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The Walfisz-like formula from Poisson's summation formula and some applications

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Abstract. The Walfisz-like formula for the number of lattice points of an arbitrary m-dimensional lattice in a hyper-ellipsoid with given semi-axes is derived from Poisson's summation formula. Applications to (i) the evaluation of certain lattice sums and (ii) the calculation of the expressions for the density of states of a single non-relativistic particle as well as of a relativistic particle enclosed in a rectangular m-dimensional box of finite size and subject to different boundary conditions are given.

1. Introduction

In order to calculate the expressions for the thermodynamic properties of an ideal non-relativistic or relativistic quantum gas contained in an enclosure of finite volume, it is necessary to know the expression for the density of single-particle states for such a system. Recently such expressions for the density of states of a single non-relativistic particle enclosed in a cubical box for the case of one, two and three dimensions and for the periodic (PBC), Dirichlet (DBC) and Neumann (NBC) boundary conditions have been derived (Baltes and Steinle 1977, Chaba 1979) by making use of the Walfisz formula (Walfisz 1924) for the number of lattice points of a simple lattice in a hypersphere of given radius. More recently, Pu (1981) has obtained the corresponding expressions for the case of an m-dimensional rectangular box with sides $L_1, L_2, \ldots, L_m$ by making use of the Poisson summation formula (PSF) (Stein and Weiss 1971) directly, but unfortunately some of these expressions are in error. Similarly in the case of a relativistic particle, such expressions for a particle enclosed in a rectangular box of different dimensionalities and in the thermodynamic limit are well known (Carvalho and Rosa Jr 1980, Dunning-Davies 1981).

In this paper we report the derivation of the more general Walfisz-like formula for the number of lattice points of an arbitrary m-dimensional lattice in a hyper-ellipsoid with given semi-axes, starting from the PSF (earlier (Chaba 1979) the PSF in one dimension was derived from the Walfisz formula and the converse could also be achieved simply by reversing the steps) and then using a special case of this for a simple lattice, we obtain the exact expressions (including finite size effects) for the density of states in the case of a single non-relativistic as well as a relativistic particle enclosed in an m-dimensional rectangular box and subject to different boundary conditions. Further, we show that some of the results obtained can be applied for doing (lattice) sums involving arbitrary lattices in any dimension and give some examples.

2. The Walfisz-like formula from Poisson's summation formula

Let $\{\boldsymbol{\tau}\}$ be a Bravais lattice in an m-dimensional Euclidean space, with volume v per lattice point and $\{\boldsymbol{\gamma}\}$ be its reciprocal, normalised by $\exp(2\pi i\boldsymbol{\gamma}\cdot\boldsymbol{\tau})=1$, then the PSF applied to summation over the lattice points (of the lattice $\{\boldsymbol{\tau}\}$) of a function $F(\boldsymbol{\tau})$ is

$$\sum_{\tau} F(\boldsymbol{\tau})=\sum_{\gamma}\mathscr{F}(\boldsymbol{\gamma}) \tag{1}$$

where $\mathscr{F}(\boldsymbol{\gamma})$ is the Fourier transform of $F(\boldsymbol{r})$.

$$\mathscr{F}(\boldsymbol{\gamma})=v^{-1}\int F(\boldsymbol{r})\exp(-2\pi i\boldsymbol{r}\cdot\boldsymbol{\gamma})\,\mathrm{d}^m r, \tag{2}$$

where $\boldsymbol{r}$, $\boldsymbol{\tau}$ and $\boldsymbol{\gamma}$ can be written as

$$\boldsymbol{r}=\sum_{p=1}^{m} x_p\boldsymbol{i}_p,\qquad \boldsymbol{\tau}=\sum_{p=1}^{m}\tau_p\boldsymbol{i}_p,\qquad \boldsymbol{\gamma}=\sum_{p=1}^{m}\gamma_p\boldsymbol{i}_p, \tag{3}$$

$\boldsymbol{i}_p$ $(p=1,2,\ldots,m)$ being the unit vectors along the cartesian coordinates of an orthogonal set of axes. We now define the vectors $\boldsymbol{R}$, $\boldsymbol{T}$ and $\boldsymbol{\Gamma}$ as

$$\boldsymbol{R}=\sum_{p=1}^{m} X_p\boldsymbol{i}_p,\qquad \boldsymbol{T}=\sum_{p=1}^{m} T_p\boldsymbol{i}_p\quad\text{and}\quad \boldsymbol{\Gamma}=\sum_{p=1}^{m}\Gamma_p\boldsymbol{i}_p \tag{4}$$

with $X_p=a_px_p$, $T_p=a_p\tau_p$ and $\Gamma_p=\gamma_p/a_p$, $(p=1,2,\ldots,m)$, where $a_p(p=1,2,\ldots,m)$ are constants. Noting that $\boldsymbol{R}\cdot\boldsymbol{\Gamma}=\boldsymbol{r}\cdot\boldsymbol{\gamma}$, we can rewrite equation (2) as

$$\mathscr{F}(\boldsymbol{\gamma})=(va_1a_2\ldots a_m)^{-1}\int F(\boldsymbol{r})\exp(-2\pi i\boldsymbol{R}\cdot\boldsymbol{\Gamma})\,\mathrm{d}^m R. \tag{5}$$

