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On the calculation of lattice sums arising in Bose–Einstein statistics of quasiparticle excitations

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Abstract. A new method for the calculation of the average occupation number of bosonic quasiparticle excitations valid for *any* type of lattice is proposed. The method is based on the recognition of the connection between lattice Green functions and generalized Watson integrals, on one hand, and on a very simple differentiation technique, which renders unnecessary and artificial to this problem more sophisticated Laplace-transform summation procedures. The mean-field approximation to Green function theories of ferromagnetism arises naturally as the zeroth term in the obtained summation formulae. The results have been specified completely for the three cubic lattices. They are new for the simple cubic and face-centred cases, whereas a certain redundancy is removed from the known body-centred cubic result. Applications of the method to more complex sums, such as, for instance, the thermodynamic sum for the total energy of the quasiparticles, are straightforward.

A new three-position recursion relation for the calculation of frequently occurring triple geometric integrals in the face-centred cubic case has also been found. It originates from a corresponding relation for a relevant Heun function.

1. The problem

The average occupation number of bosonic quasiparticle excitations is a very important quantity which is relevant to a variety of physical lattice problems (cf, for example, Tyablikov 1967, Joyce 1972a, b, Tahir-Kheli 1975, Viljoen and Lemmer 1980, Mattis 1985, and references therein). Both thermodynamic and kinetic properties depend crucially on the possibility of calculating this quantity to a satisfactory accuracy for different ranges of temperature. It seems astonishing that the problem has not received the due attention even for the highly symmetric lattices such as the cubic ones.

The sums to be calculated below are over all reciprocal-lattice vectors k in the first Brillouin zone of a crystal with N sites:

$$\Phi(Q) = \frac{1}{N}\sum_{k}\frac{1}{\exp[2Q(1-\gamma_k)]-1} \tag{1}$$

where Q is a non-negative parameter $0 \leqslant Q \leqslant \infty$

$$\gamma_k = J(k)/J(0) \tag{2}$$

and

$$J(k) = \sum_{R} J(R)\mathrm{e}^{\mathrm{i}k\cdot R}. \tag{3}$$

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In the theory of localized magnetism, $J(R)$ is the exchange coupling between moments sitting on sites f and g with $R = f - g$. The physical interpretation of the parameter Q and of the sum Φ will not be our main concern here, although some important applications and possible extensions will be briefly discussed.

Most of the work related to calculating the quantity $\Phi(Q)$ concerns lattices of cubic symmetry. There, the low- and high-temperature expansions (corresponding to large and small Q, respectively) are well known (Tahir-Kheli and ter Haar 1962, Tyablikov 1967). In an attempt to cover the *whole* range of temperatures, and not just the asymptotical limits, Flax and Raich (1969) suggested an approximate analytical procedure to calculate the sum for all Q and all cubic lattices. In fact, they considered a somewhat more complicated sum which is of importance for certain anisotropic models and which will be found in the present paper practically by inspection of our main results. Loly (1971) criticized the insufficient accuracy of their result for large Q (low temperature) and, together with Austen (Austen and Loly 1973), elaborated a numerical procedure to treat all values of Q. Wintucky (1972) extended the method of Flax and Raich and obtained the whole series (of which the latter authors had only given the first two terms), but only for the body-centred cubic (BCC) lattice. He then observed an improvement in the large-Q convergence, the checking comparison being carried out for the simplest case of lowest spin value $S = \frac{1}{2}$ only.

2. The method

The method we suggest has several advantages. First, in its general part, it applies equally well to *any* type of crystal lattice. Second, it makes contact with, and uses results from, the exhaustively studied field of lattice Green functions on different lattices (Joyce 1971a, b, 1973, Abe and Katsura 1973). Third, it is very much simpler and involves simple differentiation techniques only, whereas Flax and Raich (1969) and Wintucky (1972) applied Laplace transformations and had to deal with the resulting integrals even in the simplest cubic cases. Besides, even the known BCC lattice case acquires a more natural form and this allows for the immediate recognition of important physical facts, apart from its significance for the ensuing numerical computations.

