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Quantum particle on a circle

Relatore Prof. Paolo Ciatti Diplomando Riccardo Antonelli

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Riccardo Antonelli

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Abstract

We study the probability amplitude for a quantum particle on a circle to return to its original position after a time t. This amplitude turns out to be a tempered distribution with an intricate structure of singularities on a dense set and transformation properties reminiscent of a modular form.

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1 Introduction

Quantum mechanics includes mathematical tools routinely employed in the calculation of measurable quantities that on any remotely formal level appear nonsensical and ill-defined. The root of this widespread misbehaviour of general quantum theory would seem to trace back to the fact that quantum-mechanical observables are to be computed through expressions of the type:

$$\mathcal{O} = \left| \sum_{c} e^{i\mathcal{F}[c]} \right|^2. \tag{1}$$

The sum is over all possible configurations and can actually be a finite sum, a series, an integral, or even a functional integral, and for essentially all choices of the real functional \mathcal{F} it has very poor convergence. Nevertheless, in physics expressions like (1) are often produced and manipulated with no concerns for whether they make any sense temporarily, and are then handled with an array of regularization procedures until they are carried to a sensible final result for a desired experimental prediction.

Perhaps the most general of such regularizations is Wick rotation, in which a transformation $t \to it$ in the complex time plane is performed. Generally, computed at purely imaginary time the functionals \mathcal{F} acquire a positive imaginary part and the sum-over-paths becomes convergent. The real-time desired quantity is hopefully recovered through analytic continuation up to the real axis. This is usually understood as an occasion to cure the pathologies of quantum mechanics by defining a quantum theory simply as the result of the Wick rotation procedure. This is a practical (and almost always successful) approach but is somewhat unsatisfactory or at least unsettling, as it delegates the description of real quantities to abstract dynamics in imaginary time and also requires strong assumption of analyticity of observables.

We would like here instead to attempt a sketch of alternative meaning that can be assigned to the naively divergent oscillatory sums of quantum mechanics. For this reason we consider the simplest possible quantum system in which such unruly summations occur, a free particle on \mathbb{S}^1 . This is a sandbox even more basic than the more popular particle in a box¹, and in this context we pose the simplest question:

What is the probability that a particle left on a point on the circle will reach another given point after some given time?

This probability (density) is the squared modulus of a complex amplitude, depending on the final position and elapsed time, called the propagator, which is simply the fundamental solution to the Schrödinger equation on the circle. The answer to this apparently absolutely innocuous question is already an incredibly bizzare object. Even after being rigorously defined through regularization,

¹In fact, the box is a simple orbifold of the circle, as $[0,1] \cong \mathbb{S}^1/\{\theta \sim -\theta\}$. Thus the propagator in a box is easily obtained as a sum of two circle propagators through the method of images.

it still does not behave as a function of position and time in any naive sense. Normally, this is kept "as is" and read as a formal series, up until the point when one computes more regular observables starting from it. In this work, instead, we insist in providing an accurate description of this amplitude as it comes as an actual mathematical object (and it will turn out to be a tempered distribution of both time and space) and a study of its features.

The propagator will be found to be endowed with an intricate structure of infinite singularities and zeroes that are mapped to eachother by modular transformations, but will nonetheless be perfectly well-defined as a tempered distribution; in fact the sum-over-histories that produces it will be shown to be sensible if understood as a distributional limit. A greater attention will be provided on the time dependence of the amplitude.

Finally, after this anatomical study of the circle propagator, we will offer a possible physical understanding for the features found.

2 Quantum mechanics on \mathbb{S}^1

2.1 Schrödinger equation and propagators

Arguably, a minimal description of a quantum mechanical system is in terms of a separable complex Hilbert space \mathcal{H} , the state space, an algebra \mathcal{A} of operators acting on \mathcal{H} , and, if there is interest in studying time-evolution, a selected hermitian operator $H \in \mathcal{A}$, the Hamiltonian.

The state, representing information available about the system, is encoded as a vector² (ket) $|\Psi(t)\rangle$ in state space, where we have explicited the possibility that this knowledge is time-dependent. This possibility is realized, and information on the system at time $t = t_1$ determines the state at a later time $t = t_2$ by integration of the Schrödinger equation:

$$i\hbar \frac{\mathrm{d}}{\mathrm{d}t} |\Psi(t)\rangle = H |\Psi(t)\rangle$$
 (2)

If, in addition, we exclude that the Hamiltonian depends explicitly on time, the Schrödinger equation can immediately be integrated through an operator exponential:

$$|\Psi(t_2)\rangle = e^{-\frac{i}{\hbar}H(t_2 - t_1)} |\Psi(t_1)\rangle \tag{3}$$

²This is actually only true for *pure* (i.e., maximal) information. Imperfect/incomplete information, that is a mixed state, admits a representation as a state matrix but not as a state space vector. In addition, proportional vectors of \mathcal{H} map to the same pure state, so that the latter should better be made to correspond with rays of \mathcal{H} . Both of these points are not relevant to our present discussion.

 $U(t) = e^{-\frac{i}{\hbar}Ht}$ is the unitary time-evolution operator, and its determination coincides with the complete solution of the Schrödinger equation.

While the presentation above is absolutely general, we specialize to a very simple subcase, that of a mechanical system with finite degrees of freedom. If we have a classical Hamiltonian system whose phase space is a product $M \times TM \ni (q,p)$, where the *n*-dimensional Riemannian smooth manifold (M,g) is called the configuration space, and with some Hamiltonian function H(p,q), then the **quantization** of this system is constructed by taking as Hilbert space the set of square-normalizable complex wavefunctions on configuration space³:

$$\mathcal{H} = L^2(M) = \left\{ \psi : M \to \mathbb{C} : \int d \operatorname{vol}_M |\psi(q)|^2 < \infty \right\}. \tag{4}$$

