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The quantum Talbot effect on a sphere

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Abstract

Any quantum (Schrödinger) wavefunction on a sphere is necessarily periodic in time. The corresponding statement down one dimension, for a circular line instead, is the quantum version of the 'Talbot effect' for a diffraction grating in paraxial optics (which is fully analogous to quantum mechanics). In the circle case the 'revival' of any initial wavefunction at the period, or 'Talbot time', is accompanied by a kind of partial revival at any rational fraction of the period, increasing in complexity for less simple fractions. In particular, any piecewise constant initial wavefunction is again piecewise constant at such times. By contrast, in the sphere case, the simplest piecewise constant wave, constant on hemispheres is shown not to retain its piecewise constancy at rational fractions of the period, but instead, rather strikingly, to develop infinities at calculable locations. The calculation requires the uniform asymptotic form of the Legendre polynomials together with the Poisson sum formula leading to Gauss sums.

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Introduction

The Talbot effect [1, 2] was discovered in optics in the 1800s—the 'revival' of a spatially periodic initial wave (that through a diffraction grating) after free propagation through the 'Talbot distance'. An analogous revival effect is a consequence (and this time an *exact* consequence) of the free space Schrödinger equation in quantum mechanics—any one-dimensional initial spatially periodic wavefunction is also necessarily periodic in time—it 'revives' or repeats itself after the 'Talbot time'. The mere fact that in non-relativistic quantum mechanics the frequency is proportional to the wave number to an integer power (the square) guarantees this time periodicity.

The quadratic dependence in particular also produces striking modified revivals at all times which are rational fractions of the Talbot time. The wave is then a superposition of shifted multiples of its initial self [3]. This means, for example, that any initial wavefunction which is piecewise constant is also piecewise constant at all rational times. This case was most easily realizable in optics, being the wave through a diffraction grating—opaque, transparent, opaque, transparent, etc, so that the wave is a one-dimensional square wave. And among these the simplest case is when the segments of opaque and transparent are equal in length—the 'Ronchi grating' in optics. The permanent spatial periodicity of the wave in the Talbot effect means that, optionally, one may think of it as a wave on a circle. In the Ronchi case the initial wave is two separate constant values on two semicircles making up the whole circle. This observation prompts, by generalization, the present remarks.

On a sphere the quantum Talbot effect occurs likewise, as is obvious from the time evolution of a general wavefunction described by coefficients $c_{m,l}$. In spherical polar coordinates θ,ϕ the wave evolution is

$$\sum_{l=0}^{\infty}\sum_{m=-l}^{l} c_{m,l}\ P_l^m(\cos\theta)\exp(\mathrm{i}m\phi)\exp[-\mathrm{i}\pi l(l+1)t]. \tag{1}$$

Any initial wave exactly revives after a Talbot time, which by design here is $t = 1$ making the phase of the last exponential a multiple of 2π. (Physically the period is $2\pi mR^2/\hbar$ where m is the particle mass and R is the radius of the sphere and the Schrödinger equation is $-(\hbar^2/2mR^2)[(\sin\theta)^{-1}(\partial/\partial\theta)(\sin\theta\,\partial\psi/\partial\theta) + (\sin\theta)^{-2}(\partial^2\psi/\partial\phi^2)] = \mathrm{i}\hbar\partial\psi/\partial t$). The most fundamental case to investigate would be the time evolution of a single point δ-function initial wavefunction, supplying the 'propagator' on the sphere, but this would be more involved, being less 'well behaved' (the analogue of (7) fails to converge). We shall be content to examine a more usual, non-infinite, initial Talbot wavefunction of the type described.

By analogy one might expect some simplicity at rational fractions of this time, and there is; less simple, but perhaps more dramatic. The case analogous to the Ronchi grating, serves to illustrate the point, and we confine attention to it: the initial wavefunction is to be piecewise constant, being one constant in one hemisphere, and another constant in the other. With no loss of generality (since a superposed entirely constant wavefunction does not evolve), we take the constants to be ± 1. We have no applications of the effect in mind, but note, at least, that a physical realization of quantum mechanics on a sphere is the rotational dynamics of a diatomic molecule considered as a widthless rigid dumbell [4].

