Gauss sums and quantum mechanics

2000 J. Phys. A: Math. Gen. 33 5993

(http://iopscience.iop.org/0305-4470/33/34/305)

J. Phys. A: Math. Gen. **33** (2000) 5993–6002. Printed in the UK PII: S0305-4470(00)12116-X

Gauss sums and quantum mechanics

Vernon Armitage† and Alice Rogers‡

† Department of Mathematical Sciences, University of Durham, Science Laboratories, South Road, Durham DH1 3LE, UK

‡ Department of Mathematics, King's College London, Strand, London WC2R 2LS, UK

E-mail: `J.V.Armitage@durham.ac.uk` and `alice.rogers@kcl.ac.uk`

Received 23 February 2000, in final form 24 May 2000

Abstract. By adapting Feynman's sum over paths method to a quantum mechanical system whose phase space is a torus, a new proof of the Landsberg–Schaar identity for quadratic Gauss sums is given. In contrast to existing non-elementary proofs, which use infinite sums and a limiting process or contour integration, only finite sums are involved. The toroidal nature of the classical phase space leads to discrete position and momentum, and hence discrete time. The corresponding 'path integrals' are finite sums whose normalizations are derived, which are shown to intertwine cyclicity and discreteness to give a finite version of Kelvin's method of images.

1. Introduction

In this paper we give a new proof, using only finite sums and avoiding the need for analytic methods, of the Landsberg–Schaar formula for quadratic Gauss sums. The key idea, which springs from earlier work of one of us [1], is to apply the quantization of a quantum mechanical system whose phase space is a torus, with both position and momentum (and also time) discrete and cyclic. On adapting Feynman's 'sum over paths' method to this system a discrete and finite version of Kelvin's method of images is obtained.

The formula states that for positive integers p and q

$$\frac{1}{\sqrt{p}}\sum_{n=0}^{p-1}\exp\left(\frac{2\pi \mathrm{i} n^2 q}{p}\right)=\frac{\mathrm{e}^{\pi\mathrm{i}/4}}{\sqrt{(2q)}}\sum_{n=0}^{2q-1}\exp\left(-\frac{\pi \mathrm{i} n^2 p}{2q}\right). \tag{1}$$

In number theory this formula plays a central role, underpinning key results relating to quadratic reciprocity and characters. The formula also promises to be a useful adjunct to discrete Fourier transform methods used, for instance, in some algorithms for quantum computing [2]. In this context it essentially provides the discrete inverse quantum Legendre transformation from the free Hamiltonian to the free Lagrangian.

The standard proof of the Landsberg–Schaar formula (as given, for example, in [3]) is obtained by putting $\tau = 2\mathrm{i}q/p+\epsilon$, $\epsilon>0$, in the Jacobi identity for the theta function:

$$\sum_{n=-\infty}^{+\infty}\mathrm{e}^{-\pi n^2\tau}=\frac{1}{\sqrt{\tau}}\sum_{n=-\infty}^{+\infty}\mathrm{e}^{-\pi n^2/\tau} \tag{2}$$

and then letting $\epsilon\to 0$. This method is an example of Hecke's observation that 'exact knowledge of the behaviour of an analytic function in the neighbourhood of its singular points is a source of arithmetic theorems' [4, p 225].

While this method certainly establishes the truth of the formula, Hecke's insight notwithstanding it is somewhat unsatisfactory to have to use analytic methods and take limits when only finite sums are involved. The proof given in this paper does remain entirely in the arena of finite sums; it demonstrates the extraordinary range of Feynman's method of 'summing over histories', which here extends to the discrete and cyclic regime in a pleasing and effective way. So, in a sense, the quantum mechanics offers another example of Hecke's insight.

The key ingredient in this paper is quantization on a toroidal phase space. A first step was taken by one of us in [1], leading to a proof of the Jacobi identity by using random walks to quantize a system with cylindrical phase space. The key idea here is the observation that the series $\vartheta(\mathrm{i}t) = \sum_{n=-\infty}^{+\infty} \mathrm{e}^{-\pi n^2 \mathrm{i}t}$ is the trace of a certain quantum evolution operator $\exp -\mathrm{i}Ht/\hbar$, which converges in the distribution sense. Using path integral methods adapted to the cylinder, in particular Kelvin's method of images [3], an alternative formula for the trace is found, and equating the two expressions gives the Jacobi identity. This work is described in section 2 as an introduction to the main result in this paper.

