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The generalised Euler formula from Poisson's summation formula and some applications

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Abstract. The generalised Euler formula is derived from Poisson's summation formula. In special cases, it reduces to the ordinary Euler formula and Walfisz formula in one dimension. As an application, we use the generalised Euler formula to calculate the expression for the number of quantum states of a single non-relativistic particle in a rectangular three-dimensional box of finite size.

1. Introduction

Euler's formula for the sum of powers of natural numbers is (Gradshteyn and Ryzhik 1980)

$$\sum_{n=1}^{N} n^k = \frac{N^{k+1}}{k+1} + \frac{N^k}{2} + \frac{B_2}{2}\binom{k}{1} N^{k-1} + \frac{B_4}{4}\binom{k}{3} N^{k-3} + \frac{B_6}{6}\binom{k}{5} N^{k-5} + \ldots, \tag{1}$$

(last term contains either N or N^2), the B_n's appearing on the right-hand side of the above equation are Bernoulli numbers (Gradshteyn and Ryzhik 1980) and N is a positive integer. Roe (1941) made use of this formula to calculate the number of normal modes, $N(\nu)$, which are solutions of the Helmholtz equation, $(\nabla^2 + 4\pi^2\nu^2/c^2)\psi = 0$, with frequencies less than or equal to ν and subject to Neumann boundary conditions (NBC), $\partial\psi/\partial n = 0$, and Dirichlet boundary conditions (DBC), $\psi = 0$. He considered enclosures of various shapes which include, among others, rectangular (3D), cylindrical and spherical ones and obtained expressions which contain the bulk term ($\propto$ volume) and the surface term ($\propto$ surface area) in all cases but in the case of the rectangular box, he also obtained the edge term ($\propto$ total length of edges). In his calculations, where he employed equation (1), the numbers corresponding to N were not necessarily integers but he treated them as such, so that the results obtained by him were naturally approximate.

In this paper, in § 2, we shall derive, from the Poisson's summation formula (PSF), the generalised form of the expression for the sum on the left-hand side of equation (1) for the case when N is not necessarily an integer. We call this new result the generalised Euler's formula. The upper limit of this sum is supposed to be $[N]$, that is, the integral part of N but the result is expressed in terms of N itself. The motivation for deriving this result, clearly, came from the work of Roe referred to above. We further show that the new formula reduces to the ordinary Euler formula in the case when N is an integer and also, for $k = 0$, it reduces to the Walfisz formula (see, e.g.,

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Baltes and Steinle 1977, Chaba 1979) for the number of lattice points in an hypersphere (of given radius) in one dimension. In the end, in § 3, we present, as an application of the generalised Euler formula, the calculation for the number of single-particle quantum states of a non-relativistic particle in a 3D rectangular box and subject to Dirichlet boundary conditions (this problem is almost the same as one of the cases treated by Roe cited above) and the result obtained, which is exact, agrees with that obtained already (Freitas and Chaba 1983). Probably, using this new formula, we shall be able to improve the results in the case of cylindrical, spherical and other enclosures, treated earlier by Roe, as well.

2. The generalised Euler formula from Poisson's summation formula

The PSF in one dimension (see, e.g., Chaba 1979) is

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

If $F(x)$ be an even function of x, we can, from equation (2), easily arrive at the following alternative form of the PSF for the 'partial' sum $\Sigma_{n=1}^{\infty} F(n)$, instead of the 'complete' sum on the left-hand side of equation (2),

$$\sum_{n=1}^{\infty} F(n) = -\tfrac{1}{2}F(0) + \int_0^{\infty} F(x)\, dx + 2 \sum_{q=1}^{\infty} \int_0^{\infty} F(x) \cos(2\pi q x)\, dx. \tag{3}$$