Then the dynamics can be specified in any given atlas of M. In each chart $M \times TM \supset U \to \mathbb{R}^n \times \mathbb{R}^n$, $(q,p) \mapsto (x,p)$, we represent the classical coordinates x, p respectively by the Hermitian operators \hat{x} , \hat{p} acting as

$$\hat{x}\psi(x) := x\psi(x) \tag{5}$$

$$\hat{p}\psi(x) := -i\hbar \operatorname{grad}_{M} \psi(x) \tag{6}$$

Then finally we can write the Hamiltonian \hat{H} as simply $H(\hat{x}, \hat{p})$. In each chart, the Schrödinger equation holds:

$$i\frac{\partial}{\partial t}\psi(x,t) = \hat{H}\psi(x,t) \tag{7}$$

Physically speaking, the class of systems above is fairly broad. We can restrict it considerably to Hamiltonians of the form

$$H(p,q) = \frac{\langle p, p \rangle}{2m} \,, \tag{8}$$

which describe the dynamics of a free point particle of mass m moving on (M, g). We now choose units in which $\hbar = m = 1$. The Schrödinger equation reduces to

$$i\frac{\partial}{\partial t}\psi(x,t) = -\frac{\nabla^2}{2}\psi(x,t) \tag{9}$$

³An interesting generalization is to consider instead wavefunctions to be sections of a complex line bundle over M, perhaps topologically non-trivial. This can be seen to be equivalent to the introduction of a flat electromagnetic potential with a non-trivial holonomy, and this addition on the \mathbb{S}^1 case is a possible future extension for this work.

⁴More precisely, H(p,q) is either written as a polynomial or approximated with a family of polynomials, and the same operation is performed on the operators \hat{x} , \hat{p} to build the quantized Hamiltonian \hat{H} . Since these do not commute, ambiguities might arise, with physical implications. It is not the case for the situations we will consider, however, and we can ignore these issues.

where ∇^2 is the Laplace-Beltrami operator for the metric g.

There exists a way of understanding the time-evolution operator $\hat{U}(t)$ more explicitly in this case. Define the function $G(x_1, x_2; t)$ as the solution to the initial-value problem for equation (9) with a δ -function initial condition:

$$i\frac{\partial}{\partial t}G(x_1;x,t) = -\frac{\nabla_x^2}{2}G(x_1;x,t), \qquad (10)$$

$$G(x_1; x, 0) = \frac{1}{\sqrt{g}} \delta(x - x_1).$$
(11)

Then, since (9) is linear, the solution to the initial-value problem with initial condition $\psi(x,0)$ can be found as a convolution:

$$\psi(x,t) = G(x_1; x, t) *_{x_1} \psi(x_1, 0). \tag{12}$$

The function G is known as a fundamental solution or in more physical terms the propagator, since it coincides with the probability amplitude for a particle left at position x_1 to be found at position x after time t. (12) then describes how knowledge about the distribution of initial positions evolves as a sum over the evolutions of possible initial positions. In any case (12) is the specification of the operator $\hat{U}(t)$ as a convolution operator.

Taking a basis of eigenstates of position $|x\rangle$ normalized such that $\int dx |x\rangle \langle x|$ is the identity operator, note that

$$G(x_1; x, t) := \langle x_1 | \hat{U}(t) | x \rangle \tag{13}$$

$$= \langle x_1 | e^{-iHt} | x \rangle \tag{14}$$

$$= \langle x_1 | e^{-iHt'} e^{-iH(t-t')} | x \rangle \tag{15}$$

$$= \int dx' \langle x_1 | e^{-iHt'} | x' \rangle \langle x' | e^{-iH(t-t')} | x \rangle$$
 (16)

$$= \int dx' G(x_1; x', t') G(x'; x, t - t')$$
(17)

Expression (17) states the amplitude of propagation from an initial to a final point is equal to the sum over all possible intermediate position of the product between the amplitude of propagation from initial to intermediate and to intermediate to final position. This is a general and fundamental statement about quantum mechanics: amplitudes are sum over possible processes, each of which is a product of amplitudes of subprocesses. In general, one can always write some equality of the

form

$$\langle \text{initial} | \hat{U}(t) | \text{final} \rangle = \sum_{\text{intermediate}} \langle \text{initial} | \hat{U}(t') | \text{intermediate} \rangle \langle \text{intermediate} | U(t - t') | \text{final} \rangle ; \quad (18)$$

where f can be any general type of "sum", including even finite or infinite sums or integrals under which the intermediate states form a suitably normalized complete basis of \mathcal{H} .

2.2 Review: free particle on \mathbb{R}

Consider the quantization of the simplest possible continuous classical system: the free particle in one dimension. This is the Hamiltonian system phase space \mathbb{R}^2 (with the simple chart (p,x)) and the Hamiltonian $H(p,x) = \frac{p^2}{2}$ (having chosen units such that m=1). Configuration space is the real line. Consequently, the quantum description has as state a complex wavefunction with domain \mathbb{R} , and evolution is according to the Hamiltonian

$$H = -\frac{\partial_x^2}{2} \,. \tag{19}$$

We are interested in calculation of the propagator $G(x_1; x_2, t)$. Because of translation invariance, this quantity can only depend on the difference $x_2 - x_1$, and we can simply write G(x; t).

The most straightforward path to the propagator is through diagonalization of H. As a simple derivative operator, it's obvious a basis of eigenfunctions of H is given by the Fourier components $\phi_k(x) = e^{ikx}$. Each of them evolves according to

$$\phi_k(x;t) = \exp\left(\frac{it}{2}\partial_x^2\right)\phi_k(x;0) = e^{-ik^2t/2}e^{ikx}.$$
 (20)

Our initial wavefunction is the (non-normalizable) delta function: $\Psi(x;0) = \delta(x)$. Recalling the Fourier representation of the distribution δ :

$$\Psi(x;0) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dk \ e^{ikx}$$
 (21)

and inserting (20) we obtain the evolved state at a later time:

$$\Psi(x;t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dk \, \exp\left(-i\frac{k^2}{2}t + ikx\right) = (2\pi i t)^{-1/2} \exp\left(\frac{ix^2}{2t}\right) = G(x,t). \tag{22}$$

We note a paradoxical properties of the propagator. At any given t, $|G(t,x)|^2 \equiv \frac{1}{2\pi t}$ identically for all x. The state at time t > 0 would seem to assign uniform probability density to all positions

on the real line, and is therefore non-normalizable. This behaviour becomes more intuitive in light of the Heisenberg uncertainty principle (HUP), which states that for any state the variance of the position and momentum observables satisfy the inequality

$$\sigma_x \sigma_p \ge \frac{1}{2} \tag{23}$$

The initial δ -function state is a position eigenstate, and thus has $\sigma_x = 0$. It follows that $\sigma_p = \infty$, and indeed the Fourier transform is the constant function.

