}	7.06705×10^{-3}	
30.0	5.35277×10^{-3}	5.35277×10^{-3}	
60.0	1.87287×10^{-3}	1.87287×10^{-3}	

this method is particularly useful because it fills the gap left by the simple high and low temperature series (see Table I). In this connection we might note that Flax and Raich [3] have proposed a different method that appears to be weak for large α [14] or low temperatures; our present method may be regarded as an extended low temperature series while Flax and Raich [3] have basically extended the high temperature series.

IV. General Method for TWS and LGF for the Three Cubic Lattices

The evaluation of (1) and (2) proceeds in a similar way as for V and $T(\alpha)$. First consider the integral

$$Q_i(\alpha, \eta, l, m, n) = \frac{1}{(2\pi)^3} \int\int\int_{-\pi}^{\pi} \cos lx \cos my \cos nz \exp[-\alpha[\eta - \gamma_i(x, y, z)]]\, dx\, dy\, dz. \quad (29)$$

This integral has an asymptotic (large α) expansion:

$$Q_i(\alpha, \eta, l, m, n) \approx \frac{e^{-\alpha(\eta-1)}}{\alpha^{3/2}} \sum_{k=0}^{K} \frac{a_{k,i}^{(l,m,n)}}{\alpha^k}, \quad (30)$$

where in view of the asymptotic nature of (30) K is chosen according to the precision required [15] (for six-figure accuracy we found 10 usually appropriate), and has a small α expansion.

$$Q_i(\alpha, \eta, l, m, n) = e^{-\alpha\eta} \sum_{k=0}^{\infty} \alpha^k b_{k,i}^{(l,m,n)}, \quad (31)$$

where $a_{k,i}^{(l,m,n)}$ and $b_{k,i}^{(l,m,n)}$ are independent of α and η. The coefficients $a_{k,i}^{(l,m,n)}$ can all be obtained from the following identities:

$$I_k(t) \approx e^t \sum_{l=0}^{K} \frac{C_l^k}{t^{l+1/2}}, \text{ [11]}, \quad (32)$$

$$\frac{1}{x^n} = \frac{1}{\Gamma(n)} \int_0^{\infty} t^{n-1} e^{-xt}\, dt, \quad (33)$$

$$\frac{1}{(x+y)^p} = \frac{1}{x^p} \sum_{k=0}^{\infty} \frac{\Gamma(k+p)}{\Gamma(p)\, k!} (-y/x)^p, \qquad y < x. \quad (34)$$

Making use of (19) and (32) yields for s.c.

$$Q_1(\alpha, \eta, l, m, n) \approx e^{-\alpha(\eta-1)} \sum_{ijk=0}^{K} C_i{}^l C_j{}^m C_k{}^n (3/\alpha)^{i+j+k+3/2}. \tag{35a}$$

Successive applications of (19) and (32)–(34) yield for bcc[4] and fcc

$$\begin{aligned} Q_2(\alpha, \eta, l, m, n) & \\ \approx e^{-\alpha(\eta-1)} & \sum_{ijkrs=0}^{K} C_i{}^l C_j{}^m C_k{}^n \\ & \times \frac{\Gamma(r+i+1/2)\,\Gamma(r+j+1/2)\,\Gamma(k+s+1/2)\,\Gamma(i+j+r+s+1)}{r!\,s!\,\Gamma(i+1/2)\,\Gamma(j+1/2)\,\Gamma(k+1/2)\,\Gamma(i+j+r+1)} \\ & \times (1/\alpha)^{i+j+k+r+s+3/2}, \end{aligned} \tag{35b}$$

$$\begin{aligned} Q_3(\alpha, \eta, l, m, n) & \\ \approx e^{-\alpha(\eta-1)} & \sum_{ijkrs=0}^{K} \sum_{p=0}^{2} C_i{}^l C_j{}^m C_k{}^n \\ & \times \frac{\Gamma(k+s+1/2)\,\Gamma(j+r+s-p+1/2)\,\Gamma(r+i+p+1/2)}{2^{r+s}p!\,(s-p)!\,\Gamma(i+1/2)\,\Gamma(j+1/2)\,\Gamma(k+1/2)} \\ & \times (3/2\alpha)^{i+j+k+r+s+3/2} \end{aligned} \tag{35c}$$

for α large.

The coefficients $b_{k,i}^{(l,m,n)}$ are obtained in a straightforward manner from (29) by expanding the exponential in a power series followed by term-by-term integration. Having calculated the coefficients $a_{k,i}^{(l,m,n)}$ and $b_{k,i}^{(l,m,n)}$ for a specific integral it is straightforward to use them to calculate this integral for all α and η using the splitting technique of Sections II and III.