The starting point is to transform the sum to

$$\Phi(Q) = \frac{1}{2N} \sum_k \{\coth[Q(1 - \gamma_k)] - 1\}. \tag{4}$$

It is then converted to an integral over the Brillouin zone according to well known rules; this is harmless, because there is no condensing mode of the type encountered in Bose–Einstein condensation (Landau and Lifshitz 1969). Implementing trivial substitutions and letting the sum in the dispersion part (3) run over nearest-neighbour sites only, one has

$$\frac{1}{N} \sum_k \longrightarrow \frac{1}{\pi^3} \int\int\int_0^\pi dx_1\, dx_2\, dx_3. \tag{5}$$

One then makes use in equation (4) of the series representation (Abramowitz and Stegun 1965)

$$\coth(\pi\xi) = \frac{1}{\pi\xi} + \frac{2}{\pi} \sum_{n=1}^{\infty} \frac{\xi}{n^2 + \xi^2} \tag{6}$$

with $\xi \equiv Q(1-\gamma)/\pi$ with the result

$$\Phi(Q) = I_1(Q) + I_2(Q) - \tfrac{1}{2} \tag{7}$$

where

$$I_1(Q) = \frac{1}{2Q}\frac{1}{\pi^3}\iiint_0^\pi \mathrm{d}x_1\,\mathrm{d}x_2\,\mathrm{d}x_3(1-\gamma)^{-1} \tag{8}$$

and

$$I_2(Q) = \frac{1}{2Q}\frac{1}{\pi^3}\sum_{n=1}^{\infty}\iiint_0^\pi \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z\left[\frac{1}{1-\gamma+\mathrm{i}\frac{\pi}{Q}n} + \frac{1}{1-\gamma-\mathrm{i}\frac{\pi}{Q}n}\right]. \tag{9}$$

Let us introduce the functions $P(\xi)$

$$P(\xi) = \frac{1}{\pi^3}\iiint_0^\pi \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z\,(1-\xi\gamma)^{-1} \qquad |\xi| \leqslant 1. \tag{10}$$

Despite the uniformity of notation, the lattice type enters non-trivially via the respective γ from equation (2). With due specification, these functions are the respective lattice Green functions (Joyce 1971a, b, 1973, Abe and Katsura 1973). The $P(\xi)$'s are also known as generalized Watson integrals, because they reduce to the original Watson integrals (Watson 1939) when their argument takes the value one. Our problem is thus reduced to the Watson integrals $P(1)$ via

$$I_1(Q) = \frac{1}{2Q}P(1) \tag{11}$$

and to a sum involving their generalizations $P(\xi)$

$$I_2(Q) = \frac{1}{2Q}\sum_{n=1}^{\infty}\left[\xi_n P(\xi_n) + \xi_n^* P^*(\xi_n)\right] \tag{12}$$

where

$$\xi_n = \frac{1}{1+\mathrm{i}\frac{\pi}{Q}n} = \frac{z}{z+n} \tag{13}$$

with

$$z \equiv -\mathrm{i}Q/\pi = \mathrm{i}y \qquad y \equiv -Q/\pi. \tag{14}$$

Note that $|\xi_n| \leqslant 1$ and this holds regardless of the lattice type. One can, therefore, make use of the convergent expansion

$$P(\xi_n) = \sum_{k=0}^{\infty} A_k \cdot \xi_n^k. \tag{15}$$

The coefficients $\{A_k\}$ are defined by the respective triple trigonometric integrals:

$$A_k = \frac{1}{\pi^3}\iiint_0^\pi \mathrm{d}x_1\,\mathrm{d}x_2\,\mathrm{d}x_3\,(\gamma)^k \tag{16}$$

known also as $F(k)$ in the cubic cases (Tahir-Kheli and ter Haar 1962). The convergence of the above series on the unit circle is guaranteed by the observation, which will be repeatedly important below, that $P(\xi = 1)$ are exactly the original Watson integrals in the case of the cubic lattices (Watson 1939) or their direct analogues for other geometries. Interchanging the order of summation, one obtains from equation (12)

$$I_2(Q) = \frac{1}{2Q}\sum_{k=0}^{\infty} A_k z^{k+1} \sum_{n=1}^{\infty}\left[\frac{1}{(z+n)^{k+1}} + \frac{1}{(z^*+n)^{k+1}}\right]. \tag{17}$$

