Exploring the Propagator of a Particle in a Box

S. A. Fulling*
Departments of Mathematics and Physics, Texas A&M University, College Station, Texas, 77843-3368 USA

K. S. Güntürk†
Department of Physics, Texas A&M University, College Station, Texas, 77843-4242 USA

The propagator of a particle in a one-dimensional box is quite different from the propagator for infinite space. It has a complicated but regular structure of everywhere dense singularities. We investigate the case of periodic boundary conditions both numerically and theoretically, leaving the slightly more complicated case of reflecting boundary conditions to the suggested problems. The singularity structure is shown to match up with the fractional revivals observed by many authors in wave packet studies.

I. INTRODUCTION

The particle in a one-dimensional infinite square well is one of the most elementary problems in quantum mechanics. Recent articles by Robinett[1] and Styer[2] have shown that this simple system can still be a source of surprises. Here we take a close look at what is known as the *propagator*, which, in principle, solves the time-dependent Schrödinger equation for an arbitrary initial wave function. This Green function has mathematical properties that might fairly be described as astounding; these properties are well known to some mathematicians (mostly number theorists), but to the best of our knowledge they have not been pointed out in the physics literature, except implicitly through discussions of wave packet revivals[1–5] (see Sec. V). They raise interesting issues about how far a mathematical model can be pushed before it loses contact with the physical situation it is supposed to represent.

To streamline the algebra we consider a one-dimensional box with periodic boundary conditions, so that our particle is actually confined to a circle. (This system is called a rigid rotator in, for example, Ref. 4. In this interpretation the coordinate x is the angle of orientation of a rigid rod in a plane, rather than the position of a particle in a one-dimensional space.) Repeating the calculations for the more standard problem of a particle confined to an interval (the wave function vanishing at the ends) is a good student project.

The Schrödinger equation is

$$i\hbar\,\frac{\partial\Psi}{\partial t} = -\,\frac{\hbar^2}{2m}\,\frac{\partial^2\Psi}{\partial x^2}, \tag{1}$$

with the boundary conditions

$$\Psi(t,x-L) = \Psi(t,x+L), \qquad \frac{\partial\Psi}{\partial x}(t,x-L) = \frac{\partial\Psi}{\partial x}(t,x+L). \tag{2}$$

We note that the only mathematically independent constant in Eq. (1) is $\hbar/2m$, and we are free to choose units to give this constant any numerical value we like. This choice can be interpreted as choosing the unit of time, given a unit of length. Then we are still free to choose the unit of length arbitrarily. It turns out that the interpretation of a numerical analysis of this system is greatly facilitated by the choices

$$\frac{\hbar}{2m} = \frac{1}{\pi}\,, \qquad L = 1. \tag{3}$$

Thus our circle has circumference 2. Readers taking up the challenge of redoing everything for a true box should study a box of length 1 with boundary conditions $\Psi(t,0) = 0 = \Psi(t,1)$.

Problem 1 (discussion question). Ordinarily we are told that there are three basic physical units, those of length, mass, and time. What happened to the third unit? Hint: Try to repeat these scaling arguments when the Schrödinger equation contains a potential,

$$i\hbar\,\frac{\partial\Psi}{\partial t} = -\,\frac{\hbar^2}{2m}\,\frac{\partial^2\Psi}{\partial x^2} + \lambda V(x)\Psi \tag{4}$$

where λ is a coupling constant, such as the electron charge.

II. THE SOLUTION AND THE PROPAGATOR

We repeat the problem in our choice of natural units:

$$i\pi\,\frac{\partial\Psi}{\partial t} = -\,\frac{\partial^2\Psi}{\partial x^2}\,, \qquad \Psi(t,x-1) = \Psi(t,x+1) \tag{5}$$

and similarly for the derivative. It is convenient to refer to the related equation

$$\pi\,\frac{\partial\Psi}{\partial\tau} = \frac{\partial^2\Psi}{\partial x^2}, \qquad \Psi(\tau,x-1) = \Psi(\tau,x+1) \tag{6}$$

with $\tau > 0$, which describes the flow of heat in a circle. Note that Eq. (5) arises from Eq. (6) by the substitution $\tau = it$, so a solution of one problem can be expected to be the analytic continuation of a solution of the other to imaginary time. It is well known that Eqs. (5) and (6) can be solved exactly by two different methods, both of which are highly pertinent to the following discussion.

A. The eigenfunction expansion

This expansion is so familiar that we omit the heuristic steps. For each integer k there is a normalized eigenfunction

$$\psi_k(x) = \frac{1}{\sqrt{2}}\, e^{i\pi kx}, \tag{7}$$

with energy $E_k = \pi k^2$. The general solution of Eq. (5) is

$$\Psi(t,x) = \sum_{k=-\infty}^{\infty} c_k \psi_k(x) e^{-iE_k t}, \tag{8}$$

and the coefficients are related to the initial data by

$$c_k = \int_{-1}^{1} \psi_k(y)^* \Psi(0,y)\, dy. \tag{9}$$

When we substitute Eqs. (9) and (7) into Eq. (8) and interchange the order of integration and summation, we obtain

$$\Psi(t,x) = \int_{-1}^{1} U(t,x,y)\Psi(0,y)\, dy, \tag{10}$$

where the propagator is

$$U(t,x,y) = \frac{1}{2} \sum_{k=-\infty}^{\infty} e^{i\pi k(x-y)} e^{-i\pi k^2 t}. \tag{11}$$

We postpone a discussion of the difficulty presented by the fact that the series (11) does not converge. Note, however, that for $t = -i\tau$, we do obtain a rapidly convergent series for the Green function, $K(t,x,y)$, of the heat equation (6) (called the "heat kernel" for short).