Taking the spherical polar coordinates based on the symmetry axis, the spherical harmonics of which the wavefunction is made up are limited to $P_l^0 \equiv P_l(\cos\theta)$, the ordinary Legendre polynomials, with no ϕ dependence involved. We then have

$$\psi(\theta,t) = \sum_{l=0}^{\infty} c_l P_l(\cos\theta)\exp[-\mathrm{i}\pi l(l+1)t], \tag{2}$$

where the required coefficients c_l are found in the standard way from the ± 1 hemispheres initial wavefunction $\psi(\theta,0) = \mathrm{sgn}(\pi/2-\theta)$ by multiplying both sides of (2) with $t = 0$ by $P_j(\cos\theta)$ and integrating over the sphere

$$\int_{-1}^{1}\mathrm{sgn}(\pi/2-\theta)P_j(\cos\theta)\ \mathrm{d}\cos\theta = \int_{-1}^{1}\sum_{l=1,3,5,\ldots} c_l P_l(\cos\theta)\ P_j(\cos\theta)\ \mathrm{d}\cos\theta = \frac{c_j}{j+\frac{1}{2}}, \tag{3}$$

whence $c_l = 0$ for l even, and for l odd:

$$c_l = \frac{2\left(l+\frac{1}{2}\right)}{l+1}(-1)^{(l-1)/2}\frac{1\times 3\times 5\times\cdots\times(l-2)}{2\times 4\times 6\times\cdots\times(l-1)} = \frac{\left(l+\frac{1}{2}\right)\sin\left(\frac{1}{2}\pi l\right)\ \Gamma\left(\frac{1}{2}l\right)}{\sqrt{\pi}\,\Gamma\left(\frac{1}{2}l+\frac{3}{2}\right)}. \tag{4}$$

For large l, $c_l \sim \sin\left(\frac{1}{2}\pi l\right)2\sqrt{2/\pi l}$ for l odd, or zero for l even, which will be needed shortly (modified, with the last l replaced by $l+\frac{1}{2}$, which is just as good asymptotically).

It will turn out that for rational times, the wavefunction is not piecewise constant contrasting with the ordinary Talbot effect. Instead it has well-defined singularities (infinities) at specific values of θ, circular rings, or ridges, of infinity, as well as point infinities on the axis, and our purpose is to calculate these values, and describe the singularities, since they are the most prominent features. Lesser features such as discontinuities require more involved analysis than that presented here. The point singularities on the axis will be shown to be of inverse square-root power, while the singular rings cannot have this power since the wave must be square integrable (to the value 2), and instead they will turn out to have logarithmic divergence. These singularities are also admissible on energy grounds since the initial energy is infinite. For irrational times rather than rational ones, the wavefunction is qualitatively similar to that in the ordinary Talbot effect [3, 5] (since the summand of (2) $\sim l^{-1}$), namely it is a fractal of dimension $3/2$ as a function of θ, without any infinity. We shall not analyse this, but confine attention to the rational times.

The phenomenon of a finite initial wave giving rise to infinities is unusual, perhaps, and a preliminary indication of its origin may be helpful. The two dimensionality of the sphere (with axial symmetry) is associated with a one-sided summation ($l > 0$) in (2). This can admit infinities which the two-sided summation arising in the ordinary Talbot effect on a circle does not. As a closely related mathematical example: the sum over all odd l $(\ldots, -3, -1, 1, 3, \ldots)$ of $l^{-1}\exp[\mathrm{i}\pi(r'l + rl^2)]$, where r' and r are any rational numbers is never infinite, whereas the same sum over positive odd l only $(1, 3, 5, \ldots)$, is commonly infinite. The reason is that the exponential is periodic in l, and commonly has a non-zero complex average value (such Gauss averages are supplied in appendix A). If so, the one-sided sum is infinite, just as the simple sum of l^{-1} over odd positive l is infinite. But the two-sided sum has close cancellation between any particular period starting at a large positive l value, and the corresponding reflected period ending with that large negative l value (because of the opposite sign of l^{-1}). The result of the near cancellation is of order l^{-2} and the sum converges (albeit not absolutely). This near cancellation prevents infinities in the ordinary Talbot effect on a circle, but similar infinities to the present ones would be produced in two dimensions by an axisymmetric piecewise constant initial wave on a disc.