With a minor change of emphasis, formula (1) turns up by taking the operator that gives (2) (for $\tau = \mathrm{i}t$) and then 'looking at the system at discrete times $\tau = -2\mathrm{i}/p$'. This idea is pursued in section 3. In order to remove difficulties over convergence, and to obtain the Landsberg–Schaar formula (1), we change the problem to one in which instead of the infinite set of energy levels of the cylindrical model there is only a finite number. This is achieved, following a suggestion of Berry [5], by replacing the cylindrical phase space (with angular position θ periodic but angular momentum L unbounded) by a torus on which both θ and L are periodic. On quantization both θ and L are discrete, and moreover, as we see, discrete times are also required. Adapting the methods used in section 2 to prove the Jacobi identity in this new setting, again two expressions for the trace of the quantum evolution operator are obtained, one by working in the momentum basis in which the evolution operator is diagonal and the other by path integral methods (using a novel discrete variant on Kelvin's method of images); the equality of these two expressions gives the Landsberg–Schaar identity.

This first description of the discrete and cyclic path integral method is presented somewhat heuristically, but in a manner which should emphasize the ideas and motivation. In section 4 full details of the toroidal quantization are given together with a justification of the normalizations used in section 3.

2. Cylindrical phase space and the Jacobi identity

In this section earlier work of one of us [1] is described as a prelude to the main result of the paper, in order to demonstrate some of the novel features of the work.

Consider a rigid body constrained to rotate about a fixed axis (cf [6]). Let I denote the moment of inertia and θ denote the angle of rotation (given in radians so that it is taken mod 2π). An angular Schrödinger picture is used, with the angular momentum observable L represented as the operator

$$L = -\mathrm{i}\hbar \frac{\partial}{\partial\theta} \tag{3}$$

(where $\hbar$ as usual represents Planck's constant h divided by 2π). Using the classical expression for the energy or Hamiltonian

$$H = \frac{L^2}{2I} \tag{4}$$

the Schrödinger equation for the wavefunction $\psi(\theta, t)$ is then [7]

$$\mathrm{i}\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2I}\frac{\partial^2\psi}{\partial\theta^2}. \tag{5}$$

Using the periodic delta function

$$\dot{\delta} = \frac{1}{2\pi}\sum_{n=-\infty}^{+\infty} \mathrm{e}^{\mathrm{i}n(\theta-\theta_0)} \tag{6}$$

we obtain the kernel (or matrix element) of the evolution operator $\exp -\mathrm{i}Ht/\hbar$:

$$K(\theta, t; \theta_0, 0) = \langle\theta|\mathrm{e}^{\frac{-\mathrm{i}Ht}{\hbar}}|\theta_0\rangle = \frac{1}{2\pi}\sum_{n=-\infty}^{+\infty} \mathrm{e}^{-\frac{\mathrm{i}\hbar n^2 t}{2I}}\mathrm{e}^{\mathrm{i}n(\theta-\theta_0)} \tag{7}$$

which is convergent in the distribution sense; alternatively one can give t a small imaginary part to restore convergence. Later we shall see that when both position and momentum are cyclic, with phase space a torus, the problem of convergence does not arise.

From (7) we see that the trace of the evolution operator is

$$\mathrm{Tr}(\exp -\mathrm{i}Ht/\hbar) = \frac{1}{2\pi}\sum_{n=-\infty}^{+\infty} \mathrm{e}^{-\frac{\mathrm{i}\hbar n^2 t}{2I}} \tag{8}$$

with convergence in the sense described above.

Now, as in [1], we follow [8] adapted to the cylindrical phase space. The purpose of the section is to express the old idea of using the method of images and the universal cover of the circle in terms of path integrals, in such a way that the argument can be adapted to the toroidal phase space of section 3, obtaining a second expression for the trace of the evolution operator $\exp \mathrm{i}Ht/\hbar$, which on comparison with (8) gives the Jacobi identity.