The approach we suggest is new in two respects which can be most easily comprehended by looking at equation (17). First, a very simple calculation of the sum over n is suggested which is valid for *any* type of lattice and in which no need arises to use special summation techniques and Laplace transforms (Flax and Raich 1969, Wintucky 1972). In fact, nothing more complex than expansion (6) will be needed to carry out the said summation. Second, the A_k's for *all* cubic lattices are calculated for *any* k by making contact with work by Joyce (1973) on lattice Green functions. Note that the method is completely general with regard to the type of lattice considered, so long as one does not have to specify the coefficients A_k. In what follows, we prefer to characterize completely the physically most important cases of cubic symmetry and postpone for further investigation the cases of lower symmetry.

3. General and simple calculation of $\Phi(Q)$

Having recognized, in equation (17), the general and particular parts of the mathematical problem we are facing, in this section, we proceed as far as we can without loss of generality, i.e. no special type of lattice is envisaged. Remembering that $z = \mathrm{i}y = -\mathrm{i}Q/\pi$ (equation (14)), one easily rewrites the expression as

$$I_2(Q) = \frac{1}{2Q}\sum_{k=0}^{\infty} A_k y^{k+1} \sum_{n=1}^{\infty}\left[\frac{1}{(y+\mathrm{i}n)^{k+1}} + \frac{1}{(y-\mathrm{i}n)^{k+1}}\right]. \tag{18}$$

The crucial observation is that, by simple differentiation rules,

$$\frac{1}{(y \pm \mathrm{i}n)^{k+1}} = \frac{(-1)^k}{k!}\frac{\partial^k}{\partial y^k}\left(\frac{1}{y \pm \mathrm{i}n}\right) \tag{19}$$

whereby

$$I_2(Q) = \frac{1}{2Q}\sum_{k=0}^{\infty}(-1)^k A_k \frac{y^{k+1}}{k!}\frac{\mathrm{d}^k}{\mathrm{d}y^k}\left[\sigma(y)\right] \tag{20}$$

with the definition

$$\sigma(y) \equiv \sum_{n=1}^{\infty}\left(\frac{1}{y+\mathrm{i}n} + \frac{1}{y-\mathrm{i}n}\right) = \sum_{n=1}^{\infty}\frac{2y}{y^2+n^2}. \tag{21}$$

From equation (6), this time used in the opposite direction,

$$\sigma(y) = \pi\mathcal{L}(\pi y) \tag{22}$$

where $\mathcal{L}(x)$ is the Langevin function, $\mathcal{L}(x) \equiv \coth x - 1/x$. Since $y = -Q/\pi$, one has

$$\sigma(Q) = -\pi\mathcal{L}(Q)$$

and

$$\frac{\mathrm{d}^k}{\mathrm{d}y^k} = (-\pi)^k \frac{\mathrm{d}^k}{\mathrm{d}Q^k}.$$

Thus, we find that for *any* lattice

$$I_2(Q) = \frac{1}{2Q}\sum_{k=0}^{\infty}(-1)^k A_k \frac{Q^{k+1}}{k!}\frac{\mathrm{d}^k}{\mathrm{d}Q^k}\mathcal{L}(Q). \tag{23}$$

If the last expression is inserted into equation (7), one would obtain for all cubic lattices the type of result which Wintucky (1972) reported for the BCC lattice. The final expression would, however, be somewhat redundant if kept in the resulting form. First and qualitatively, the persistence of the Langevin function in a *quantum* statistical problem such as the calculation of the sum $\Phi(Q)$ would signal a *classical* (spin quantum number $S \to \infty$) character to the assumptions of the underlying theory, which is not the case. Second, the reported BCC result (Wintucky 1972) involves one and the same quantity, namely the original Watson integral $P(1)$ for the BCC lattice (Watson 1939), which appears twice in different disguises and with opposite signs. More precisely, it seems to have been overlooked that

$$\frac{4K^2(1/\sqrt{2})}{\pi^2} - \sum_{k=0}^{\infty} A_k \cdot 1^k \equiv 0 \tag{24}$$

where $K(k)$ is the complete elliptic integral of the first kind.