Poisson summation

Essentially just one mathematical manoeuvre is needed to show the claimed effects and calculate the singularities, namely application of the Poisson sum formula to the sum (2) representing the wave $\psi(\theta, t)$. The Poisson sum formula equates a function sampled with a periodic δ-comb (to form a sum) to its Fourier transform sampled with another periodic δ-comb (the Fourier transform of the original one, to form another sum). Schematically, in general

$$\int \text{Function}(x) \times (\cdots\_\uparrow\_\_\uparrow\_\_\uparrow\_\_\uparrow\_\_\cdots)\,\mathrm{d}x$$
$$= \int \text{Fourier transform}(y) \times (\cdots\_\Uparrow\_\Uparrow\_\Uparrow\_\Uparrow\_\Uparrow\_\Uparrow\cdots)\,\mathrm{d}y. \tag{5}$$

The reason why such an alternative sum is desirable is that the singularities (infinities) in the present sum arise from failure of the sum to converge for the specific θ values sought (singularity locations). The locations and nature of the singularities will be much clearer if the infinities arise instead as individual infinite terms in an otherwise convergent sum. The Poisson sum will be such, but the Legendre polynomials prevent its direct application.

First the wave needs to be split, $\psi = \psi_{<\infty} + \psi_\infty$, into a non-infinite background function of lesser interest $\psi_{<\infty}$, plus a simpler function ψ_∞ containing the infinities. The simpler function involves the asymptotic form for the Legendre polynomial. Since the singularities can occur at the endpoints $\theta = 0$ and π, and/or elsewhere, it is necessary to use the form that is uniformly valid for all θ. Actually since our wave is permanently an odd function under reflection in the equator plane $\theta = \pi/2$, we can restrict attention to the range $0 < \theta < \pi/2$, then for large l the uniform asymptotic approximation [6] of the Legendre polynomials is

$$P_l(\cos\theta) \sim \sqrt{\frac{\theta}{\sin\theta}} J_0\left(\left(l + \frac{1}{2}\right)\theta\right). \tag{6}$$

We choose to define ψ_∞ as the sum over all positive integers l of this form, with a suitable coefficient, namely the asymptotic form of c_l given earlier. The difference of the true and asymptotic versions $\psi - \psi_\infty$ yields a sum $\psi_{<\infty}$ which is always and everywhere absolutely convergent (since the difference of the sides of (6) $\sim l^{-1}$), that is, free of infinities.

$$\psi_{<\infty}(\theta, t) = \sum_{l=1,3,5,\ldots} \left[c_l P_l(\cos\theta) - \left(\sin\left(\frac{1}{2}\pi l\right) 2\sqrt{\frac{2}{\pi}}\sqrt{\frac{1}{l+1/2}}\right)\sqrt{\frac{\theta}{\sin\theta}} J_0\left(\left(l+\frac{1}{2}\right)\theta\right)\right] \times \exp[-\mathrm{i}\pi l(l+1)t]. \tag{7}$$

Here the sum has been explicitly restricted to the non-zero contributions, $l = $ odd. The more interesting singular part then is, re-written with a convenient separation into the product of two braces,

$$\psi_\infty(\theta, t) = 2\sqrt{\frac{2}{\pi}}\sqrt{\frac{\theta}{\sin\theta}} \sum_{l=1,3,5,\ldots}\left\{\sqrt{\frac{1}{l+1/2}} J_0\left(\left(l+\frac{1}{2}\right)\theta\right)\right\}\left\{\sin\left(\frac{1}{2}\pi l\right)\exp[-\mathrm{i}\pi l(l+1)t]\right\}. \tag{8}$$