B. The method of images, or sum over classical paths

We turn now to the second method of constructing $U(t,x,y)$. If the configuration space of the particle were the entire real line, the counterpart of Eq. (11) would be

$$U_\infty(t,x,y) = \frac{1}{\sqrt{4it}}\, e^{i\pi(x-y)^2/4t}, \tag{12}$$

where the correct interpretation of the branch of the square-root function is

$$\frac{1}{\sqrt{it}} = e^{-i(\operatorname{sgn} t)\pi/4} |t|^{-1/2}. \tag{13}$$

The easiest way to arrive at Eqs. (12)–(13) is to start from the better known Green function for the heat equation,

$$\begin{aligned} K_\infty(\tau,x,y) &= \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ik(x-y)} e^{-k^2\tau/\pi}\, dk \\ &= \frac{1}{\sqrt{4\tau}}\, e^{-\pi(x-y)^2/4\tau}, \end{aligned} \tag{14}$$

and let $\tau = it$. K_∞ is a solution of the heat equation with the initial data $K_\infty(0,x,y) = \delta(x-y)$; in particular, $K_\infty(0,x,y) = 0$ for $x \neq y$. Similarly, U_∞ is a solution of the Schrödinger equation, and should satisfy

$$\lim_{t\to 0} U_\infty(t,x,y) = \delta(x-y). \tag{15}$$

Although $U_\infty(t,x,y)$ for $x \neq y$ does not literally approach 0 for small t — instead, it oscillates increasingly rapidly — it can be shown that Eq. (15) is true in an "effective" or "distributional" sense:[6] $\Psi(t,x)$ constructed in analogy to Eq. (10) does reduce properly to $\Psi(0,x)$ in the limit of small t.

We now argue that the sum

$$U(t,x,y) \equiv \sum_{n=-\infty}^{\infty} U_\infty(t,x,y+2nL) \tag{16}$$

is periodic in x with period $2L$ $(= 2)$ and hence satisfies the boundary conditions in Eq. (2). Furthermore, it satisfies the correct differential equation (1), and for x and y both between $-L$ and L it has the right initial data, because the term for $n = 0$ reproduces the needed delta function and the other terms go to zero in the sense described above. Therefore, it must be the correct propagator for Eq. (5): U as defined by

$$U(t,x,y) = \frac{1}{\sqrt{4it}} \sum_{n=-\infty}^{\infty} e^{i\pi(x-y-2n)^2/4t} \tag{17}$$

must be equal to U as defined by Eq. (11). (Again, Eq. (17) has convergence trouble but there is no problem with its heat analog.)

Problem 2. Derive Eq. (17) by an alternative route (which some students might find more convincing): Solve the Schrödinger equation (1) on the entire real line by Fourier transforms, assuming[7] that $\Psi(0,x) = 0$ outside the interval $-L < x \leq L$. Call this solution $\Psi_\infty(t,x)$. Form the sum

$$\Psi(t,x) = \sum_{n=-\infty}^{\infty} \Psi_\infty(t,x-2nL). \tag{18}$$

Observe that Ψ solves the periodic problem (Eqs. (1) and (2)) and has the correct initial data $\Psi(0,x)$ inside the interval $-L < x \leq L$. (Ignore convergence questions unless you are a math major.) Interchange the summation and integration in your expression (and set $L = 1$) to obtain Eq. (10) with Eq. (17).

Problem 3. Construct the propagator for the true box problem, where Eq. (2) is replaced by $\Psi(t,0) = 0 = \Psi(t,1)$, by both the eigenfunction and the image method. The term "image" is perhaps more apt in this case than in the periodic case, because the displaced source points are reflections of the original source point y through the walls of the box.

A modern alternative way of looking at the image method, which generalizes better to more complicated problems, is to regard the image sum (17) as a sum over all paths by which a particle could travel from the source point y to the field point x, obeying classical mechanics. That is, instead of regarding $y + 2n$ as the coordinate of a copy of y in a distant region of an "unrolled" space, we may interpret $x - y - 2n$ as the separation between x and the *original* source point y along a path that winds around the original circular space several times. In addition to traveling directly, the particle could zip around the circle an arbitrary number of times in either direction before arriving; hence the variety of distances $|x-y-2n|$ in Eq. (17). (In the true box, one needs to sum over all possible ways the particle could bounce off the walls.) Because we are doing nonrelativistic quantum mechanics, we are not supposed to worry about the fact that the speed of these paths becomes arbitrarily large as $|n|$ increases. It is perhaps reassuring that the terms with large $|n|$ are highly oscillatory and thus less important in the final sum. Classical path analysis has no necessary connection with the Feynman formulation of quantum mechanics in terms of a sum over *all* paths, although it arises very naturally within the latter.

III. NUMERICAL INVESTIGATION OF THE PROPAGATOR

Problem 4. Use a computer algebra system or numerical software package to plot the heat kernel $K(\tau, x, y)$ as a function of x for various fixed τ and y. Also look at K as a function of τ for fixed x and y; of course, $x = y$ is special. Try both Eqs. (11) and (17) (with $t = -i\tau$). Do they agree? Which series converges faster? (It should be obvious from the equations how the answer to that question will depend upon τ.)