It is, therefore, much more appealing and technically important to proceed as below. One uses the fact that

$$\mathcal{L}^{(k)}(Q) = (\coth Q)^{(k)} - (-1)^k k!/Q^{k+1}$$

and finds from equation (23) that

$$I_2(Q) = \frac{1}{2}\sum_{k=0}^{\infty}(-1)^k A_k \frac{Q^k}{k!}\frac{\mathrm{d}^k}{\mathrm{d}Q^k}(\coth Q) - \frac{1}{2Q}P(1). \tag{25}$$

The second term is precisely equal to $I_1(Q)$ of equation (7) so that

$$\Phi(Q) = \frac{1}{2}\sum_{k=0}^{\infty}(-1)^k A_k \frac{Q^k}{k!}\frac{\mathrm{d}^k}{\mathrm{d}Q^k}(\coth Q) - \tfrac{1}{2}. \tag{26}$$

According to equation (16), $A_0 = 1$ for all types of lattice. This simple observation provides for an equivalent and physically more appealing form of $\Phi(Q)$, namely

$$\Phi(Q) = \Phi_0 + \frac{1}{2}\sum_{k=1}^{\infty}(-1)^k A_k \frac{Q^k}{k!}\frac{\mathrm{d}^k}{\mathrm{d}Q^k}(\coth Q) \tag{27}$$

where

$$\Phi_0 = \frac{1}{\exp(2Q) - 1}. \tag{28}$$

In fact, Φ_0 corresponds exactly to the mean-field approximation in the theory of ferromagnetism (Callen and Shtrikman 1965), whereas $\coth(x)$ is a function which typically arises in a number of quantum statistical *bosonized* problems (Abrikosov *et al* 1965, Landau and Lifshitz 1969). At the same time, the identification of the mean-field approximation sheds light on the physical interpretation of the parameter Q: it is essentially the generalized effective field (Callen and Shtrikman 1965).

Furthermore, $\Phi(Q)$ can be cast into the form of an operator expression. Defining the operator

$$\hat{D} \equiv Q\frac{\mathrm{d}}{\mathrm{d}x}$$

one can rewrite equation (26) as

$$\Phi(Q) = \tfrac{1}{2}[\hat{F}(Q)\coth x]_{|x=Q} - \tfrac{1}{2} \tag{29}$$

where the operator $\hat{F}$ is given by

$$\hat{F}(Q) = \sum_{k=0}^{\infty}(-1)^k A_k \frac{(\hat{D})^k}{k!} \tag{30}$$

(for the very interesting specification for the BCC case, see below).

4. The coefficients A_k

As discussed at the end of section 2, it is here that one first has to specify the type of lattice and, thus, reduce the generality of treatment in order to obtain definite lattice-specific results. Below, we concentrate on the three lattices of cubic symmetry: body-centred cubic (BCC), simple cubic (SC), and face-centred cubic (FCC). From the definition of A_k (16), we have explicitly

$$A_k(\mathrm{BCC}) = \frac{1}{\pi^3}\int\int\int_0^{\pi} \mathrm{d}x_1\,\mathrm{d}x_2\,\mathrm{d}x_3\,(\cos x_1 \cdot \cos x_2 \cdot \cos x_3)^k \tag{31}$$

$$A_k(\mathrm{SC}) = \frac{1}{\pi^3}\frac{1}{3^k}\int\int\int_0^{\pi} \mathrm{d}x_1\,\mathrm{d}x_2\,\mathrm{d}x_3\,(\cos x_1 + \cos x_2 + \cos x_3)^k \tag{32}$$

$$A_k(\mathrm{FCC}) = \frac{1}{\pi^3}\frac{1}{3^k}\int\int\int_0^{\pi} \mathrm{d}x_1\,\mathrm{d}x_2\,\mathrm{d}x_3\,(\cos x_1\cos x_2 + \cos x_2\cos x_3 + \cos x_3\cos x_1)^k. \tag{33}$$

The specification of γ for the three cubic cases is obvious from the above three equations and comes about by carrying out the summation over nearest neighbours in equation (3) in the respective cases. The A_k's for the lowest values of k are easily computed, but we need a general expression for any k. A common property shared by the lattice Green functions for the BCC and SC cases is that they are symmetric under reflection. Hence, for both lattices, the A_k's vanish identically for $k = 2p + 1$. This property does not hold for the FCC lattice.