If any possible value of the momentum is equally likely, it makes sense that after any small time the particle could have moved to any point on the real line with equal probability. This statement of dubious rigorousness is as far as it is possible to go in the attempt to make physical sense of the propagator as an actual solution. In reality, physically realizable initial states are normalizable and will remain so as they evolve in time; nevertheless it will be possible to model such evolution through convolution with the Schrödinger kernel:

$$\Phi(x;t) = (\Phi(0) * G(t))(x) := \int_{-\infty}^{\infty} dx' \Phi(x',0) G(x-x',t)$$
(24)

and since the kernel is a tempered distribution⁵, if $\Phi(x,0)$ is taken to be Schwartz so will be $\Phi(x,t)$. Thus the state will be normalizable at all times.

As an instructive example, consider a more regular initial state, such as the Gaussian $\Phi(x;0) = N \exp\left(-\frac{x^2}{2\sigma^2}\right)$, with N such that $\int dx |\Phi(x)|^2 = 1$. The wavefunction at time t is then

$$\Phi(x;t) = (\Phi(0) \star G(t))(x) = \int dy \Phi(y;0)G(x-y,t)$$
 (25)

$$= N\sqrt{\frac{\sigma^2}{\sigma^2 + it}}e^{-\frac{x^2}{2(\sigma^2 + it)}}.$$
 (26)

The final state is still smooth and normalizable; in fact $|\Phi(x;t)|^2$ is still a gaussian with finite (but growing in time) standard deviation $\sigma^2/(\sigma^4+t^2)$.

heat equation

2.3 Free particle on the circle

Let us consider now the case of interest for this work: a particle moving on the circle \mathbb{S}^1 . A change of units can fix the radius of the circle to any desired value; we take the circumference to be 1. In

⁵For positive times, G(x;t) is a smooth bounded function, so it defines a tempered distribution. For t=0, it equals a δ -function by definition, again a tempered distribution.

a local chart, for example using an angle coordinate $x \in [0, 1]$, the Schrödinger equation takes the form

$$-i\partial_t \Psi(x;t) = -\frac{\partial_x^2}{2} \Psi(x;t) \tag{27}$$

$$\Psi(0;t) = \Psi(1;t), \quad \partial_x \Psi(0;t) = \partial_x \Psi(1;t) \tag{28}$$

Boundary conditions (28) should be obvious intuitively; formally they can be derived easily by considering a second overlapping chart and imposing the Schrödinger equation applies there too.

Again the goal is to determine the propagator, that is to say the generalized solution corresponding to a δ -function initial condition.

One way of integrating the equation is by exploiting the known non-compact solution through a method of images. The circle is interpreted as $\mathbb{S}^1 = \mathbb{R}/\mathbb{Z}$, that is the quotient of \mathbb{R} through the identification of points that differ by an integer. Thus, a free particle starting on a point x_1 in the circle at time 0 and ending on another point x_2 after a certain time interval t is equivalent to a free particle on \mathbb{R} starting on $x_1 \in \mathbb{R}$ and ending up on any representative $x_2 + n$, $n \in \mathbb{Z}$, of the class of x_2 under the equivalence relation. The index n of the representative corresponds to the winding number, that is the number of turns around the circle performed by the particle before reaching x_2 . (See figure 1).

In accordance with (18) the amplitude for the particle on \mathbb{S}^1 to move from x_1 to x_2 is equal to the sum over all images for the particle on \mathbb{R} to move from x_1 to that image over the same time interval. Therefore, setting again $x_1 = 0$ by translation invariance, the circle propagator is given by the sum over "unwrapped" propagators:

$$A(x;t) := A(0,x;0,t) = \sum_{n=-\infty}^{\infty} G(x+n;t).$$
 (29)

Naively ignoring convergence issues, we would then obtain the sum

$$A(x;t) = (2\pi i t)^{-1/2} \sum_{n=-\infty}^{\infty} \exp\left(i\frac{(x+n)^2}{2t}\right).$$
 (30)

Defining the variables⁶ $\tau := -2\pi t$ and z := -x, this becomes

$$A(x;t) = \exp\left(\frac{ix^2}{2t}\right) \frac{1}{\sqrt{2\pi it}} \sum_{n=-\infty}^{\infty} \exp\left(\frac{in^2}{2t} + \frac{ixn}{t}\right)$$
(31)

⁶The reasoning behind the nature of the redefinitions will become apparent in the next section.

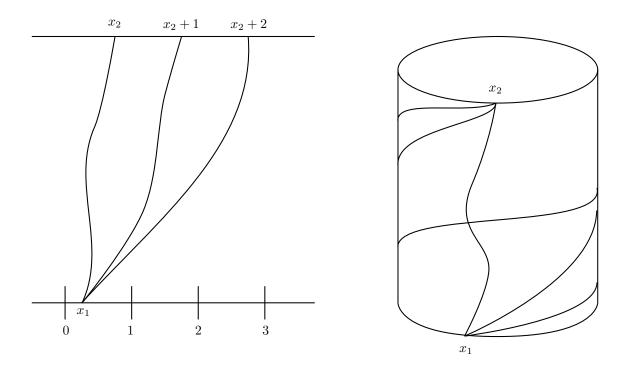


Figure 1: A few trajectories on \mathbb{R} from x_1 to $x_2 + n$ and their images under the quotient $\mathbb{S}^1 = \mathbb{R}/\mathbb{Z}$, which are paths from x_1 to x_2 with winding number n.

$$=e^{-i\pi z^2\tau}\frac{1}{\sqrt{-i\tau}}\sum_{n=-\infty}^{\infty}\exp\left(-\frac{\pi in^2}{\tau} + \frac{2\pi inz}{\tau}\right);$$
(32)

in particular, the probability amplitude (density) for the particle to return to its original position (x = 0) is

$$A(0;t) = \frac{1}{\sqrt{-i\tau}} \sum_{n=-\infty}^{\infty} e^{-i\pi n^2/\tau} =: \vartheta(\tau).$$
(33)

The issue with the above is that the sum of oscillatory terms does not converge in any simple sense. (In fact, we will prove in proof!! it almost never does converge pointwise). It does however converge in the sense of distributions in t to a tempered distribution with highly singular behaviour. Our goal is to provide a complete description of the structure of this distribution. Since the x-dependence of the amplitude is not as fascinating as that on τ , we will limit most of our considerations to the x = 0 case, with no real loss of qualitative structure. We will recover the x dependence after, in the discussion of fractional revivals and the physical interpretation of the amplitude.