Denote by

$$S(\theta(t)) = \int_0^t \mathcal{L}(\dot{\theta}, \theta; t)\,\mathrm{d}t \tag{9}$$

the classical action, where $\mathcal{L}$ is the Lagrangian, and then we obtain the evolution amplitude from $(\theta_0, 0)$ to (θ, t) as

$$K(\theta, t; \theta_0, 0) \sim \sum_{\text{periodic paths from } (\theta_0,0) \text{ to } (\theta,t)} \mathrm{e}^{\mathrm{i}S(\theta)/\hbar} \tag{10}$$

where '$\sim$' indicates that a normalization factor (cf (11)) is required. In order to carry out the path integral sum we carry out the integration on the universal covering space, $\mathbb{R}$, of S^1, that is, we lift the homotopy classes to the universal covering space [1,6]. Corresponding to paths from θ_0 to θ in S^1, we have paths from some fixed θ_0^* in $\nu^{-1}(\theta_0)$ (here ν denotes the covering projection from $\mathbb{R}$ to S^1) to each of the θ_j^* in $\nu^{-1}(\theta)$, where the index j runs through the fundamental group ($\cong\mathbb{Z}$) of S^1. It follows (this is of course Kelvin's method of images) that

$$K(\theta, t; \theta_0, 0) = \sum_{n=-\infty}^{+\infty}\left(\frac{I}{2\pi\mathrm{i}\hbar t}\right)^{\frac{1}{2}}\exp\left(\frac{\mathrm{i}I}{2\hbar t}(\theta-\theta_0-2\pi n)^2\right). \tag{11}$$

(The normalization factor is taken from [8].) A full treatment of this path integral calculation may be found in the book of Schulman [9].

On equating the expressions for the trace in (8) and (11) we obtain

$$\sum_{n=-\infty}^{+\infty} \mathrm{e}^{\frac{(\mathrm{i}\hbar n^2 t)}{2I}} = \left(\frac{2\pi I}{\mathrm{i}\hbar t}\right)^{\frac{1}{2}}\sum_{n=-\infty}^{+\infty} \mathrm{e}^{\frac{-2\hbar^2 n^2 I}{\hbar\mathrm{i}t}}. \tag{12}$$

(As already observed, care is needed over convergence, which is intended in the distributional sense.) If we arrange that $2\pi I = \hbar$, $\tau = \mathrm{i}t$, then we obtain formally the usual Jacobi identity (2) for $\vartheta(\mathrm{i}t)$.

After this work was presented [1] it was suggested by Berry [5] that the way forward to obtaining the Landsberg–Schaar formula by similar means might be to consider a system where the angular momentum, as well as the angle, was cyclic so that the phase space was compact and the quantized observables would not only be discrete but also have a finite range. This approach, which does indeed lead to the Landsberg–Schaar formula, is developed in the following section.

3. Toroidal phase space and the Landsberg–Schaar formula

In this section we adapt the methods of the preceding section to a toroidal phase space on which both L and θ are periodic. On quantization this gives discreteness to both these variables, and makes it possible (provided that suitable values are used for the various constants involved) to have only a finite number of energy eigenstates. Time, too, becomes quantized as emerges when evolution is considered. In this section we concentrate on ideas, obtaining the Landsberg–Schaar formula by proceeding in the manner of a physicist, while in the next section the quantization scheme is fully described and normalization factors are derived.

Suppose that the phase space of our system is a torus, with angular momentum L of period P and angle of rotation θ of period 2π. Quantization in L and θ, when both θ and L are periodic, gives, respectively,

$$L = n\hbar \qquad \theta = \frac{2\pi m\hbar}{P} \qquad m, n \in \mathbb{Z}. \tag{13}$$

The phase space is quantized to a lattice on the torus, and the small rectangles with sides $\hbar$ and $\frac{2\pi\hbar}{P}$ fit a whole number of times into the phase space torus area. The area of the phase space torus is $2\pi P$. So $2\pi P = 2\pi N\hbar$, ($P = N\hbar$, $N \in \mathbb{Z}$) and so the small rectangles fit N^2 times into the phase space torus.

There are precisely N energies, E_n, $1 \leqslant n \leqslant N$, and so the trace of the evolution operator is given by

$$\begin{aligned}\mathrm{Tr}(\exp -\mathrm{i}Ht/\hbar) &= \frac{1}{2\pi}\sum_{n=1}^{N} \mathrm{e}^{-\frac{\mathrm{i}E_n t}{\hbar}} \\ &= \frac{1}{2\pi}\sum_{n=1}^{N} \mathrm{e}^{-\frac{\mathrm{i}\hbar n^2 t}{2I}}.\end{aligned} \tag{14}$$

Now we turn to the L-periodicity and show that it implies a restriction on the times, t, of 'looking at the system'.