Now, we assume that the function $F(\boldsymbol{r})$ has a special form and its dependence on $\boldsymbol{r}$ is only through the magnitude R of $\boldsymbol{R}$. In this case, it can be easily seen that $\mathscr{F}(\boldsymbol{\gamma})$ depends on $\boldsymbol{\gamma}$ only through the magnitude Γ of $\boldsymbol{\Gamma}$ and, in this case, we can rewrite equation (5) as

$$\mathscr{F}(\Gamma)=(va_1a_2\ldots a_m)^{-1}\int F(R)\exp(-2\pi i\boldsymbol{R}\cdot\boldsymbol{\Gamma})\,\mathrm{d}^m\boldsymbol{R}, \tag{6}$$

and the PSF, in this special case, takes the form,

$$\sum_{\tau} F(T)=\sum_{\gamma}\mathscr{F}(\Gamma). \tag{7}$$

Now the relation $R^2=\Sigma_{p=1}^m X_p^2=\Sigma_{p=1}^m a_p^2x_p^2$ can be rewritten as

$$\sum_{p=1}^{m} x_p^2/(R/a_p)^2=1, \tag{8}$$

which is the equation of an m-dimensional hyper-ellipsoid with semi-axes $A_p=R/a_p$ $(p=1,2,\ldots,m)$, the variable R determining the size of the hyper-ellipsoid. Now, for the sake of simplicity in calculating $\mathscr{F}(\Gamma)$ from equation (6), we choose $\boldsymbol{\Gamma}$ along the unit vector $\boldsymbol{i}_1$, so that $\boldsymbol{R}\cdot\boldsymbol{\Gamma}=X_1\Gamma$. Also, we may write $\mathrm{d}^m\boldsymbol{R}=\mathrm{d}X_1\,\mathrm{d}^{m-1}\boldsymbol{R}'$, where the vector $\boldsymbol{R}'=\Sigma_{p=2}^m X_p\boldsymbol{i}_p$. Integrating over the directions of $\boldsymbol{R}'$, we can write $\mathrm{d}^{m-1}\boldsymbol{R}'=S_{m-1}(R')\,\mathrm{d}R'$, $S_{m-1}(R')$ being the surface area of an $(m-1)$-dimensional sphere

(Pathria 1972) and then we have

$$\mathscr{F}(\Gamma)=(va_1a_2\ldots a_m)^{-1}2\pi^{(m-1)/2}[\Gamma(m-1)/2]^{-1}$$
$$\times\int_{X_1=-\infty}^{\infty}\int_{R'=0}^{\infty}F(R)\exp(-2\pi\mathrm{i}\Gamma X_1)R'^{m-2}\,\mathrm{d}X_1\,\mathrm{d}R'. \tag{9}$$

Now, putting $X_1=R\cos\theta$, $R'=R\sin\theta$, $\mathrm{d}X_1\,\mathrm{d}R'=R\,\mathrm{d}R\,\mathrm{d}\theta$ (where θ varies from 0 to π) and integrating over the angle θ, we obtain

$$\mathscr{F}(\Gamma)=2\pi(va_1a_2\ldots a_m)^{-1}\int_0^{\infty}F(R)R^{m/2}J_{(m-2)/2}(2\pi\Gamma R)/\Gamma^{(m-2)/2}\,\mathrm{d}R, \tag{10}$$

where $J_\nu(z)$ occurring inside the integral is a Bessel function of the first kind and of order ν (Abramowitz and Stegun 1965). Now, using equations (7) and (10), we get

$$\sum_{\tau}F(T)=2\pi(va_1a_2\ldots a_m)^{-1}\int_0^{\infty}\mathrm{d}R\,R^{m/2}F(R)\sum_{\gamma}J_{(m-2)/2}(2\pi\Gamma R)/\Gamma^{(m-2)/2},$$

