17/3/83

UFPB - DF- 01/83

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

J de Freitas and A N Chaba

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

Abstract

Walfisz-like formula for the number of lattice points of an arbitrary m-dimensional lattice in a hyperellipsoid with given semi-axes is derived from the 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. (Author)

BR8511495

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's formula (Walfisz 1924) for the number of lattice points of a simple lattice in a hypersphere of given radius. More recently, Pu (1983) 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's summation formula (PSF) (Stein and Weiss 1971) directly but unfortunately some of these expressions are in error. Also 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 hyperellipsoid with given semi-axes, starting from the PSF (Earlier (Chaba 1979), the PSF in one dimension was derived from the Walfisz's formula and the converse could also be done just 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. Walfisz-like formula from Poisson's summation formula

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

$$\sum_{\vec{\tau}} F(\vec{\tau}) = \sum_{\vec{\gamma}} \mathfrak{F}(\vec{\gamma}) \tag{1}$$

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

$$\mathfrak{F}(\vec{\gamma}) = v^{-1} \int F(\vec{r}) \exp(-2\pi i\, \vec{r}.\vec{\gamma})\, d^m\vec{r}, \tag{2}$$

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

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

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

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

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

$$\mathfrak{J}(\vec{\gamma}) = (va_1 a_2 \ldots a_m)^{-1} \int F(\vec{r}) \exp(-2\pi i \vec{R}.\vec{\Gamma}) d^m R. \tag{5}$$

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

$$\mathfrak{J}(\Gamma) = (va_1 a_2 \ldots a_m)^{-1} \int F(R) \exp(-2\pi i \vec{R}.\vec{\Gamma}) d^m \vec{R}, \tag{6}$$

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

$$\sum_{\vec{\tau}} F(T) = \sum_{\vec{\Upsilon}} \mathfrak{J}(\Gamma) \tag{7}$$

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

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

which is the equation of an m-dimensional hyperellipsoid with semi-axes $A_p = R/a_p$ $(p=1,2,\ldots,m)$, the variable R determining the size of the hyperellipsoid. Now, for the sake of simplicity in calculating $\mathfrak{J}(\Gamma)$ from Eq. (6), we choose $\vec{\Gamma}$ along the unit vector $\vec{I}_1$, so that $\vec{R}.\vec{\Gamma} = X_1\Gamma$. Also, we may write $d^m\vec{R} = dX_1 d^{m-1}R'$, where the vector $\vec{R}' = \sum_{p=2}^{m} X_p \vec{I}_p$. Integrating over the directions of R', we can write $d^{m-1}R' = S_{m-1}(R')dR'$, $S_{m-1}(R')$ being the surface area of an (m-1)-dimensional sphere (Pathria 1972) and then, we have

$$\mathfrak{J}(\Gamma) = (va_1a_2\ldots a_m)^{-1} 2\pi^{(m-1)/2} (\Gamma(m-1)/2)^{-1} \int_{X_1=-\infty}^{\infty}\int_{R'=0}^{\infty} F(R)\exp(-2\pi i\Gamma X_1) R'^{m-2} dX_1 dR'. \tag{9}$$

Now, putting $X_1 = R\cos\theta$, $R' = R\sin\theta$, $dX_1 dR' = RdRd\theta$ (where θ varies from 0 to π) and integrating over the angle θ, we obtain

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

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

$$\sum_{\vec{\tau}} F(T) = 2\pi (v a_1 a_2 \ldots a_m)^{-1} \int_0^\infty dR\, R^{m/2} F(R) \sum_{\vec{\gamma}} J_{(m-2)/2}(2\pi \Gamma R)/\Gamma^{(m-2)/2},$$

which can be rewritten as

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

where

$$n_m(R) dR = 2\pi (v a_1 a_2 \ldots a_m)^{-1} R^{m/2} \sum_{\vec{\gamma}} J_{(m-2)/2}(2\pi \Gamma R)/\Gamma^{(m-2)/2} dR, \tag{12}$$

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

$$\begin{aligned} N_m(\rho/a_1,\rho/a_2,\ldots,\rho/a_m) &= \int_0^\rho n_m(R) dR \\ &= (v a_1 a_2 \ldots a_m)^{-1} \rho^{m/2} \sum_{\vec{\gamma}} J_{m/2}(2\pi \Gamma \rho)/\Gamma^{m/2}. \end{aligned} \tag{13}$$

