Poisson's summation formula, Walfisz's formula, and certain lattice sums occurring in the study of a system of ideal bosons

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The equivalence of the results is pointed out for certain lattice sums occurring in the study of a system of ideal bosons derived by the use of the Poisson's summation formula with those obtained by using the expression for the density of single-particle states, given recently by Baltes and Steinle, and arrived at by the use of Walfisz's formula for the number of lattice points in a hypersphere of p dimensions. Further, expressions are given for the density of single-particle states in one and two dimensions for periodic, Dirichlet, and Neumann boundary conditions. In the end the equivalence is shown between the Poisson's summation formula and Walfisz's formula directly.

From the recent work of Baltes and Steinle,[1] one can write the following expression for the density of single-particle states, derived by the use of the Walfisz's[2] formula on the number of lattice points in a hypersphere of p dimensions, for a particle enclosed in a cubical box of length L. (It may be noted that the notation used here is slightly different from that in Ref. 1):

$$a_3(k)=\frac{L^3k^2}{2\pi^2}\sum_{l_{1,2,3}=-\infty}^{+\infty}\frac{\sin[(1+\theta^2)Llk]}{(1+\theta^2)Llk}+\theta\frac{3L^2k}{4\pi}\sum_{m_{1,2}=-\infty}^{+\infty}J_0(2Lmk)+\theta^2\frac{3L}{4\pi}\sum_{q=-\infty}^{+\infty}\cos(2Lqk)+\frac{\theta^3}{8}\delta(k), \tag{1}$$

where $l=(l_1^2+l_2^2+l_3^2)^{1/2}$, $m=(m_1^2+m_2^2)^{1/2}$, $\theta=0$, -1, and $+1$ for the periodic, Dirichlet, and Neumann boundary conditions, PBC, DBC, and NBC, respectively (in Ref. 1, the expression is given for Dirichlet and Neumann boundary conditions only), J_0 is the Bessel function of order zero, and k is related to the single-particle energy ε by $\varepsilon=\hbar^2k^2/2M$, where M is the mass of the particle.

Using Eq. (1), the expression is calculated for the number of bosons N in a finite three-dimensional cubical box as follows:

$$\begin{aligned}N&=\sum_i\langle n_i\rangle=\sum_i(e^{\alpha+\beta\epsilon_i}-1)^{-1}\\&=\sum_i\sum_{j=1}^{\infty}e^{-j(\alpha+\beta\epsilon_i)}\\&=\sum_{j=1}^{\infty}e^{-j\alpha}\sum_i e^{-j\lambda^2k_i^2/4\pi},\end{aligned} \tag{2}$$

where, $\langle n_i\rangle$ is the mean occupation number in a single-particle state of energy ε_i, $\alpha=-\mu/KT$, $\beta=1/KT$, μ being the chemical potential, K the Boltzmann constant, T the absolute temperature of the system and $\lambda=h/(2MKT)^{1/2}$ is the mean thermal wavelength of the particles. Now to do the sum over i, one replaces it by an integral and uses Eq. (1) for the density of states and obtains

$$\begin{aligned}\sum_i e^{-j\lambda^2k_i^2/4\pi}&=\int_0^{\infty}e^{-j\lambda^2k^2/4\pi}a_3(k)\,dk\\&=\frac{L^3}{\lambda^3}\frac{1}{j^{3/2}}\sum_{l_{1,2,3}=-\infty}^{+\infty}e^{-y^2l^2/j\alpha}\\&\quad+\theta\frac{3}{2}\frac{L^2}{\lambda^2}\frac{1}{j}\sum_{m_{1,2}=-\infty}^{+\infty}e^{-y^2m^2/j\alpha}\\&\quad+\theta^2\frac{3L}{4\lambda}\frac{1}{j^{1/2}}\sum_{q=-\infty}^{+\infty}e^{-y^2q^2/j\alpha}+\frac{\theta^3}{8},\end{aligned} \tag{3}$$

where $y=(1+\theta^2)(\pi\alpha)^{1/2}(L/\lambda)$. Using Eq. (3) in Eq. (2), separating the terms corresponding to $l=0$, $m=0$, and $q=0$, and introducing Bose-Einstein functions[3] $g_\nu(\delta)$, one gets