Thus, the main focus of our attention is directed towards the $\vartheta(\tau)$ "function".

3 Deconstructing $\vartheta(\tau)$

 $breve\ introduzione$

3.1 A resummation formula

We will first simplify $\vartheta(t)$ considerably. We recall the Poisson resummation formula: if f(x) and $\hat{f}(k)$ are Fourier transforms⁷ of eachother, then

$$\sum_{n=-\infty}^{\infty} f(n) = \sum_{\xi=-\infty}^{\infty} \hat{f}(2\pi\xi), \qquad (34)$$

provided any of the two series converges at least distributionally. Taking $f(x) = e^{-i\frac{\pi}{\tau}x^2}$, and thus $\hat{f}(k) = \sqrt{-i\tau}e^{i\frac{\tau}{4\pi}k^2}$, the equality reads (renaming dummy ξ to n):

$$\sum_{n=-\infty}^{\infty} e^{-i\frac{\pi}{\tau}n^2} = \sqrt{-i\tau} \sum_{n=-\infty}^{\infty} e^{i\tau\pi n^2} , \qquad (35)$$

so that the $\vartheta(\tau)$ amplitude is rewritten as

$$\vartheta(\tau) = \sum_{n = -\infty}^{\infty} e^{i\tau\pi n^2} \tag{36}$$

3.2 $\operatorname{Im}\{\tau\} > 0$ and the modular group

It seems natural to try and promote t, or equivalently τ , to complex variables. If τ is in the upper half plane the series is absolutely convergent pointwise, as

$$|\exp(\pi i n^2 \tau)| \le e^{-\pi n^2 \operatorname{Im} \tau}. \tag{37}$$

In fact, the series converges to a function holomorphic on the upper half-plane, the Jacobi theta function:

$$\vartheta(z;\tau) := \sum_{n=-\infty}^{\infty} \exp(\pi i n^2 \tau + 2\pi i n z).$$
 (38)

⁷Note we use the "physicist's" convention with $\hat{f}(k) = \int dx \, e^{-ikx} f(x)$, so the argument of \hat{f} is the wavenumber and ξ is the inverse wavelength.

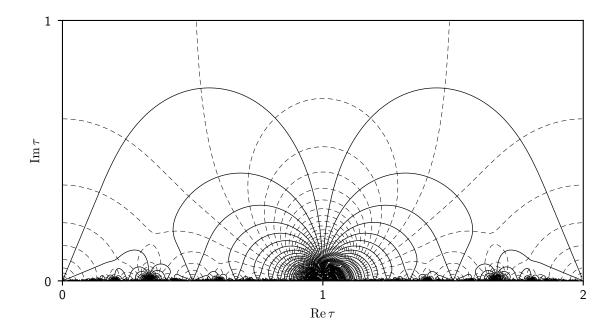


Figure 2: Plot of $\vartheta(\tau)$ over the upper-half plane. Contours of $|\vartheta(\tau)|$ (dashed) and $\arg(\vartheta(\tau))$ (solid) are depicted.

The issue is that $\vartheta(\tau)$ coincides with the theta function computed on the real axis, outside of its domain of convergence. We argue $\vartheta(t)$ can be constructed as the limit $\lim_{\epsilon \to 0} \vartheta(0; \tau + i\epsilon)$, where the limit is taken distributionally; that is to say the distribution is specified by the following action on a test function $\varphi(t)$:

$$\int_{-\infty}^{\infty} dt \, \vartheta(t)\varphi(t) := \lim_{\epsilon \to 0} \int_{-\infty}^{\infty} dt \, \vartheta(0; \tau + i\epsilon)\varphi(t)$$
(39)

We will prove there is convergence in this sense in section 3.5.

 $\vartheta(0;\tau)$ has remarkable transformation properties which carry over to $\vartheta(\tau)$. These can be summarized in the following two identities that are of particular interest for the study of $\vartheta(\tau)$:

$$\vartheta(0; \tau + 2) = \vartheta(0; \tau), \tag{40}$$

$$\vartheta(0; -\frac{1}{\tau}) = \sqrt{-i\tau}\,\vartheta(0;\tau)\,. \tag{41}$$

The first is evident from the derived expression. That the function is periodic of period 2 in τ means that the propagator at time $t^* = \frac{1}{\pi}$, or recovering units $t^* = 4\pi \frac{mR^2}{\hbar}$, is equal to the propagator at time 0. In other words, any quantum state on the circle repeats every t^* . This fact is less remarkable if one recalls that all energy eigenvalues on the circle, forming a complete basis,

evolve in time with the simple phase factor e^{int/t^*} , with $n \in \mathbb{N}$, so that all wavefunctions must also share the same periodicity in time. Still, it means a quantum particle placed exactly at one point on a circle (that is, in a position eigenstate) will return to the original position with probability 1 every t^* .

The second relation is however especially important in combination with the first. The two transformations in terms of τ belong to the modular group $PSL(2,\mathbb{Z})$, which is composed of all maps of the form

$$\tau \to \frac{a\tau + b}{c\tau + d}, \quad a, b, c, d \in \mathbb{Z}, \ ad - bc = 1.$$
 (42)

These are all diffeomorphisms from the upper half-plane to itself. They can also be extended to act on the real axis, provided the latter is compactified with a point at infinity as $\hat{\mathbb{R}} = \mathbb{R} \cup \{\infty\}$. The modular group is also realizable as a matrix group: if a modular transformation is represented by the unitary integer matrix

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix} \tag{43}$$

then composition of modular maps is seen to coincide with matrix multiplication; this translates into a homomorphism from the modular group to $SL(2,\mathbb{Z})$. Since opposite matrices A and -A yield the same modular transformation, this can be turned into an isomorphism by quotienting the sign ambiguity: $SL(2,\mathbb{Z})/\mathbb{Z}_2 = PSL(2,\mathbb{Z})$ is therefore the modular group.