Substituting ρ/a_p by $\Lambda_p (p=1,2,\ldots m)$ and noting that $\Gamma \rho = (\sum_{p=1}^{m} \Lambda_p^2 \gamma_p^2)^{1/2}$, we finally obtain the following Walfisz-like formula for the number of lattice points of the lattice $\{\vec{\tau}\}$ in an m-dimensional hyperellipsoid of semi-axes $\Lambda_1,\Lambda_2,\ldots,\Lambda_m$,

$$N_m(\Lambda_1,\Lambda_2,\ldots,\Lambda_m) = \Lambda_1 \Lambda_2 \ldots \Lambda_m v^{-1} \sum_{\vec{\gamma}} J_{m/2}(2\pi (\sum_{p=1}^{m} \Lambda_p^2 \gamma_p^2)^{1/2}) / (\sum_{p=1}^{m} \Lambda_p^2 \gamma_p^2)^{m/4}. \tag{14}$$

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

(i) For a simple lattice (Square in the case of two dimensions, 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

$$N_m(\lambda_1,\lambda_2,\ldots,\lambda_m)=\lambda_1\lambda_2\ldots\lambda_m\sum_{(q_p)=-\infty}^{\infty} J_{m/2}(2\pi(\sum_{p=1}^{m}\lambda_p^2q_p^2)^{1/2})/(\sum_{p=1}^{m}\lambda_p^2q_p^2)^{m/4}, \quad (15)$$

which, in the case of hypersphere of radius ρ, becomes

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

where $q=(\sum_{p=1}^{m} q_p^2)^{1/2}$. Eqs. (15) and (16) are justly Walfisz's formulae.

(ii) For the case of an arbitrary lattice $\{\vec{\tau}\}$, the number of lattice points in a hypersphere of radius ρ is obtained from Eq. (14) by putting $a_1=a_2=\ldots=a_m=1$, so that $\lambda_1=\lambda_2\ldots=\lambda_m=\rho$ and thus we have

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

$\gamma=(\sum_{p=1}^{D}\gamma_p^2)^{1/2}$ being the magnitude of the reciprocal lattice vector $\vec{\gamma}$, and, in this case, Eqs. (11) and (12) become, respectively,

$$\sum_{\vec{\tau}}F(\tau) = \int_0^{\infty}dR\, F(R)n_m(R) \quad (18)$$

and

$$n_m(R)dR= (2\pi/v)R^{m/2}\sum_{\vec{\gamma}} J_{(m-2)/2}(2\pi\gamma R)/\gamma^{(m-2)/2}dR, \quad (19)$$

where the expression in Eq. (19) represents the number of lattice points of the lattice $\{\vec{\tau}\}$ in a hyperspherical shell of radius R and thickness dR. In case of further specialization to the case of a simple lattice, Eq. (17) reduces to Eq. (16), as it should, and Eq. (19) becomes

$$n_m(R)dR=2\pi R^{m/2} \sum_{\{q_p\}=-\infty}^{\infty} J_{(m-2)/2}(2\pi Rq)/q^{(m-2)/2}dR, \qquad (20)$$

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

3. Applications

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

i) Evaluation of lattice sums in arbitrary dimensions.

Firstly, we notice that in order to do the lattice sum $\sum_{\vec{\tau}} F(\tau)$ for a certain dimensionality, we can use Eq. (18) along with Eq. (19) for $n_m(R)dR$ 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 procedure given here is much simpler. We may further point out that this procedure can also be regarded as an application of Walfisz-like formula (Eq. (17)) because Eq. (19) can be obtained from Eq. (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 to other methods. First, we take up the two-dimensional sum $\sum'_{\{l_p\}=-\infty}^{\infty} K_o(\mu(l_1^2+l_2^2)^{1/2})$, $\mu > o$, involving a simple lattice, prime on the summation meaning that the term $l_1 = l_2 = 0$ is excluded from it. As a first step, using Eq. (18), we do the summation