After this warmup exercise, we want to investigate the propagator $U(t, x, y)$ numerically, but we know better than to throw the infinite sums (11) and (17) directly onto a computer. Those series actually converge *distributionally*, which means in practice[6] that if we first apply each term to a sufficiently well-behaved initial wave packet as in Eq. (10) and *then* do the summation, we will obtain a convergent series that yields the correct wave function at time t. (For a fixed initial packet, the terms will become small at sufficiently large k or n, because of the increasingly oscillatory nature of the integrals involved.)

Roughly speaking, anything a physicist would want to do with the series (11) and (17) can be rigorously justified by the theory of distributions and/or careful analysis of limits, but that is not the subject of this paper. Theoretical physics can go a long way with formal manipulations of such series. But when we hit the hard metal of the computer, the failure of numerical convergence can no longer be ignored. The punishment would be meaningless numbers or perhaps an error message.

A time-honored method for dealing with such series is to give t a small negative imaginary part so that the series converges, and then investigate the limit as this cutoff parameter goes to 0. (Recall that if we take t all the way to the negative imaginary axis, we obtain the heat kernel. Now, however, we want to keep the real part of t as a variable.) Some of the most interesting results are obtained by considering $U(t, x, y)$ as a function of t with $x = y$. Because U in the periodic system depends on x and y only through the combination $x - y$, there is no loss of generality in taking $y = 0$ in our numerical experiments:

$$U(t, x, y) = U(t, x - y, 0). \tag{19}$$

(This property no longer holds for the true box.) So, we will study

$$U_{\text{eigen}}(t - i\epsilon, 0, 0) = \frac{1}{2} + \sum_{k=1}^{\infty} e^{-i\pi k^2 (t - i\epsilon)} \tag{20}$$

and

$$U_{\text{image}}(t - i\epsilon, 0, 0) = \frac{1}{\sqrt{it + \epsilon}} \left[\frac{1}{2} + \sum_{n=1}^{\infty} e^{i\pi n^2/(t - i\epsilon)} \right] \tag{21}$$

(with t real and ϵ positive). These quantities should be exactly equal, but in practice we have to truncate the sums at some finite values of k and n and there will be some numerical error. Therefore, we plot both functions on the same graph and let the discrepancy indicate the accuracy of the computations.

Problem 5 (project). Develop systematic error estimates for the series (20) and (21), so that you can learn in advance how many terms must be added to obtain an accurate numerical result for a fixed, nonzero ϵ.

In Fig. 1 we present graphs of the real part of U for various intervals of t and values of ϵ, with $k_{\max}$ and $n_{\max}$ chosen sufficiently large in each case to force good agreement between the eigen and image sums. As ϵ decreases, the graph develops increasingly complicated local structure. Indeed, it soon becomes clear that we face an infinite task: Zooming in on a small interval gives the temporary illusion of progress, but taking ϵ still smaller shows that we have not reached a limit. A tall spike develops around $t = 2$, whereas around $t = 1$ there is a peculiar flat spot. Smaller spikes seem to be associated with simple fractional values of t. Indeed, in Sec. IV we show that $U(t - i\epsilon, 0, 0)$ as $\epsilon \to 0$ has a singularity at *every rational number* $t = p/q$ with p and q not both odd;[8] the size of the spike decreases as q increases. Our motivation for the unusual normalization conventions (3) rather than $\hbar/2m = 1$ and $L = \pi$ was to put these singularities at rational numbers, rather than rational multiples of π.

Problem 6 (various options). Use the *Mathematica* or *Maple* code for these computations available at the authors' Web site[9] to zoom in on other values of t, to plot the imaginary part or the modulus (absolute value) of U, or to plot $U(t,x,0)$ as a function of t with $x \neq 0$.

Problem 7 (high-priority project). Study $U(t,x,0)$ as a function of x at fixed t. Do you observe anything interesting? Be alert to possibilities for streamlining the computation by avoiding redundant values of the variables. (For instance, there is no reason to plot U at negative x.)

Problem 8 (project). Do similar computations for the true box, or infinite square well, of length 1. There is a lot of variety here, because now the value of y matters — whether it is near the walls or somewhere in the middle of the box. Note that many conclusions about the periodic propagator can be carried over to the square-well propagator by noting that the latter is the "odd part" of the former:

$$U_{\rm box}(t,x,y) = U(t,x,y) - U(t,x,-y). \qquad (22)$$

To appreciate how astounding the box propagators are, compare their properties with some other simple systems whose propagators are exactly calculable. The propagator of a free particle (12) is a completely smooth function of all its variables as long as t is nonzero; in fact, it varies rather slowly unless $|t|$ is small. The well known propagator of the harmonic oscillator[10] is smooth except when t is an integer multiple of half the period. At those times the initial delta-function singularity reforms; this reflects the existence of a *caustic* — the fact that the classical paths departing from y with various momenta all refocus at a particular point $x = \pm y$ at those times. (Of course, the free particle in infinite space has no caustics, because there is always a unique trajectory going from y to x in time t.) The box propagator (with either periodic or reflection boundary conditions) is singular at *all* (real) times. In a sense, these systems *have caustics everywhere*, because there are always *infinitely many classical paths* that travel from y to x in time t. Finally, the analogous Green functions for the wave equation in a box are singular only if a classical ray can travel at the wave speed from y to x exactly in time t; so when $x = y$ such singularities are separated by the time needed by a "photon" to travel around the circle (or bounce off the wall, as the case may be). (Our investigations were triggered by a short remark about this distinction in a mathematical paper.[11])

IV. THE THETA FUNCTION

Is there any hope that the thicket of complications visible in our computations can be penetrated by descending to a small enough scale with sufficiently accurate numerical analysis? The answer is no, and a theoretical analysis shows that the propagator has, to speak loosely for the moment, little infinite spikes *everywhere*; the closer we look with the graphical microscope, the more spikes we will see. The reader may find the details of this section more dificult to follow than the mathematics in the rest of the paper. What is important is the conclusion.

