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DENSITY OF STATES, POISSON'S FORMULA OF SUMMATION AND WALFISZ'S FORMULA *

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ABSTRACT

Using Poisson's formula for summation, we obtain an expression for density of states of d-dimensional scalar Helmoholtz's equation under various boundary conditions. Likewise, we also obtain formulas of Walfisz's type. It becomes evident that the formulas obtained by Pathria *et al*. in connection with ideal bosons in a finite system are exactly the same as those obtained by utilizing the formulas for density of states.

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In order to study the statistical properties of a system of finite volume, it is necessary to know the density of states of the system. For a rectangular body satisfying the **periodic** boundary condition (PBC), Neumann boundary condition (NBC) and Dirichlet boundary condition (DBC) for dimensionality $d = 1,2,3$, the expressions for density of states are given in Refs.1 to 3. They are derived indirectly from a temporal coherent function of a finite black body. It had been pointed out [2)] that this expression can follow from Walfisz's formula of lattice summation which was known more than fifty years ago. It was clarified further in Ref.3 that the formulas for a finite system of ideal bosons obtained by Pathria *et al*. [4)-6)] with the help of Poisson's formula of summation are exactly the same as those derived from the formula for density of states. Also, the Poisson formula itself is nothing but the one-dimensional Walfisz formula. In this short communication we have obtained not only the general formula for density of states for any dimension d by using Poisson's formula of summation but also showed that Walfisz's type formulas can be readily derived from Poisson's formula. The method of Pathria *et al*. [4)-6)] is to apply Poisson's formula to the function to be summed, while in obtaining these formulas from that of density of states we must sum the delta function at the beginning. The two methods are naturally equivalent.

Starting from the corresponding one-dimensional Poisson formula, it is not difficult to show by induction that the d-dimensional Poisson equations are

$$\sum_{l_1,\cdots l_d=-\infty}^{\infty} f(l_1,\cdots,l_d) = \sum_{n_1,\cdots n_d=-\infty}^{\infty} \int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty} f(x_1,\cdots x_d)\, e^{2\pi i(n_1x_1+\cdots+n_dx_d)}\, dx_1\cdots dx_d \quad , \tag{1}$$

$$\sum_{l_1,\cdots l_d=\frac{1}{2}(1-\eta)}^{\infty} f(l_1,\cdots,l_d) = \left(\frac{\eta}{2}\right)^d f(0,\cdots,0) + \sum_{s=1}^{d}\left(\frac{\eta}{2}\right)^{d-s} \sum_{1\le j_1<\cdots j_s\le d}\ \sum_{n_{j_1},\cdots n_{j_s}=-\infty}^{\infty} \int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty} f(0,\cdots x_{j_1}\cdots 0,\cdots x_{j_s}\cdots 0)\, \exp\left\{2\pi i\sum_{p=1}^{s} n_{j_p}x_{j_p}\right\} \prod_p dx_{j_p} \quad . \tag{2}$$

The summation in the above equations are restricted to integers. In formula (2) $\eta = \pm 1$ and when $\eta = 1$ the sum at the left-hand side begins from zero, for $\eta = -1$, it begins from one. $f(x_1,\dots,x_d)$ is a function of d variables. If

$$f(x_{p1},\dots,x_{pd}) = f(x_1,\dots,x_d) \tag{3}$$

for all permutations P applying on $(1,\dots,d)$ and

$$f(x_1,\dots,-x_j,\dots,x_d) = f(x_1,\dots,x_j,\dots,x_d) \tag{4}$$

then (2) becomes

$$\sum_{\ell_1,\dots\ell_d=\frac{1}{2}(1-\eta)}^{\infty} f(\ell_1,\dots\ell_d) = \left(\frac{\eta}{2}\right)^d f(0,\dots,0) + \left(\frac{\eta}{2}\right)^d \sum_{s=1}^{d} \eta^s \binom{d}{s}$$

$$\sum_{n_1,\dots n_s=-\infty}^{\infty} \int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty} f(x_1,\dots x_s,0,\dots 0)\, e^{2\pi i(n_1x_1+\dots+n_sx_s)}\, dx_1\dots dx_s \,. \tag{5}$$

The scalar Helmholtz equation in the rectangular region $L_1 \times \dots \times L_d$ is

$$\left\{ (\partial_1^2 + \dots + \partial_d^2) + k^2 \right\} \psi(x_1,\dots,x_d) = 0 \,. \tag{6}$$

For PBC, the wave vector k is equal to

$$k = 2\pi \sqrt{\frac{\ell_1^2}{L_1^2} + \dots + \frac{\ell_d^2}{L_d^2}} \,, \tag{7}$$

where $\ell_1,\dots,\ell_d$ are integers. For NBC

$$k = \pi \sqrt{\frac{\ell_1^2}{L_1^2} + \dots + \frac{\ell_d^2}{L_d^2}} \,, \tag{8}$$

where $\ell_1,\dots,\ell_d$ are integers from 0 to ∞. For DBC the same formula applies but $\ell_1,\dots,\ell_d$ are integers from 1 to ∞.