Any quantum mechanical state $\psi(\theta, t)$ has an expansion

$$\psi(\theta, t) = \sum_{k=-\infty}^{+\infty} a_k \mathrm{e}^{\mathrm{i}(k\theta - \frac{\hbar k^2 t}{2I})} \qquad a_k = a_{k+N} \tag{15}$$

with the usual observations about convergence. Now take the Fourier transform in θ of (15) to go from position (angle) space to momentum space. We obtain (here $\hat{\psi}$ denotes the Fourier transform in the variable θ)

$$\hat{\psi}(L, t) = \int_{-\infty}^{+\infty} \psi(\theta, t)\mathrm{e}^{-\mathrm{i}p\theta/\hbar}\,\mathrm{d}\theta \tag{16}$$

and we use $\mathcal{F}[\mathrm{e}^{\mathrm{i}k\theta}] = \delta(L - k\hbar)$

$$\hat{\psi}(L, t) = \sum_{k=-\infty}^{+\infty} a_k \mathrm{e}^{-\frac{\mathrm{i}\hbar k^2 t}{2I}} \delta(L - k\hbar) \tag{17}$$

where δ denotes the Dirac delta distribution, and

$$\begin{aligned} \hat{\psi}(L + P, t) &= \sum_{k=-\infty}^{+\infty} a_k \mathrm{e}^{-\frac{\mathrm{i}\hbar k^2 t}{2I}} \delta(L + P - k\hbar) \\ &= \sum_{k=-\infty}^{+\infty} a_k \mathrm{e}^{-\frac{\mathrm{i}\hbar (k+N)^2 t}{2I}} \delta(L - k\hbar). \end{aligned} \tag{18}$$

Thus periodicity of period P in L, that is $\hat{\psi}(L + P, t) = \hat{\psi}(L, t)$, implies

$$1 = \mathrm{e}^{-\mathrm{i}\hbar t(N^2+2kN)/(2I)} \tag{19}$$

so that (assuming N is even, as is required later)

$$t = \frac{2\pi m I}{N\hbar} \qquad m \in \mathbb{Z}. \tag{20}$$

On substituting from (20) in (14) we obtain

$$\begin{aligned} \mathrm{Tr}(\exp -\mathrm{i}Ht/\hbar) &= \frac{1}{2\pi} \sum_{n=0}^{N} \mathrm{e}^{-\mathrm{i}\hbar n^2 \frac{2\pi m I}{N\hbar 2I}} \\ &= \frac{1}{2\pi} \sum_{n=0}^{N} \mathrm{e}^{-\mathrm{i}\hbar\pi n^2 \frac{m}{N}}. \end{aligned} \tag{21}$$

We have to compute

$$\sum_{\text{periodic paths}} \mathrm{e}^{\mathrm{i}S(\theta)/\hbar} \tag{22}$$

where the sum is now over all periodic paths on the torus. At the nth energy level, p_n is constant:

$$E_n = \frac{p_n^2}{2I} \qquad I\dot{\theta}_n = p_n \qquad I\theta = p_n t. \tag{23}$$

Hence, for the 'time of looking' given in (20),

$$|I\theta| \leqslant p_n \cdot \frac{2|m|\pi I}{N\hbar} \leqslant |m| \cdot 2\pi I. \tag{24}$$

On repeating the argument given in section 2, but now restricting θ as in (24), we obtain in place of (11)

$$K(\theta, t) = \sum_{n=0}^{m-1} \left(\frac{I}{2\pi \mathrm{i}\hbar t}\right)^{\frac{1}{2}} \exp\left(\frac{\mathrm{i}I}{2\hbar t}(\theta - 2\pi n)^2\right) \tag{25}$$

where as before

$$t = \frac{2\pi m I}{N\hbar}. \tag{26}$$

(The normalization factor used is taken from (11), and is justified in section 4; while it might seem simpler to derive this by the method used by Davison [10] than by the methods of section 4, in fact there is a crucial step (equation (3.5) of Davison's paper) which would require knowledge of the Gauss sums under study.)

It follows from (25) that the propagator trace is

$$\mathrm{Tr}(\exp -\mathrm{i}Ht/\hbar) = \left(\frac{N}{4\pi^2\mathrm{i}m}\right)^{\frac{1}{2}} \sum_{n=0}^{m-1} \exp\left(\frac{\mathrm{i}n^2}{(\frac{2\hbar\cdot 2m\pi}{N\hbar})}\right)$$
$$= \left(\frac{N}{\mathrm{i}m}\right)^{\frac{1}{2}} \sum_{n=0}^{m-1} \mathrm{e}^{\mathrm{i}\pi n^2 N/m}. \tag{27}$$

