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Equivalence between the methods involving Fourier series and the Poisson's summation formula and evaluation of a class of lattice sums in arbitrary dimensions

Mirabeau Dias and A N Chaba

Universidade Federal da Paraíba, Departamento de Física, CCEN, João Pessoa, Paraíba, Brasil

Abstract. ~~We bring out~~ The similarities between the Fourier series method and the Poisson's summation formula method (are brought out) by evaluating the lattice sum $g(\vec{r}) \equiv \sum_{\vec{\tau}} \exp(-\lambda\,|\vec{r}-\vec{\tau}|)/|\vec{r}-\vec{\tau}|$ over a Bravais lattice $\{\vec{\tau}\}$ in three dimensions, λ and $\vec{r}$ being independent of $\vec{\tau}$. It is ~~We~~ shown that the two approaches are actually equivalent by proving that the Poisson's summation formula (in any dimensionality) can, itself, be derived from the Fourier series method. ~~Also we present~~ An expression (is also presented) ready for quick use, for a class of lattice sums $\sum_{\vec{\tau}} F(|\vec{r}-\vec{\tau}|)$ over a Bravais lattice $\{\vec{\tau}\}$ in arbitrary dimensions. (Author)

1. Introduction

Many authors (Born and Huang 1954, Ziman 1964, Ahrony and Fisher 1973, Medeiros e Silva and Hokross 1980) use the Fourier series (FS) method for evaluating lattice sums or transforming a sum over a direct lattice into one over a reciprocal lattice which is required as an intermediate step in the well known Ewald's method. Others (Hall 1976, Chaba 1980, Freitas and Chaba 1983) use the Poisson's summation formula (PSF) (Stein and Weiss 1971) method for similar purposes. It appears that some workers are aware of only the former approach and others only of the latter. The PSF method also involves the use of Fourier transform and, therefore, the calculations in the two methods are expected to be quite a bit similar to each other. In section 2, we bring out this similarity by doing the lattice sum

$$g(\vec{r}) \equiv \sum_{\vec{\tau}} \exp(-\lambda|\vec{r} - \vec{\tau}|)/|\vec{r} - \vec{\tau}| \qquad (1)$$

over any Bravais lattice $\{\vec{\tau}\}$ in three dimensions, λ and $\vec{r}$ (position vector) being independent of $\vec{\tau}$. The result of this sum was earlier quoted by Dias and Chaba (1983) in their work on the Screened Wigner lattice model.

One of the main purposes of this paper is to establish a relation between the two approaches mentioned above. In section 3, we show that the two approaches are, in fact, equivalent. We do so by proving that the PSF in arbitrary dimensions can, itself, be derived from the FS method. In section 4, we derive an expression for a class of lattice sums $\sum_{\vec{\tau}} F(|\vec{r} - \vec{\tau}|)$ over a

Bravais lattice $\{\vec{\tau}\}$ in arbitrary dimensions. This expression is of immediate applicability and represents a generalization of a result earlier given by Freitas and Chaba (1983). In section 5, we derive the result for the lattice sum $\sum_{\tau}' \exp(-\lambda\tau)/\tau$ (where prime on the summation sign means that the term corresponding to $\vec{\tau}=0$ is excluded from it) considered as a special case of the sum $g(\vec{r})$ in equation (eqn.)(1). In the appendix, we derive certain results needed for this purpose.

2. Evaluation of lattice sum $g(\vec{r})$

In the sum $g(\vec{r})$ in eqn.(1), $\{\vec{\tau}\}$ is a Bravais lattice in three dimensions with volume Ω per lattice point and while performing the sum over $\vec{\tau}$, λ and $\vec{r}$ (position vector) are regarded as constants. Let $\{\vec{\gamma}\}$ be the reciprocal lattice vectors normalized by the relation $\exp(2\pi i\vec{\tau}.\vec{\gamma})=1$. In the following, we evaluate this sum by two different methods, (a) the Poisson's summation formula method and (b) the Fourier series method and then we compare the two.