4.1. The BCC case

This is the simplest case and the result for A_k is easy to obtain. Namely,

$$A_{2k+1} = 0 \qquad A_{2k} = (a_k)^3 \qquad a_k = \frac{\Gamma(k+1/2)}{\sqrt{\pi}\Gamma(k+1)} \tag{34}$$

or, more pragmatically,

$$a_{k+1} = \frac{(2k+1)!!}{(2k+2)!!} = \frac{2k+1}{2k+2}a_k \qquad a_0 = 1 \tag{35}$$

($\Gamma(z)$ is the gamma function). The third power arises because of the trivial factorization of the corresponding trigonometric integral in this case. The A_k's up to $k = 6$ are given in table 1. One then reads the final result for the BCC case from equations (27) and (34):

$$\Phi(Q)|_{\mathrm{BCC}} = \Phi_0 + \frac{1}{2}\sum_{k=1}^{\infty} A_{2k}\frac{Q^{2k}}{(2k)!}\frac{\mathrm{d}^{2k}}{\mathrm{d}Q^{2k}}(\coth Q). \tag{36}$$

It is in this case that the operator form (30) is especially intriguing. In fact, doing some straightforward manipulations on equation (26), the most involved being the duplication formula for the gamma-function (Abramowitz and Stegun 1965), one obtains a *closed-form operator expression of the hypergeometric type*:

$$\Phi(Q)|_{\mathrm{BCC}} = \tfrac{1}{2}\,{}_2F_3(\tfrac{1}{2}, \tfrac{1}{2}; 1, 1, 1; \tfrac{1}{4}\hat{D}^2)(\coth x)|_{x=Q} - \tfrac{1}{2} \tag{37}$$

where ${}_2F_3$ is a generalized hypergeometric function (Slater 1966) which acts here as an operator because of the nature of its argument. Note that the 'ordinary' function ${}_2F_3(\frac{1}{2}, \frac{1}{2}; 1, 1, 1; t^2/4)$ is precisely the Laplace transform of the function (Joyce 1971b)

$$R(\zeta) \equiv \frac{1}{\zeta}P\left(\frac{1}{\zeta}\right). \tag{38}$$

This is an indication of the possibility of another derivation, since the initial summation in equation (12) runs precisely over $R(\xi_n^{-1})$. We believe that the simple calculation reported above is sufficiently clear and convincing, although the connection with $R(\zeta)$ and the operator expression might still be useful in generalizations and might offer new insights.

Table 1. The coefficients A_k for the three cubic lattices up to $k = 6$; the c_k's are given for the FCC case only.

k	A_{2k}(BCC)	A_{2k}(SC)	c_k(FCC)	A_k(FCC)
0	1	1	1	1
1	$\left(\frac{1}{2}\right)^3$	$\frac{1}{3^1}\frac{1}{2}$	0	0
2	$\left(\frac{3}{8}\right)^3$	$\frac{1}{3^2}\frac{5}{8}$	$\frac{1}{24}$	$\frac{1}{3^2}\frac{3}{4}$
3	$\left(\frac{5}{16}\right)^3$	$\frac{1}{3^3}\frac{155}{144}$	$\frac{1}{72}$	$\frac{1}{3^3}\frac{3}{4}$
4	$\left(\frac{35}{128}\right)^3$	$\frac{1}{3^4}\frac{2485}{1152}$	$\frac{7}{576}$	$\frac{1}{3^4}\frac{135}{64}$
5	$\left(\frac{63}{256}\right)^3$	$\frac{1}{3^5}\frac{3619}{768}$	$\frac{7}{864}$	$\frac{1}{3^5}\frac{135}{32}$
6	$\left(\frac{231}{1024}\right)^3$	$\frac{1}{3^6}\frac{902761}{82944}$	$\frac{805}{124416}$	$\frac{1}{3^6}\frac{165}{16}$