This is now ready for the Poisson sum formula to be applied to reveal the infinities. The procedure is to insert a δ-comb inside the last brace, selecting odd l only, and replace the sum by an integral over l considered as a continuous variable. If a unit step function Θ, selecting positive $l + \frac{1}{2}$ only, is included in the first brace, then the integral can be taken as over all l, which is necessary. Each brace will then be a Fourier transform which can be evaluated analytically. We start, then, with

$$\psi_\infty(\theta, t) \equiv 2\sqrt{\frac{2}{\pi}}\sqrt{\frac{\theta}{\sin\theta}} \int_{-\infty}^{\infty} \left\{\int_{-\infty}^{\infty} \sqrt{\frac{1}{l'+1/2}}\, J_0\left(\left(l'+\frac{1}{2}\right)\theta\right)\Theta\left(l'+\frac{1}{2}\right) \mathrm{e}^{\mathrm{i}2\pi m l'}\,\mathrm{d}l'\right\} \times \left\{\int_{-\infty}^{\infty} \sin\left(\frac{1}{2}\pi l''\right)\exp[-\mathrm{i}\pi l''(l''+1)t]\delta_{\mathrm{odd}}(l'')\,\mathrm{e}^{-\mathrm{i}2\pi m l'}\,\mathrm{d}l''\right\}\mathrm{d}m. \tag{9}$$

Performing the m integral here would go backwards to (8) interpreted as an integral as described. Proceeding forwards instead we need to evaluate the two braces; the first, $\{'\}$, will be given by complete elliptic integrals K, and the second, $\{''\}$, will, for rational t, be a periodic δ-comb again. To evaluate the first, one can set $r^2 = l + \frac{1}{2}$, and write the Bessel function as its trigonometric integral representation, and then reverse the order of integration

$$\begin{aligned}\{'\} &= \mathrm{e}^{-\mathrm{i}\pi m}\int_0^\infty\left[\int_0^{2\pi}\exp[\mathrm{i}r^2\theta\cos\chi]\frac{1}{2\pi}\,\mathrm{d}\chi\right]\exp[\mathrm{i}2\pi m r^2]2\,\mathrm{d}r \\ &= \mathrm{e}^{-\mathrm{i}\pi m}\int_0^{2\pi}\sqrt{\frac{\mathrm{i}\pi}{\theta\cos\chi + 2\pi m}}\frac{1}{2\pi}\,\mathrm{d}\chi \\ &= \Theta(2\pi\,|m| - \theta)\,\mathrm{e}^{-\mathrm{i}\pi m}\,\mathrm{e}^{\mathrm{i}\pi\,\mathrm{sgn}\,m/4}\frac{2}{\sqrt{\pi}}\frac{1}{\sqrt{\theta}}\frac{1}{\sqrt{1+2\pi\,|m|/\theta}}K\left(\frac{2}{1+2\pi\,|m|/\theta}\right) \\ &\quad + \Theta(\theta - 2\pi\,|m|)\,\mathrm{e}^{-\mathrm{i}\pi m}\,\mathrm{e}^{\mathrm{i}\pi/4}\frac{2}{\sqrt{\pi}}\frac{1}{\sqrt{2}}\frac{1}{\sqrt{\theta}}\left[K\left(\frac{1+2\pi m/\theta}{2}\right) - \mathrm{i}K\left(\frac{1-2\pi m/\theta}{2}\right)\right],\end{aligned} \tag{10}$$