The Poisson's summation formula method

The Poisson's summation formula for the lattice sum $\sum_{\vec{\tau}} F(\vec{\tau})$ in three dimensions is written as

$$\sum_{\vec{\tau}} F(\vec{\tau}) = \sum_{\vec{\gamma}} \mathcal{F}(\vec{\gamma}) , \qquad (2)$$

where $\mathcal{F}(\vec{\gamma})$ is the Fourier transform of the function $F(\vec{R})$, corresponding to the summand in the left hand side of eqn(2), with

$$\mathcal{F}(\vec{\gamma}) = \Omega^{-1}\int F(\vec{R})\,\exp(-2\pi i\vec{R}.\vec{\gamma})d^3R\ , \qquad (3)$$

where the integral is over the whole lattice which is taken to be of infinite size and Ω appearing outside the integral is the volume per lattice point. To do the sum $g(\vec{r})$, we put

$$F(\vec{R}) = \exp(-\lambda|\vec{r} - \vec{R}|)/|\vec{r} - \vec{R}| \qquad (4)$$

and, then, from eqn.(3), we obtain

$$\mathcal{F}(\vec{\gamma}) = \Omega^{-1}\int\left[\exp(-\lambda|\vec{r}-\vec{R}|)/|\vec{r}-\vec{R}|\right]\exp(-2\pi i\vec{R}.\vec{\gamma})d^3R$$

$$= \Omega^{-1}\exp(-2\pi i\vec{r}.\vec{\gamma})\int\left[\exp(-\lambda|\vec{r}-\vec{R}|)/|\vec{r}-\vec{R}|\right]\exp\left[2\pi i(\vec{r}-\vec{R}).\vec{\gamma}\right]d^3R$$

By changing the variable of integration from $\vec{R}$ to $\vec{\rho}$ by the relation $\vec{r} - \vec{R} = \vec{\rho}$, we can rewrite $\mathcal{F}(\vec{\gamma})$ as

$$\mathcal{F}(\vec{\gamma}) = \Omega^{-1}\exp(-2\pi i\vec{r}.\vec{\gamma})\int\left[\exp(-\lambda\rho)/\rho\right]\exp(2\pi i\vec{\rho}.\vec{\gamma})d^3\rho \qquad (5)$$

$$= \Omega^{-1}\exp(-2\pi i\vec{r}.\vec{\gamma})\int_{\rho=0}^{\infty}\int_{\theta=0}^{\pi}\int_{\phi=0}^{2\pi}\left[\exp(-\lambda\rho)/\rho\right]\exp(2\pi i\rho\gamma\cos\theta)\rho^2\sin\theta\,d\rho d\theta d\phi\ ,$$

where, we have used polar coordinates, with z-axis along the vector $\vec{\gamma}$. Doing the angular integrations, we get

$$\mathcal{F}(\vec{\gamma}) = 2(\Omega\gamma)^{-1}\exp(-2\pi i\vec{r}.\vec{\gamma})\int_0^\infty d\rho\exp(-\lambda\rho)\sin(2\pi\gamma\rho), \tag{6}$$

which leads to

$$\mathcal{F}(\vec{\gamma}) = 4\pi\Omega^{-1}\exp(-2\pi i\vec{r}.\vec{\gamma})/(\lambda^2 + 4\pi^2\gamma^2), \tag{7}$$

and substituting this expression for $\mathcal{F}(\vec{\gamma})$ and $F(\vec{\tau})$ from eqn.(4) in eqn.(2), we finally, obtain

$$g(\vec{r}) \equiv \sum_{\vec{\tau}} \exp(-\lambda|\vec{r} - \vec{\tau}|)/|\vec{r} - \vec{\tau}| = 4\pi\Omega^{-1}\sum_{\vec{\gamma}} \exp(-2\pi i\vec{r}.\vec{\gamma})/(\lambda^2 + 4\pi^2\gamma^2), \tag{8}$$

which is exactly the result quoted by Dias and Chaba (1983) (see their eqn.(7)) though written in a slightly different form.

Fourier series method

The sum $g(\vec{r})$ in eqn.(1) is a periodic function of $\vec{r}$, with the periodicity of the lattice and, therefore, we can expand it as a Fourier series

$$g(\vec{r}) \equiv \sum_{\vec{\tau}}\exp(-\lambda|\vec{r} - \vec{\tau}|)/|\vec{r} - \vec{\tau}| = \sum_{\vec{\gamma}} A_{\vec{\gamma}}\exp(2\pi i\vec{r}.\vec{\gamma}), \tag{9}$$

where, the Fourier co-eficients $A_{\vec{\gamma}}$ are given by

$$A_{\vec{\gamma}} = V^{-1}\int g(\vec{r})\exp(-2\pi i\vec{r}.\vec{\gamma})d^3r. \tag{10}$$