In order to evaluate $T_i(\alpha, \eta, l, m, n)$ one makes use of the identity

$$\frac{1}{e^x - 1} = \sum_{j=1}^{\infty} e^{-jx} \tag{36}$$

to express (2) as

$$T_i(\alpha, \eta, l, m, n) = \sum_{j=1}^{\infty} Q_i(j\alpha, \eta, l, m, n). \tag{37}$$

[4] Joyce [8] has developed recurrence relationships for the $a_{k,2}^{(0,0,0)}$ which are much more economical to use than (35b); however, for many problems the general expressions we use (35a–c) are quite adequate.

Splitting this sum in a similar manner to (20) and using (30) and (31), (37) becomes

$$T_i(\alpha, \eta, l, m, n) = \sum_{j=1}^{N-1} e^{-j\alpha\eta} \sum_{k=0}^{\infty} (j\alpha)^k b_{k,i}^{(l,m,n)}$$

$$+ \frac{1}{\alpha^{3/2}} \sum_{k=0}^{K} \frac{a_{k,i}^{(l,m,n)}}{\alpha^k} \zeta_N(k + 3/2, \alpha(\eta - 1)), \tag{38}$$

where

$$\zeta_N(p, x) = \sum_{m=N}^{\infty} \frac{e^{-mx}}{m^p} \tag{39}$$

and N is given by (18) (see Appendix).

$W_i(\eta, l, m, n)$ can be expressed in terms of Q_i in the following manner (see (33)):

$$W_i(\eta, l, m, n) = \int_0^{\infty} Q_i(t, \eta, l, m, n)\, dt. \tag{40}$$

Splitting the domain of integration by introducing a parameter s (analogous to N in (38)) and using (30) and (31), we obtain

$$W_i(\eta, l, m, n) = \sum_{k=0}^{\infty} b_{k,i}^{(l,m,n)} \int_0^{s} e^{-t\eta} t^k\, dt$$

$$+ \sum_{k=0}^{K} a_{k,i}^{(l,m,n)} \int_s^{\infty} \frac{e^{-t(\eta-1)}}{t^{k+3/2}}\, dt. \tag{41}$$

In (38) and (41) the infinite sum in the first term has good convergence and corresponds to the power series expansion which would be used to evaluate the Bessel functions in the first terms of (13) and (25).

Conclusion

We have developed procedures for the precision evaluation of generalized TWS and generalized LGF for all the cubic lattices. Many applications to physical problems are now possible. Prior to this work there has been very little discussion of TWS, attention having been concentrated on LGF. Moreover, the concentration there has been on the sc lattice for restricted values of l, m, n. In going beyond the integrals discussed in this work one would probably be involved in more complicated dispersion functions such as those resulting from longer-ranged interactions and then the expansions may become too tedious. For those cases, results to an accuracy better than 1 % may be achieved readily with a more direct numerical integration scheme such as that proposed by Loly and Huett [16].

Appendix

To use the method described in the preceding sections it is important to be able to calculate truncated Riemann zeta functions accurately. This may be achieved by the following rearrangements which overcome the slow convergence of (39) for small x.

$$\begin{aligned}
\zeta_N(p, x) &= \sum_{m=N}^{\infty} (e^{-mx}/m^p) \\
&= \sum_{m=1}^{\infty} \sum_{l=1}^{N} \left[\frac{e^{-(2Nm-l)x}}{(2Nm-l)^p} + \frac{e^{-(2Nm+l-1)x}}{(2Nm+l-1)^p}\right] \\
&= \sum_{m=1}^{\infty} \sum_{l=1}^{N} \sum_{r=0}^{\infty} \frac{e^{-2Nmx}}{(2Nm)^{p+r}} \frac{\Gamma(p+r)}{r!\,\Gamma(p)} [l^r e^l x + (1-l)^r e^{(1-l)x}] \\
&= \frac{1}{N^p} \sum_{r=0}^{\infty} \frac{\zeta(p+r, 2Nx)}{2^{p+r}} \frac{\Gamma(p+r)}{r!\,\Gamma(p)} \left[\sum_{l=1}^{N} \left(\frac{l}{N}\right)^r e^{lx} + \left(\frac{1-l}{N}\right)^r e^{(1-l)x}\right].
\end{aligned}$$

We have finally a rapidly converging series expansion in terms of the usual Riemann zeta functions.

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