The series (11) and (17), and even the special cases in Eqs. (20) and (21), cannot be evaluated in terms of elementary functions. Nevertheless, the function $U(t,x,0)$ with t in the lower half of the complex plane is the principal example of a *Jacobi theta function*, a class of objects about which entire books have been written, the most elementary of which is by Bellman.[12] In this section we treat t as a complex variable; that is, t now means what was called $t - i\epsilon$ in Sec. III.

Theorem 1. Let $U(t) \equiv U(t,0,0)$ for $\operatorname{Im} t < 0$ be defined by either of the equivalent equations (20) and (21). This function has the following properties:

- *Periodicity.* For any integer N,
$$U(t+2N) = U(t). \qquad (23)$$
- *Reflection.*
$$U(-t^*) = U(t)^*. \qquad (24)$$
(Note that the minus sign and the complex conjugation must occur together to keep the number in the correct half-plane.)
- *Inversion.*
$$U\left(-\tfrac{1}{t}\right) = \sqrt{it}\, U(t). \qquad (25)$$

Problem 9. Derive Eqs. (23) and (24) from Eq. (20).

Problem 10. Show that

$$U(2 - t^*) = U(t)^* \qquad (26)$$

and interpret this property as a reflection symmetry about $t = 1$.

The most interesting part of the theorem is the inversion property (25), which is proved starting from Eq. (21):

$$\begin{aligned} U(t) &= \frac{1}{\sqrt{it}}\left[\frac{1}{2} + \sum_{n=1}^{\infty} e^{i\pi n^2/t}\right] \\ &= \frac{1}{\sqrt{it}}\left[\frac{1}{2} + \sum_{k=1}^{\infty} e^{-i\pi k^2\left(\frac{-1}{t}\right)}\right] \\ &= \frac{1}{\sqrt{it}} U\left(-\frac{1}{t}\right). \qquad (27) \end{aligned}$$

It is tempting to push Eqs. (25) and (24) right onto the real axis and to conclude, for example, that $U(1/N)$ is larger in absolute value than $U(N)$ by a factor $\sqrt{N}$. This conclusion is a case where nonrigorous mathematics can lead to a totally false conclusion. In fact, careful attention to the imaginary parts moves the $\sqrt{N}$ from the numerator to the denominator, as we now show.

Let us revert momentarily to the notation $t-i\epsilon$, where t and ϵ are real ($\epsilon > 0$), and consider $t > 1$. Then Eq. (25) says that

$$U\left(\frac{-1}{t-i\epsilon}\right) = \sqrt{it+\epsilon}\,U(t-i\epsilon). \tag{28}$$

After expanding the argument on the left-hand side in a geometric series and introducing $\delta = \epsilon/t^2$, we have

$$U\left(-\frac{1}{t} - i\delta + O(\delta^2)\right) = \sqrt{it+\delta t^2}\,U(t-i\delta t^2). \tag{29}$$

Now suppose that we know that $U(t-i\epsilon)$ behaves for small ϵ like $C\epsilon^{-1/2}$, where C is a constant. (It will soon become clear why this particular behavior is of interest.) It follows from Eq. (29) that $U\left(-\frac{1}{t} - i\delta\right)$ behaves for small δ like

$$\sqrt{it}\,C(\delta t^2)^{-1/2} = \sqrt{i}\,Ct^{-1/2}\delta^{-1/2}. \tag{30}$$

Note that this calculation does not actually require that δ be real, only that $\operatorname{Re}\delta > 0$ and $|\delta|$ be small.

We are now ready for the main point. Let t be a rational number between 0 and 1. Then we have[8] $t = p/q$ with $p < q$. The inversion and reflection properties relate U near t to U near $1/t = q/p$. Then the periodicity formula (23) relates that time to some time $q/p - 2N$ in the interval $(0, 2)$. If necessary, we use reflection about $t = 1$ (Eq. (26)) to move this point into the interval $(0, 1)$. In either case, we are now looking at U near a t of the form

$$\frac{2pM \pm q}{p} \equiv \frac{r}{p}\,, \tag{31}$$

where $r < p$ and r has the same parity as q. Now repeat the entire process, relating r/p by inversion and reflection to some number greater than 1 and then by periodicity and possibly reflection to a number s/r, where $s < r$ and s has the same parity as p. If we keep going, we must eventually hit bottom, when p, or r, or s, or ... becomes equal to 1. Then after one more inversion, we arrive at t equal to an integer, which is odd if p and q are both odd, and is even if one of them is even. A final translation by Eq. (23) brings us to either 1 or 0, respectively. But we know that $U(t)$ has a square-root singularity at $t = 0$, arising from the first term in Eq. (21) and tracing all the way back to Eq. (14). Moving backwards through the chain of transformations, we see that $U(t)$ *must have a singularity proportional to*

$$\frac{1}{\sqrt{t - p/q}} \tag{32}$$

in the vicinity of any rational number p/q with p and q not both odd.