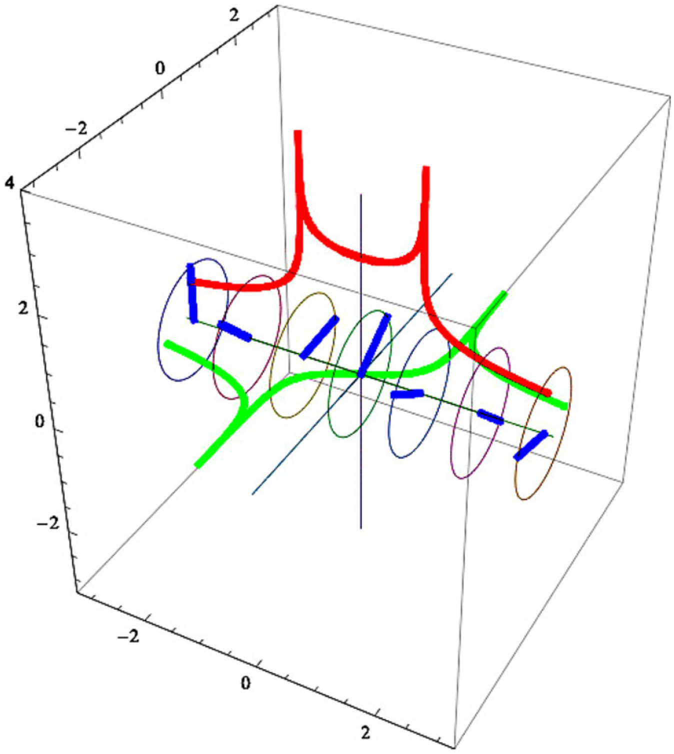

Figure 1. A representation of the Poisson sum supplying the wavefunction on the sphere at a chosen value of θ, at a chosen time (a rational fraction $a/4b$ of the period or 'Talbot time'). The horizontal axis (of the discs) is an auxiliary real variable m. A specific continuous complex function ((10) without the $\exp(-\mathrm{i}\pi m)$ prefactor) of this variable has real and imaginary parts shown in a vertical and a horizontal plane, viewed perspectively. It is sampled by an infinite comb of δ-functions with phase factors (disc radii vectors, which differ, but are periodic) forming the sum ((14), with an extra prefactor $\exp(-\mathrm{i}\pi m)$). The continuous function has logarithmic singularities, and does not depend on θ, but the δ-comb has spacing inversely proportional to θ. So when $\theta = 0$ the spacing is infinite (i.e. absent unless one of the δ-functions is at the origin), and as θ increases, the comb shrinks inwards along the axis, yielding the value infinity whenever a δ-function passes either of the two singularities of the continuous function.

where care has been taken to ensure that the correct square root (that with the positive real part) has been used in the last integration. The result is presented with all the arguments of the K's being between zero and one so that the values of the K's are real and positive (recalling that θ is positive, indeed $0 < \theta < \pi/2$). The result is, as it must be, $\exp(-\mathrm{i}\pi m)/\sqrt{\theta}$ times a function of $2\pi m/\theta$ only which is shown in figure 1. The important features of the function are the logarithmic singularities at $2\pi|m|/\theta = 1$ since $K(k) \sim -\log\sqrt{1-k^2}$ as k approaches 1 from below, and the inverse square-root decay for large $2\pi|m|/\theta$ from the prefactor of the first K (whose value $K(0) = \pi/2$).

Turning to the second brace of (9)

$$\{''\} = \int_{-\infty}^{\infty} \sin\left(\frac{1}{2}\pi l''\right) \exp[-\mathrm{i}\pi l''(l''+1)t]\delta_{\mathrm{odd}}(l'')\,\mathrm{e}^{-\mathrm{i}2\pi m l'}\,\mathrm{d}l''$$
$$= \sum_n -(-1)^n \exp[-\mathrm{i}\pi 2n(2n-1)t]\exp[-\mathrm{i}2\pi m(2n-1)], \qquad (11)$$

where $l'' = 2n - 1$ has been used to count odd l'' only. Simplifying

$$\{''\} = \mathrm{e}^{\mathrm{i}2\pi m} \sum_n - \exp[-\mathrm{i}\pi 4n^2 t] \exp[-\mathrm{i}\pi n(4m - 2t + 1)]. \tag{12}$$

For irrational times t, the sum is infinite for almost all values of m (but (9) is not infinite since m is summed over). For any rational time written as $t = a/4b$, with a and b sharing no factors (this is always possible), the sum is

$$\{''\} = \mathrm{e}^{\mathrm{i}2\pi m} \sum_n - \exp[-\mathrm{i}\pi n^2 a/b] \exp[-\mathrm{i}\pi (n/b)(4mb - a/2 + b)]. \tag{13}$$

This is a Gauss sum and yields a δ-comb in m with a periodic phase modulation. The δ-comb has constant spacing $1/2b$ between the δ-functions, and all have a coefficient of constant magnitude. The actual locations of the δ-functions are where $(4mb - a/2 + b)$ is an even integer if ab is even, or an odd integer if ab is odd. The phase factor coefficients are number theoretic ([7] gives an early application in a similar context), and are given by ($2b$ times) the Gauss average supplied in appendix A. The result of the average is of the form $(1/\sqrt{b})\exp(\mathrm{i}\pi$ integer/4) (exp(iπ integer $c^2/4b$), where $c = (4mb - a/2 + b)$, and the integers depend on a and b, but not c (i.e. not m).

