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Some generalisations of the Poisson summation formula

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Abstract. Some useful generalisations of the Poisson summation formula are presented with proofs. These extend the formula to finite sums over arbitrary intervals and to sums of derivatives. The results are indicated as being of importance in the treatment of scattering in semiclassical quantum theory.

1. Introduction

In the following we suggest some useful generalisations of the Poisson summation formula that do not appear to be widely known. In particular, the formula is extended to finite sums over arbitrary intervals, and to sums of derivatives. The proofs given here are based on the Fourier series method (e.g. Courant and Hilbert 1937) rather than the contour-integral method[†] (e.g. Morse and Feshbach 1953). Both methods of proof are valid for Dirichlet functions.

Let $f(x)$ be a function of a real variable x such that $f(x)$ possesses a Fourier series expansion over any unit interval in the range $n - \frac{1}{2} - \alpha < x < N + 1 - \alpha$ where n and N are integers such that $n \leq N$. It is sufficient for $f(x)$ to be a Dirichlet function[‡] for $n - 1 < x < N + 1$. We shall prove the following:

$$\sum_{l=n}^N f(l) = \sum_{m=-\infty}^{\infty} \exp[2m\pi i(\alpha - \frac{1}{2})] \int_n^{N+1} f(\lambda + \alpha - \frac{1}{2}) \exp(2m\pi i\lambda) d\lambda \quad (1)$$

for any real α such that $|\alpha| < \frac{1}{2}$. The sum on the left-hand side of (1) is over integer values of l in the range $n \leq l \leq N$, while that on the right-hand side is over all integer values of m [†]. If, in addition, the k th derivative, $f^k(x) = d^k f/dx^k$, of $f(x)$ exists at each of the points $x = l = n, n + 1, n + 2, \dots, N$ (as would be the case if $f^k(x)$ is Dirichlet), then we can also prove that

$$\sum_{l=n}^N f^k(l) = \sum_{m=-\infty}^{\infty} (-2m\pi i)^k \exp[2m\pi i(\alpha - \frac{1}{2})] \int_n^{N+1} f(\lambda + \alpha - \frac{1}{2}) \exp(2m\pi i\lambda) d\lambda$$

$$\alpha \in \mathbb{R}, \quad |\alpha| < \frac{1}{2}. \quad (2)$$

These results can be extended to infinite sums by taking the appropriate limit(s). The formulae then remain valid if the sums and integrals are convergent.

[†] See note added in proof.

[‡] If $f(x)$ and its first derivatives are bounded and continuous, save possibly for a finite number of points, for $a < x < b$, and $f(x) = \lim_{\epsilon \rightarrow 0} \frac{1}{2}[f(x + \epsilon) + f(x - \epsilon)]$ for all x in (a, b) , then $f(x)$ is a Dirichlet function for x in (a, b) .

The special case of (1) when $n = 0$, $N = \infty$, $\alpha = 0$ is well known and has been extensively applied to treatments of partial-wave series representations of quantal and semiclassical scattering amplitudes (e.g. Berry and Mount 1972, Frahn 1975, Rowley and Marty 1976, Brink 1978, Schaeffer 1978, Crowley 1978a, b).

A more general case of (1) arises in the context of general angular-momentum quantisation in the semiclassical theory of Crowley (1979) which provides a globally-valid uniform approximation to the quantal wavefunction for scattering by a central field. The derivation, which is based upon a diffraction-integral representation embodying classical Hamilton-Jacobi theory and in which angular-momentum quantisation is *not* a prerequisite, leads to an expression for the asymptotic wavefunction having the form of:

$$\psi(r, \theta, \phi) \underset{r \rightarrow \infty}{\sim} \frac{1}{kr} \sum_{m=-\infty}^{\infty} \exp(-m\pi\alpha/2) \int_0^{\infty} \exp[\pi i(\lambda - \frac{1}{2})/2] \{ \exp[-i(kr - \frac{1}{2}\pi(\lambda + \frac{1}{2}))] \\ + S(\lambda) \exp[i(kr - \frac{1}{2}\pi(\lambda + \frac{1}{2}))] \} \exp(2m\pi i\lambda) F(\lambda, \theta) \lambda \, d\lambda,$$

where α is a constant so far undetermined, $S(\lambda)$ is the complete semiclassical s matrix, and $F(\lambda, \theta)$ is related to a Legendre polynomial $P_l(x)$ by $F(l + \frac{1}{2}, \theta) = P_l(\cos \theta) + O(1/l)$ for $l = \text{integer} \gg 1$. By application of the theorem (1), the above becomes