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

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

$$n_2(R)dR = \{2\pi R + 2\pi R \sum'_{\{q_p\}=-\infty}^{\infty} J_o(2\pi qR)\} dR,$$

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

$$\sum'_{\{l_p\}=-\infty}^{\infty} K_o(\mu(l_1^2+l_2^2)^{1/2}) = 2\pi/\mu^2 + (1/2)\ln(\mu^2/4\pi) + C$$

$$-(\mu^2/2\pi) \sum'_{\{q_p\}=-\infty}^{\infty} (q_1^2+q_2^2)^{-1} \{\mu^2+4\pi^2(q_1^2+q_2^2)\}^{-1}, \qquad (21)$$

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, Hohenberg and Pincus 1966; Chaba and Pathria 1975), in connection with different physical problems. As a second example, we do the three-dimensional sum $\sum_{\vec{\tau}}' e^{-a\tau}/\tau$, again the prime on the sum means that the term corresponding to $\tau=0$ is excluded from it. As a first step, using Eq. (18), we do the sum

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

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

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

and doing the integration, we get

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

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

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

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 $\vec{\tau}$ has already (Chaba and Pathria 1978) appeared 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 the Ewald's method for doing this sum. We may point out that the form of our result (Eq.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 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's 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 Walfisz-like formula or from the PSF.

ii) 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 by 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 $\epsilon = \hbar^2 k^2/2m$, where

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

with $l_{1,2,\ldots,m} = 0, \pm 1, \pm 2, \ldots$ (23)

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

$$N_m^P(K) = (L_1L_2\ldots L_m K^{m/2}/(2\pi)^{m/2}) \sum_{\{l_p\}=-\infty}^{\infty} J_{m/2}(K(\sum_{p=1}^{m} q_p^2L_p^2)^{1/2})/(\sum_{p=1}^{m} q_p^2L_p^2)^{m/4}, \quad (24)$$

which exactly agrees with Eq. (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 Walfisz's formula whereas we have reserved this name for Eqs. (15) and (16) and Walfisz-like formulae for Eqs. (14) and (17) (All these expressions deal with the number of lattice points in a hypersphere or hyperellipsoid). 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 generalizing it to m dimensions,

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

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

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

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

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

In this case, Eq. (26) becomes

$$N_m^{D/N}(K;L_1,L_2,\ldots,L_m)=(1/2)^m(\eta^m\theta(K)+$$

$$\sum_{s=1}^{m}\eta^{m-s}\sum_{1\leq j_1<j_2\ldots<j_s\leq m}N_s^P(K;2L_{j_1},2L_{j_2},\ldots,2L_{j_s})) , \qquad (28)$$

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 $k\leq K$ 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

$$N_m(K)=(1+\eta^2)^{-m}(\eta^m\theta(K)+$$

$$\sum_{s=1}^{m}\eta^{m-s}\sum_{1\leq j_1<j_2\ldots<j_s\leq m}N_s^P(K;(1+\eta^2)L_{j_1},(1+\eta^2)L_{j_2},\ldots(1+\eta^2)L_{j_s})) , \qquad (29)$$

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

$$N_m(K)=(1+\eta^2)^{-m}(\eta^m\theta(K)+$$

$$\sum_{s=1}^{m}\eta^{m-s}\sum_{1\leq j_1<j_2\ldots<j_s\leq m}\frac{(1+\eta^2)^{s/2}L_{j_1}L_{j_2}\ldots L_{j_s}K^{s/2}}{(2\pi)^{s/2}}\sum_{(q_{j_p})=-\infty}^{\infty}\frac{J_{s/2}(K(1+\eta^2)(\sum_{n=1}^{s}q_{j_n}^2L_{j_n}^2)^{1/2})}{(\sum_{p=1}^{s}q_{j_p}^2L_{j_p}^2)^{s/4}}). \qquad (30)$$