In equation (3), one needs the form of the function $F(x)$ only for $x \geqslant 0$. On the other hand, however, if we are given $F(x)$ for $x \geqslant 0$, we can always define $F(x)$ for $x < 0$ in such a way that $F(x)$ is an even function, so that the above result is valid for any function $F(x)$. Now, we shall make use of the PSF in the form given in equation (3) to do the summation $\Sigma_{n=1}^{N} n^k$, where, now, N is not necessarily an integer. Firstly, we rewrite this sum as

$$\sum_{n=1}^{N} n^k = \sum_{n=1}^{\infty} n^k \theta(N-n), \tag{4}$$

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

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

Now using equation (3) in equation (4), we obtain

$$\begin{aligned} \sum_{n=1}^{N} n^k &= -\tfrac{1}{2}\delta_{k,0} + \int_0^{\infty} x^k \theta(N-x)\, dx + 2 \sum_{q=1}^{\infty} \int_0^{\infty} x^k \theta(N-x) \cos(2\pi q x)\, dx \\ &= -\tfrac{1}{2}\delta_{k,0} + \int_0^{N} x^k\, dx + 2 \sum_{q=1}^{\infty} \int_0^{N} x^k \cos(2\pi q x)\, dx. \end{aligned} \tag{5}$$

Using the result in the tables (Gradshteyn and Ryzhik 1980) for the last integral in equation (5), we get

$$\sum_{n=1}^{N} n^k = \frac{N^{k+1}}{k+1} + \frac{N^k}{\pi} \sum_{l=0}^{k} l! \binom{k}{l} \frac{1}{(2\pi N)^l} \sum_{q=1}^{\infty} \frac{\sin(2\pi q N + l\pi/2)}{q^{l+1}} - \tfrac{1}{2}\delta_{k,0}$$
$$- \frac{2(k!)}{(2\pi)^{k+1}} \sin(k\pi/2)\zeta(k+1), \tag{6}$$

where $\zeta(n)$ is the Riemann's zeta function. Equation (6) can also be written as

$$\sum_{n=1}^{N} n^k = \frac{N^{k+1}}{k+1} + \frac{N^k}{\pi} \left(\sum_{m=0}^{[k/2]} (2m)! \binom{k}{2m} \frac{(-1)^m}{(2\pi N)^{2m}} \sum_{q=1}^{\infty} \frac{\sin(2\pi q N)}{q^{2m+1}} \right.$$
$$\left. + \sum_{m=0}^{[(k-1)/2]} (2m+1)! \binom{k}{2m+1} \frac{(-1)^m}{(2\pi N)^{2m+1}} \sum_{q=1}^{\infty} \frac{\cos(2\pi q N)}{q^{2m+2}} \right)$$
$$- \tfrac{1}{2}\delta_{k,0} - \frac{2(k!)}{(2\pi)^{k+1}} \sin(k\pi/2)\zeta(k+1), \tag{7}$$

where the double summation involving cosines should appear only when $k \geqslant 1$. Equation (6) or (7) is the generalised Euler formula. Now we shall study two special cases of equations (6) and (7), namely, (i) when N is an integer and (ii) when $k = 0$.

(i) When N is an integer

First we define ε, the fractional part of N, as

$$\varepsilon = N - [N], \qquad 0 \leqslant \varepsilon < 1, \tag{8}$$

then equation (7) can be rewritten as

$$\sum_{n=1}^{N} n^k = \frac{N^{k+1}}{k+1} + \frac{N^k}{\pi} \left(\sum_{m=0}^{[k/2]} (2m)! \binom{k}{2m} \frac{(-1)^m}{(2\pi N)^{2m}} \sum_{q=1}^{\infty} \frac{\sin(2\pi q \varepsilon)}{q^{2m+1}} \right.$$
$$\left. + \sum_{m=0}^{[(k-1)/2]} (2m+1)! \binom{k}{2m+1} \frac{(-1)^m}{(2\pi N)^{2m+1}} \sum_{q=1}^{\infty} \frac{\cos(2\pi q \varepsilon)}{q^{2m+2}} \right)$$
$$- \tfrac{1}{2}\delta_{k,0} - \frac{2(k!)}{(2\pi)^{k+1}} \sin(k\pi/2)\zeta(k+1).$$