$$\psi(r, \theta, \phi) \underset{r \rightarrow \infty}{\sim} \frac{1}{kr} \sum_{l=0}^{\infty} \exp[\pi i(l - \frac{1}{2} + \alpha/4)/2] \{ \exp[-i(kr - \frac{1}{2}\pi(l + \frac{1}{2} + \alpha/4))] \\ + S(l + \alpha/4) \exp[i(kr - \frac{1}{2}\pi(l + \frac{1}{2} + \alpha/4))] \} F(l + \alpha/4, \theta) (l + \alpha/4) \\ = \frac{1}{kr} \sum_{l=0}^{\infty} (2l + \frac{1}{2}\alpha) F(l + \alpha/4) \exp[\pi i(l + \alpha/4 - \frac{1}{2})/2] \cos[kr - \pi(l + \alpha/4 + \frac{1}{2})/2] \\ + [\exp(ikr)/2ikr] \sum_{l=0}^{\infty} (2l + \alpha/4) [S(l + \alpha/4) - 1] F(l + \alpha/4, \theta).$$

The condition that, when $S(\lambda) \equiv 1$, the above must yield an asymptotic representation of a plane-wave leads to the assignment, $\alpha = 2$, and hence to angular-momentum quantisation in the form of

$$\lambda - \frac{1}{2} = l = \text{integer}$$

where λ is the classical angular momentum in units of \hbar . In this way it is shown that angular momentum quantisation and the Langer Modification (Berry and Mount 1972) are natural consequences of a complete semiclassical theory. Such a theory leads to partial-wave representations of a continuum (scattering) wavefunction and the s matrix that closely resemble those of the exact theory.

Equation (2) has recently been applied to the treatment of sums arising in a description of the effect of a quasimolecular resonance on a direct-reaction process (Crowley 1978b, § 5). The transition amplitude t for a direct-reaction process dominated by a quasimolecular (potential) resonance in the elastic scattering is derived semiclassically in the form,

$$t = \sum_{m=-\infty}^{\infty} m \exp[i(\nu - 1)m\pi] \int_0^{\infty} f(\lambda) \exp(2\pi i m \lambda) \, d\lambda$$

where ν is an integer equal to the change, in units of \hbar , in the angular-momentum

component normal to the scattering plane; and $f(\lambda)$ is a continuous bounded differentiable function of λ for $\infty \geq \lambda > 0$ but is not differentiable at $\lambda = 0$ where $f(\lambda)$ has a zero and a branch point (see note added in proof). Each term in the sum over m in the above gives the contribution from trajectories which make m complete circuits of the origin. That such a contribution increases in proportion to m is consistent with the transition probability being proportional to the interaction time. Application of equation (2) enables the transition rate t to be re-expressed as a partial-wave sum in one of the following ways:

(i) $\nu = \text{even}$, when

$$\begin{aligned} t &= \sum_{m=-\infty}^{\infty} m \exp(-m\pi i) \int_0^{\infty} f(\lambda) \exp(2m\pi i\lambda) d\lambda \\ &= \frac{i}{2\pi} \sum_{l=0}^{\infty} f'(l + \frac{1}{2}) \end{aligned}$$

by application of (2) with $\alpha = 0$. The validity of the theorem depends upon $f'(\lambda) = \partial f(\lambda)/\partial \lambda$ existing at each of the points $\lambda = l + \frac{1}{2}$, $l = 0, 1, 2, \dots$ and upon $f(\lambda)$ possessing a Fourier series expansion over any unit interval in the range $0 < \lambda \leq \infty$. In this case the function $f(\lambda)$ is given as satisfying both these conditions.

(ii) $\nu = \text{odd}$.

This case is more tricky on account of $f(\lambda)$ not being differentiable at $\lambda = 0$. However, we can make use of the fact that $f(\lambda)$ is bounded throughout the closed interval $0 \leq \lambda \leq \infty$ and determine t from

$$\begin{aligned} t &= \sum_{m=-\infty}^{\infty} \lim_{\epsilon \rightarrow 0^+} \int_{\epsilon}^{\infty} m f(\lambda) \exp(2\pi i m \lambda) d\lambda \\ &= \lim_{\epsilon \rightarrow 0^+} \sum_{m=-\infty}^{\infty} m \int_{\epsilon}^{\infty} f(\lambda) \exp(2\pi i m \lambda) d\lambda \end{aligned}$$

(for the sense in which this limit exists, see note added in proof.)