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

$$
\begin{aligned}
D_m(k) &= dN_m(k)/dk \\
&= (1+\eta^2)^{-m}\{\eta^m \delta(k) + \\
&\sum_{s=1}^{m} \eta^{m-s} \sum_{1 \le j_1 < j_2 \ldots j_s \le m} \frac{(1+\eta^2)^{(s+2)/2} L_{j_1} L_{j_2} \ldots L_{j_s} k^{s/2}}{(2\pi)^{s/2}} \sum_{(q_{j_p})=-\infty}^{\infty} \frac{J_{(s-2)/2}\left(k(1+\eta^2)\left(\sum_{p=1}^{s} q_{j_p}^2 L_{j_p}^2\right)^{1/2}\right)}{\left(\sum_{p=1}^{s} q_{j_p}^2 L_{j_p}^2\right)^{(s-2)/4}}\}
\end{aligned}
\tag{31}
$$

Although Eqs. (30) and (31) are somewhat similar to Eqs. (21) and (16) of Pu (1981) respectively, 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 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 Eq. (26) is invariant under all permutations of its arguments whereas in our problem f given in Eq. (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 Eq. (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.

(iii) 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 Eq. (23).
The number of states $N^P(E)$ 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 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 hyperellipsoid with semi-axes $KL_p/2\pi$ (p=1,2,...,m), and, therefore, using Walfisz's formula, Eq. (15), we obtain

$$C_m^P(\varepsilon)=V(\varepsilon^2-m_0^2c^4)^{m/4}(c\hbar)^{-m/2}\sum_{\{q_p\}=-\infty}^{+\infty}{}' J_{m/2}\left((c\hbar)^{-1}(\varepsilon^2-m_0^2c^4)^{1/2}\left(\sum_{p=1}^{m}q_p^2L_p^2\right)^{1/2}\right)\Big/\left(\sum_{p=1}^{m}q_p^2L_p^2\right)^{m/4}. \quad (34)$$

Now, we can get the expression for the density of states $D_m^P(\varepsilon)$ by differentiating Eq. (34),

$$D_m^P(\varepsilon)=\partial C_m^P(\varepsilon)/\partial\varepsilon$$

$$=2\pi V(c\hbar)^{-(m+2)/2}\varepsilon(\varepsilon^2-m_0^2c^4)^{(m-2)/4}\sum_{\{q_p\}=-\infty}^{+\infty}{}' J_{(m-2)/2}\left((c\hbar)^{-1}(\varepsilon^2-m_0^2c^4)^{1/2}\left(\sum_{p=1}^{m}q_p^2L_p^2\right)^{1/2}\right)\Big/$$

$$\left(\sum_{p=1}^{m}q_p^2L_p^2\right)^{(m-2)/4},$$

which can be rewritten as

$$D_m^P(\varepsilon)=2\pi^{m/2}V(c\hbar)^{-m}(\Gamma(m/2))^{-1}\varepsilon(\varepsilon^2-m_0^2c^4)^{(m-2)/2}$$

$$+2\pi V(c\hbar)^{-(m+2)/2}\varepsilon(\varepsilon^2-m_0^2c^4)^{(m-2)/4}\sum_{\{q_p\}=-\infty}^{+\infty}{}' J_{(m-2)/2}\left((c\hbar)^{-1}(\varepsilon^2-m_0^2c^4)^{1/2}\left(\sum_{p=1}^{m}q_p^2L_p^2\right)^{1/2}\right)\Big/$$

$$\left(\sum_{p=1}^{m}q_p^2L_p^2\right)^{(m-2)/4}. \quad (35)$$

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

$$D_1^P(\varepsilon)=2L\varepsilon(c\hbar)^{-1}(\varepsilon^2-m_0^2c^4)^{-1/2}+2L\varepsilon(c\hbar)^{-1}(\varepsilon^2-m_0^2c^4)^{-1/2}\sum_{q=-\infty}^{+\infty}{}'\cos\left(qL(c\hbar)^{-1}(\varepsilon^2-m_0^2c^4)^{1/2}\right), \quad (36)$$

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

$$D_3^P(\varepsilon)=4\pi V(c\hbar)^{-3}\varepsilon(\varepsilon^2-m_0^2c^4)^{1/2}+2V(c\hbar)^{-2}\varepsilon\sum_{q_{1,2,3}=-\infty}^{+\infty}{}' \sin\{(c\hbar)^{-1}(\varepsilon^2-m_0^2c^4)^{1/2}(q_1^2L_1^2+q_2^2L_2^2+q_3^2L_3^2)^{1/2}\}/$$
$$(q_1^2L_1^2+q_2^2L_2^2+q_3^2L_3^2)^{1/2}. \quad (38)$$