Comparing eqn.(10) for $A_{\vec{\gamma}}$ with eqn.(3) for $\mathcal{F}(\vec{\gamma})$, we notice that both the integrals are over the whole lattice (and, so, on the whole space) and have somewhat similar structure. On the other hand, $F(\vec{R})$ in eqn.(3) corresponds to the summand in the left hand side of eqn.(2) whereas eqn.(10) contains the whole sum $g(\vec{r})$ in eqn.(9) and, further, the volume of the whole lattice, V occurs outside the integral in eqn.(10) instead of the volume per lattice point, Ω, in eqn.(3). Writing $g(\vec{r})$ explicitly in eqn.(10) we have,

$$A_{\vec{\gamma}} = V^{-1}\int\left[\sum_{\vec{\tau}}\exp(-\lambda|\vec{r} - \vec{\tau}|)/|\vec{r} - \vec{\tau}|\right]\exp(-2\pi i\vec{r}.\vec{\gamma})d^3r.$$

Interchanging the integral and the sum and using the normalization $\exp(2\pi i\vec{\tau}.\vec{\gamma}) = 1$, we can rewrite $A_{\vec{\gamma}}$ as

$$A_{\vec{\gamma}} = V^{-1}\sum_{\vec{\tau}}\int\left[\exp(-\lambda|\vec{r} - \vec{\tau}|)/|\vec{r} - \vec{\tau}|\right]\exp\left[-2\pi i(\vec{r} - \vec{\tau}).\vec{\gamma}\right]d^3(\vec{r} - \vec{\tau}). \quad (11)$$

As all the lattice points are equivalent due to the symmetry of the lattice, the integral has the same value for any $\vec{\tau}$. We choose $\vec{\tau} = 0$ and, then, the sum over $\vec{\tau}$ can be replaced by a multiplying factor N, the total number of lattice points in the lattice. Writing $V/N = \Omega$, we get

$$A_{\vec{\gamma}} = \Omega^{-1}\int\left[\exp(-\lambda r)/r\right]\exp(-2\pi i\vec{r}.\vec{\gamma})d^3r,$$

or on replacing the vector $\vec{r}$ by $-\vec{\rho}$, we get

$$\tilde{A}_{\vec{\gamma}} = \Omega^{-1}\int\left[\exp(-\lambda\rho)/\rho\right]\exp(2\pi i\vec{\rho}.\vec{\gamma})d^3\rho \ . \qquad (12)$$

Note that the integral in eqn.(12) is the same as the one occurring in eqn.(5) and we can write $A_{\vec{\gamma}}$ as

$$A_{\vec{\gamma}} = \mathcal{J}(\vec{\gamma})\exp(2\pi i\vec{r}.\vec{\gamma}) \ , \qquad (13)$$

and using the expression for $\mathcal{J}(\vec{\gamma})$, already calculated, in eqn. (7), we get

$$A_{\vec{\gamma}} = 4\pi\Omega^{-1}(\lambda^2 + 4\pi^2\gamma^2)^{-1} \ ,$$

which, on substitution in eqn.(9) and changing $\vec{\gamma}$ into $-\vec{\gamma}$ in the summand, leads to the result already obtained in eqn.(8).

Comparing the two procedures, we notice that there is a great similarity in the calculations and, of course, the results are identical. We notice that there are differences, as well. For example, the symmetry argument after eqn.(11) occurring in the FS method is not required in the PSF method. Of course, the reason for this is that when we derive the PSF from the FS method, as is done in the next section, we do make use of such an argument which, therefore, is inbuilt in the PSF.