$$\begin{aligned} &\equiv \lim_{\epsilon \rightarrow 0^+} \sum_{m=-\infty}^{\infty} m \exp(-2\pi i m) \int_0^{\infty} f(\lambda + \epsilon) \exp[2\pi i m(\lambda + \epsilon)] d\lambda \\ &\equiv \lim_{\epsilon \rightarrow 0^+} \sum_{m=-\infty}^{\infty} m \exp[-2\pi i m(1 - \epsilon)] \int_0^{\infty} f(\lambda + \epsilon) \exp(2\pi i m \lambda) d\lambda. \end{aligned}$$

Theorem (2) is applicable provided we choose α so that $\alpha = \epsilon - \frac{1}{2}$, whence

$$\begin{aligned} t &= \lim_{\epsilon \rightarrow 0^+} \sum_{m=-\infty}^{\infty} m \exp[2\pi i m(\alpha - \frac{1}{2})] \int_0^{\infty} f(\lambda + \alpha + \frac{1}{2}) \exp(2m\pi i \lambda) d\lambda \\ &= \frac{i}{2\pi} \sum_{l=0}^{\infty} f'(l + 1) \end{aligned}$$

provided that $f'(\lambda) = \partial f/\partial \lambda$ exists and is continuous at each of the points $\lambda = l + 1 = 1, 2, 3, \dots$

The partial-wave representations of t thus obtained may be subsequently treated using the Watson-Regge transformation in which only the resonant (pole) contributions from the elastic s matrix are included.

2. Proofs

We begin by proving (1) given that the function $f(x)$ satisfies the conditions set out prior to equation (1). By considering the Fourier series expansion of the function $g(x) = f(x+l)$, for $n - \frac{1}{2} < \alpha + l < N + \frac{1}{2}$ and $\alpha - \frac{1}{2} < x < \alpha + \frac{1}{2}$, we find that

$$f(x+l) = \sum_{m=-\infty}^{\infty} \left[\int_{\alpha-\frac{1}{2}}^{\alpha+\frac{1}{2}} f(y+l) \exp[2m\pi i(y-\alpha)] dy \right] \exp[-2m\pi i(x-\alpha)], \tag{3}$$

where the sum on the right-hand side is over all integer values of m . In particular, if $|\alpha| < \frac{1}{2}$, setting $x = 0$ yields

$$\begin{aligned} f(l) &= \sum_{m=-\infty}^{\infty} \int_{\alpha-\frac{1}{2}}^{\alpha+\frac{1}{2}} f(y+l) \exp(2m\pi iy) dy \\ &= \sum_{m=-\infty}^{\infty} \int_l^{l+1} f(\lambda + \alpha - \frac{1}{2}) \exp[2m\pi i(\lambda + \alpha - \frac{1}{2})] d\lambda, \quad l \in \mathbb{N}. \end{aligned} \tag{4}$$

Finally, summing both sides of (4) over integer values of l in the range $n \leq l \leq N$ yields

$$\begin{aligned} \sum_{l=n}^N f(l) &= \sum_{m=-\infty}^{\infty} \exp[2m\pi i(\alpha - \frac{1}{2})] \sum_{l=n}^N \int_l^{l+1} f(\lambda + \alpha - \frac{1}{2}) \exp(2m\pi i\lambda) d\lambda \\ &= \sum_{m=-\infty}^{\infty} \exp[2m\pi i(\alpha - \frac{1}{2})] \int_n^{N+1} f(\lambda + \alpha - \frac{1}{2}) \exp(2m\pi i\lambda) d\lambda \end{aligned}$$

which is the result (1).

The proof of (2) when $f^k(x)$ exists and is continuous at each of the points $x = l = n, n + 1, \dots, N$, follows by differentiating both sides of (3) k times with respect to x and proceeding as before. This proof breaks down, for example, if $f^k(x)$ is Dirichlet and has a discontinuity at one or more of the points $x = l$. In this case we can make use of the first result (1) by noting that the right-hand side contains a redundant parameter α which may take on any real value in the range $|\alpha| < \frac{1}{2}$. Differentiating both sides of (1) with respect to α yields:

$$\begin{aligned} 0 &= \sum_{m=-\infty}^{\infty} 2\pi im \exp[2m\pi i(\alpha - \frac{1}{2})] \int_n^{N+1} f(\lambda + \alpha - \frac{1}{2}) \exp(2m\pi i\lambda) d\lambda \\ &\quad + \sum_{m=-\infty}^{\infty} \exp[2m\pi i(\alpha - \frac{1}{2})] \int_n^{N+1} f^1(\lambda + \alpha - \frac{1}{2}) \exp(2m\pi i\lambda) d\lambda. \end{aligned}$$

