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A Generalization of the Euler-Maclaurin Sum Formula

Giiti Iwata

Department of Physics, Faculty of Science,
Ochanomizu University, Tokyo
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The Euler-Maclaurin sum formula, which is formulated with respect to a function of one variable, is generalized so as to be applicable to a function of several variables with the aid of periodic Bernoulli functions.

§ 1. Periodic Bernoulli functions

The Bernoulli polynomial of order k may be expanded as a Fourier series[1)]

$$B_k(x) = -k!\,\Sigma'(2\pi ir)^{-k}\exp(2\pi irx) \tag{1}$$

for $0<x<1$, the prime indicating that the term corresponding to $r=0$ is omitted. Following the lead of this representation, we define periodic Bernoulli function of order k by

$$G_k(\mathbf{r}) = -\Sigma'\exp(2\pi i\mathbf{r}\cdot\mathbf{n})\cdot(2\pi i\mathbf{n})^{-2k} \tag{2}$$

where $\mathbf{r}$ is a point $(x_1, x_2, \cdots, x_d)$ in a d-dimensional euclidean space and $\mathbf{n}=(n_1, n_2, \cdots, n_d)$ ranges over all lattice points except the origin. The periodic Bernoulli functions have the following properties

1° Periodicity $G_k(\mathbf{r}+\mathbf{n})=G_k(\mathbf{r})$.

2° $G_k(\mathbf{r})$ is symmetric in $x_1, x_2, \cdots, x_d$ and even in any of $x_1, \cdots, x_d$.

3° $G_k(\mathbf{r})$ is continuous everywhere for $k>d/2$.

4° $G_k(\mathbf{r})$ is singular at lattice points for $k\leqq d/2$.

5° $G_0(\mathbf{r})=1-\sum\delta(\mathbf{r}-\mathbf{n})$.

6° $\Delta G_k(\mathbf{r})=G_{k-1}(\mathbf{r})$, Δ=Laplace operator.

7° $$G_k(x_1, \cdots, x_{d-1}, 0) = \frac{(-)^{k-1}B_k}{(2k)!} + \frac{1}{(2\pi)^{2k}}\frac{1}{(k-1)!} \times\Sigma'\exp(2\pi i\mathbf{n}^*\cdot\mathbf{r})\cdot\left(\frac{\partial}{\partial(n^*)^2}\right)^{k-1}\frac{\pi\operatorname{Cot}\pi n^*}{n^*}. \tag{3}$$

B_k: Bernoulli number, $n^*=(n_1, n_2, \cdots, n_{d-1}, 0)$, $n^*=|\mathbf{n}^*|$

$$G_k(x_1, \cdots, x_{d-1}, 1/2) = \frac{(-)^k B_k}{(2k)!}(1-2^{1-2k}) + \frac{1}{(2\pi)^{2k}} \frac{1}{(k-1)!}$$

$$\times \Sigma' \exp(2\pi i \mathbf{n}^* \cdot \mathbf{r}) \cdot \left(\frac{\partial}{\partial (n^*)^2}\right)^{k-1} \frac{\pi}{n^* \operatorname{Sin} \pi n^*} . \tag{4}$$

The summation Σ' excludes the term $n_1 = n_2 = \cdots = n_{d-1} = 0$.

8° $\left(\frac{\partial G_k(\mathbf{r})}{\partial x_i}\right)_{x_i=1/2} = 0$ for any i.

9° For $d=1$, $G_k(x) = \frac{B^*_{2k}(x)}{(2k)!}$, $\frac{dG_k(x)}{dx} = \frac{B^*_{2k-1}(x)}{(2k-1)!}$

where $B^*_k(x)$ is redefined to be periodic by the Fourier series (1).

These properties follow at once from the definition (2). In particular, the property 5° is derived with the aid of the well-known Lighthill summation formula[2)]

$$\sum_{\mathbf{n}} \delta(\mathbf{r}-\mathbf{n}) = \sum_{\mathbf{n}} \exp(i2\pi \mathbf{r} \cdot \mathbf{n})$$

§ 2. The Euler-Maclaurin sum formula

If we integrate the product of $G_0(\mathbf{r})$ and a continuous function $f(\mathbf{r})$ over a domain D, we have the relation

$$\int_D G_0(\mathbf{r}) f(\mathbf{r}) d\mathbf{r} = \int_D f(\mathbf{r}) d\mathbf{r} - \sum_{\mathbf{n} \in D} f(\mathbf{n}) \tag{5}$$

where $\mathbf{n}$ ranges over lattice points in D. On the other hand, with the aid of the property 6° in § 1 and the Green formula, we have