In general, this singularity is not as strong as the one at $t = 0$. We can determine the numerical coefficient multiplying the singularity by collecting the $t^{-1/2}$ factors that have accumulated from repeated use of Eq. (30):

$$\sqrt{\frac{p}{q}}\sqrt{\frac{r}{p}}\sqrt{\frac{s}{r}}\cdots = \frac{1}{\sqrt{q}}\,. \tag{33}$$

The singularity also has a phase, which is more tedious to calculate. In view of the remark after Eq. (30), what we are seeing in Fig. 1 around a rational point with small q is the emergence of this singularity (Eq. (32) times Eq. (33) times the phase), cluttered by infinitely many, even more indistinct and embryonic, nearby smaller spikes corresponding to larger values of q. An alternative proof of Eq. (33), using mathematics (finite Fourier series) closely related to that appearing in Refs. 3 and 5, can be extracted with some difficulty from Sec. 19 of Ref. 12 or pp. 65–73 of Ref. 13.

Finally, for $t = 1$ (and hence whenever p and q are both odd), Eq. (20) reduces to

$$U(t-i\epsilon) = \frac{1}{2} + \sum_{k=1}^{\infty}(-1)^k e^{-\pi k^2 \epsilon}, \tag{34}$$

and it is known[14] that this quantity approaches 0 as $\epsilon \to 0$.

For completeness we state the "off-diagonal" generalization of Theorem 1:

Theorem 2: Let $U(t,x) \equiv U(t,x,0)$ for $\operatorname{Im} t < 0$ be defined by either of the equivalent equations (11) and (17). This function has the following properties:

- *Periodicity.* For any integer N,

$$U(t, x+2N) = U(t,x), \quad U(t+2N, x) = U(t,x). \tag{35}$$

- *Reflection.* For x real,

$$U(t,-x) = U(t,x), \quad U(-t^*, x) = U(t,x)^*. \tag{36}$$

- *Inversion.*

$$U(t,x) = \frac{1}{\sqrt{it}}\,e^{i\pi x^2/4t}\,U\left(-\frac{1}{t}, \frac{x}{t}\right). \tag{37}$$

Problem 11. Notice that on the right side of Eq. (37) the x argument has become slightly complex. How must one modify Eq. (36) to handle this? (Prove the appropriate reflection identities starting from Eq. (11).)

V. IMPLICATIONS

By this time an alarm bell might have gone off in the alert reader's mind. In the real world, where physical quantities can be measured only to finite accuracy, can anything of genuine physical significance depend on whether a time coordinate is rational or irrational? When a model develops such rococo features, does that not indicate that it has been pushed beyond its regime of validity?

If we were dealing with a discontinuous index of refraction, for instance, and discovered implausible behavior in the solutions of the wave equation at very short wavelengths, we would say that the problem arose from neglect of the atomic nature of matter; nature does not really contain infinitely sharp boundaries. But the box with periodic boundary conditions is so simple and so fundamental that this kind of excuse does not seem pertinent. As we've seen, there are not even any numerical parameters in the theory that are modeling something. Everything is absolute.

Let us return to first principles. The quantum propagator is a complete description of the dynamics of the system, via Eq. (10). Admittedly, this statement is somewhat like saying that in principle a whole book can be read at one glance if it is printed on a stack of transparent paper. Staring at a formula for the propagator itself, even in a case like Eq. (12) where the formula is simple, may not be very enlightening. One needs to follow the fate of particular example wave packets $\Psi(0, y)$ to gain an intuition for the dynamical content of $U(t, x, y)$.

Recently wave packets in the infinite square well have been extensively studied with special attention to fractional revivals.[1,2,4,5] Consider an initial wave packet that is sufficiently localized that one can speak of its position, but also sufficiently localized in momentum that it will not instantly disperse. Then for a short time the evolved packet $\Psi(t, x)$ closely follows a classical trajectory, but eventually it will spread out to a length comparable to the whole box. However, the periodicity theorem (23) implies that after a time

$$T = \frac{4mL^2}{\pi\hbar} = 2 \quad \text{(in our units)}, \tag{38}$$

the packet must "refocus" or "revive" precisely to its original form. (For comparison, the period of a single classical orbit for a particle with energy equal to the kth eigenvalue is

$$T_k = 2L\sqrt{\frac{m}{2E_k}} = \frac{1}{2k}\,T, \tag{39}$$

and the spreading time for a Gaussian packet of initial width $\Delta x \ll L = 1$ is of the order of

$$T_{\text{disp}} = \frac{4m}{\hbar}\,L\Delta x = 2\pi\Delta x \ll T, \tag{40}$$

as follows by a short calculation from Eq. (18) in Ref. 1 and the equation above it.) Furthermore, both numerical and analytical calculations reveal that at times $pT/2q$, simple fractions of the full revival time, the packet undergoes a partial revival, refocusing into q equally spaced copies of its original shape. These revivals (at least for small q) are real physics, not just mathematical curiosities; analogous phenomena have been predicted and observed in realistic physical systems, notably Rydberg atoms (electrons in highly excited Bohr orbits). For references to this experimental work, consult Refs. 1–5.