4.2. The SC case

Here, once again, $A_{2k+1} = 0$, because of the reflection symmetry of the respective lattice Green function $P(\xi)$. The result for A_{2k} can be read off from work by Joyce (1973):

$$A_{2k} = \frac{1}{3^{2k}} \frac{\Gamma(k+1/2)}{\Gamma(k+1)} {}_3F_2(\tfrac{1}{2}, -k, -k; 1, 1; 4) \tag{39}$$

where ${}_3F_2(\frac{1}{2}, -k, -k; 1, 1; 4)$ is a terminating hypergeometric series (Slater 1967). A practically more useful result with regard to the application of our final results is the three-position recursion relation (Joyce 1973):

$$A_{2(k+1)} = \frac{1}{36(k+1)^3}\{2(2k+1)(10k^2+10k+3)A_{2k} - k(4k^2-1)A_{2(k-1)}\} \tag{40}$$

with $A_{-2} \equiv 0$ and $A_0 = 1$ ($k \geqslant 0$).

In fact, the derivation of the recursion (40) by Joyce (1973) was based on a relation due to Watson (1910). Here we suggest an alternative recursion formula which derives from known properties of certain Heun functions for the lattice problem under discussion. The same procedure is then used for the FCC case below so that the A_k's in the SC and FCC cases are treated on an equal footing, the underlying common feature being the fact that in both cases the respective lattice Green functions $P(\xi)$ can be cast as the square of a Heun function.

In particular, for the SC case, one has (Joyce 1973)

$$P(\xi)|_{SC} = [F(9, -\tfrac{3}{4}; \tfrac{1}{4}, \tfrac{3}{4}, 1, \tfrac{1}{2}; x)]^2 \qquad x = \xi^2. \tag{41}$$

On the other hand, F is defined for small x by the series

$$F(a, b; \alpha, \beta, \gamma, \delta; \xi^2) = \sum_{n=0}^{\infty} c_n \xi^{2n} \tag{42}$$

where the coefficients $\{c_n\}$ satisfy another three-position recursion relation

$$a(n+1)(n+\gamma)c_{n+1} = \{(a+1)n^2 + [\gamma + \delta - 1 + (\alpha + \beta - \delta)a]n - b\}c_n - (n - 1 + \alpha)(n - 1 + \beta)c_{n-1} \qquad (n \geqslant 0) \tag{43}$$

with $c_{-1} \equiv 0$ and $c_0 = 1$ (Joyce 1973). Therefore,

$$P(\xi)|_{SC} = \sum_{m,n=0}^{\infty} c_m c_n \xi^{2(m+n)} = \sum_{p=0}^{\infty} \left(\sum_{q=0}^{p} c_{p-q} c_q \right) \xi^{2p} = \sum_{k=0}^{\infty} A_{2k} \xi^{2k} \tag{44}$$

where the double infinite summation by rows and columns is converted to summation by diagonals (Whittaker and Watson 1962). A trivial change of the summation index ($p \to k$) was used in the last step, while the coefficients of the (now) single infinite summation are identified as A_{2k} by virtue of the uniqueness of the convergent expansion for $P(\xi)$ ($|\xi| \leqslant 1$). That is,

$$A_{2k}(SC) = \sum_{q=0}^{k} c_{k-q} c_q \tag{45}$$

where, specifying equation (43) to the SC case of equation (41), one computes the c_n's from

$$c_{n+1} = \frac{1}{9 \cdot 16 \cdot (n+1)^2}[4(40n^2 + 20n + 3)c_n - (4n-3)(4n-1)c_{n-1}] \quad (46)$$

with $c_{-1} \equiv 0$ and $c_0 = 1$.