$$\begin{aligned}N=\frac{L^3}{\lambda^3}\Bigg[&g_{3/2}(\alpha)+{\sum_{l_{1,2,3}=-\infty}^{+\infty}}'\sum_{j=1}^{\infty}\frac{e^{-j\alpha}}{j^{3/2}}e^{-y^2l^2/j\alpha}\\&+\theta\frac{3\lambda}{2L}\left(g_1(\alpha)+{\sum_{m_{1,2}=-\infty}^{+\infty}}'\sum_{j=1}^{\infty}\frac{e^{-j\alpha}}{j}e^{-y^2m^2/j\alpha}\right)\\&+\theta^2\frac{3\lambda^2}{4L^2}\left(g_{1/2}(\alpha)+{\sum_{q=-\infty}^{+\infty}}'\sum_{j=1}^{\infty}\frac{e^{-j\alpha}}{j^{1/2}}e^{-y^2q^2/j\alpha}\right)\\&+\theta^3\frac{\lambda^3}{8L^3}g_0(\alpha)\Bigg],\end{aligned} \tag{4}$$

where primes on the sums means that the terms corresponding to $l=0$, $m=0$, and $q=0$ are excluded from them. Following Greenspoon and Pathria,[4] I replace the summations over j by integrations and doing them, I finally obtain

$$N=\frac{L^3}{\lambda^3}\Bigg[g_{3/2}(\alpha)+\frac{(\pi\alpha)^{1/2}}{y}\sum_{l_{1,2,3}=-\infty}^{+\infty}{}' \frac{e^{-2yl}}{l} + \theta\,\frac{3\lambda}{2L}\left(g_1(\alpha)+2\sum_{m_{1,2}=-\infty}^{+\infty}{}' K_0(2ym)\right) + \theta^2\,\frac{3\lambda^2}{4L^2}[g_{1/2}(\alpha)+2(\pi/\alpha)^{1/2}g_0(2y)] + \theta^3\,\frac{\lambda^3}{8L^3}\,g_0(\alpha)\Bigg], \quad (5)$$

where $K_0(Z)$ is a modified Bessel function. Ziff *et al.*[5] have shown that the replacement of sums over j by integrations introduces errors of order $O[\exp(-L/\lambda)]$ which, for $L\gg\lambda$, are negligible. We observe that for $\theta=0$ (PBC), Eq. (5) agrees with the result of Greenspoon and Pathria[4] [see their Eqs. (A12) and (A13)], and for $\theta=-1$ (DBC) and $\theta=+1$ (NBC) this equation agrees with the corresponding results of Zasada and Pathria[6] [see their Eq. (9)]. [Also see Eq. (8) of Chaba and Pathria,[7] for DBC].

In view of the result contained in Eq. (5) and the procedure used to obtain it, I wish to make the following two comments:

(i) The term involving $g_{3/2}(\alpha)$ in Eq. (5) is the customary bulk term and, earlier, it was noted[7] that the other terms involving $g_\nu(\alpha)$ in Eq. (5) come from the modification[8] (of the Weyl term), due to the finite size of the system, in the expression for the density of states, which was taken[8] to be

$$a_3(k)=L^3k^2/2\pi^2+\theta 3L^2k/4\pi + \theta^2 3L/4\pi+\theta^3\delta(k)/8, \quad (6)$$

this expression agreeing with non oscillatory terms of Eq. (1), that is, $l=0$, $m=0$, $q=0$ terms in the three summations along with the last term in Eq. (1). Further it was felt that the remaining terms in Eq. (5) arise explicitly from the discreteness of states and due to the summation procedure which was used rather than replacing the sum by integration and using expression (6) for the density of states. But now we note that if we use the more accurate expression in Eq. (1) for the density of states, all the finite-size effects are completely obtained from this alone.