In this equation, first we do the summations over q involving cosines and sines which are tabulated (Gradshteyn and Ryzhik 1980) and the results are given in terms of Bernoulli's polynomials, $B_n(x)$. These results are valid for $0 < \varepsilon < \frac{1}{2}$. But for our purposes, it is enough, because actually we are interested in the case $\varepsilon \to +0$. After doing these summations, the two summations over m can be combined and we obtain

$$\sum_{n=1}^{N} n^k = \frac{N^{k+1}}{k+1} - N^k \sum_{i=0}^{k} \binom{k}{i} \frac{(-1)^i B_{i+1}(\varepsilon)}{(i+1)N^i} - \tfrac{1}{2}\delta_{k,0} - \frac{2(k!)}{(2\pi)^{k+1}} \sin(k\pi/2)\zeta(k+1).$$

When N approaches an integral value from above, $\varepsilon \to +0$ and Bernoulli's polynomials are just Bernoulli's numbers, $B_n(\varepsilon) = B_n$. Then, the above equation becomes

$$\sum_{n=1}^{N} n^k = \frac{N^{k+1}}{k+1} - N^k \sum_{i=0}^{k} \binom{k}{i} \frac{(-1)^i B_{i+1}}{(i+1)N^i} - \tfrac{1}{2}\delta_{k,0} - \frac{2(k!)}{(2\pi)^{k+1}} \sin(k\pi/2)\zeta(k+1), \tag{9}$$

or writing the first few terms in the summation over i explicitly and noting that $B_1 = -\frac{1}{2}$

and $B_3=0$, we get,

$$\sum_{n=1}^{N} n^k=\frac{N^{k+1}}{k+1}+\frac{N^k}{2}+\frac{B_2}{2}\binom{k}{1}N^{k-1}+\frac{B_4}{4}\binom{k}{3}N^{k-3}+\cdots$$
$$-\tfrac{1}{2}\delta_{k,0}-\frac{2(k!)}{(2\pi)^{k+1}}\sin(k\pi/2)\zeta(k+1). \tag{10}$$

Equation (9) or (10) is just the ordinary Euler formula which is valid for integer N. Comparing equations (10) and (1), we see that the last two terms in (10) substitute the phrase 'last term contains either N or N^2' at the end of equation (1).

(ii) When $k=0$

In this case, equation (6) reduces to

$$\sum_{n=1}^{x} 1=x+\frac{1}{\pi}\sum_{q=1}^{\infty}\frac{\sin(2\pi qx)}{q}-\tfrac{1}{2} \tag{11}$$

where we have replaced N by x which is not necessarily an integer. Therefore, the number of lattice points, $n_1(x)$, in a hypersphere of radius x in one dimension, which is actually equal to the number of lattice points between $-x$ and $+x$ can be written as

$$n_1(x)=1+2\sum_{n=1}^{x} 1.$$

On using equation (11) here, we obtain

$$n_1(x)=2x+\frac{1}{\pi}\sum_{q=-\infty}^{+\infty}{}' \frac{\sin(2\pi qx)}{q}, \tag{12}$$

where the prime on the summation over q means that the term $q=0$ is excluded from it. Equation (12) is the Walfisz formula (see, e.g., Chaba 1979) in one dimension.

3. Applications

As an application of the generalised Euler formula, we shall calculate the number of single-particle quantum states of a non-relativistic particle enclosed in a 3D rectangular box with L_1, L_2 and L_3 as the lengths of its edges and the eigenfunctions, ψ, being subject to the DBC ($\psi=0$) on the walls of the box. These eigenfunctions are the solutions of the Schrödinger equation

$$\nabla^2\psi+k^2\psi=0, \qquad k^2=2mE/\hbar^2 \tag{13}$$

and have the form

$$\psi(x,y,z)=A\sin(n_1\pi x/L_1)\sin(n_2\pi y/L_2)\sin(n_3\pi z/L_3), \tag{14}$$

and the eigenvalues k are given by

$$k=\pi(n_1^2/L_1^2+n_2^2/L_2^2+n_3^2/L_3^2)^{1/2}, \qquad n_1, n_2, n_3=1,2,3\ldots. \tag{15}$$