 $PSL(2,\mathbb{Z})$ has an obvious but powerful property of mapping rationals to rationals (or better, extended rationals $\hat{\mathbb{Q}} = \mathbb{Q} \cup \{\infty\}$), and moreover this action is transitive, in the sense that given rationals r and s there exists a modular map sending $r \mapsto s$. The modular group is generated by the two transformations:

$$T: \tau \to \tau + 1, \quad T = \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix}$$
 (44)

$$S: \tau \to -1/\tau, \quad S = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$$
 (45)

The Jacobi theta function $\vartheta(z,\tau)$ has well-defined transformation properties under T and S, implying the same holds for general modular transformations. However, the transformation under T involves a shift in the variable z, which is not especially useful for our purposes. The transformations that do keep z constant are generated by maps (40) and (41):

$$T^2: \tau \to \tau + 2, \quad T^2 = \begin{pmatrix} 1 & 2 \\ 0 & 1 \end{pmatrix}$$
 (46)

$$S: \tau \to -1/\tau \,, \quad S = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \tag{47}$$

These do generate a proper subgroup of $PSL(2,\mathbb{Z})$, as we will show now, which we call Λ . Define the notion of parity of a reduced fraction p/q as the parity of pq. (The parity of $\infty \in \hat{\mathbb{Q}}$ is taken to be the same as 0, so even). It's clear this parity is invariant under action of Λ ; moreover since at least two rationals of opposite parity exist (e.g. 0 and 1), transitivity implies Λ and $PSL(2,\mathbb{Z})$ cannot coincide.

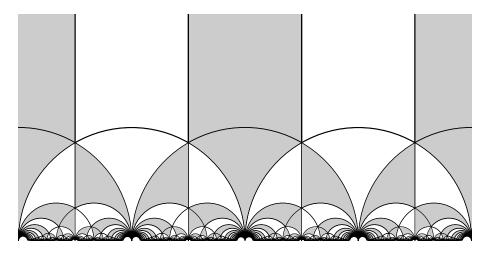


Figure 3: A representation of the action of $PSL(2,\mathbb{Z})$ on the upper half-plane \mathbb{H}^2 as a tessellation of ideal trangles with angles $(30^\circ, 30^\circ, 0^\circ)$. Any of the triangles acts as a fundamental domain; the ideal 0° vertices lie on the real axis at rational points. The shading depicts the two orbits of the subgroup $\Lambda \subset PSL(2,\mathbb{Z})$

What is more useful is that there are *only* two orbits, in the sense that any rational r can be mapped through an element of Λ to either 0 or 1 depending on its parity. We consider the following explicit algorithm.

Taken a rational $r=\pm \frac{p}{q}$ in lowest terms, $r\neq 0,1,$

- if r < -1 or r > 1, apply relevant power of T^2 to place it in [-1,1]
- \bullet apply S

The above procedure has the property of always decreasing the magnitude of either p or q. Since these are positive integers, iteration of the procedure has to reach 0 or 1 in a finite number of

steps. A couple examples:

$$\frac{13}{4} \xrightarrow{(T^2)^{-2}} -\frac{3}{4} \xrightarrow{S} \xrightarrow{4} \xrightarrow{(T^2)^{-1}} -\frac{2}{3} \xrightarrow{S} \xrightarrow{3} \xrightarrow{(T^2)^{-1}} -\frac{1}{2} \xrightarrow{S} \xrightarrow{2} \xrightarrow{(T^2)^{-1}} 0 \tag{48}$$

$$\frac{7}{9} \xrightarrow{S} -\frac{9}{7} \xrightarrow{(T^2)^1} \xrightarrow{5} \xrightarrow{S} -\frac{5}{5} \xrightarrow{S} \xrightarrow{T^2)^1} \xrightarrow{3} \xrightarrow{S} -\frac{5}{3} \xrightarrow{(T^2)^1} \xrightarrow{1} \xrightarrow{S} -3 \xrightarrow{(T^2)^2} \xrightarrow{1} (49)$$

Returning to our physical object of interest, the amplitude, we see that properties (40) and (41) relate the behaviour of ϑ at a rational time⁸ with the behaviour at time 0 or 1 depending on the parity. Therefore ϑ has a sort of self-similar structure, and any qualitative features present at the points 0 and 1 will be repeated infinitely in two dense sets. For example, we anticipate (though this will be studied more precisely) that the amplitude has a $\tau^{-1/2}$ singularity for τ close to zero, since for very small time the propagator on a circle is expected to reduce to that of the free particle. If so, then there must also be a similar singularity at all even rationals; therefore ϑ has a dense set of singularities.

3.3 Even rationals

It is easy to show ϑ "should" have a $\sim \tau^{-1/2}$ singularity near $\tau=0$ [2]. Indeed, applying (41):

$$\vartheta(\tau) = \sqrt{\frac{i}{\tau}} \sum_{n = -\infty}^{\infty} e^{-i\pi n^2 \frac{1}{\tau}}.$$
 (50)

Naively, all terms in the sum except n=0 are oscillatory and supposedly cancel for small times, and $\vartheta(\tau) \sim \sqrt{\frac{i}{\tau}}$. This corresponds to physical intuition: the propagator should reduce to the free particle propagator for very short times, in which the particle has not yet "probed" the global structure of the circle. If this is true, however, then similar singularities should be repeated at any even rational point. Thus ϑ would have infinite singularities, and thus be unbounded, in any given interval. This makes it impossible for it to be ever asymptotic to $\tau^{-1/2}$ in the first place.

The asymptotic behaviour must not of course be interpreted as direct but in a distributional sense. In particular, a more sensible definition is that for a family of Schwartz functions $f_{\sigma}(\tau) = f(\tau/\sigma)$ the evaluation of ϑ on f_{σ} is asymptotic to that of f_{σ} on the tempered distribution $At^{-1/2}$ for some constant A. In integration against a Schwartz function we expect the secundary singularities at each even rational to matter less and less as we approach the main singularity at $\tau = 0$. We now test explicitly ϑ against a family of shrinking Gaussians and verify this intuition.

⁸We are, of course, here referring to the normalized time τ for simplicity.