The expressions (40) and (45) of course give identical results, as can easily be checked for the lowest values of k. The first several coefficients are given in table 1. From equations (27), (45) and (46), one finds the relevant solution for this case as

$$\Phi(Q)|_{SC} = \Phi_0 + \frac{1}{2}\sum_{k=1}^{\infty} A_{2k}\frac{Q^{2k}}{(2k)!}\frac{d^{2k}}{dQ^{2k}}(\coth Q). \quad (47)$$

4.3. The FCC case

As noted above, now $P(\xi)$ is no longer an even function of its argument so that, in principle, all A_k's from equation (15) can be non-zero. To our knowledge, there are no closed-form or recursion-type expressions for the A_k's available in the literature for this case. We, therefore, implement the Heun-function procedure which was just described for the SC case. One has (Joyce 1973)

$$P(\xi)_{FCC} = [F(-3, 0; \tfrac{1}{2}, 1, 1, 1; \xi)]^2. \quad (48)$$

Using the expansion $F(a, b; \alpha, \beta, \gamma, \delta; \xi) = \sum_{n=0}^{\infty} c_n \xi^n$ as above, one finds

$$P(\xi)_{FCC} = \sum_{k=0}^{\infty} A_k \xi^k$$

with

$$A_k = \sum_{q=0}^{k} c_{k-q} c_q.$$

The difference now is that the c_n's are defined by another three-position recursion relation:

$$c_{n+1} = \frac{n}{6(n+1)^2}[(4n+1)c_n + (2n-1)c_{n-1}]. \quad (49)$$

This straightforward way of calculating the coefficients A_k(FCC) for any k has escaped attention and is, in fact, new. Note that the proper triple trigonometric integrals

$$A_k^{\Gamma}(\text{FCC}) \equiv 3^k \pi^3 A_k(\text{FCC})$$

can be easily obtained for *any* k. Thus, the adopted procedure leads naturally to an important by-product. The c_k's and the A_k's for several values of k are collected in table 1 together with the A_{2k}'s for the other cubic lattices. With the A_k's thus specified and from equations (27) and (49), the final result for the FCC case reads

$$\Phi(Q)_{FCC} = \Phi_0 + \frac{1}{2}\sum_{k=1}^{\infty}(-1)^k A_k \frac{Q^k}{k!}\frac{d^k}{dQ^k}(\coth Q). \quad (50)$$

5. Generalizations

A more general sum which has been evaluated by Wintucky (1972) for the BCC case only can easily be found essentially by inspection of the above procedures. The sum is

$$\Phi(Q,\eta)=\frac{1}{N}\sum_k \frac{1}{\exp[2Q(1-\eta\gamma_k)]-1} \qquad 0\leqslant\eta\leqslant 1. \tag{51}$$

Starting with equation (1), the effect of $\eta\neq 1$ in equations (7)–(10) is to appear as an extra factor multiplying γ:

$$\gamma \longrightarrow \eta\gamma.$$

By inspection of equation (10), one traces down that

$$\xi \longrightarrow \eta\xi$$

and, hence,

$$\tilde{\xi}_n(0\leqslant\eta\leqslant 1)=\eta\xi_n(\eta=1)=\eta\frac{z}{z+n}. \tag{52}$$

The extended ($\eta\neq 1$) expressions for $I_{1,2}(Q,\eta)$ now read:

$$I_1(Q,\eta)=\frac{1}{2Q\eta} \tag{53}$$

$$I_2(Q,\eta)=\frac{1}{2Q\eta}\sum_{n=1}\{\tilde{\xi}_n P(\tilde{\xi}_n)+\tilde{\xi}_n^* P(\tilde{\xi}_n^*)\}. \tag{54}$$

As $\eta\leqslant 1$, the convergence of expansion (15) is only improved. The sums over k acquire a factor of η^{2k+1}, while the crucial expression $\sigma_k(y)$ from equation (22) remains unaltered. Therefore, one immediately arrives at the final result

$$\Phi(Q,\eta)=\Phi_0+\frac{1}{2}\sum_{k=1}^{\infty}(-1)^k A_k\frac{(\eta Q)^k}{k!}\frac{\mathrm{d}^k}{\mathrm{d}Q^k}(\coth Q) \tag{55}$$

for any type of lattice. The particularization to the cubic lattices proceeds as above.