So, on equating (14) and (27), we obtain

$$\sum_{n=0}^{N} \mathrm{e}^{-\frac{2\pi\mathrm{i}n^2}{N}} = \left(\frac{N}{\mathrm{i}m}\right)^{\frac{1}{2}} \sum_{n=0}^{m-1} \mathrm{e}^{\mathrm{i}\pi n^2 N/m}. \tag{28}$$

Finally in (28) we take $N = 2q$, $m = p$, $\mathrm{i}^{-1} = -\mathrm{e}^{\pi\mathrm{i}/2}$ to obtain

$$\frac{\mathrm{e}^{\pi\mathrm{i}/4}}{\sqrt{(2q)}} \sum_{n=0}^{2q-1} \exp\left(-\frac{\pi\mathrm{i}n^2 p}{2q}\right) = \frac{1}{\sqrt{p}} \sum_{n=0}^{p-1} \exp\left(\frac{2\pi\mathrm{i}n^2 q}{p}\right) \tag{29}$$

which is the Landsberg–Schaar formula (1).

4. Normalization of the discrete path integral

In this section details are given of the quantum mechanical system whose path integration is used in the previous section to prove the Landsberg–Schaar formula (1). The necessary path integral formula is derived by adapting the original approach of Feynman [8] to the discrete and cyclic setting. Because all sums are finite in this case there are no convergence or other analytic difficulties, so that a precise result is obtained with well defined normalization. This confirms the validity of the more heuristic, but geometrically and arithmetically well motivated, use of the Feynman principle in the previous section.

The starting point is the classical phase space of the system, which is taken to be toroidal with coordinates θ, L of periodicity 2π and P respectively. As Hilbert space for our system we take $\mathcal{H} = \mathbb{C}^N$ (where N is a positive integer) realized as

$$\left\{ f : \mathbb{R} \to \mathbb{C} | f(\theta) = \sum_{n=1}^{N} a_n \exp\left(\frac{2\pi\mathrm{i}n\theta}{N}\right) \right\}$$

where each a_n is a complex number.

One basis of $\mathcal{H}$ is then plainly $\{f_k : k = 0, \ldots, N-1\}$ with $f_k(\theta) = \frac{1}{\sqrt{N}} \exp(\frac{2\pi\mathrm{i}k\theta}{N})$. This is the angular momentum basis, that is, each f_k is an eigenvector of the angular momentum operator L (defined now by $L = -\mathrm{i}\frac{N}{2\pi}\frac{\partial}{\partial\theta}$) with eigenvalue k. Using Dirac notation, we write f_k as $|k\rangle$. For simplicity we use units in which $\hbar$ takes the value 1.

Another basis is $\{b_r : r = 1, \ldots, N\}$ with

$$b_r(\theta) = \frac{1}{N} \sum_{k=0}^{N-1} \exp\left(\frac{2\pi\mathrm{i}(\theta - r)k}{N}\right). \tag{30}$$

The inner product on $\mathcal{H}$ is defined by

$$\langle f | g \rangle = \sum_{j=0}^{N-1} f(j)^* g(j). \tag{31}$$

With this inner product both of these bases are orthonormal.

The b_r may be regarded as the position basis if one restricts the domain of the elements f of $\mathcal{H}$ to $\mathbb{Z}_N = \{0, 1, \dots, N-1\}$ and defines the (exponentiated angular) position operator $\hat{x}$ by

$$\hat{x} f(\theta) = \exp\left(2\pi \mathrm{i}\frac{\theta}{N}\right) f(\theta) \tag{32}$$

since then

$$\hat{x} b_r = \exp\left(2\pi \mathrm{i}\frac{r}{N}\right) b_r \tag{33}$$

so that b_r is an eigenstate of $\hat{x}$, with eigenvalue $\exp(2\pi \mathrm{i}\frac{r}{N})$. (In Dirac notation we write b_r as $|r\rangle$.)

Now the proof of the Landsberg–Schaar identity essentially involves calculating the trace of $\exp -\mathrm{i}Ht$ (with $H = \frac{L^2}{2I}$ and $t = \frac{2\pi m I}{N}$ as before) in these two different bases. From the outset we will set $m = p$, where p is one of the two integers in the Landsberg–Schaar formula.

Method 1 is the direct way, that is, working in the momentum basis in which H is diagonal. We have $Ht|k\rangle = \frac{\pi k^2 p}{N}|k\rangle$ so that

$$\mathrm{Tr}(\exp -\mathrm{i}Ht) = \sum_{k=0}^{N-1} \exp\left(-\frac{\mathrm{i}\pi k^2 p}{N}\right). \tag{34}$$

Method 2 uses discrete, cyclic 'path integrals'. We consider $\langle r|\exp -\mathrm{i}Ht|s\rangle$.