We may mention that the results in Eqs (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 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 to the first term except for the case of m=1. Thus except for m=1, the first term in Eq. (35) (which contains Eqs. (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, complete expression in Eq. (36) has to be used even in this limit. The first term of Eq. (35), which corresponds to the Weyl's 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 Eq. (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 the Eqs. (32) and (33) is again given by Eq. (25). Now using Eq. (34) in Eq. (29) which is valid in the present case also, we get

$$N_m(E)=(1+\eta^2)^{-m}\{\eta^m\theta((c\hbar)^{-1}(E^2-m_0^2c^4)^{1/2})+\sum_{s=1}^{m}\eta^{m-s}\sum_{1\leq j_1<j_2\ldots<j_s\leq m}(1+\eta^2)^{s/2}L_{j_1}L_{j_2}\ldots L_{j_s}(E^2-m_0^2c^4)^{s/4}\cdots$$

$$(c\hbar)^{-s/2}\sum_{\{q_{j_p}\}=-\infty}^{\infty}J_{s/2}\{(1+\eta^2)(c\hbar)^{-1}(E^2-m_0^2c^4)^{1/2}(\sum_{p=1}^{s}q_{j_p}^2L_{j_p}^2)^{1/2}\}/(\sum_{p=1}^{s}q_{j_p}^2L_{j_p}^2)^{s/4}\}. \quad (39)$$

Now we can obtain the espression for the density of states $D_m(\epsilon)$, for the PBC, the DBC and the NBC by differentiating Eq. (39).

$$D_m(\epsilon)=dN_m(\epsilon)/d\epsilon$$

$$=(1+\eta^2)^{-m}\{\eta^m\epsilon(\epsilon^2-m_0^2c^4)^{-1/2}\delta((\epsilon^2-m_0^2c^4)^{1/2})$$

$$+\sum_{s=1}^{m}\eta^{m-s}\sum_{1\leq j_1<j_2\ldots<j_s\leq m}2\pi(c\hbar)^{-(s+2)/2}(1+\eta^2)^{(s+2)/2}L_{j_1}L_{j_2}\ldots L_{j_s}\,\epsilon(\epsilon^2-m_0^2c^4)^{(s-2)/4}$$

$$\sum_{\{q_{j_p}\}=-\infty}^{\infty}J_{(s-2)/2}\{(c\hbar)^{-1}(1+\eta^2)(\epsilon^2-m_0^2c^4)^{1/2}(\sum_{p=1}^{s}q_{j_p}^2L_{j_p}^2)^{1/2}\}/(\sum_{p=1}^{s}q_{j_p}^2L_{j_p}^2)^{(s-2)/4}\}. \quad (40)$$

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

One of the authors (A N C) takes this opportunity of thanking the Conselho Nacional de Desenvolvimento e Tecnologico of Brazil for the financial support for this research.

References

Abramowitz M and Stegan I A 1965 Handbook of Mathematical Functions (Dover, New York) p. 360

Baltes H P and Steinle B 1977 J. Math. Phys. 18 1275 - 6

Carvalho C A D and Rosa Jr. S.G. 1980 J. Phys. A: Math. Gen. 13 3233 - 41

Chaba A N 1979 Phys. Rev. A 20 1292 - 94

________ 1980 J. Phys. A: Math. Gen. 13 3037 - 47

Chaba A N and Pathria R K 1975 Phys. Rev. B12 3697 - 704

________ 1978 Phys. Rev. A18 1277 - 81

Dunning-Davies J 1981 J. Phys. A: Math. Gen. 14 3005 - 12

Fetter A L, Hohenberg P C and Picus P 1966 Phys. Rev. 147 140 - 52

Fu F 1981 Phys. Lett. 81A 127 - 31

Medeiros e Silva J and Mokross B J 1980 Phys. Rev. B21 2972 - 76

Pathria R K 1972 Statistical Mechanics (Pergamon, New York) p. 502

Stein E M and Weiss G 1971 Fourier Analysis on Euclidean Spaces (Princeton, N J: Princeton University Press) p. 253

Walfisz A 1924 Math. Z. 19 300 - 07