3. Derivation of the Poisson's summations formula in arbitrary dimensions from Fourier series method

In order to derive the PSF in any dimensionality n from the FS method, we consider the following sum

$$G(\vec{r}) \equiv \sum_{\tau} F(\vec{r} - \vec{\tau}) \ , \tag{14}$$

where $\{\vec{\tau}\}$ is a Bravais lattice in the n-dimensional space. In order to do this sum, we follow the procedure similar to the one used in the second half of the last section for the particular sum $g(\vec{r})$ of eqn.(1) in three dimensions. The sum $G(\vec{r})$ is a periodic function of $\vec{r}$, with the periodicity of the lattice $\vec{\tau}$ and, therefore, we can expand it as a Fourier series,

$$G(\vec{r}) \equiv \sum_{\tau} F(\vec{r} - \vec{\tau}) = \sum_{\gamma} A_{\vec{\gamma}} \exp(2\pi i \vec{r}.\vec{\gamma}), \tag{15}$$

where $\{\vec{\gamma}\}$ is a reciprocal lattice, normalized by $\exp(2\pi i \vec{\tau}.\vec{\gamma}) = 1$ and the Fourier co-efficients $A_{\vec{\gamma}}$ are given by

$$A_{\vec{\gamma}} = V^{-1} \int G(\vec{r}) \exp(-2\pi i \vec{r}.\vec{\gamma}) d^n r$$

$$= V^{-1} \int \sum_{\tau} F(\vec{r} - \vec{\tau}) \exp(-2\pi i \vec{r}.\vec{\gamma}) d^n r \ ,$$

where, the integral is over the whole lattice (considered infinite) in n dimensions and V is the total volume of the lattice. Interchanging the integral and the sum and using the normalization condition, we can rewrite $A_{\vec{\gamma}}$ as

$$A_{\vec{\gamma}} = V^{-1}\sum_{\vec{\tau}}\int F(\vec{r}-\vec{\tau})\exp\left[-2\pi i(\vec{r}-\vec{\tau}).\vec{\gamma}\right]d^n(\vec{r}-\vec{\tau}). \qquad (16)$$

Due to the symmetry of the lattice, all the lattice points are equivalent and, therefore, the integral occurring here has the same value for any $\vec{\tau}$. We choose $\vec{\tau} = 0$ and, then, the sum over $\vec{\tau}$ can be replaced by a multiplying factor N, the total number of lattice points in the lattice. Writing $V/N = \Omega$, we get

$$A_{\vec{\gamma}} = \Omega^{-1}\int F(\vec{r})\exp(-2\pi i\vec{r}.\vec{\gamma})d^n r = \mathcal{F}'(\vec{\gamma}) , \qquad (17)$$

where it should be noted that $\mathcal{F}'(\vec{\gamma})$ is the Fourier transform of $F(\vec{r})$ (or of $F(\vec{\tau})$ with respect to $\vec{\tau}$) and not of the summand $F(\vec{r}-\vec{\tau})$ in eqn.(14) with respect to $\vec{\tau}$, which we call $\mathcal{F}(\vec{\gamma})$ (see eqns.(3)-(5) in three dimensions). That also explains why eqn.(13) does not have the same form as eqn.(17), as $\mathcal{F}'(\vec{\gamma})$ and $\mathcal{F}(\vec{\gamma})$ are not the same. In fact, eqn.(13) should be a special case of eqn.(17) which is shown to be the case. In order to do so, we derive the relation between $\mathcal{F}'(\vec{\gamma})$ and $\mathcal{F}(\vec{\gamma})$, where

$$\mathcal{F}(\vec{\gamma}) = \Omega^{-1}\int F(\vec{r}-\vec{R})\exp(-2\pi i\vec{R}.\vec{\gamma})d^n R$$

$$= \Omega^{-1}\exp(-2\pi i\vec{r}.\vec{\gamma})\int F(\vec{r}-\vec{R})\exp\left[2\pi i(\vec{r}-\vec{R}).\vec{\gamma}\right]d^n R.$$

Changing the variable $\vec{R}$ of integration to $\vec{\rho}$ by the relation $\vec{r} - \vec{R} = \vec{\rho}$, we get

$$\mathcal{F}(\vec{\gamma}) = \Omega^{-1}\exp(-2\pi i\vec{r}.\vec{\gamma})\int F(\vec{\rho})\exp(2\pi i\vec{\rho}.\vec{\gamma})d^n\rho$$

$$= \mathcal{F}'(-\vec{\gamma})\exp(-2\pi i\vec{r}.\vec{\gamma}) \qquad (18.a)$$

or

$$\mathcal{F}'(\vec{\gamma}) = \mathcal{F}(-\vec{\gamma})\exp(-2\pi i\vec{r}.\vec{\gamma}) \ , \qquad (18b)$$

and combining it with eqn.(17), we get

$$A_{-\vec{\gamma}} = \mathcal{F}(\vec{\gamma})\exp(2\pi i\vec{r}.\vec{\gamma}) \ . \qquad (19)$$