which can be rewritten as

$$\sum_{\tau}F(T)=\int_0^{\infty}\mathrm{d}R\,F(R)n_m(R), \tag{11}$$

where

$$n_m(R)\,\mathrm{d}R=2\pi(va_1a_2\ldots a_m)^{-1}R^{m/2}\sum_{\gamma}J_{(m-2)/2}(2\pi\Gamma R)/\Gamma^{(m-2)/2}\,\mathrm{d}R, \tag{12}$$

can be interpreted as the number of lattice points of the lattice $\{\tau\}$ between two hyper-ellipsoids with semi-axes R/a_p and $(R+\mathrm{d}R)/a_p (p=1,2,\ldots,m)$. The expression for the number $N_m(\rho/a_1,\rho/a_2,\ldots,\rho/a_m)$ of lattice points in a hyper-ellipsoid of semi-axes $\rho/a_p (p=1,2,\ldots,m)$ can be obtained by integrating equation (12),

$$N_m(\rho/a_1,\rho/a_2,\ldots,\rho/a_m)=\int_0^{\rho}n_m(R)\,\mathrm{d}R$$
$$=(va_1a_2\ldots a_m)^{-1}\rho^{m/2}\sum_{\gamma}J_{m/2}(2\pi\Gamma\rho)/\Gamma^{m/2}. \tag{13}$$

Substituting ρ/a_p by A_p $(p=1,2,\ldots,m)$ and noting that $\Gamma_\rho=(\Sigma_{p=1}^{m}A_p^2\gamma_p^2)^{1/2}$, we finally obtain the following Walfisz-like formula for the number of lattice points of the lattice $\{\tau\}$ in an m-dimensional hyper-ellipsoid of semi-axes $A_1, A_2,\ldots,A_m$,

$$N_m(A_1,A_2,\ldots,A_m)=A_1A_2\ldots A_m v^{-1}\sum_{\gamma}J_{m/2}\left[2\pi\left(\sum_{p=1}^{m}A_p^2\gamma_p^2\right)^{1/2}\right]\Big/\left(\sum_{p=1}^{m}A_p^2\gamma_p^2\right)^{m/4}. \tag{14}$$

Now we shall discuss the special cases of equation (14).

(i) For a simple lattice (square in the case of two dimensions, simple cubic in the case of three dimensions, etc) with primitive lattice vectors of unit magnitude, $v=1$ and $\gamma_p=q_p$ are integers. In this case, the above expression becomes

$$N_m(A_1,A_2,\ldots,A_m)$$
$$=A_1A_2\ldots,A_m\sum_{\{q_p\}=-\infty}^{\infty}J_{m/2}\left[2\pi\left(\sum_{p=1}^{m}A_p^2q_p^2\right)^{1/2}\right]\Big/\left(\sum_{p=1}^{m}A_p^2q_p^2\right)^{m/4}, \tag{15}$$

which, in the case of a hyper-sphere of radius ρ, becomes

$$N_m(\rho) = \rho^{m/2} \sum_{\{q_p\}=-\infty}^{\infty} J_{m/2}(2\pi\rho q)/q^{m/2}, \tag{16}$$

where $q = (\Sigma_{p=1}^{m} q_p^2)^{1/2}$. Equations (15) and (16) are just the Walfisz formulae.

(ii) For the case of an arbitrary lattice $\{\boldsymbol{\tau}\}$, the number of lattice points in a hyper-sphere of radius ρ is obtained from (14) by putting $a_1 = a_2 = \ldots = a_m = 1$, so that $A_1 = A_2 \ldots = A_m = \rho$ and thus we have

$$N_m(\rho) = \rho^{m/2} v^{-1} \sum_{\boldsymbol{\gamma}} J_{m/2}(2\pi\rho\gamma)/\gamma^{m/2}, \tag{17}$$

$\gamma = (\Sigma_{p=1}^{m} \gamma_p^2)^{1/2}$ being the magnitude of the reciprocal lattice vector $\boldsymbol{\gamma}$, and, in this case, equations (11) and (12) become, respectively,

$$\sum_{\boldsymbol{\tau}} F(\tau) = \int_0^{\infty} \mathrm{d}R\, F(R) n_m(R) \tag{18}$$

and

$$n_m(R)\,\mathrm{d}R = (2\pi/v) R^{m/2} \sum_{\boldsymbol{\gamma}} J_{(m-2)/2}(2\pi\gamma R)/\gamma^{(m-2)/2}\,\mathrm{d}R, \tag{19}$$

where the expression in equation (19) represents the number of lattice points of the lattice $\{\boldsymbol{\tau}\}$ in a hyperspherical shell of radius R and thickness $\mathrm{d}R$. In the case of further specialisation to that of a simple lattice, (17) reduces to (16), as it should, and (19) becomes

$$n_m(R)\,\mathrm{d}R = 2\pi R^{m/2} \sum_{\{q_p\}=-\infty}^{\infty} J_{(m-2)/2}(2\pi R q)/q^{(m-2)/2}\,\mathrm{d}R, \tag{20}$$

where $q = (\Sigma_{p=1}^{m} q_p^2)^{1/2}$.