(ii) Here we have obtained Eq. (5) for N, making use of the expression in Eq. (1) for the density of states which is itself derived by using the Walfisz formula, whereas in Ref. 4, 6, and 7, identical results were obtained, for the corresponding boundary conditions, by making use of the Poisson summation formula, so that, we may say that these two approaches provide alternate but equivalent ways of doing such sums. We have verified that when one uses the former approach to do the sums involved in the internal energy of the finite three-dimensional system of ideal bosons, $U=\sum_i \varepsilon_i\langle n_i\rangle$ (or the pressure) and the logarithm of the grand partition function

$$\ln Z=-\sum_i \ln(1-e^{-(\alpha+\beta\epsilon_i)}),$$

we again arrive at the same results, for the corresponding boundary conditions, as obtained earlier by the latter approach[4,5,7].

The expressions for the density of single-particle states in the case of two-dimensional (square of each side L) and one-dimensional (of length L) enclosures may also be written down as follows:

$$a_2(k)=\frac{L^2k}{2\pi}\sum_{m_{1,2}=-\infty}^{+\infty} J_0[kmL(1+\theta^2)] + \theta\,\frac{L}{\pi}\sum_{q=-\infty}^{+\infty}\cos(2kLq)+\frac{\theta^2}{4}\,\delta(k) \quad (7)$$

and

$$a_1(k)=\frac{L}{\pi}\sum_{q=-\infty}^{+\infty}\cos[kLq(1+\theta^2)]+\frac{\theta}{2}\,\delta(k). \quad (8)$$

Again, using Eqs. (7) and (8), one can obtain expressions for N, U, and $\ln Z$ which are identical with the corresponding results[5,9,10] already obtained by the other approach.

From the equivalence of the results obtained by the two approaches, one suspects that there is some basic and direct connection (or equivalence) between the Poisson summation formula and the Walfisz formula, in the spirit discussed above, as is actually seen to be the case. The Walfisz formula for the number of lattice points $N_p(x)$ in a hypersphere of p dimensions and of radius x is

$$N_p(x)=\frac{\pi^{p/2}}{\Gamma(1+p/2)}\,x^p + x^{p/2}\sum_{l_{1,2,\dots,p}=-\infty}^{+\infty}{}' l^{-p/2}J_{p/2}(2\pi xl), \quad (9)$$

where $l=(l_1^2+l_2^2+\cdots+l_p^2)^{1/2}$ and this for a one-dimensional case can be written

$$N_1(x)=\sum_{q=-\infty}^{+\infty}\frac{\sin(2\pi xq)}{\pi q}; \quad (10)$$

so that, the density of lattice points is given by

$$n_1(x)=\frac{dN_1(x)}{dx}=\sum_{q=-\infty}^{+\infty} 2\cos(2\pi q x). \tag{11}$$

Here $n_1(x)\,dx$ includes the number of lattice points in the interval $(x, x+dx)$ as well as $(-x, -x-dx)$. If $a_1(x)$ is the density of lattice points between x and $x+dx$ only, then due to the symmetry of the lattice points about the origin, we can write

$$a_1(x)=\sum_{q=-\infty}^{+\infty}\cos(2\pi q x)=\sum_{q=-\infty}^{+\infty} e^{-2\pi q x i}. \tag{12}$$

Now in order to do the sum $\Sigma_{n=-\infty}^{+\infty} F(n)$, we replace it by integration and make use of Eq. (12) for the density of states, that is,

$$\sum_{n=-\infty}^{+\infty} F(n) \rightarrow \int_{-\infty}^{+\infty} F(x)a_1(x)\,dx$$
$$=\sum_{q=-\infty}^{+\infty}\int_{-\infty}^{+\infty} F(x)e^{-2\pi q x i}\,dx.$$

Thus we arrive at the result,

$$\sum_{n=-\infty}^{+\infty} F(n)=\sum_{q=-\infty}^{+\infty}\mathfrak{F}(q), \tag{13}$$

where $\mathfrak{F}(q)$ is the Fourier transform of $F(x)$:

$$\mathfrak{F}(q)=\int_{-\infty}^{+\infty} F(x)e^{-2\pi q x i}\,dx. \tag{14}$$

Equation (13) is just the Poisson summation formula and it has been shown that this formula is exactly equivalent to replacing the sum in $\sum_{n=-\infty}^{+\infty} F(n)$ by integration and using the expression for the density of states given in Eq. (12) which itself is obtained from the Walfisz formula. It is, then, not surprising that the results arrived at by the two approaches referred to above are identical.

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