Now we can easily show that eqn.(13) is a special case of eqn.(19) by noting from eqn.(17) that when $F(\vec{r})$ depends only on the magnitude of $\vec{r}$, $A_{-\vec{\gamma}} = A_{\vec{\gamma}}$ and then eqn.(19) leads to eqn.(13). Now on substituting eqn.(17) in eqn.(15), we get

$$\sum_{\tau} F(\vec{r} - \vec{\tau}) = \sum_{\gamma} \mathcal{F}'(\vec{\gamma})\exp(2\pi i\vec{r}.\vec{\gamma}). \qquad (20)$$

Putting $\vec{r} = 0$ and noting that $\sum_{\tau} F(-\vec{\tau}) = \sum_{\tau} F(\vec{\tau})$, we get

$$\sum_{\tau} F(\vec{\tau}) = \sum_{\gamma} \mathcal{F}(\vec{\gamma}) \ , \qquad (21)$$

where we have replaced $\mathcal{F}'(\vec{\gamma})$ by $\mathcal{F}(\vec{\gamma})$ which now is the Fourier transform with respect to $\vec{\tau}$ of the summand $F(\vec{\tau})$ in the sum in the left hand side of eqn.(21) (see eqn.(17)) and is given by

$$\mathcal{F}(\vec{\gamma}) = \Omega^{-1}\int F(\vec{r})\exp(-2\pi i\vec{r}.\vec{\gamma})d^n r. \qquad (22)$$

Eqn.(21) with eqn.(22) is the desired Poisson's summation formula in n dimensions.

We have seen that eqn.(21) follows from eqn.(20), which, therefore, can be considered as generalization of the former. However, eqn.(20) can also be derived from eqn.(21), as can be seen by replacing $F(\vec{\tau})$ by $F(\vec{r} - \vec{\tau})$ and substituting from eqn.(18a) for $\mathcal{F}(\vec{\gamma})$ in eqn.(21) and changing the sign of $\vec{\gamma}$ everywhere in the summand. We may point out, however, that for certain lattice sums, eqn.(20) may serve as a better starting point than eqn.(21), as we shall see in the next section where we treat a special class of lattice sums.

4. Evaluation of a class of lattice sums $\sum_{\vec{\tau}} F(|\vec{r} - \vec{\tau}|)$ in arbitrary dimensions

This a special case of the sum $G(\vec{r})$ defined in eqn.(14) where the function F in the summand, now, depends on the modulous of its argument $(\vec{r} - \vec{\tau})$. We can directly use eqns.(20) and (17) which, respectively, become in this case

$$F(|\vec{r} - \vec{\tau}|) = \sum_{\vec{\gamma}}{}' \mathcal{J}(\vec{\gamma})\exp(2\pi i\vec{r}.\vec{\gamma}) \qquad (23)$$

and

$$\mathcal{F}'(\vec{\gamma}) = \Omega^{-1}\int F(\rho)\exp(-2\pi i\vec{\rho}.\vec{\gamma})d^n\rho \ , \qquad (24)$$

where the function F depends on the modulous ρ of $\vec{\rho}$. The integral in eqn.(24) also appeared in the recent work of Freitas and Chaba (1983) (see their eqns.(6) and (10)) where they performed the angular integrations (in spherical coordinates) leaving only one integration over ρ. Making use of their result, we get

$$\mathcal{F}'(\vec{\gamma}) = 2\pi\Omega^{-1}\int_0^\infty d\rho\ F(\rho)\rho^{n/2}J_{(n-2)/2}(2\pi\gamma\rho)/\gamma^{(n-2)/2}, \qquad (25)$$

where $J_\nu(z)$ occurring inside the integral is a Bessel function of the first kind and order ν (Abramovitz and Stegun 1965). Using eqn. (25) in eqn.(23), we, finally, obtain

$$\sum_{\vec{\tau}} F(|\vec{r} - \vec{\tau}|) = 2\pi\Omega^{-1}\sum_{\vec{\gamma}}\exp(2\pi i\vec{r}.\vec{\gamma})\gamma^{-(n-2)/2}\int_0^\infty d\rho\rho^{n/2}F(\rho)J_{(n-2)/2}(2\pi\gamma\rho); \qquad (26)$$