A further generalization is the calculation of the sum which gives, up to a factor which is irrelevant to the present discussion, the *total* energy as a sum over the energy of the individual quasiparticles:

$$\tilde{\Phi}(Q,\eta)=\frac{1}{N}\sum_k \frac{\gamma_k}{\exp[2Q(1-\eta\gamma_k)]-1}. \tag{56}$$

Apart from its fundamental thermodynamic significance, the sum is important in the improved Callen decoupling scheme of the Green function approach to ferromagnetism where the renormalization of the energy spectrum of the excitations is non-trivial and is dominated by the total energy, and not by the net magnetization, over a certain range of temperatures (Callen 1963, Tahir-Kheli 1975). It is plain to see that the presence of the extra factor of γ_k in the numerator of equation (56) raises by one the power of the dispersion factor γ_k in the integrals A_k in equations (31)–(33). The same method works unrestrictedly, while the minute adjustments can be carried out easily.

6. Summary

A new method for the calculation of the average occupation number $\Phi(Q)$ of bosonic quasiparticle excitations for any type of lattice has been presented. The method is very simple and, in its general part, is valid for *all* types of crystal lattice. Its crucial components are: (i) simple differentiation technique in taking the summation over k in equation (17) which completely avoids former sophisticated methods such as Laplace transformations and additional integrations arising thereupon—in fact, no special knowledge beyond expansion (6) for $\coth x$ is required; and (ii) the recognition of the connection with the theory of the lattice Green functions and the implementation of work done in this field.

The general new result is given by equation (27) and is characterized in detail for the BCC, SC and FCC cases separately (only the BCC result in a redundant form was known before). The mean-field approximation arises naturally as the zeroth term of the series representation of $\Phi(Q)$ and reveals the physical interpretation of the parameter Q; up to a numerical spin-dependent factor, it is the generalized effective field in magnetic theory.

An operator formulation of the general result has been presented. It is particularly intriguing in the BCC case, where the sum Φ can be cast as a closed-form *operator* hypergeometric function ${}_2\hat{F}_3$. Its ordinary (non-operator) counterpart is the Laplace transform of the function $R(\zeta) = \frac{1}{\zeta}P(\frac{1}{\zeta})$ studied previously in lattice statistical problems.

The required coefficients A_k and, hence, the frequently occurring triple trigonometric integrals, have been systematized. While the A_k's in the BCC case are well known and there is a recursion relation for them in the SC case, a novel procedure valid for both the SC and FCC cases has been developed. It is based on previous knowledge about the respective Heun functions the squares of which give the lattice Green functions $P(\xi)_{\mathrm{SC}}$ and $P(\xi)_{\mathrm{FCC}}$; the calculation of the A_k's for *any* k involves a straightforward summation over the coefficients c_n (equations (46) and (49)) which are calculated from simple three-position recursion relations. The results for $A_k(\mathrm{FCC})$ for general k have not been reported so far.

The generalization to the more complex sum $\Phi(Q, \eta)$ with $0 \leqslant \eta \leqslant 1$ (equation (51)) is then found by inspection. This sum is relevant to the Green function theory of anisotropic ferromagnets where the parameter η measures the strength of the anisotropy ($\eta = 1$ corresponding to the isotropic case). The additional total-energy sum $\tilde{\Phi}(Q, \eta)$ of equation (56), which is relevant to more elaborate decoupling schemes of the Green function approach to the theory of ferromagnetism, can be derived from the reported results without any difficulty.

Finally, the particular interest in calculating as completely as possible the average occupation number of quasiparticle excitations is motivated by the desire to go beyond the mean-field approximation in determining the temperature dependence of magnetic anisotropy and magnetostriction coefficients within the very general theory of Callen and Callen (1965) (du Tremolet 1993) which was recently extended and supplemented by an efficacious parametric approach (Millev and Fähnle 1994a, b). Preliminary work in this direction is under way (Millev and Fähnle 1994c).

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