The propagator itself may be regarded as the time development of an infinitely sharp initial wave packet. Although the infinite spread of momentum in such a packet makes visualization of the motion difficult, the counterpart of the fractional revivals is easily observable. By now, it is hoped, some students will have made progress on Problem 7 and obtained graphs like those in Fig. 2. When t is a rational number p/q with fairly small q, the plot of $U(t - i\epsilon, x, 0)$ as a function of x displays a family of tall, evenly spaced peaks. When computations are done with t equal to p/π or a random string of decimal digits, the pattern is irregular and less concentrated. (Of course, to a computer all numbers are rational; but a randomly chosen number is likely to have a rather large q, and the associated periodic pattern will not show up clearly until ϵ is very small.)

A close examination shows that the locations of the peaks agree with those observed in the wave packet studies. In particular, when p and q are both odd, there is no peak at $x = 0$, which instead falls halfway between peaks. (Some other peaks that do exist are not visible in plots of the real part of U because they have purely imaginary phase.) A comparison with the paper of Aronstein and Stroud[5] is particularly instructive, but requires some notational adjustment. First, their box has reflecting walls instead of periodic boundary conditions; in our context, the spatially reversed packets in their figures should be thought of as traveling on the "far side" of our circle, which is being viewed edge on. Second, the fraction they write as p/q is *half* the number denoted by p/q in the present paper; thus Case 2 of Ref. 5 corresponds in our terminology to p and q both odd, Case 1 to p even, and Case 3 to q even.

For a packet of a given width Δx, the revivals are difficult to observe for large q. The many copies of the initial pulse will overlap, and because their phases vary, they will usually interfere destructively. As remarked in Ref. 5, it is necessary to have[15]

$$\lim_{q\to\infty} \Psi(1/q, x) = \Psi(0, x), \tag{41}$$

although $\Psi(1/q, x)$ is also a superposition of q spaced-out copies of $\Psi(0, x)$! The larger the ratio $L/\Delta x$, the more noticeable the high-q revivals will be. In principle, all the rational numbers are potentially significant. If we think of Δx as being fixed at, say, the Compton wavelength of the particle, $\hbar/mc$ (below which nonrelativistic quantum mechanics becomes suspect), then the fine structure of the propagator becomes more important as L becomes larger, that is, in the more nearly classical regime. (This observation is in keeping with the fact that the sum over classical paths, although exact in this simple problem, is in general a semiclassical approximation.) Note that the particle's mass, which we found earlier to be totally irrelevant to the internal mathematics of the theory, reappears here in the context of the physical interpretation of the theory: It sets the length scale that defines quantum (versus classical) behavior.

VI. ANTIDERIVATIVES OF THE PROPAGATOR

Another way of dealing with a singular generalized function such as the theta function at real t is to integrate its definition until we obtain a genuine function. For example, Eq. (11) yields

$$\int U(t,x,0)\,dt = \sum_{k\neq 0} \frac{i}{2\pi k^2} e^{ikx} e^{-i\pi k^2 t} + \frac{t}{2} + C(x), \quad (42)$$

where $C(x)$ is a constant of integration. This series is convergent (absolutely and uniformly) and hence defines a continuous function. Note that the cutoff parameter ϵ is no longer necessary. (Of course, to evaluate the sum numerically we still have to choose an arbitrary maximum value of k.)

Similarly, integrating U twice with respect to x yields a continuous function. To cut a long story short, we define

$$P(t,x) = \sum_{k=1}^{\infty} \frac{1}{\pi k^2} \cos(\pi k x)\bigl(1 - e^{-i\pi k^2 t}\bigr), \quad (43)$$

and note that

$$U(t,x) = \frac{1}{2} - i\frac{\partial P}{\partial t}(t,x)\,, \quad (44)$$

and

$$U(t,x) = \delta(x) + \frac{1}{\pi}\frac{\partial^2 P}{\partial x^2}(t,x). \quad (45)$$

Problem 12. Verify Eqs. (44) and (45). Hint: First derive the Fourier cosine series

$$\sum_{k=1}^{\infty} \frac{1}{\pi k^2} \cos(\pi k x) = \pi\left(\frac{x^2}{4} - \frac{x}{2} + \frac{1}{6}\right) \quad (46)$$

(for $0 \leq x \leq 1$) and the distribution identity

$$\delta(x) = \frac{d}{dx}\,\frac{1}{2}\operatorname{sgn} x = \frac{d}{dx}\,\frac{x}{2|x|} = \frac{d^2}{dx^2}\,\frac{|x|}{2}\,. \quad (47)$$

When we plot $P(t,0)$ (see Fig. 3), what do we see? Batman! Batman has little Batmen on his shoulders (at points with $q = 3$), and presumably so ad infinitum, in keeping with the self-similar character of U observed in Sec. IV. More seriously, the curve has numerous cusps where two pieces of graph with the same concavity meet at a common vertical tangent. With the advantage of knowing the answer beforehand, we can identify these as square-root singularities, proportional to $\left|t - \frac{p}{q}\right|^{1/2}$, whose derivatives are the singularities (32) of $U(t,0)$.