which is a generalization of the results of Freitas and Chaba (1983), as on putting $\vec{r} = 0$ in eqn.(26), we recover their eqn.(18) together with eqn.(19). Eqn.(26) represents an expression, ready for quick use, for the evaluation of a class of lattice sums of the form $\sum_{\vec{\tau}} F(|\vec{r} - \vec{\tau}|)$ in any dimensionality n and in this expression, only one integral with respect to ρ remains to be done. For exemple, if we use this equation for the sum $g(\vec{r})$ in eqn.(1), we directly obtain (on putting $n = 3$ and $F(\rho) = \exp(-\lambda\rho)/\rho$)

$$g(\vec{r}) \equiv \sum_{\vec{\tau}} \exp(-\lambda|\vec{r}-\vec{\tau}|)/|\vec{r}-\vec{\tau}| = 2\pi\Omega^{-1}\sum_{\vec{\gamma}}\gamma^{-1/2}\exp(2\pi i\vec{r}.\vec{\gamma})\int_0^\infty d\rho\rho^{1/2}\exp(-\lambda\rho)J_{1/2}(2\pi\gamma\rho),$$

or, on putting $J_{1/2}(x) = (2/\pi x)^{1/2}\sin(x)$, and changing $\vec{\gamma}$ into $-\vec{\gamma}$ in the summand, it leads to

$$g(\vec{r}) \equiv \sum_{\vec{\tau}} \exp(-\lambda|\vec{r}-\vec{\tau}|)/|\vec{r}-\vec{\tau}| = 2\Omega^{-1}\sum_{\gamma}\gamma^{-1}\exp(-2\pi i\vec{r}.\vec{\gamma})\int_0^\infty d\rho\sin(2\pi\gamma\rho)\exp(-\lambda\rho),$$

which agrees with the result obtained by substituting eqn.(6) in eqn.(2).

5. Evaluation of the sum $\sum_{\vec{\tau}}'\exp(-\lambda\tau)/\tau$

This is a sum over the lattice $\{\vec{\tau}\}$ in three dimensions. The prime on the sum means that the term corresponding to $\vec{\tau} = 0$ is excluded from the sum. We treat this sum as a special case of the sum $g(\vec{r})$ in eqn.(1) and write it as

$$\sum_{\tau}'\exp(-\lambda\tau)/\tau = \lim_{r\to 0}\left[\sum_{\tau}\exp(-\lambda|\vec{r}-\vec{\tau}|)/|\vec{r}-\vec{\tau}| - \exp(-\lambda r)/r\right]. \qquad (27)$$

Substituting for the sum on the right hand side from eqn.(8) and after slight rearrangement, we obtain

$$\sum_{\tau}'\exp(-\lambda\tau)/\tau = 4\pi(\Omega\lambda^2)^{-1} - \lambda^2(\pi\Omega)^{-1}\sum_{\gamma}'\gamma^{-2}(\lambda^2+4\pi^2\gamma^2)^{-1}$$
$$+\lim_{r\to 0}\left[(\pi\Omega)^{-1}\sum_{\gamma}'\gamma^{-2}\exp(-2\pi i\vec{r}.\vec{\gamma}) - \exp(-\lambda r)/r\right]. \qquad (28)$$

In order to calculate the limit of the expression in square brackets, we substitute for the sum over $\vec{\gamma}$ from eqn.(A.6) [obtained by replacing $\vec{\tau}$ by $\vec{\gamma}$, Ω by $1/\Omega$ and $\vec{\epsilon}$ by $-\vec{r}$] and obtain

$$\sum_{\tau}{}' \exp(-\lambda\tau)/\tau = 4\pi(\Omega\lambda^2)^{-1} + J_\gamma(0,1,3)(\pi\Omega^{1/3})^{-1} + \lambda$$

$$- \lambda^2(\pi\Omega)^{-1}\sum_{\gamma}{}'\gamma^{-2}(\lambda^2 + 4\pi^2\gamma^2)^{-1}, \qquad (29)$$

which is the desired result. The constant $J_\gamma(0,1,3)$ can be obtained more quickly from eqn.(A.2) [than from eqn.(29) itself] by giving a suitable particular value to λ and doing the sums numerically, the same way as was done by Chaba and Pathria (1975) (see after their eqn.(26)) to calculate the constant C, in their work on lattice sums. Recently, the result in eqn.(29) was obtained directly (without going through eqn.(A.2)) by Freitas and Chaba (1983) by a much shorter method using Walfisz formula but then the constant $J_\gamma(0,1,3)$ has to be obtained from the eqn.(29) itself. We may mention that this sum occurred recently in the work of Medeiros e Silva and Mokross (1980) in connection with their study of the Screened Wigner lattice where they did this sum by the Ewald's method, our result being much more elegant. Also this sum for a particular case of simple cubic lattice had earlier appeared in the work of Chaba and Pathria (1978) in their study of Bose-Einstein condensation in finite systems.