For PBC, the density of states $D_d(k)$ is, by definition, equal to

$$D_d(k) = \sum_{\ell_1,\dots\ell_d}^{\infty} \delta\left(k - 2\pi\sqrt{\frac{\ell_1^2}{L_1^2} + \dots + \frac{\ell_d^2}{L_d^2}}\right) \,. \tag{9}$$

From (1) it follows that

$$D_d(k) = \sum_{n_1,\dots n_d=-\infty}^{\infty} \int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty} \delta\left(k - 2\pi\sqrt{\frac{x_1^2}{L_1^2} + \dots + \frac{x_d^2}{L_d^2}}\right)$$

$$\exp 2\pi i(n_1x_1 + \dots + n_dx_d)\, dx_1\dots dx_d \,. \tag{10}$$

Introducing the d-dimensional spherical co-ordinate system $(y,\theta_1,\dots,\theta_{d-1})$, $0 \leq y < \infty$, $0 \leq \theta_i \leq \pi$, $i = 1,\dots,d-2$, $0 \leq \theta_{d-1} \leq 2\pi$ and taking θ_1 as the angle between vectors $(x_1/L_1,\dots,x_d/L_d)$ and $(L_1n_1,\dots,L_dn_d)$ we have

$$D_d(k) = \frac{L_1\cdots L_d}{(2\pi)^d} k^{d-1} \Omega_{d-1} \sum_n \int_{-1}^{1} e^{ink\gamma} (1-\gamma^2)^{\frac{d-3}{2}} d\gamma \tag{11}$$

where $n = \sqrt{n_1^2L_1^2 + \dots + n_d^2L_d^2}$. $\sum_n$ represents that $n_1,\dots,n_d$ are taken over all integers from $-\infty$ to ∞ and Ω_{d-1} is the solid angle subtended by a (d-1) dimensional sphere. From the integral representation of the Bessel function, it gives

$$D_d(k) = \frac{L_1\cdots L_d}{(2\pi)^d} k^{d-1} \Omega_d \sum_n \Gamma\left(\frac{d}{2}\right) \frac{J_{\frac{d}{2}-1}(nk)}{(nk/2)^{d/2-1}} \,, \tag{12}$$

which can be written as

$$= \frac{L_1\cdots L_d}{(2\pi)^d} k^{d-1}\Omega_d + \frac{L_1\cdots L_d}{(2\pi)^d} k^{d-1}\Omega_d \sum_n{}' \Gamma\left(\frac{d}{2}\right) \frac{J_{\frac{d}{2}-1}(nk)}{(nk/2)^{d/2-1}} \tag{13}$$

the first term is the Weyl term which forms the essential part and the second term is the oscillatory part. The meaning attached to each of them is evident.

For NBC and DBC, the density of states $D^\eta(k)$ is, by definition, equal to

$$D_d^\eta(k) = \sum_{l_1,\cdots l_d=\frac{1}{2}(1-\eta)}^{\infty} \delta\left(k - \pi\sqrt{\frac{l_1^2}{L_1^2}+\cdots+\frac{l_d^2}{L_d^2}}\right), \tag{14}$$

while for NBC, $\eta = 1$ and for DBC, $\eta = -1$.

Because conditions (3) and (4) are satisfied, we may apply Eq.(5) to obtain

$$D_d^\eta(k) = \left(\frac{\eta}{2}\right)^d \left\{ \delta(k) + \sum_{s=1}^{d} \eta^s \binom{d}{s} D_s(k; 2L_1, \cdots 2L_s)\right\}. \tag{15}$$

Thus the density of states for NBC and DBC can be expressed in terms of that for PBC. It should be noted that each side of the rectangular is doubled in the corresponding expression for PBC. This is denoted explicitly in Eq.(15). Substituting Eq.(12) in (15), we have

$$D_d^\eta(k) = \left(\frac{\eta}{2}\right)^d \left\{ \delta(k) + \sum_{s=1}^{d} \eta^s \binom{d}{s} \frac{L_1\cdots L_s}{\pi^s} k^{s-1}\Omega_s \right.$$
$$\left. \sum_n \Gamma\left(\frac{s}{2}\right) \frac{J_{\frac{s}{2}-1}(2nk)}{(nk)^{s/2-1}} \right\}. \tag{16}$$

When $d = 1,2,3$ the results in Refs.1 to 3 are obtained from Eqs.(16) and (12).

Now, we calculate the total number of states with the magnitude of a vector less than k in wave vector space. For PBC, it is given by definition that

$$N_d(k) = \sum_{l_1,\cdots l_d=-\infty}^{\infty} \theta\left(k - 2\pi\sqrt{\frac{l_1^2}{L_1^2}+\cdots+\frac{l_d^2}{L_d^2}}\right), \tag{17}$$

where θ is the usual step function defined by

$$\theta(k) = \begin{cases} 1 & k > 0 \\ 0 & k \leq 0 \end{cases}.$$

At $k = 0$, $\theta(k)$ can be either defined as $\frac{1}{2}$, 1 or 0 with the understanding that the states situated at the boundary are counted $\frac{1}{2}$, counted or not counted, respectively.