3. Applications

Now we shall consider the applications of some of the results obtained above.

3.1. Evaluation of lattice sums in arbitrary dimensions

Firstly, we notice that in order to do the lattice sum $\Sigma_{\boldsymbol{\tau}} F(\tau)$ for a certain dimensionality, we can use equation (18) along with equation (19) for $n_m(R)\,\mathrm{d}R$ with a suitable value of m. The result thus obtained would be exact and would be the same as that arrived at by the direct application of PSF but the proceudre given here is much simpler. We may further point out that this procedure can also be regarded as an application of the Walfisz-like formula (equation (17)), because equation (19) can be obtained from equation (17) just by differentiation. We shall now illustrate this method by doing two lattice sums which have already appeared in the literature in order to show how direct and straightforward the present approach is as compared with other methods. First, we take up the two-dimensional sum $\Sigma'^{\infty}_{\{l_p\}=-\infty} K_0[\mu(l_1^2 + l_2^2)^{1/2}]$, $\mu > 0$, involving a simple lattice, the prime on the summation indicating that the term $l_1 = l_2 = 0$ is excluded from it. As a first step, using equation (18), we do the summation

$$\sum_{\{l_p\}=-\infty}^{\infty} (l_1^2 + l_2^2)^{1/2} K_1[\mu(l_1^2 + l_2^2)^{1/2}] = \int_0^{\infty} R K_1(\mu R) n_2(R)\,\mathrm{d}R,$$

where, $n_2(R)\,dR$ is obtained from equation (20) for a simple lattice by putting $m=2$, with the result

$$n_2(R)\,dR=\left(2\pi R+2\pi R\sum_{\{q_p\}=-\infty}^{\infty}{}' J_0(2\pi qR)\right)dR,$$

and doing the integration, we get

$$\sum_{\{l_p\}=-\infty}^{+\infty}(l_1^2+l_2^2)^{1/2}K_1[\mu(l_1^2+l_2^2)^{1/2}]=4\pi/\mu^3+4\pi\mu\sum_{\{q_p\}=-\infty}^{\infty}{}'[\mu^2+4\pi^2(q_1^2+q_2^2)]^{-2}.$$

Separating out the $l_1=l_2=0$ term from the sum on the left-hand side and integrating with respect to μ, we get

$$\begin{aligned}\sum_{\{l_p\}=-\infty}^{\infty}{}' K_0[\mu(l_1^2+l_2^2)^{1/2}]&\\ &=2\pi/\mu^2+(1/2)\ln(\mu^2/4\pi)+C\\ &\quad-(\mu^2/2\pi)\sum_{\{q_p\}=-\infty}^{\infty}{}'(q_1^2+q_2^2)^{-1}[\mu^2+4\pi^2(q_1^2+q_2^2)]^{-1},\end{aligned}\qquad(21)$$

where C is the constant of integration and can be obtained numerically by giving a suitable particular value to μ. This sum has already appeared in the literature (Fetter *et al* 1966, Chaba and Pathria 1975), in connection with different physical problems. As a second example, we do the three-dimensional sum $\Sigma_\tau' e^{-a\tau}/\tau$, again the prime on the sum means that the term corresponding to $\tau=0$ is excluded from it. As a first step, using equation (18), we do the sum

$$\sum_\tau e^{-a\tau}=\int_0^\infty e^{-aR}n_3(R)\,dR,$$

where $n_3(R)\,dR$ is obtained from equation (19) for an arbitrary lattice by putting $m=3$, with the result

$$n_3(R)\,dR=\left[(4\pi R^2/v)+(2R/v)\sum_\gamma{}'\sin(2\pi\gamma R)/\gamma\right],$$

and doing the integration, we get

$$\sum_\tau e^{-a\tau}=(8\pi a/v)\sum_\gamma(a^2+4\pi^2\gamma^2)^{-2}.$$

Separating out the terms corresponding to $\tau=0$ and $\gamma=0$ from the two sides and integrating with respect to a, we get

$$\sum_\tau{}' e^{-a\tau}/\tau=4\pi/(va^2)+J_\gamma(0,1,3)/(\pi v^{1/3})+a-(a^2/\pi v)\sum_\gamma{}'\gamma^{-2}(a^2+4\pi^2\gamma^2)^{-1},\qquad(22)$$