$$\int_D G_0(\mathbf{r}) f(\mathbf{r}) d\mathbf{r} = \sum_{k=1}^{m} \int_C \left(\Delta^{k-1} f(\mathbf{r}) \frac{\partial G_k(\mathbf{r})}{\partial \nu} - \frac{\partial \Delta^{k-1} f(\mathbf{r})}{\partial \nu} G_k(\mathbf{r})\right) d\mathbf{s}$$

$$+ \int_D \Delta^m f(\mathbf{r}) \cdot G_m(\mathbf{r}) d\mathbf{r} \tag{6}$$

where C is the boundary of D, $d\mathbf{s}$ stands for the surface element of C, and $\partial/\partial \nu$ denotes the outward normal derivative on C. m is any positive integer. Hence we have a generalized Euler-Maclaurin sum formula

$$\sum_{\mathbf{n} \in D} f(\mathbf{n}) = \int_D f(\mathbf{r}) d\mathbf{r} - \sum_{k=1}^{m} \int_C \left(\Delta^{k-1} f(\mathbf{r}) \frac{\partial G_k(\mathbf{r})}{\partial \nu} - \frac{\partial \Delta^{k-1} f(\mathbf{r})}{\partial \nu} G_k(\mathbf{r})\right) d\mathbf{s}$$

$$- \int_D \Delta^m f(\mathbf{r}) \cdot G_m(\mathbf{r}) d\mathbf{r} . \tag{7}$$

When $d=1$ and the domain $D=(1/2, n+1/2)$, we have

$$\sum_{r=1}^{n} f(r)=\int_{1/2}^{n+1/2} f(x)dx+\sum_{k=1}^{m}\frac{(-)^k B_k}{(2k)!}(1-2^{1-2k})\left\{f^{(2k-1)}\left(n+\frac{1}{2}\right)-f^{(2k-1)}\left(\frac{1}{2}\right)\right\}$$
$$-\frac{1}{(2m)!}\int_{1/2}^{n+1/2} B_{2m}^*(x)f^{(2m)}(x)dx\ .$$

When $d=1$ and the domain D is $(0, n)$, we have the well-known Euler-Maclaurin sum formula[3]

$$\sum_{r=1}^{n-1} f(r)+\frac{1}{2}(f(0)+f(n))=\int_0^n f(x)dx-\sum_{k=1}^{m}\frac{(-)^k B_k}{(2k)!}\{f^{(2k-1)}(n)-f^{(2k-1)}(0)\}$$
$$-\frac{1}{(2m)!}\int_0^n B_{2m}^*(x)f^{(2m)}(x)dx\ .$$

When the boundary C is composed of planes $x_i=\text{integer}+1/2$, $i=1, 2, \cdots, d$, the formula (7) becomes simpler since $\partial G_k(\mathbf{r})/\partial\nu$ vanishes at the boundary for any k.

§ 3. Generalized Zeta funcfions

For the later use, we introduce a generalized Zeta function $Z(s)$ in a d-dimensional space defined by

$$Z(s)=\Sigma'\frac{1}{(\mathbf{n}^2)^s} \qquad \text{for } \mathscr{R}s>d/2 \tag{8}$$

where $\mathbf{n}$ ranges over all lattice points except the origin. The function $Z(s)$ has the following properties similar to those of the Riemann Zeta function.[4),5)]

1° $\pi^{-s}\Gamma(s)Z(s)=\Sigma'\int_0^\infty \exp(-\pi\mathbf{n}^2t)\cdot t^{s-1}dt,\quad \mathscr{R}s>d/2.$

2° $\pi^{-s}\Gamma(s)Z(s)=\dfrac{1}{s-d/2}-\dfrac{1}{s}+\Sigma'\int_1^\infty \exp(-\pi\mathbf{n}^2t)\cdot(t^{d/2-s}+t^s)t^{-1}dt.$

3° $\pi^{-s}\Gamma(s)Z(s)=\pi^{-(d/2-s)}\Gamma(d/2-s)Z(d/2-s).$

4° $Z(s)$ has a simple pole at $s=d/2$ with the residue $\pi^{d/2}/\Gamma(d/2)$.

5° $Z(s)$ has zeros at $s=-1, -2, -3, \cdots$.

6° $Z(0)=-1$.

7° $Z'(0)=-\gamma-\log\pi-\dfrac{2}{d}+\Sigma'\int_1^\infty \exp(-\pi\mathbf{n}^2t)\cdot(1+t^{d/2})t^{-1}dt.$

$\gamma=$Euler constant.

The property 1° is obvious. The property 2° follows from 1° when the range of integration is divided into two parts at $t=1$ and the variable t is changed into $1/t$ in one part. The properties 3°

through 7° follow from 2°.