Breaking the time interval down into p steps $\Delta t = \frac{t}{p}$, and using s_i to label basis elements b_{s_i} at the ith step, we have

$$\langle r|\exp -\mathrm{i}Ht|s\rangle = \langle r|\exp -\mathrm{i}H\Delta t|s_{p-1}\rangle\langle s_{p-1}|\exp -\mathrm{i}H\Delta t|s_{p-2}\rangle \cdots \langle s_1|\exp -\mathrm{i}H\Delta t|s\rangle \tag{35}$$

(with summation from 0 to $N-1$ over each of the intermediate s_i, $i = 1, \dots, p-1$). We thus need to consider $\langle s_i|\exp -\mathrm{i}H\Delta t|s_{i-1}\rangle$. Now

$$\begin{aligned}\langle s_i|\exp -\mathrm{i}H\Delta t|s_{i-1}\rangle &= \sum_{k=0}^{N-1}\langle s_i|k\rangle\langle k|s_{i-1}\rangle \exp\left(-\frac{\pi \mathrm{i}k^2}{N}\right)\\ &= \sum_{k=0}^{N-1}\frac{1}{N}\exp\left(\frac{2\pi \mathrm{i}k(s_i - s_{i-1})}{N}\right)\exp\left(-\frac{\pi \mathrm{i}k^2}{N}\right)\end{aligned} \tag{36}$$

using the fact that

$$\langle r|k\rangle = \frac{1}{\sqrt{N}}\exp\left(\frac{2\pi kr}{N}\right). \tag{37}$$

Thus

$$\langle s_i|\exp -\mathrm{i}H\Delta t|s_{i-1}\rangle = \sum_{k=0}^{N-1}\frac{1}{N}\exp\left(-\frac{\pi \mathrm{i}}{N}(k - (s_i - s_{i-1}))^2\right)\exp\left(\pi \mathrm{i}\frac{(s_i - s_{i-1})^2}{N}\right). \tag{38}$$

Again, as in section 3, we set $N = 2q$, so that in particular N is even and we have

$$\begin{aligned}\langle s_i|\exp -\mathrm{i}HT|s_{i-1}\rangle &= \sum_{k=0}^{N-1}\frac{1}{N}\exp\left(-\frac{2\pi \mathrm{i}}{2N}(k - (s_i - s_{i-1}))^2\right)\exp\left(2\pi \mathrm{i}\frac{(s_i - s_{i-1})^2}{2N}\right)\\ &= \frac{1}{\sqrt{\mathrm{i}N}}\exp\left(2\pi \mathrm{i}\frac{(s_i - s_{i-1})^2}{2N}\right)\end{aligned} \tag{39}$$

by equation (47) of the appendix. Thus

$$\langle r|\exp -\mathrm{i}HT|s\rangle = (\mathrm{i}N)^{-p/2}\sum_{s_1=0}^{N-1}\cdots\sum_{s_{p-1}=0}^{N-1}\exp\left(2\pi\mathrm{i}\frac{\sum_{i=1}^{p}(s_i-s_{i-1})^2}{2N}\right) \tag{40}$$

where $s_0 = r$, $s_p = s$.

At this stage we assume that p and q are coprime and that p is odd, so that p and $N = 2q$ are coprime; we observe that

$$\sum_{l=0}^{N-1}\sum_{k=0}^{p-1}\exp\left(2\pi\mathrm{i}\frac{(kN+lp)^2}{2Np}\right) = \sum_{t=0}^{Np-1}\exp\frac{2\pi\mathrm{i}t^2}{2Np} = \sqrt{\mathrm{i}Np} \tag{41}$$

where we have used the result (46) from the appendix. (Because p and N are coprime the expression $kN + lp$ takes all Np distinct values (mod Np) as k ranges from 0 to $p-1$ and l ranges from 0 to $N-1$.) This result allows us to insert in the expression for $\langle r|\exp -\mathrm{i}Ht|s\rangle$ the extra summations $\sum_{l=0}^{N-1}\sum_{k=0}^{p-1}\exp\left(2\pi\mathrm{i}\frac{(kN+lp)^2}{2Np}\right)$ together with the compensating factor $1/\sqrt{\mathrm{i}Np}$. This step effectively allows the winding number k for a path to be shared over the p steps in the path.