We shall calculate the total number of states $N(K)$ with all allowed $k\leqslant K$ or

$$n_1^2/L_1^2+n_2^2/L_2^2+n_3^2/L_3^2\leqslant K^2/\pi^2. \tag{16}$$

We shall closely follow the procedure of Roe (1941), except that we shall use our generalised rather than the ordinary Euler formula used by him. We define n_1', n_2', n_3' as

$$n_1' = KL_1/\pi, \tag{17a}$$

$$n_2' = L_2(K^2/\pi^2 - n_1^2/L_1^2)^{1/2}$$
$$= (L_2/L_1)(n_1'^2 - n_1^2)^{1/2} = l_{21}(n_1'^2 - n_1^2)^{1/2} \tag{17b}$$

and

$$n_3' = L_3(K^2/\pi^2 - n_1^2/L_1^2 - n_2^2/L_2^2)^{1/2}$$
$$= (L_3/L_2)(n_2'^2 - n_2^2)^{1/2} = l_{32}(n_2'^2 - n_2^2)^{1/2}, \tag{17c}$$

where $l_{ij} = L_i/L_j$. Here n_1', n_2', n_3' are not necessarily integers but, as was said before, Roe regarded them as such, leading him to the results which were only approximately correct. In terms of these, we can write $N(K)$, which is equal to the number of lattice points in an octant of an ellipse in the $\boldsymbol{n}$ space, as

$$N(K) = \sum_{n_1=1}^{n_1'} \sum_{n_2=1}^{n_2'} \sum_{n_3=1}^{n_3'} 1. \tag{18}$$

First we do the sum over n_3 by using the generalised Euler formula and substitute for n_3' from (17c),

$$N(K) = \sum_{n_1=1}^{n_1'} \sum_{n_2=1}^{n_2'} \left(-\frac{1}{2} + \sum_{q_3=-\infty}^{+\infty} \frac{\sin(2\pi q_3 n_3')}{2\pi q_3} \right)$$
$$= \sum_{n_1=1}^{n_1'} \left(-\frac{1}{2} \sum_{n_2=1}^{n_2'} 1 + \sum_{q_3=-\infty}^{+\infty} \frac{1}{2\pi q_3} \sum_{n_2=1}^{n_2'} \sin[2\pi q_3 l_{32}(n_2'^2 - n_2^2)^{1/2}] \right). \tag{19}$$

The summation over n_2 involving sines is somewhat tricky and in order to do it, we first expand it in powers of $n_2^2/n_2'^2$ by the Taylor series expansion and then use the generalised Euler formula in the form of equation (6). After doing some algebra, we arrive at the following result:

$$\sum_{n=1}^{n'} \sin[2\pi ql(n'^2 - n^2)^{1/2}]$$
$$= -\tfrac{1}{2}\sin(2\pi qln') + \frac{\pi n' lq}{2} \sum_{q'=-\infty}^{+\infty} J_1[2\pi n'(l^2q^2 + q'^2)^{1/2}]/(l^2q^2 + q'^2)^{1/2}. \tag{20}$$

Using equation (20) and also equation (17b) for n_2' in equation (19), we get

$$N(K) = \tfrac{1}{4} \sum_{n_1=1}^{n_1'} 1 - \tfrac{1}{2}\left(\sum_{q_2=-\infty}^{+\infty} (1/2\pi q_2) \sum_{n_1=1}^{n_1'} \sin[(2\pi q_2 l_{21}(n_1'^2 - n_1^2)^{1/2}] \right.$$
$$\left. + \sum_{q_3=-\infty}^{+\infty} \frac{1}{2\pi q_3} \sum_{n_1=1}^{n_1'} \sin[2\pi q_3 l_{31}(n_1'^2 - n_1^2)^{1/2}] \right)$$
$$+ \frac{l_{31}}{4} \sum_{q_{2,3}=-\infty}^{+\infty} (l_{32}^2 q_3^2 + q_2^2)^{-1/2} \sum_{n_1=1}^{n_1'} (n_1'^2 - n_1^2)^{1/2}$$
$$\times J_1(2\pi l_{21}(n_1'^2 - n_1^2)^{1/2}(l_{32}^2 q_3^2 + q_2^2)^{1/2}), \tag{21}$$