§ 4. Spherically symmetric Bernoulli functions

When both the function $f(\mathbf{r})$ and the domain D are spherically symmetric, we may use spherically symmetric Bernoulli functions $\bar{G}_k(r)$, which are defined to be the average of $G_k(\mathbf{r})$ on the spherical surface $|\mathbf{r}|=r$. The formula (7) becomes then

$$\sum_{\mathbf{n}\in D} f(n)=\omega\int_a^b f(r)r^{d-1}dr-\omega\sum_{k=1}^m\left[\left\{\Delta^{k-1}f(r)\cdot\frac{\partial\bar{G}_k(r)}{\partial r}-\frac{\partial\Delta^{k-1}f(r)}{\partial r}\bar{G}_k(r)\right\}r^{d-1}\right]_a^b$$
$$-\omega\int_a^b \Delta^m f(r)\cdot\bar{G}_m(r)r^{d-1}dr\ . \tag{9}$$

It is to be understood here that the domain D is bounded by two spherical surfaces of radius a and b, and that ω is the surface area of the unit sphere, or $\omega=2\pi^{d/2}/\Gamma(d/2)$.

Since the average of $\exp(i2\pi r\cdot\mathbf{n})$ on the spherical surface $|\mathbf{r}|=r$ is given by

$$\langle\exp(i2\pi\mathbf{r}\cdot\mathbf{n})\rangle=\int\delta(r^2-\mathbf{r}^2)\exp(i2\pi\mathbf{r}\cdot\mathbf{n})d\mathbf{r}\Big/\int\delta(r^2-\mathbf{r}^2)d\mathbf{r}$$
$$=\Gamma(d/2)J_{d/2-1}(2\pi nr)\cdot(\pi nr)^{1-d/2}$$
$$=\frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty}\frac{\Gamma(d/2)\Gamma(s)}{\Gamma(d/2-s)}(\pi nr)^{-2s}ds\ ,$$
$$0<c=\mathscr{R}s<(d+1)/4\ ,$$ [6]

we have an integral representation of $\bar{G}_k(r)$

$$\bar{G}_k(r)=\frac{(-)^{k-1}}{(2\pi)^{2k}}\frac{1}{2\pi i}\int\frac{\Gamma(d/2)\Gamma(s)}{\Gamma(d/2-s)}(\pi r)^{-2s}Z(k+s)ds\ ,$$
$$d/2<\mathscr{R}s<(d+1)/4\ . \tag{10}$$

The integrand has a pole at $s=d/2-k$, and poles at $s=0, -1, -2, \cdots, -k$.

On the other hand we deduce from 5° and 6° in § 1 that

$$\bar{G}_0(r)=1-\sum\frac{\delta(r-n)}{\omega r^{d-1}}$$

and

$$\Delta\cdot\bar{G}_k(r)=\bar{G}_{k-1}(r)\ ,\qquad \Delta=\frac{1}{r^{d-1}}\frac{\partial}{\partial r}r^{d-1}\frac{\partial}{\partial r}\ . \tag{11}$$

Solving the equation (11) successively with the aid of the integral representation (10) for determining undetermined solutions of the homogeneous Laplace equation $\Delta u=0$, we have for $d=2$

$$\bar{G}_1(r)=\frac{r^2}{4}+\frac{1}{4\pi}\left(\frac{2\Gamma'(1)}{\Gamma(1)}-2\log\pi+c_1\right)$$
$$-\frac{1}{2\pi}\log r+\frac{1}{2\pi}\Sigma'(\log n-\log r)\in(r-n)$$
$$\bar{G}_2(r)=\frac{r^4}{64}+\frac{r^2}{16\pi}\left(\frac{2\Gamma'(1)}{\Gamma(1)}-2\log\pi+c_1\right)-\frac{1}{8\pi}r^2(\log r-1)-\frac{Z(2)}{(2\pi)^4}$$
$$+\frac{1}{2\pi}\Sigma'\left(\frac{r^2}{2}(\log n-\log r)+\frac{r^2-n^2}{4}\right)\in(r-n)$$
$$\left[c_1=\lim_{s\to1}\left(\pi^{-s}\Gamma(s)Z(s)-\frac{1}{s-1}\right),\quad \in(x)=1 \text{ for } x>0\ ,\quad \in(x)=0 \text{ for } x<0\right]$$

and for $d=3$

$$\bar{G}_1(r)=\frac{r^2}{6}+\frac{Z(1)}{4\pi^2}+\frac{1}{4\pi r}-\frac{1}{4\pi}\Sigma'\left(\frac{1}{n}-\frac{1}{r}\right)\in(r-n)$$
$$\bar{G}_2(r)=\frac{r^4}{120}+\frac{Z(1)r^2}{24\pi^2}+\frac{r}{8\pi}-\frac{Z(2)}{(2\pi)^4}-\frac{1}{4\pi}\Sigma'\frac{(r-n)^3}{6nr}\in(r-n)$$

where the Σ' means the summation over all lattice points except the origin. For practical uses one may need tables of $\bar{G}_k(r)$.

References

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