$$\{''\} = -\mathrm{e}^{\mathrm{i}2\pi m} \left\langle \exp\left[-\mathrm{i}\frac{\pi}{b}(an^2 + cn)\right]\right\rangle_n 2b\, \delta_{\text{even}}(c - ab) \tag{14}$$

leading to the exact expression for the wavefunction in terms of (7), (10) and (14),

$$\psi(\theta, a/4b) = \psi_{<\infty} + 2\sqrt{\frac{2}{\pi}}\sqrt{\frac{\theta}{\sin\theta}} \int_{-\infty}^{\infty} \{'\}(-1)\, \mathrm{e}^{\mathrm{i}2\pi m} \times \left\langle \exp\left[-\mathrm{i}\frac{\pi}{b}(an^2 + cn)\right]\right\rangle_n 2b\, \delta_{\text{even}}(c - ab)\, \mathrm{d}m. \tag{15}$$

Interpretation of the result

An important feature of the new δ-comb (14), contrasting with the one from which it originated (its Fourier transform, the integrand within the second brace of (9)), is that the average of the coefficients of the δ-functions must be zero because the original comb has no δ-function at zero, only odd integers. Actually what matters is that the average of the coefficients times $\exp(-\mathrm{i}\pi m)$ is zero, where this exponential is taken from the first brace result (10). This too is true, because the extra phase factor shifts the whole original comb (odd integers) by half a unit, and still there is no δ-function at the origin. The importance is as follows.

Inserting the two braces (10), and (14) into (9), the wave $\psi(\theta, a/4b)$ at the rational time $a/4b$ is the sum obtained by sampling the elliptic integrals function (10) at regular spacings $1/2b$ in m, with the δ-comb (14). This is the 'Poisson summed' form of $\psi(\theta, a/4b)$. The zero average just mentioned means that the Poisson sum converges because with the terms grouped into periods, the decay of the groups for large m is like $m^{-3/2}$ rather than $m^{-1/2}$. The sum can only yield infinity if some individual term is infinite (unlike the original sum (8), as mentioned earlier, which becomes infinite by failure to converge).

In figure 1, which has horizontal axis $2\pi m/\theta$, the grid of sampling points shrinks inwards towards the origin $m = 0$ as θ increases from 0 to $\pi/2$. Each time a δ-function passes ± 1 a logarithmic singularity can be expected. The locations of the logarithmic infinities are $2\pi m = \pm\theta$ that is, 2π even $+ \pi a - 2\pi b = \pm 4b\theta$ if ab is even and 2π odd $+ \pi a - 2\pi b = \pm 4b\theta$ if ab is odd. This amounts to the following: if a is odd (whether b is odd or even), the logarithmic singularities are expected at $4b\theta/\pi =$ odd. If a is even (so b is odd), they are expected at