Repeating the calculations, we have

$$N_d(k) = \frac{L_1\cdots L_d}{(2\pi)^d}\,\Omega_{d-1} \sum_n \int_0^k \frac{\Gamma(1/2)\,\Gamma((d-1)/2)}{(nw)^{d/2-1}}\, 2^{d/2-1} J_{d/2-1}(nw)\, w^{d-1} dw . \tag{18}$$

Utilizing the formula for Bessel functions

$$\frac{d}{dz} z^\nu J_\nu(z) = z^\nu J_{\nu-1}(z)$$

and completing the integral with respect to w, we obtain

$$N_d(k) = \frac{L_1\cdots L_d}{(2\pi)^d}\, V_d \sum_n \Gamma\left(\frac{d}{2}+1\right) \frac{J_{d/2}(nk)}{(nk/2)^{d/2}}, \tag{19}$$

where V_d is the volume of a d-dimensional sphere of radius k. This is just the Walfisz formula. For NBC ($\eta = 1$) and DBC ($\eta = -1$), the number of states $N_d^\eta(k)$ with magnitude less than k is given by

$$N_d^\eta(k) = \sum_{l_1,\cdots l_d=\frac{1}{2}(1-\eta)}^{\infty} \theta\left(k - \pi\sqrt{\frac{l_1^2}{L_1^2}+\cdots+\frac{l_d^2}{L_d^2}}\right). \tag{20}$$

Similarly we have

$$N_d^\eta(k) = \left(\frac{\eta}{2}\right)^d \left\{ \theta(k) + \sum_{s=1}^{d} \eta^s \binom{d}{s} N_d(k; 2L_1, \cdots, 2L_s)\right\}$$
$$= \left(\frac{\eta}{2}\right)^d \left\{ \theta(k) + \sum_{s=1}^{d} \eta^s \binom{d}{s} \frac{L_1\cdots L_s}{\pi^s} V_d \right.$$
$$\left. \sum_n \Gamma\left(\frac{s}{2}+1\right) \frac{J_{s/2}(2nk)}{(nk)^{s/2}} \right\}. \tag{21}$$

These are formulas of the Walfisz type. From the point of view of the lattice summation, it can be interpreted as the number of lattice points in the first quadrant in a sphere with radius k in wave number space. For $\eta = 1$, the points on the co-ordinate plane is taken into account in the first quadrant. For $\eta = -1$, it is not taken into account. The term $\theta(k)$ comes from the contribution of the vertex, terms with $s = 1,2,\ldots$ come from the boundary line, boundary plane. From definitions, it follows that

$$\frac{d}{dk} N_d(k) = D_d(k)$$

and

$$\frac{d}{dk} N_d^\eta(k) = D_d^\eta(k)$$

which may be verified readily from Eqs.(12), (19), (16) and (21).

The technique [4)-6)] used by Pathria et al. is to apply Poisson's summation formula directly to the function $f(k) = f\left(2\pi\sqrt{\frac{l_1^2}{L_1^2}+\cdots+\frac{l_d^2}{L_d^2}}\right)$

i.e.

$$\sum_{l_1,\cdots l_d}^{\infty} f\left(2\pi\sqrt{\frac{l_1^2}{L_1^2}+\cdots+\frac{l_d^2}{L_d^2}}\right) = \sum_{n_1,\cdots n_d}^{\infty}\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty} f\left(2\pi\sqrt{\frac{x_1^2}{L_1^2}+\cdots+\frac{x_d^2}{L_d^2}}\right)$$

$$\exp\left\{2\pi i\left(n_1x_1+\cdots+n_dx_d\right)\right\} dx_1\cdots dx_d \quad .$$

Repeating the calculations performed above, we have

$$\sum_{l_1,\cdots l_d=-\infty}^{\infty} f\left(2\pi\sqrt{\frac{l_1^2}{L_1^2}+\cdots+\frac{l_d^2}{L_d^2}}\right) =$$

$$= \int_0^{\infty} f(k)\,\frac{L_1\cdots L_d}{(2\pi)^d}\,k^{d-1}\Omega_d\sum_n \Gamma\left(\frac{d}{2}\right)\frac{J_{d/2-1}(nk)}{(nk/2)^{d/2-1}}\,dk \quad . \qquad (22)$$

This result is certainly the same as that obtained from

$$\sum_{l_1,\cdots l_d}^{\infty} f\left(2\pi\sqrt{\frac{l_1^2}{L_1^2}+\cdots+\frac{l_d^2}{L_d^2}}\right) = \int_0^{\infty} f(k)\,D_d(k)\,dk$$

by substituting into it the $D_d(k)$ given by Eq.(12). While in obtaining Eq.(12) for $D_d(k)$, the Poisson formula is applied to the delta function.

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