where $J_1(x)$ is the Bessel function of the first kind and of order one. The summation over n_1 involving J_1 is also done in the same way as the sum over sines discussed above, with the result that

$$\sum_{n=1}^{n'} (n'^2-n^2)^{1/2} J_1(a(n'^2-n^2)^{1/2})$$
$$= -(n'/2)J_1(an') + \sum_{q=-\infty}^{+\infty} \{a(a^2+4\pi^2q^2)^{-3/2}\sin[n'(a^2+4\pi^2q^2)^{1/2}]$$
$$-n'a(a^2+4\pi^2q^2)^{-1}\cos[n'(a^2+4\pi^2q^2)^{1/2}]\}. \tag{22}$$

Using equations (20) and (22) for the relevant summations in equation (21), we finally get

$$N(K) = \frac{L_1L_2L_3}{16\pi^2} \sum_{q_{1,2,3}=-\infty}^{+\infty} \left(\frac{\sin[2K(q_1^2L_1^2+q_2^2L_2^2+q_3^2L_3^2)^{1/2}]}{(q_1^2L_1^2+q_2^2L_2^2+q_3^2L_3^2)^{3/2}} \right.$$
$$\left. -\frac{2K\cos[2K[q_1^2L_1^2+q_2^2L_2^2+q_3^2L_3^2)^{1/2}]}{(q_1^2L_1^2+q_2^2L_2^2+q_3^2L_3^2)} \right)$$
$$-\frac{K}{8\pi}\left(L_1L_2 \sum_{q_{1,2}=-\infty}^{+\infty} \frac{J_1(2K(q_1^2L_1^2+q_2^2L_2^2)^{1/2})}{(q_1^2L_1^2+q_2^2L_2^2)^{1/2}} \right.$$
$$+L_3L_1 \sum_{q_{3,1}=-\infty}^{+\infty} \frac{J_1(2K(q_3^2L_3^2+q_1^2L_1^2)^{1/2})}{(q_3^2L_3^2+q_1^2L_1^2)^{1/2}}$$
$$\left. +L_2L_3 \sum_{q_{2,3}=-\infty}^{+\infty} \frac{J_1(2K(q_2^2L_2^2+q_3^2L_3^2)^{1/2})}{(q_2^2L_2^2+q_3^2L_3^2)^{1/2}} \right)$$
$$+\frac{1}{4}\left(\sum_{q_1=-\infty}^{+\infty} \frac{\sin(2Kq_1L_1)}{2\pi q_1} + \sum_{q_2=-\infty}^{+\infty} \frac{\sin(2Kq_2L_2)}{2\pi q_2} \right.$$
$$\left. + \sum_{q_3=-\infty}^{+\infty} \frac{\sin(2Kq_3L_3)}{2\pi q_3} \right) - \frac{1}{8}. \tag{23}$$

This result is exact and agrees with the special case, for the rectangular 3D box, of the more general result derived earlier by Freitas and Chaba (see equation (30) of Freitas and Chaba 1983) by making use of the Walfisz formula for the dimensionality d. The terms corresponding to $q_1 = q_2 = q_3 = 0$ in the triple summation, $q_1 = q_2 = 0$, etc, in the double summations and $q_1 = 0$, etc, in the single summations in equation (23) agree with the bulk, surface and edge terms of Roe's result. In addition to these, there is one K-independent term $(-\frac{1}{8})$ and the rest of the terms are of oscillatory nature and these last terms were qualitatively foreseen by Roe who referred to them as the fluctuating terms. According to him these terms are unimportant but we wish to point out that in problems where small k's are important, as in the study of Bose-Einstein condensation in finite systems, these oscillatory terms (especially in the triple summation in equation (23)) have a very important role to play (see, e.g., Chaba (1979) together with Chaba and Pathria (1978)).

By slightly modifying the above procedure, we can calculate $N(K)$ in the case of NBC on the walls of the rectangular box in three dimensions and also for other dimensionalities. Also, we hope to apply the generalised Euler formula to calculate $N(K)$ for other enclosures like the cylinder and sphere treated earlier by Roe.

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