where, $J_\gamma(0,1,3)/(\pi v^{1/3})$ is the constant of integration and this notation is adopted to be consistent with that used earlier (Chaba 1980). This sum with simple lattice $\boldsymbol{\tau}$ has already appeared (Chaba and Pathria 1978) in connection with the study of the phenomenon of Bose–Einstein condensation in a three-dimensional system of ideal bosons. More recently, it has occurred again in the work of Medeiros e Silva and Mokross (1980) on the screened Wigner Lattice, where they used Ewald's method for doing this sum. We may point out that the form of our result (equation (22)) is much more elegant and also is easier to work with. Before ending this discussion on the lattice sums, we wish to make one more comment. Whereas in the references Chaba (1979) and Pu (1981), it was shown that the sums in the k-space can be done by using the relevant expressions for density of states obtained from the Walfisz formula (the results being identical with those obtained by using PSF), here we have shown that we can do sums involving any arbitrary lattice (in the real space or the k-space) by using the expression for the density of lattice points obtained from the Walfisz-like formula or from the PSF.

3.2. *Density of states of a non-relativistic particle*

Now we shall derive expressions for the density of states of a single non-relativistic particle in an m-dimensional rectangular box of finite size and of sides $L_1, L_2, \ldots, L_m$ and subject to PBC, NBC and DBC. Such expressions have already been derived Pu (1981) but contain an error. So we have taken up this application in order to give the correct results, obtained using a somewhat different approach, for ready reference. We take up the case of PBC first. In this case, the single-particle energy eigenvalues ε are given by $\varepsilon = \hbar^2 k^2/2m$, where

$$k = 2\pi\left(\sum_{p=1}^{m} l_p^2/L_p^2\right)^{1/2} \qquad \text{with } l_{1,2\ldots,m} = 0, \pm 1, \pm 2, \ldots. \tag{23}$$

The number of states $N^P(K)$ with $k \leqslant K$ or with $\Sigma_{p=1}^{m} l_p^2/L_p^2 \leqslant K^2/4\pi^2$, is, clearly, equal to the number of lattice points of a simple m-dimensional lattice in a hyper-ellipsoid with semi-axes $KL_p/2\pi (p = 1, 2, \ldots, m)$ and, therefore, using the Walfisz formula, equation (15), we obtain

$$N_m^P(K) = [L_1L_2 \ldots L_m K^{m/2}/(2\pi)^{m/2}] \sum_{\{q_p\}=-\infty}^{\infty} J_{m/2}\left[K\left(\sum_{p=1}^{m} q_p^2 L_p^2\right)^{1/2}\right] \bigg/ \left(\sum_{p=1}^{m} q_p^2 L_p^2\right)^{m/4}, \tag{24}$$

which exactly agrees with equation (19) of Pu (1981) who derived it by using the PSF directly. Further, we feel that he incorrectly called this expression (which deals with the *number of single-particle states* of a non-relativistic particle in a rectangular box) as the Walfisz formula whereas we have reserved this name for equations (15) and (16) and the Walfisz-like formulae for equations (14) and (17) (All these expressions deal with *the number of lattice points in a hypersphere or hyper-ellipsoid*). Now we take up the cases of the DBC and the NBC. In these cases, k is given by

$$k = \pi\left(\sum_{p=1}^{m} l_p^2/L_p^2\right)^{1/2},$$

where, for the DBC

$$l_{1,2,\ldots,m} = 1, 2, 3, \ldots,$$

and, for the NBC

$$l_{1,2,\ldots,m} = 0, 1, 2, 3, \ldots. \tag{25}$$

Now, if $f(x_1, x_2, \ldots, x_m)$ is an even function in all of its arguments, then we can obtain the following result by first doing it in one, two, and three dimensions and then generalising it to m dimensions,

$$\sum_{\{l_p\}=(1-\eta)/2}^{\infty} f(l_1, l_2, \ldots, l_m) = (1/2)^m\Big(\eta^m f(0, 0, \ldots, 0) + \sum_{s=1}^{m} \eta^{m-s} \sum_{1\leqslant j_1<j_2\ldots<j_s\leqslant m} \sum_{\{l_{j_p}\}=-\infty}^{+\infty} f(l_{j_1}, l_{j_2}\ldots, l_{j_p}, \ldots l_{j_s})\Big) \tag{26}$$

where $\eta = \pm 1$. Now we choose

$$f(l_1, l_2, \ldots, l_m) = \theta\Big(K - \pi\Big(\sum_{p=1}^{m} l_p^2/L_p^2\Big)^{1/2}\Big), \tag{27}$$

where $\theta(x)$ is the step-function defined by

$$\theta(x) = \begin{cases} 1, & \text{when } x \geqslant 0 \\ 0, & \text{when } x < 0. \end{cases}$$