Now, since $f^1(x)$ is a Dirichlet function, the second sum on the right is, by (1), a valid representation of the sum,

$$\sum_{l=n}^N f^1(l).$$

Hence

$$\sum_{l=n}^N f^1(l) = \sum_{m=-\infty}^{\infty} -2m\pi i \exp[2m\pi i(\alpha - \frac{1}{2})] \int_n^{N+1} f(\lambda + \alpha - \frac{1}{2}) \exp(2m\pi i\lambda) d\lambda, \tag{5}$$

which completes the proof for $k = 1$. The proof for general k follows by induction.

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Note added in proof. It should be noted that, throughout this paper $\sum_{m=-\infty}^{\infty}$ is used in a special sense as follows: If $f(m)$ is a function for which $\exp[\pm(-\gamma m)]f(m) \rightarrow 0$ as $m \rightarrow \infty$, $\forall \gamma > 0$, then

$$\sum_{m=-\infty}^{\infty} f(m) = f(0) + \lim_{\gamma \rightarrow 0^+} \sum_{m=1}^{\infty} [f(m) + f(-m)] e^{-m\gamma}. \quad (\text{N.1})$$

In this way, sums over m may be treated as if uniformly convergent (provided that the limit $\gamma \rightarrow 0^+$ exists). In particular, it can be shown that

$$\sum_{m=-\infty}^{\infty} \exp(2m\pi iz) = \lim_{\gamma \rightarrow 0^+} \frac{1}{2i} \left(\frac{\exp[-i\pi(z-i\gamma)]}{\sin[\pi(z-i\gamma)]} - \frac{\exp[-i\pi(z+i\gamma)]}{\sin[\pi(z+i\gamma)]} \right) \quad (\text{N.2})$$

for $z \in \mathbb{R}$, which, when applied to the sum over m on the RHS of (1) yields the Watson (W) transform,

$$\sum_{l=n}^N f(l) = \frac{1}{2i} \oint_{C(\alpha)} f(\lambda) e^{-\lambda\pi i} \operatorname{cosec}(\pi\lambda) d\lambda, \quad (\text{N.3})$$

where the contour $C(\alpha)$ is a simple closed Jordan curve encircling, in a positive sense, the segment of real (λ) axis between $\lambda = n - \frac{1}{2} + \alpha$ and $\lambda = N + \frac{1}{2} + \alpha$. Evaluating the integral directly, by application of Cauchy's theorem, reveals a direct correspondence between the poles of $\operatorname{cosec}(\pi\lambda)$ lying within C and terms of the sum on the LHS of (N.3). The above thus express the right-hand sides of equations (1, 2, 4 etc) as Dirichlet functions of α , for any $\alpha \in \mathbb{R}$. (For non-half-integer values of α , the same result follows by setting $x = n$, $n \in \mathbb{N}$, in equation (3) when the RHS of (4) yields $f(l+n)$ for $|\alpha - n| < \frac{1}{2}$). When α takes on half-integer values, the contour C passes through a pole of $\operatorname{cosec}(\pi\lambda)$ giving rise to a contribution equal to one-half of the residue ($\times 2\pi i$). Thus, at such a point, the function of α has a Dirichlet-type discontinuity. For example, setting $\alpha = \pm \frac{1}{2}$ in (4) yields $\frac{1}{2}[f(l) + f(l \pm 1)]$ respectively. However, when $f(x)$ possesses branch points, the functions on the right-hand sides of (1, 2, 4 etc) are defined only for values of α for which the contour C is closed on the Riemann surface (i.e. C does not cross cuts). Branch points (and associated cuts) must always lie outside C and therefore give rise to no contribution even when α is allowed to approach a limit in which a branch point lies on C .

In this manner one can achieve an alternative proof of § 1(ii) by considering the W -transform of $\sum_{l=n}^{\infty} f(l)$ with the contour taken to the right of the branch point of $f(l)$ at $\lambda = 0$. Integration by parts yields a contour integral involving $f(\lambda)$, after which the contour may be taken arbitrarily close to the branch point without actually enclosing it. Finally, reversing the above procedure, whereby the W -transform was obtained from (1), yields the original expression for t (as given in § 1(ii)) with the limit $\epsilon \rightarrow 0^+$ outside the sum.

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