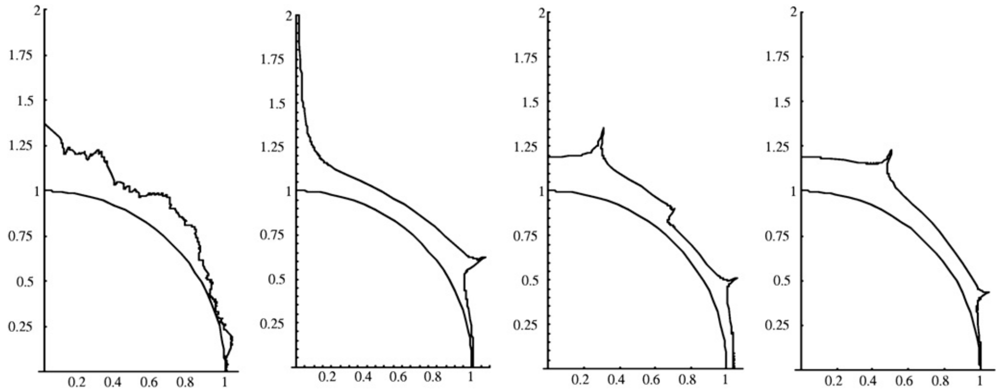

Figure 2. Depicting the wavefunction on the sphere at various different times chosen to illustrate the four possible cases. The wavefunction starts as a constant (not shown) in the upper hemisphere and minus the constant in the lower hemisphere, and 'revives' to this again at the 'Talbot time'. By symmetry, between these times, it remains axisymmetric about the vertical axis, and reflection antisymmetric about the equator circle, but has radically different character at irrational fractions of the Talbot time, and at rational ones. In the former (e.g. $1/\pi$, left) the wave is fractal with dimension 3/2 as in the ordinary Talbot effect for irrational times, but at the latter it exhibits rings of logarithmic infinity (little peaks) and/or inverse square-root divergences about the axis points. If the rational fraction is denoted $a/4b$, where a and b are integers sharing no factors, the three cases (respectively $(a, b) = (2, 3)$, $(4, 7)$ and $(1, 2)$ in the pictures) are, a even but not divisible by four, and a divisible by four and a odd. The angle gaps between the infinities are constant, respectively π/b, $2\pi/b$ and $\pi/2b$. In all cases the equator is midway between infinities, fixing their positions. In the a even but not divisible by four case (second picture) there is an inverse square-root divergence at the top point. In the a divisible by four case (third picture), there is a cancelled infinity on the equator and at every midway angle, leaving a visible step.

$4b\theta/\pi = a + 2 \bmod 4$, i.e. if $a = 0 \bmod 4$ they are at $4b\theta/\pi = 2, 6, 10, \ldots$, or if $a = 2 \bmod 4$ they are expected at $4b\theta/\pi = 0, 4, 8, \ldots$ etc. The $a =$ odd case is uncomplicated and there is a logarithmic infinity at all the expected locations.

In each of the two $a =$ even cases, though, there is a simultaneous passage of a δ-function passed the singularities at ± 1, and therefore there is the possibility of the pair cancelling each other since the δ-functions have different phases. This cancellation is easily shown to happen (appendix B) in the case $a = 0 \bmod 4$ only, and there, the possible singularity at $\theta = \pi/2$ is cancelled out, together with every alternate possible singularity (figure 2). The $a = 2 \bmod 4$ case has no cancellation but instead is accompanied by a stronger singularity at $\theta = 0$ (and also, therefore, negatively at $\theta = \pi$) which arises as follows.

The appearance of the extra singularity depends on whether or not there is a δ-function at the origin in figure 1 (which will not 'move' as θ increases and the comb spacing shrinks). If there is not, then $\psi(0, a/4b)$ is finite (not infinite) by the Fourier argument: the average value of the δ-function coefficients in the original comb (9) is zero, so that the original sum converges by periodic grouping (correspondingly, the sampling in the new δ-comb of (14) is infinitely wide, countering the inverse square root of θ in the prefactor of (10)). But if and only if $a = 2 \bmod 4$ (and b is therefore odd), there is a δ-function of the new comb (14) fixed at the origin, and as θ tends to zero (wide sampling), it alone samples the elliptic integrals function with its $1/\sqrt{\theta}$ prefactor. Consequently there is this inverse square-root singularity at the location $\theta = 0$ (and by symmetry a negative one at $\theta = \pi$). This inverse square-root singularity dominates, or eliminates the logarithmic singularity at $\theta = 0$ that necessarily accompanies it since $a = 2 \bmod 4$.

Acknowledgments

This work began as a final year undergraduate project at the University of Bristol. We thank M R Dennis for useful discussions.

Appendix A

The Gauss average in (14) is over all integers n, and the results copied from [7] are listed here.

$$\begin{aligned}
&\left\langle \exp\left[-\mathrm{i}\frac{\pi}{b}(an^2+cn)\right]\right\rangle_n \\
&\quad = \frac{1}{\sqrt{b}}\left(\frac{a}{b}\right)\exp\left[\mathrm{i}\frac{\pi}{4}(b-1)\right]\exp\left[i\frac{\pi a}{b}(a\backslash b)^2\left(\frac{c}{2}\right)^2\right] \quad \text{for } a \text{ even, } b \text{ odd, } c \text{ even} \\
&\quad = \frac{1}{\sqrt{b}}\left(\frac{b}{a}\right)\exp\left[-\mathrm{i}\frac{\pi}{4}a\right]\exp\left[\mathrm{i}\frac{\pi a}{b}(a\backslash b)^2\left(\frac{c}{2}\right)^2\right] \quad \text{for } a \text{ odd, } b \text{ even, } c \text{ even} \\
&\quad = \frac{1}{\sqrt{b}}\left(\frac{a}{b}\right)\exp\left[\mathrm{i}\frac{\pi}{4}(b-1)\right]\exp\left[\mathrm{i}\frac{\pi 4a}{b}(4a\backslash b)^2c^2\right] \quad \text{for } a \text{ odd, } b \text{ odd, } c \text{ odd} \\
&\quad = \text{zero otherwise,}
\end{aligned} \tag{A.1}$$