In this case equation (26) becomes

$$N_m^{\mathrm{D/N}}(K; L_1, L_2, \ldots, L_m) = (1/2)^m\Big(\eta^m\theta(K) + \sum_{s=1}^{m} \eta^{m-s} \sum_{1\leqslant j_1<j_2\ldots<j_s\leqslant m} N_s^{\mathrm{P}}(K; 2L_{j_1}, 2L_{j_2}, \ldots, 2L_{j_s})\Big), \tag{28}$$

where

$$\eta = \begin{cases} +1, & \text{for the NBC} \\ -1, & \text{for the DBC} \end{cases}$$

and $N_m(K; L_1, L_2, \ldots, L_m)$ is the number of states with $k \leqslant K$ for a particle in a rectangular box of sides $L_1, L_2, \ldots, L_m$, for the boundary conditions indicated by the superscripts P for PBC, D for DBC and N for NBC. For all the three boundary conditions, the results can be written together as

$$N_m(K) = (1+\eta^2)^{-m}\Big(\eta^m\theta(K) + \sum_{s=1}^{m} \eta^{m-s} \sum_{1\leqslant j_1<j_2\ldots<j_s\leqslant m} N_s^{\mathrm{P}}[K; (1+\eta^2)L_{j_1}, \times(1+\eta^2)L_{j_2}, \ldots, (1+\eta^2)L_{j_s}]\Big), \tag{29}$$

where $\eta = 0$ for the PBC. Now substituting equation (24) in equation (29), we get

$$N_m(K) = (1+\eta^2)^{-m}\Big(\eta^m\theta(K) + \sum_{s=1}^{m} \eta^{m-s} \sum_{1\leqslant j_1<j_2\ldots<j_s\leqslant m} \frac{(1+\eta^2)^{s/2} L_{j_1}L_{j_2}\ldots L_{j_s}K^{s/2}}{(2\pi)^{s/2}} \times \sum_{\{q_{i_p}\}=-\infty}^{\infty} \frac{J_{s/2}[K(1+\eta^2)(\Sigma_{p=1}^{s} q_{i_p}^2 L_{j_p}^2)^{1/2}]}{(\Sigma_{p=1}^{s} q_{i_p}^2 L_{j_p}^2)^{s/4}}\Big). \tag{30}$$

In the case of the PBC, $\eta = 0$ and, therefore, only one term in the summations over s and the j_p's corresponding to $s = m$ and $j_1 = 1$, $j_2 = 2, \ldots j_m = m$ survives and we recover equation (24). Now we can obtain the expression for the density of states $D_m(k)$ by differentiating equation (30).

$$D_m(k) = \mathrm{d}N_m(k)/\mathrm{d}k$$

$$= (1+\eta^2)^{-m}\left(\eta^m \delta(k) + \sum_{s=1}^{m} \eta^{m-s} \sum_{1\leq j_1<j_2\ldots j_s\leq m} \frac{(1+\eta^2)^{(s+2)/2} L_{j_1} L_{j_2}\ldots L_{j_s} k^{s/2}}{(2\pi)^{s/2}}\right.$$
$$\left.\times \sum_{\{q_{j_p}\}=-\infty}^{\infty} \frac{J_{(s-2)/2}[k(1+\eta^2)(\Sigma_{p=1}^{s} q_{j_p}^2 L_{j_p}^2)^{1/2}]}{(\Sigma_{p=1}^{s} q_{j_p}^2 L_{j_p}^2)^{(s-2)/4}}\right). \tag{31}$$

Although equations (30) and (31) are somewhat similar to (21) and (16) respectively of Pu (1981), there is a slight difference in that in his results there occurs a combinatorial factor $\binom{m}{s}$ as multiplier instead of the sum over the j's in our results. This error in his equations arose because Pu assumed that the function $f(x_1, x_2, \ldots, x_m)$ occurring in equation (26) is invariant under all permutations of its arguments whereas in our problem f given in equation (27) does not have the above property for a rectangular box, in general, though it does possess that property in the case of a 'cubical' box. That is why the special cases of equation (16) of Pu (1981) for $m=2$ and 3 did agree with the corresponding results in Chaba (1979) which were valid only in the case of the 'cubical' box.