Consider the normalized Gaussian $g_{\sigma}(\tau) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{\tau^2}{2\sigma^2}\right)$. The integral of $g_{\sigma}(\tau)$ against $A\tau^{-1/2}$ is

$$\left\langle \tau^{-1/2} \middle| g_{\sigma} \right\rangle = A \int_{-\infty}^{\infty} d\tau \, g_{\sigma}(\tau) \tau^{-1/2} = \frac{2A}{\sigma \sqrt{2\pi}} 2^{1/4} \sqrt{\sigma} \int_{0}^{\infty} dx e^{-x} x^{-3/4} = \frac{A\Gamma(\frac{1}{4})}{2^{1/4} \sqrt{\pi \sigma}} \,. \tag{51}$$

On the other hand, if $g_{\sigma}(\tau)$ is integrated against ϑ , we obtain

$$\langle \vartheta | g_{\sigma} \rangle = \sum_{n = -\infty}^{\infty} \int d\tau \frac{1}{\sigma \sqrt{2\pi}} e^{-\frac{\tau^2}{2\sigma^2} + i\pi\tau n^2} = \sum_{n = -\infty}^{\infty} \exp(-\pi^2 \sigma^2 n^4 / 2); \qquad (52)$$

only the asymptotic behaviour for small σ is relevant. Defined $N^4 := 2\pi^{-2}\sigma^{-2}$, the summand is slowly-varying for large N. Thus we can approximate as an integral:

$$= N \sum_{n=-\infty}^{\infty} \frac{1}{N} \exp\left(-\frac{n^4}{N^4}\right) \sim N \int_{-\infty}^{\infty} d\xi \, e^{-\xi^4} = 2N \,\Gamma(\frac{5}{4}) = \frac{2^{-3/4}}{\sqrt{\pi\sigma}} \Gamma(\frac{1}{4}) \,. \tag{53}$$

It is therefore seen that the action of ϑ on a Schwartz function shrinking around $\tau = 0$ is asymptotic to that of the distribution $\sqrt{\frac{i}{\tau}}$.

Now that the existence of this singularity has been ascertained, let us verify a reduced copy of it exists at any even rational. Imagine the even rational a gets mapped to the even rational b by one step of the iterative procedure described in section 3.2. Assume it is known that in the vicinity of b there is an inverse square-root singularity:

$$\vartheta(b + \delta \tau') \sim K \delta \tau^{-1/2} \tag{54}$$

Now, if a and b are related by a simple translation $(T^2)^n$, then it's obvious this singularity is copied with no change in the constant K by the periodicity property (40). If instead they are related by the map S, and b = -1/a, then

$$\vartheta(a+\delta\tau) = \sqrt{\frac{i}{a}}\vartheta\left(-\frac{1}{a+\delta\tau}\right) \sim \sqrt{\frac{i}{a}}\vartheta(b+\frac{\delta\tau}{a^2}) = \sqrt{ia}K\delta\tau^{-1/2}\,,\tag{55}$$

so that a inherits the singularity of b but suppressed by a factor of \sqrt{a} . By simple induction, a singularity appears at any even rational $\pm p/q$, and the constant of proportionality $K_{p/q}$ is equal to the square root of the product of all rational encountered in the procedure towards $\tau = 0$ at each application of S; it's clear this is simply $|K_{p/q}| = 1/\sqrt{q}$. So, in the vicinity of p/q the distribution ϑ behaves as

$$\vartheta(\tau) \sim \frac{1}{\sqrt{p - q\tau}} \tag{56}$$

è possibile anche fare un calcolo della fase delle singolarità? Credo di sì

Forse no... forse è equivalente al calcolo delle fasi nella (85), che coinvolge number theory e potrebbe non essere fattibile nel caso generale

3.4 Odd rationals

The point $\tau = 1$ is equally peculiar. We argue ϑ vanishes there along with all of its distributional derivatives $\frac{d^k}{dt^k}\vartheta(\tau)$. Again, the statement as it stands is non-sensical unless it is reformulated in distributional language because of the dense set of singularities. To express it we introduce again a family of shrinking Schwartz functions $f_{\sigma}(\tau) = f((\tau - 1)/\sigma)$, this time centered around 1. We claim that, for all $k \in \mathbb{N}$,

$$\lim_{\sigma \to 0} \left\langle \frac{\mathrm{d}^k}{\mathrm{d}t^k} \vartheta \middle| f_\sigma \right\rangle = 0 \tag{57}$$

As before, it suffices to test against shrinking normalized Gaussians $g_{\sigma}(\tau) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{\tau^2}{2\sigma^2}\right)$. We find

$$\left\langle \frac{\mathrm{d}^k}{\mathrm{d}t^k} \vartheta \middle| g_\sigma \right\rangle = \sum_{n=-\infty}^{\infty} (i\pi n^2)^k \frac{1}{\sigma\sqrt{2\pi}} \int_{-\infty}^{\infty} d\tau e^{-\frac{(\tau-1)^2}{2\sigma^2} + i\pi\tau n^2} = \sum_{n=-\infty}^{\infty} (i\pi n^2)^k \exp\left(-\frac{\pi^2\sigma^2 n^4}{2} + i\pi n^2\right)$$
(58)

$$= (i\pi)^k \sum_{n=-\infty}^{\infty} n^{2k} (-1)^n e^{-\pi^2 \sigma^2 n^4/2} =: (i\pi)^k S_k(\sigma). \qquad (0^0 = 1)$$
 (59)

The series (59) is absolutely convergent for any positive σ and natural k. Defined again $N^4 := 2/(\pi^2 \sigma^2)$, we intend to show $\lim_{N\to\infty} S_k = 0$. First we recognize that S_k it is a residue sum for the poles of the meromorphic function

$$F_{k,N}(z) = \frac{\pi}{\sin \pi z} z^{2k} \exp\left(-\frac{z^4}{N^4}\right),$$
 (60)

which indeed has poles at all $n \neq 0$ with residue $(-1)^n n^{2k} e^{-n^4/N^4}$, and another pole at 0 with residue 1 for k = 0 only, so that there is match with S_k for any k. By the residue theorem, a partial sum for S_k is $1/(2\pi i)$ the contour integral of F around a loop circling the relevant poles; in the limit the entire sum is equal to the integral along a pair of lines:

$$2\pi i S_k = -\int_{-\infty}^{\infty} F_{k,N}(\rho + it) d\rho + \int_{\infty}^{\infty} F_{k,N}(\rho - it) d\rho;$$
 (61)