Using these facts, we see that

$$\begin{aligned}
&\langle r|\exp -\mathrm{i}Ht|s\rangle \\
&\quad= \frac{(\mathrm{i}N)^{-p/2}}{\sqrt{\mathrm{i}aNp}}\sum_{s_1=0}^{N-1}\cdots\sum_{s_{p-1}=0}^{N-1}\sum_{l=0}^{N-1}\sum_{k=0}^{p-1}\exp\left(2\pi\mathrm{i}\left(\sum_{i=1}^{p}\frac{(s_i-s_{i-1})^2}{2N}+\frac{(kN+lp)^2}{2Np}\right)\right)\\
&\quad= \frac{(\mathrm{i}N)^{-p/2}}{\sqrt{\mathrm{i}aNp}}\sum_{s_1=0}^{N-1}\cdots\sum_{s_{p-1}=0}^{N-1}\sum_{l=0}^{N-1}\sum_{k=0}^{p-1}\\
&\quad\quad\times\exp\left(2\pi\mathrm{i}\left(\sum_{i=1}^{p}\left(\frac{(s_i-s_{i-1})^2}{2N}+\frac{l^2}{2N}\right)+\frac{k^2q}{p}\right)\right)\\
&\quad= \frac{(\mathrm{i}N)^{-p/2}}{\sqrt{\mathrm{i}aNp}}\sum_{s_1=0}^{N-1}\cdots\sum_{s_{p-1}=0}^{N-1}\sum_{l=0}^{N-1}\sum_{k=0}^{p-1}\exp\left(2\pi\mathrm{i}\left(\sum_{i=1}^{p}\frac{(s_i-s_{i-1}+l)^2}{2N}+\frac{(k^2q)}{p}\right)\right)
\end{aligned} \tag{42}$$

provided that $r - s \equiv 0 \pmod N$.

Now let $u_1 = s_1 - s_0 + l = s_1 - r + l$, $u_2 = s_2 - s_1 + l$ and so on, with $u_p = s_p - s_{p-1} + l = s - s_{p-1} + l$. Then $\sum_{i=1}^{p} u_i = r - s + lp$ so that $u_p = r - s + lp - \sum_{i=1}^{p-1} u_i$. Thus if p and N are coprime and $s_1, \ldots, s_{p-1}$ are fixed the integer variable u_p will take each value $0, 1, \ldots, N-1$ mod N precisely once as l ranges from 0 to $N-1$, so that

$$\begin{aligned}
&\langle r|\exp -\mathrm{i}HT|s\rangle \\
&\quad= \frac{(\mathrm{i}N)^{-p/2}}{\sqrt{\mathrm{i}Np}}\sum_{u_1=0}^{N-1}\cdots\sum_{u_p=0}^{N-1}\sum_{k=0}^{p-1}\exp\left(2\pi\mathrm{i}\left(\sum_{i=1}^{p}\frac{u_i^2}{2N}\right)\right)\exp\left(2\pi\mathrm{i}\frac{(k^2q)}{p}\right)\\
&\quad= \frac{(\mathrm{i}N)^{-p/2}}{\sqrt{\mathrm{i}Np}}(N\mathrm{i})^{p/2}\sum_{k=0}^{p-1}\exp\left(2\pi\mathrm{i}\frac{(k^2q)}{p}\right)\ \text{by (46)}\\
&\quad= \frac{1}{\sqrt{\mathrm{i}pN}}\sum_{k=0}^{p-1}\exp\left(2\pi\mathrm{i}\frac{(k^2q)}{p}\right).
\end{aligned} \tag{43}$$

Hence

$$\begin{aligned}
\mathrm{Tr}(\exp \mathrm{i}Ht) &= \sum_{s=0}^{N-1} \langle s| \exp \mathrm{i}Ht |s\rangle \\
&= \frac{N}{\sqrt{\mathrm{i}pN}} \sum_{k=1}^{p} \exp\left(2\pi \mathrm{i} \frac{(k^2 q)}{p}\right) \\
&= \frac{\sqrt{2q}}{\sqrt{\mathrm{i}p}} \sum_{k=1}^{p} \exp\left(2\pi \mathrm{i} \frac{(k^2 q)}{p}\right) \qquad (\text{since } N = 2q) \qquad (44)
\end{aligned}$$

so that by (34) we have the Landsberg–Schaar formula for the case where p and q are coprime and p is odd.