3.3. *Density of states of a relativistic particle*

Now we shall derive the expression for the density of states of a single relativistic particle enclosed in an m-dimensional 'rectangular' box of finite size and of sides L_1, $L_2, \ldots, L_m$ (and of volume $V = L_1 L_2 \ldots L_m$) and subject to PBC. In this case, the single-particle energy eigenvalues ε are given by

$$\varepsilon^2 = m_0^2 c^4 + c^2 \hbar^2 k^2 \tag{32}$$

which can also be written as

$$k = (\varepsilon^2 - m_0^2 c^4)^{1/2}/c\hbar \tag{33}$$

where k is again given by equation (23).

The number of states $N^{\mathrm{P}}(E)$ with $\varepsilon \leq E$ or $k \leq K = (E^2 - m_0^2 c^4)^{1/2}/c\hbar$ is given by the number of different sets $\{l_p\}$ of the values of the l_p's, satisfying

$$\sum_{p=1}^{m} l_p^2/L_p^2 \leq K^2/4\pi^2$$

and is clearly equal to the number of lattice points of a simple m-dimensional lattice in a hyper-ellipsoid with semi-axes $KL_p/2\pi\,(p=1,2,\ldots,m)$, and, therefore, using the Walfisz formula, equation (15), we obtain

$$N_m^{\mathrm{P}}(E) = V(E^2 - m_0^2 c^4)^{m/4}(c\hbar)^{-m/2}$$
$$\times \sum_{\{q_p\}=-\infty}^{+\infty} J_{m/2}\left((c\hbar)^{-1}(E^2 - m_0^2c^4)^{1/2}\left(\sum_{p=1}^{m} q_p^2 L_p^2\right)^{1/2}\right)\Big/\left(\sum_{p=1}^{m} q_p^2 L_p^2\right)^{m/4}. \tag{34}$$

Now we can get the expression for the density of states $D_m^{\mathrm{P}}(\varepsilon)$ by differentiating equation (34),

$$D_m^{\mathrm{P}}(\varepsilon)=\mathrm{d}N_m^{\mathrm{P}}(\varepsilon)/\mathrm{d}\varepsilon=2\pi V(c\hbar)^{-(m+2)/2}\varepsilon(\varepsilon^2-m_0^2c^4)^{(m-2)/4}\sum_{\{q_p\}=-\infty}^{+\infty}J_{(m-2)/2}$$

$$\times\left[(c\hbar)^{-1}(\varepsilon^2-m_0^2c^4)^{1/2}\left(\sum_{p=1}^{m}q_p^2L_p^2\right)^{1/2}\right]\Big/\left(\sum_{p=1}^{m}q_p^2L_p^2\right)^{(m-2)/4},$$

which can be rewritten as

$$\begin{aligned}D_m^{\mathrm{P}}(\varepsilon)=&\,2\pi^{m/2}V(ch)^{-m}[\Gamma(m/2)]^{-1}\varepsilon(\varepsilon^2-m_0^2c^4)^{(m-2)/2}\\&+2\pi V(ch)^{-(m+2)/2}\varepsilon(\varepsilon^2-m_0^2c^4)^{(m-2)/4}\\&\times\sum_{\{q_p\}=-\infty}^{+\infty}{}'J_{(m-2)/2}\left[(c\hbar)^{-1}(\varepsilon^2-m_0^2c^4)^{1/2}\right.\\&\left.\times\left(\sum_{p=1}^{m}q_p^2L_p^2\right)^{1/2}\right]\Big/\left(\sum_{p=1}^{m}q_p^2L_p^2\right)^{(m-2)/4}.\end{aligned}\tag{35}$$

For ready reference, we write below the results for the special cases of $m=1$, 2 and 3

$$\begin{aligned}D_1^{\mathrm{P}}(\varepsilon)=&\,2L\varepsilon(ch)^{-1}(\varepsilon^2-m_0^2c^4)^{-1/2}+2L\varepsilon(ch)^{-1}(\varepsilon^2-m_0^2c^4)^{-1/2}\\&\times\sum_{q=-\infty}^{+\infty}{}'\cos[qL(c\hbar]^{-1}(\varepsilon^2-m_0^2c^4)^{1/2}],\end{aligned}\tag{36}$$

$$D_2^{\mathrm{P}}(\varepsilon)=2\pi A\varepsilon(ch)^{-2}+2\pi A\varepsilon(ch)^{-2}\sum_{q_{1,2}=-\infty}^{+\infty}{}'J_0[(c\hbar)^{-1}(\varepsilon^2-m_0^2c^4)^{1/2}(q_1^2L_1^2+q_2^2L_2^2)^{1/2}],\tag{37}$$

$$\begin{aligned}D_3^{\mathrm{P}}(\varepsilon)=&\,4\pi V(ch)^{-3}\varepsilon(\varepsilon^2-m_0^2c^4)^{1/2}+2V(ch)^{-2}\varepsilon\\&\times\sum_{q_{1,2,3}=-\infty}^{+\infty}{}'\sin[(c\hbar)^{-1}(\varepsilon^2-m_0^2c^4)^{1/2}\\&\times(q_1^2L_1^2+q_2^2L_2^2+q_3^2L_3^2)^{1/2}]/(q_1^2L_1^2+q_2^2L_2^2+q_3^2L_3^2)^{1/2}.\end{aligned}\tag{38}$$