And this limit is sensible since F(z) is exponentially decaying for $|z| \to \infty$ as long as $\arg z \neq (m + \frac{1}{2})\frac{\pi}{2}$. Using F(-z) = -F(z) we reduce the integral to the half-line:

$$-\pi i S_k = \int_{it}^{it+\infty} \frac{\pi}{\sin \pi z} z^{2k} \exp\left(-\frac{z^4}{N^4}\right) dz, \qquad (62)$$

Then, with the substitution $z = N\xi$:

$$= N^{1+2k} \int_{it/N}^{it/N+\infty} \frac{\pi}{\sin \pi N \xi} \xi^{2k} \exp(-\xi^4) d\xi.$$
 (63)

Note t was arbitrary, so we can choose to fix a constant it/N =: K. In addition, for large enough N, $|\sin(\pi N \xi)| = |\sin(\pi N (\operatorname{Re} \xi + iK))| \ge C e^{\pi N K}$ for some constant C. Thus the absolute value of the integral is bounded:

$$\pi |S_k| \le N^{1+2k} \frac{\pi}{C} e^{-\pi NK} \int_0^\infty |\xi|^{2k} \exp(-\operatorname{Re}\{\xi^4\}) d\operatorname{Re}\xi,$$
 (64)

and the last integral is a finite constant depending only on K. We can finally send $N \to \infty$ while keeping K constant. Therefore $S_k \to 0$ for $N \to \infty$, for all k.

Having ascertained the existence of the "flat point" of ϑ in $\tau = 1$, it is now trivial to verify this structure is copied at all odd rationals through the action of the group Λ .

3.5 Distributional convergence

We are now set to prove that there is convergence in the sense of tempered distributions of the series

$$\vartheta(\tau) = \sum_{n=-\infty}^{\infty} e^{i\pi\tau n^2} \,. \tag{65}$$

By this, we mean that defined $\vartheta_N(\tau)$ as the partial sum with |n| < N, given any Schwartz function $f(\tau)$ the evaluation of ϑ_N over f converges to a finite value for $N \to \infty$. The partial sum evaluations however are

$$\int_{-\infty}^{\infty} d\tau \,\vartheta_N(\tau) f(\tau) = \sum_{|n| < N} \int_{-\infty}^{\infty} d\tau \, e^{i\pi\tau n^2} f(\tau) = \sum_{|n| < N} \hat{f}(-\pi n^2) \,, \tag{66}$$

having recognized the Fourier transform of $f(\tau)$. We recall that the Fourier transform of a Schwartz function is itself Schwartz. This means $\|\hat{f}\|_{1,0} = \sup_{\tau} |\tau \hat{f}(\tau)|$ is finite, and thus $|\hat{f}(\tau)| \leq C/|\tau|$

for some C > 0, so that the above series is absolutely convergent. Thus, $\vartheta(\tau)$ is a well-defined tempered distribution.

Equivalently, we have just proven that the Fourier transform of the $\vartheta(\tau)$ distribution, which is the "quadratic δ comb":

$$\hat{\vartheta}(\omega) = \sum_{n = -\infty}^{\infty} \delta(\omega + \pi n^2) \tag{67}$$

is a well-defined tempered distribution.

 $Segue\ dimostrazione\ alternativa\ con\ l'integrale,\ magari\ spostare\ in\ una\ sezione\ apposita\ con\ grafico\ di\ B$

Consider the following series for real τ :

$$B(\tau) = \frac{1}{i\pi} \sum_{n = -\infty}^{\infty} \frac{e^{i\pi\tau n^2}}{n^2}$$
 (68)

The series is absoutely convergent and limited as a function of τ , as $\sum_{n=0}^{\infty} \frac{1}{n^2} = \frac{\pi^2}{6}$. Therefore, $B(\tau)$ is a well-defined function in $L_{1,\text{loc}}$.

4 The theta function propagator

Having now satisfyingly examined the qualitative structure of the propagator for x = 0 as a function of time, we now return back to our original formulation to include the spatial dependence.

Recovering (32), and recalling the definition (38) of the Jacobi theta function, we recognize

$$A(z,\tau) = e^{-i\pi z^2 \tau} \frac{1}{\sqrt{-i\tau}} \vartheta\left(\frac{z}{\tau}; -\frac{1}{\tau}\right)$$
(69)

The full Jacobi theta function has more general modular transformation properties than the subcase $\vartheta(\tau) = \vartheta(0; \tau)$ we studied before. In particular, it holds that

$$\vartheta(z+1;\tau) = \vartheta(z;\tau) \tag{70}$$

$$\vartheta(z;\tau+1) = \vartheta(z+\frac{1}{2};\tau) \tag{71}$$

$$\vartheta\left(\frac{z}{\tau}; -\frac{1}{\tau}\right) = \sqrt{-i\tau} \exp\left(\frac{\pi}{\tau}iz^2\right) \vartheta(z; \tau) \tag{72}$$

Equations (70) and (71) are immediate; (72) can again be proven by means of Poisson resummation[thetamodular]; we omit the derivation for the sake of brevity.

Relation (72) immediately implies that the fundamental solution A is directly a theta function:

$$A(z,\tau) = \vartheta(z;\tau) \tag{73}$$

The Jacobi theta for real values of the period is thus reinterpreted physically as the quantum propagator on the circle. There is an enlightening analogy with a better-known case; consider again the Schrödinger equation for a particle moving on some Riemannian manifold M:

$$i\frac{\partial}{\partial t}\Psi = -\frac{\nabla^2}{2}\Psi\,, (74)$$

where ∇^2 is the Laplace-Beltrami operator on M, and perform the substitution $t \mapsto it$; this yields

$$\frac{\partial}{\partial t}\Psi = -\frac{\nabla^2}{2}\Psi\,,\tag{75}$$

i.e. the heat / diffusion equation on M. Indeed, it is well-known $\vartheta(z;it)$ (much more regular than its real-period counterpart studied in this work) is the fundamental solution to the heat equation on the circle. This can be understood physically as diffusion being the Wick-rotated, or imaginary-time, counterpart of the Schrödinger equation. This, in fact, is to be seen as a minimal example of a general phenomenon in quantum theories in which the Wick-rotated theory (a statistical-mechanical system) has better converging observables; and observables in the quantum theory, only formally specified by non-converging oscillatory integrals, can be defined by analytic continuation of the imaginary-time observables.