Appendix

Here, we derive a result [eqn.(A.6)] which is needed in section 5 of the text. Starting from the Poisson's summation formula (PSF) in three dimensions, we can easily show that

$$\sum_{\vec{\tau}} \exp(-a\tau^2) = \Omega^{-1}(\pi/a)^{3/2} \sum_{\vec{\gamma}} \exp(-\pi^2\gamma^2/a). \quad \text{(A.1)}$$

Separating the terms corresponding to $\vec{\tau} = 0$ and $\vec{\gamma} = 0$ from the respective sums on the two sides of eqn.(A.1) and integrating with respect to 'a', we obtain

$$\sum_{\vec{\tau}}{}' \exp(-a\tau^2)/\tau^2 = 2\pi^{3/2}(\Omega a^{1/2})^{-1} + J_{\tau}(0,1,3)\Omega^{-2/3} + a - \pi\Omega^{-1}\sum_{\vec{\gamma}}{}'\gamma^{-1}\,\mathrm{erfc}(\pi\gamma/\sqrt{a}), \quad \text{(A.2)}$$

where

$$J_{\tau}(0,1,3) = \Omega^{2/3}\lim_{a\to 0}\left[\sum_{\vec{\tau}}{}' \exp(-a\tau^2)/\tau^2 - 2\pi^{3/2}(\Omega a^{1/2})^{-1}\right], \quad \text{(A.3)}$$

and the primes on the sums over $\vec{\tau}$ and $\vec{\gamma}$ (here and elsewhere) mean that the terms corresponding to $\vec{\tau} = 0$ and $\vec{\gamma} = 0$ are excluded from the respective sums. The eqn.(A.2) represents a generalization to an arbitrary lattice of a result earlier given by Chaba and Pathria (1975) (see their eqn.(23)) for a simple cubic lattice.

Again, starting from the PSF in three dimensions, we can show that

$$\sum_{\vec{\tau}} \exp(-a\tau^2 + 2\pi i\vec{\varepsilon}.\vec{\tau}) = \Omega^{-1}(\pi/a)^{3/2} \sum_{\vec{\gamma}} \exp(-\pi^2|\vec{\gamma} - \vec{\varepsilon}|^2/a), \qquad (A.4)$$

and separating the term corresponding to $\vec{\tau} = 0$ from the sum on the left hand side and integrating with respect to 'a', we get

$$\sum_{\vec{\tau}}{}' \exp(-a\tau^2 + 2\pi i\vec{\varepsilon}.\vec{\tau})/\tau^2 = a + \sum_{\vec{\tau}}{}' \exp(2\pi i\vec{\varepsilon}.\vec{\tau})/\tau^2 - \pi\Omega^{-1} \sum_{\vec{\gamma}} \mathrm{erfc}(\pi a^{-1/2}|\vec{\gamma} + \vec{\varepsilon}|)/|\vec{\gamma} + \vec{\varepsilon}|.$$

(A.5)

Comparing eqns. (A.5) and (A.2) one obtains the asymptotic behaviour of the sum $\sum_{\vec{\tau}}{}' \exp(2\pi i\vec{\varepsilon}.\vec{\tau})/\tau^2$:

$$\lim_{\varepsilon \to 0} \sum_{\vec{\tau}}{}' \exp(2\pi i\vec{\varepsilon}.\vec{\tau})/\tau^2 = \pi(\Omega\varepsilon)^{-1} + J_\tau(0,1,3)\Omega^{-2/3} + O(\varepsilon^2). \qquad (A.6)$$

We may remark that the eqns. (A.5) and (A.6) also represent generalizations to any lattice of the corresponding results given earlier by Chaba and Pathria (1976) (see their eqns.(48) and (51)) for a simple cubic lattice.

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