Problem 13. Plot $P(t,x)$ as a function of x for various values of t, and interpret the results in view of what we know from Sec. V and Eq. (47). Two examples are shown in Fig. 4; note that the qualitative difference between rational and "irrational" t is not very noticeable. To obtain good plots it is necessary to choose the horizontal and (especially) the vertical plot ranges very judiciously. If the vertical range is too large, the curve appears structureless; if it is too small, the graph is dominated by oscillations specific to a particular Fourier partial sum that have nothing to do with the function being approximated.

The utility of equations such as (44) and especially (45) is that the action of a distribution on a sufficiently smooth function can be calculated by an integration by parts:

$$\int_{-1}^{1} \frac{\partial^2 P}{\partial x^2}(t,x)\Psi(x)\,dx = \int_{-1}^{1} P(t,x)\frac{\partial^2 \Psi}{\partial x^2}(x)\,dx. \quad (48)$$

(Here the right-hand side *defines* the left-hand side; see endnote 6.) Thus an antiderivative of a distribution contains the same information as the distribution itself, encoded in a less singular form.

Problem 14 (discussion question and possible project). Can Eq. (48) (with Eqs. (10) and (45)) be used as a practical method of evolving wave packets numerically, competitive with those cited in Sec. V? Does Simpson's rule apply to a function as rough as P? Would it help to integrate with respect to x several more times?

VII. SUMMARY

The propagator of a particle in a box is not a function, but rather a distribution with everywhere dense singularities. Therefore, it is impossible to compute and examine directly. We have discussed three ways of getting at it indirectly: analytic continuation to slightly complex time (Secs. III and IV), application to smooth initial wave packets of finite width (Sec. V), and indefinite integration (Sec. VI). These methods are complementary and combine to reveal a surprisingly rich structure in this simple quantum system.

* Electronic address: `fulling@math.tamu.edu`; URL: `http://www.math.tamu.edu/~fulling`

† Electronic address: `k-gunturk@rainbow.physics.tamu.edu`

[1] R. W. Robinett, "Visualizing the collapse and revival of wave packets in the infinite square well using expectation values," Am. J. Phys. **68** (5), 410–420 (2000).

[2] D. F. Styer, "Quantum revivals versus classical periodicity in the infinite square well," Am. J. Phys. **69** (1), 56–62 (2001).

[3] I. Sh. Averbukh and N. F. Perelman, "Fractional revivals: Universality in the long-term evolution of quantum wave packets beyond the correspondence principle dynamics," Phys. Lett. A **139**, 449–453 (1989); "Fractional revivals of wave packets," Acta Phys. Polon. A **78**, 33–40 (1990).

[4] R. Bluhm, V. A. Kostelecký, and J. A. Porter, "The evolution and revival structure of localized quantum wave packets," Am. J. Phys. **64** (7), 944–953 (1996).

[5] D. L. Aronstein and C. R. Stroud, "Fractional wavefunction revivals in the infinite square well," Phys. Rev. A **55**, 4526–4537 (1997).

[6] One way among many of constructing $\delta(x)$ is to define $\delta_t(x)$ by the right-side of either Eq. (12) or Eq. (14) and then to define $\delta(x) = \lim_{t\downarrow 0} \delta_t(x)$ by the instruction to integrate a function $\Psi(x)$ over δ_t and only later take the limit $t \to 0$. In each case it can be proved that this limit is $\Psi(0)$, as desired. More generally, a *distribution* is a linear function whose independent variable is a function (say $\Psi(x)$) and whose dependent variable is a number (such as $\Psi(0)$). The action of the distribution on Ψ is generally written in integral notation, as in $\delta[\Psi] = \int \delta(x)\Psi(x)\,dx$, although there is no actual function $\delta(x)$ that fulfills this role. All calculus operations on distributions are defined by the principle demonstrated above: "integrate over a function and only later take the limit." For example, a sum such as $\sum_{n=-\infty}^{\infty} e^{in(x-y)}/2\pi$ may diverge (in the literal, pointwise sense), but if we multiply it by $\Psi(y)$ and integrate term by term, we obtain the Fourier series of $\Psi(x)$; thus the sum converges in the distributional sense to the periodic extension of the Dirac delta function.

[7] To avoid technical issues, assume that $\Psi(0, x)$ is continuous inside the interval and that its limit as x approaches $-L$ is equal to $\Psi(0, L)$.

[8] Whenever we write $t = p/q$, we shall assume that the fraction is in lowest terms. Thus the case of p and q both even does not need to be considered.

[9] `http://www.math.tamu.edu/~fulling/box/` . The figures in this paper were made with *Mathematica*. Some computations also were done with *Maple*. *Mathematica* produces compact graphics that are more suitable for publication. *Maple* produces larger graphics whose greater detail was sometimes easier to interpret on the screen and in printouts.

[10] F. U. Chaos and L. Chaos, "Comment on 'The harmonic oscillator propagator,' by Barry R. Holstein [Am. J. Phys. **66** (7), 583–589 (1998)]," Am. J. Phys. **67** (7), 643 (1999); N. S. Thornber and E. F. Taylor, "Propagator for the simple harmonic oscillator," Am. J. Phys. **66** (11), 1022–1024 (1998).

[11] J. J. Duistermaat and V. W. Guillemin, "The spectrum of positive elliptic operators and periodic bicharacteristics," Invent. Math. **29**, 39–79 (1975), esp. pp. 45–56.

[12] R. Bellman, *A Brief Introduction to Theta Functions* (Holt–Rinehart-Winston, New York, 1961).