We may mention that the results in equations (35)–(38) are new, so far as we know. We notice that the first term in each of these equations varies monotonically with ε but that the subsequent terms are of oscillatory character and it can be easily verified that in the thermodynamic limit, the oscillatory terms become negligible as compared with the first term except for the case of $m=1$. Thus except for $m=1$, the first term in equation (35) (which contains equations (37) and (38)) represents the result in the thermodynamic limit, the subsequent terms in the summations involving Bessel functions, being the finite-size corrections. For the case of $m=1$, the oscillatory terms are of the same order of magnitude as the first term, even in the thermodynamic limit and, therefore, the complete expression in (36) has to be used even in this limit. The first term of (35), which corresponds to the Weyl term in the case of a non-relativistic particle in a three-dimensional box, is the one used by Dunning-Davies (1981) for the (so-called) exact calculation of the thermodynamic properties of an ideal relativistic Bose gas, in the thermodynamic limit. Also the first term in (38) for the density of states was used by Carvalho and Rosa Jr (1980) in their study of the relativistic Bose gas in three dimensions and in the thermodynamic limit. Clearly, one will have to use the complete expressions given above in order to include the finite-size effects.

Now we take up the cases of the DBC and the NBC. In these cases, k in (32) and (33) is again given by (25). Now using (34) in (29) which is valid in the present case also, we get

$$N_m(E) = (1+\eta^2)^{-m}\Big\{\eta^m\theta[(c\hbar)^{-1}(E^2-m_0^2c^4)^{1/2}] + \sum_{s=1}^{m}\eta^{m-s} \times \sum_{1\leq j_1<j_2\ldots<j_s\leq m} (1+\eta^2)^{s/2}L_{j_1}L_{j_2}\ldots L_{j_s}(E^2-m_0^2c^4)^{s/4}(ch)^{-s/2} \times \sum_{\{q_{j_p}\}=-\infty}^{\infty} J_{s/2}\Big[(1+\eta^2)(c\hbar)^{-1}(E^2-m_0^2c^4)^{1/2}\Big(\sum_{p=1}^{s} q_{j_p}^2L_{j_p}^2\Big)^{1/2}\Big] \times\Big(\sum_{p=1}^{s} q_{j_p}^2L_{j_p}^2\Big)^{-s/4}\Big\}. \tag{39}$$

Now we can obtain the expression for the density of states $D_m(\varepsilon)$, for the PBC, the DBC and the NBC by differentiating equation (39)

$$D_m(\varepsilon) = \mathrm{d}N_m(\varepsilon)/\mathrm{d}\varepsilon = (1+\eta^2)^{-m}\Big\{\eta^m\varepsilon(\varepsilon^2-m_0^2c^4)^{-1/2}\delta[(\varepsilon^2-m_0^2c^4)^{1/2}] + \sum_{s=1}^{m}\eta^{m-s} \sum_{1\leq j_1<j_2\ldots<j_s\leq m} 2\pi(ch)^{-(s+2)/2}(1+\eta^2)^{(s+2)/2}L_{j_1}L_{j_2}\ldots L_{j_s} \times\varepsilon(\varepsilon^2-m_0^2c^4)^{(s-2)/4} \times \sum_{\{q_{j_p}\}=-\infty}^{\infty} J_{(s-2)/2}\Big[(c\hbar)^{-1}(1+\eta^2)(\varepsilon^2-m_0^2c^4)^{1/2}\Big(\sum_{p=1}^{s} q_{j_p}^2L_{j_p}^2\Big)^{1/2}\Big] \times\Big(\sum_{p=1}^{s} q_{j_p}^2L_{j_p}^2\Big)^{-(s-2)/4}\Big\}. \tag{40}$$

In the case of PBC, $\eta=0$ and, therefore, only one term in the summations over s and the j_p's corresponding to $s=m$ and $j_1=1$, $j_2=2,\ldots,j_m=m$ in equations (39) and (40) survives and we recover equations (34) and (35) respectively.

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