where the column brackets are the Jacobi symbol of number theory, and the symbol $(a\backslash b)$ stands for the integer inverse of a with respect to b, that is, the unique integer between 1 and $b - 1$ such that $a\,(a\backslash b) = 1 \bmod b$. In terms of Euler's totient function, $(a\backslash b) = a^{\phi(b)-1} \bmod b$.

Appendix B

This appendix calculates the circumstances in which cancellation of a pair of 'simultaneous' singularities (infinities) occurs. The conclusion will be that cancellation only happens at fractional times $a/4b$ with $a = 0 \bmod 4$, in which case alternate singularities in θ are eliminated, starting with that at $\theta = \pi/2$.

The ratio of the value of $\{'\}$ in (10) at $2\pi m/\theta = 1$ to that at $2\pi m/\theta = -1$ is $\exp(-\mathrm{i}\theta + \mathrm{i}\pi/2)$. For cancellation, therefore, the ratio of the complementary brace $\{''\}$ at these locations must be minus the reciprocal of this, namely $\exp(\mathrm{i}\theta + \mathrm{i}\pi/2)$. The expressions for the brace $\{''\}$ at the two locations are, from the prefactor of the delta function in (14), $\exp(\mathrm{i}\theta)\,\langle\,\rangle$ with $c = 2\theta b/\pi - a/2 + b$ and $\exp(-\mathrm{i}\theta)\,\langle\,\rangle$ with $c = -2\theta b/\pi - a/2 + b$. The difference of the squares of these two c values is $(2b - a)4\theta b/\pi = (2b - a)(2c - 2b + a) = 4(b - a/2)(c - b + a/2)$, where c denotes the first value above and the brackets are both integers. The ratio of the expressions required is thus $\exp(\mathrm{i}\theta)\exp[\mathrm{i}\pi(c - b + a/2)/2b]\exp[\mathrm{i}\pi a(a/b)^2(b - a/2)(c - b + a/2)/b] = \exp(\mathrm{i}\theta)\exp(-\mathrm{i}\pi/2)\exp[\mathrm{i}\pi(c + a/2)/2b]\exp[\mathrm{i}\pi a(a\backslash b)^2(-a/2)(c + a/2)/b] = \exp(\mathrm{i}\theta)\exp(-\mathrm{i}\pi/2)\exp[\mathrm{i}\pi(c + a/2)(1 - a^2(a\backslash b)^2)/2b]$, where the bs in the numerator have been simplified (using the fact that a is even). Next the product $a(a\backslash b)$ can be simplified because by the definition (of the integer inverse) $a(a\backslash b) = 1 +$ multiple of b. In fact the multiple must be odd since a is even, so $1 - a^2(a\backslash b)^2 = -\mathrm{odd}^2\, b^2 - \mathrm{odd}\, b$. Cancelling the b in numerator and denominator of the exponent, the ratio is $\exp(\mathrm{i}\theta)\exp(-\mathrm{i}\pi/2)\exp[\mathrm{i}\pi(c + a/2)\mathrm{odd}/2]$. If $a = 2 \bmod 4$ this expression cannot equal $\exp(\mathrm{i}\theta)\exp(\mathrm{i}\pi/2)$. If $a = 0 \bmod 4$, then alternate even values of c satisfy the equality and there is cancellation. Finally we can verify that the singularity at $\theta = \pi/2$ is always among those cancelled. At $\theta = \pi/2$, we have $c + a/2 = 2b$ so the ratio is $\exp(\mathrm{i}\theta)\exp(-\mathrm{i}\pi/2)\exp[\mathrm{i}\pi b\ \mathrm{odd}]$. Since b is odd this directly equals $\exp(\mathrm{i}\theta)\exp(\mathrm{i}\pi/2)$ and the result is verified.

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