By a similar procedure, but using negative time steps, we obtain

$$\sum_{k=0}^{2q'-1} \exp\left(\pi \mathrm{i} \frac{k^2 p'}{2q'}\right) = \frac{\sqrt{2q'\mathrm{i}}}{\sqrt{p'}} \sum_{k=0}^{p'-1} \exp\left(-2\pi \mathrm{i} \frac{(k^2 q')}{p'}\right) \qquad (45)$$

again assuming that p' and q' are coprime and that p' is odd. Doubling the range on each side simply doubles the value on each side, so that setting $p = 4q'$ and $q = p'$ in the above gives the Lansberg–Schaar formula for the case where p and q are coprime with $p \equiv 0 \bmod 4$. If p and q are coprime with $p \equiv 2 \bmod 4$ then both sides of the Landsberg–Schaar formula are zero. Thus we have established the formula for all cases where p and q are coprime, the general case following on setting $p = mp''$, $q = mq''$ with p'', q'' coprime.

Appendix

The two formulae below may be proved by elementary means [11, 12]:

$$\sum_{n=0}^{2r-1} \exp\left(\frac{2\pi \mathrm{i}(n-s)^2}{4r}\right) = \sqrt{2r\mathrm{i}} \qquad (46)$$

$$\sum_{k=0}^{2r-1} \exp\left(-2\pi \mathrm{i} \frac{(k-s)^2}{4r}\right) = \sqrt{\frac{2r}{\mathrm{i}}} \qquad (47)$$

where we use $\sqrt{\mathrm{i}} = \frac{\sqrt{2}}{2}(1+\mathrm{i})$. Given such an elementary evaluation of the Gauss sum, together with an elementary proof of the quadratic reciprocity law:

$$\left(\frac{p}{q}\right)\left(\frac{q}{p}\right) = (-1)^{\frac{p-1}{2}\frac{q-1}{2}} \qquad (48)$$

where $(\frac{p}{q})$ denotes the Legendre symbol and p and q are odd primes, one could prove (1) by evaluating each side and then appealing to the reciprocity law and its extensions (to $p = 2$ and $p = -1$). Whether such a proof would provide insight into why the result is true is another matter.

Again, there is another proof of the theta function identity (2), due to Polya [13], which depends on an identity involving binomial coefficients, identities which are in turn related to the Markov chain approach to diffusion processes considered in [1].

The approach adopted in this paper presupposes an elementary proof of the evaluation of Gauss sums in (46) and (47), but not of the reciprocity law. It is perhaps tempting therefore to regard the present approach as a substitute, in some sense, for the reciprocity law, but we prefer to see it as a quantum mechanical equivalent of Hecke's observation, in which Feynman's 'sum over histories' in discrete time replaces the limiting process that derives (1) from (2).

References

[1] Armitage J V 1987 Gauss sums and Markov chains *Lecture given at LMS Symp. on Number Theory and Dynamical Systems (York, UK)*

[2] Shor P W 1994 Algorithms for quantum computation: discrete logarithms and factorising *Proc. 35th Ann. Symp. on Foundations of Computer Science* ed S Goldwasser (Los Alimitos, CA: IEEE Computer Society Press) p 124

[3] Dym H and McKean H P 1972 *Fourier Series and Integrals* (New York: Academic)

[4] Hecke E 1923 *Vorlesungen über die Theorie der Algebraischen Zahlen* (Leipzig: Akademie) (Engl. Transl. 1981 *Lectures on the Theory of Algebraic Numbers* (New York: Springer))

[5] Berry M 1987 Private communication

[6] Schulman L 1968 A path integral for spin *Phys. Rev.* **176** 1558–69

[7] Schiff L 1968 *Quantum Mechanics* 3rd edn (New York: McGraw-Hill)

[8] Feynman R P and Hibbs A 1965 *Quantum Mechanics and Path Integrals* (New York: McGraw-Hill)

[9] Schulman L S 1981 *Techniques and Applications of Path Integration* (New York: Wiley)

[10] Davison B 1954 On Feynman's 'integral over all paths' *Proc. R. Soc.* A **225** 252–63

[11] Landau E 1927 *Elementare Zahlentheorie Vorlesungen über Zahlentheorie* section 1 (Leipzig: Hirzel) 1950 Reprinted (New York: Chelsea)

[12] Waterhouse W C 1970 The sign of the Gaussian sum *J. Number Theor.* **2** 363

[13] Polya G 1927 Elementare beweis eine thetaformel *Sitz. der Phys.–Math. Klasse* (Berlin) pp 158–61