We now show a remarkable structure of the theta function propagator that should clarify the nature of the singularities in the time dependence. Fixed a rational time $\tau = p/q$ in least terms, without loss of generality between 0 and 1, rewrite the summation index n as n = aq + b, for $a \in \mathbb{Z}$, $b = 0, \ldots, q - 1$. The amplitude becomes:

$$\vartheta(z;\tau) = \sum_{a=-\infty}^{\infty} \sum_{b=0}^{q-1} \exp\left(\pi i \frac{p}{q} (aq+b)^2 + 2\pi i (aq+b)z\right)$$
 (76)

$$= \left(\sum_{b=0}^{q-1} e^{i\pi\frac{pb^2}{q} + 2\pi ibz}\right) \sum_{a=-\infty}^{\infty} (-1)^{pqa} e^{2\pi iaq}$$
 (77)

We recognize the sum over a as the Fourier series for a Dirac comb, i.e. a periodic array of δ functions:

$$III_T(z) := \sum_{n = -\infty}^{\infty} \delta(z - nT) = \frac{1}{T} \sum_{k = -\infty}^{\infty} e^{2\pi i k z}, \qquad (78)$$

so that the sum over a reduces to

$$\frac{1}{q} \coprod_{\frac{1}{q}} (z + \Delta), \tag{79}$$

where $\Delta = 0$ if p/q is even, and $\Delta = \frac{1}{2}$ if it's odd. Thus we have the remarkable fact that at any fixed rational time $\tau = p/q$, the theta function amplitude is a sum of q δ -functions equally spaced around the circle; the Dirac deltas are then weighted by the phase factor

$$\sum_{b=0}^{q-1} \left(e^{i\pi/q} \right)^{pb^2 + 2bzq} \tag{80}$$

Since $\coprod_{\frac{1}{q}}$ only has support in $z=\frac{c+\Delta}{q}$ for $c=0,\ldots,q-1$ (understood mod 1), this factor is

$$\beta_{p,q,c} = \sum_{b=0}^{|q|-1} \left(e^{i\pi/q} \right)^{pb^2 + 2bc + 2\Delta b} , \tag{81}$$

Expression (81) is a generalized quadratic Gauss sum, and its determination is extremely complex. It is however sufficient for our purposes to ascertain the norm $|\beta_{p,q,c}|$. We lift the restriction on p and q to be positive and for p < q for the purpose of the proof. Immediately:

$$\beta_{p+2kq,q,c} = \beta_{p,q,c} \,, \tag{82}$$

so that p can be taken to have |p| < |q|. In addition, we make use of the reciprocity formula for generalized quadratic Gauss sums[1]:

$$|\beta_{p,q,c}| = \sqrt{\left|\frac{q}{p}\right|} |\beta_{-q,p,c}|. \tag{83}$$

Having in addition noted that $|\beta_{p,1,c}| = 1$ for all p, c, we can induct over all pairs (p,q) and conclude⁹

$$|\beta_{p,q,c}| = \sqrt{q} \tag{84}$$

Thus, the fundamental solution at fractional time becomes

$$\vartheta\left(z; \frac{p}{q}\right) = \frac{1}{\sqrt{q}} \sum_{c=0}^{q-1} \phi_{p,q,c} \,\delta\left(z - \frac{c}{q}\right) \,, \tag{85}$$

for some phases $\phi_{p,q,c}$, a characterization which will become extremely useful when attempting a physical interpretation of time evolution of an initial state.

We just comment that the prefactor $1/\sqrt{q}$ is expected on the face of unitarity, or conservation of information. The time evolution operator of the Schrödinger equation is unitary, and preserves the L^2 norm of the wavefunction. Taken an initial smooth wavefunction $\psi(z)$ with compact support in an interval around 0 smaller than $\frac{1}{2q}$, and normalized such that $\int_{\mathbb{S}^1} dx |\psi(z)|^2 = 1$, time evolution by a fractional time p/q is equivalent with convolution with the $\vartheta(z; p/q)$ kernel, which results by (85) in q non-overlapping copies of the original wavefunction, with some phases and rescaled by $1/\sqrt{q}$. The final squared norm of the wavefunction is thus

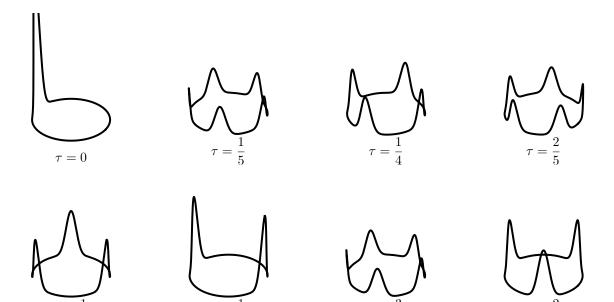
$$\frac{1}{q} \sum_{c=0}^{q-1} 1 = 1. (86)$$

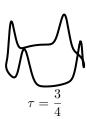
5 Physical interpretation

5.1 Fractional revivals and antirevivals

Spiegazione della struttura a tempi razionali: a tempo razionale pari la funzione d'onda viene "rivitalizzata" in q copie, mentre a tempo razionale dispari le copie rivitalizzate sono sfasate di 1/(2q) (antirevivals)

⁹We remark the reasoning is strongly reminiscent of that employed in section 3.3, suggesting the calculations are connected. Indeed, a proof of the reciprocity formula can also be provided starting from the modular properties of the theta function[1].





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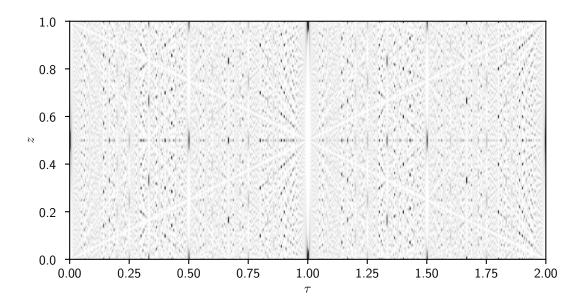


Figure 4: $|\psi(z,\tau)|^2$ for an initial Gaussian state over a full revival period.