[13] H. Helson, *Harmonic Analysis* (Addison-Wesley, Reading, 1983).

[14] G. H. Hardy, *Divergent Series* (Chelsea, New York, 1991), Sec. 4.10.

[15] Mathematical experts will note that Eq. (41) is not a complete triviality. It will hold in some reasonable topology, which may depend on the smoothness of $\Psi(0, x)$.

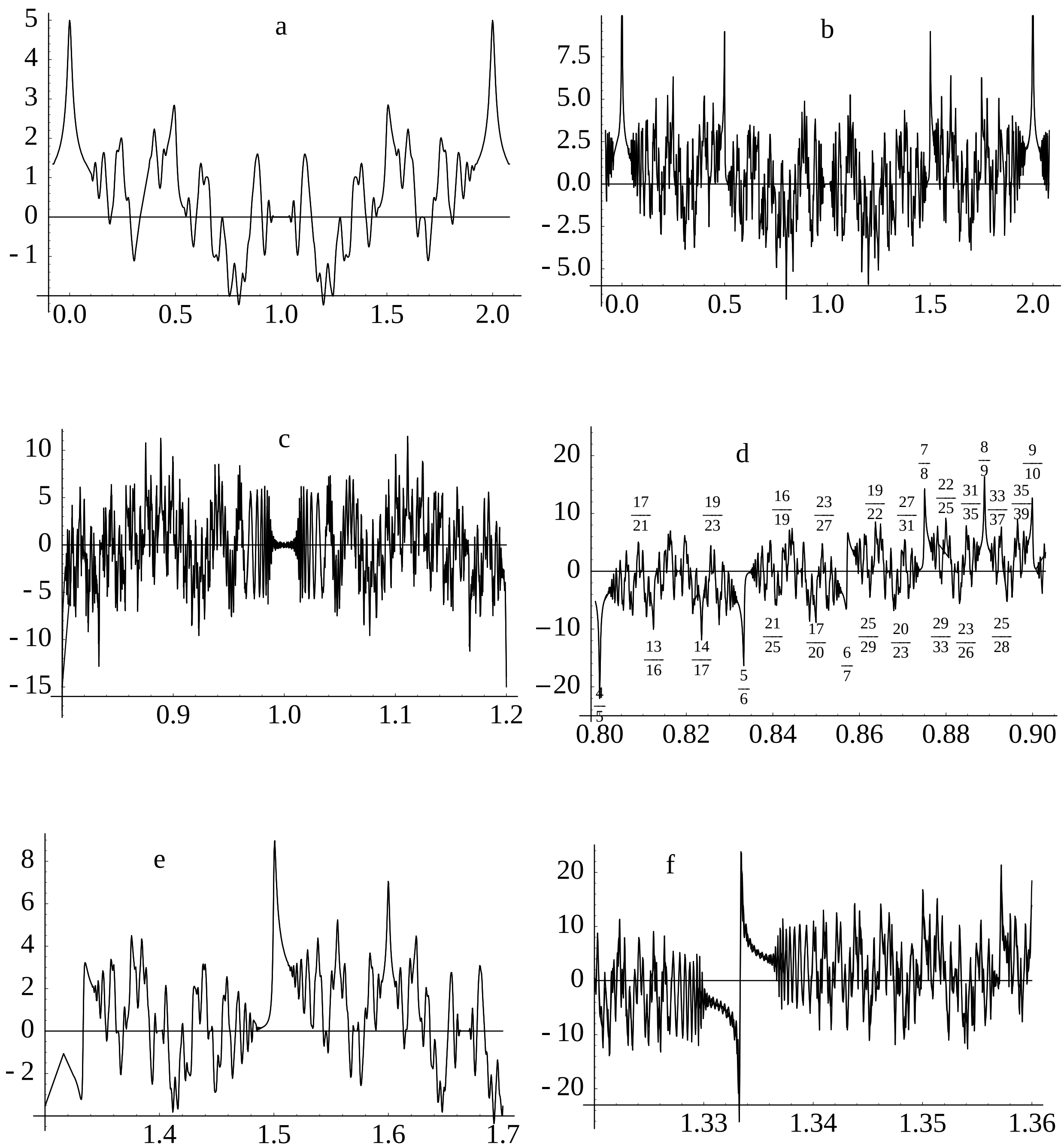

FIG. 1: $\mathrm{Re}\,U(t - i\epsilon, 0, 0)$ as a function of t. In comparing graphs, it is important to note the changes of vertical scale. (a) $\epsilon = 0.01$ ($n_{\max} = k_{\max} = 50$). (b) $\epsilon = 0.001$ ($n_{\max} = k_{\max} = 50$). (c) $0.8 \le t \le 1.2$, $\epsilon = 0.0001$ ($n_{\max} = k_{\max} = 40$). (d) $0.8 \le t \le 0.9$, $\epsilon = 0.0001$ ($n_{\max} = k_{\max} = 100$); simple fractional values of t are marked. (e) $1.3 \le t \le 1.7$, $\epsilon = 0.001$ ($n_{\max} = k_{\max} = 100$); peaks at $t = 3/2$ and $8/5$ are prominent. (f) $1.32 \le t \le 1.36$, $\epsilon = 0.00001$ ($n_{\max} = k_{\max} = 100$); the peak at $t = 4/3$ is seen "sideways" because of its complex phase.

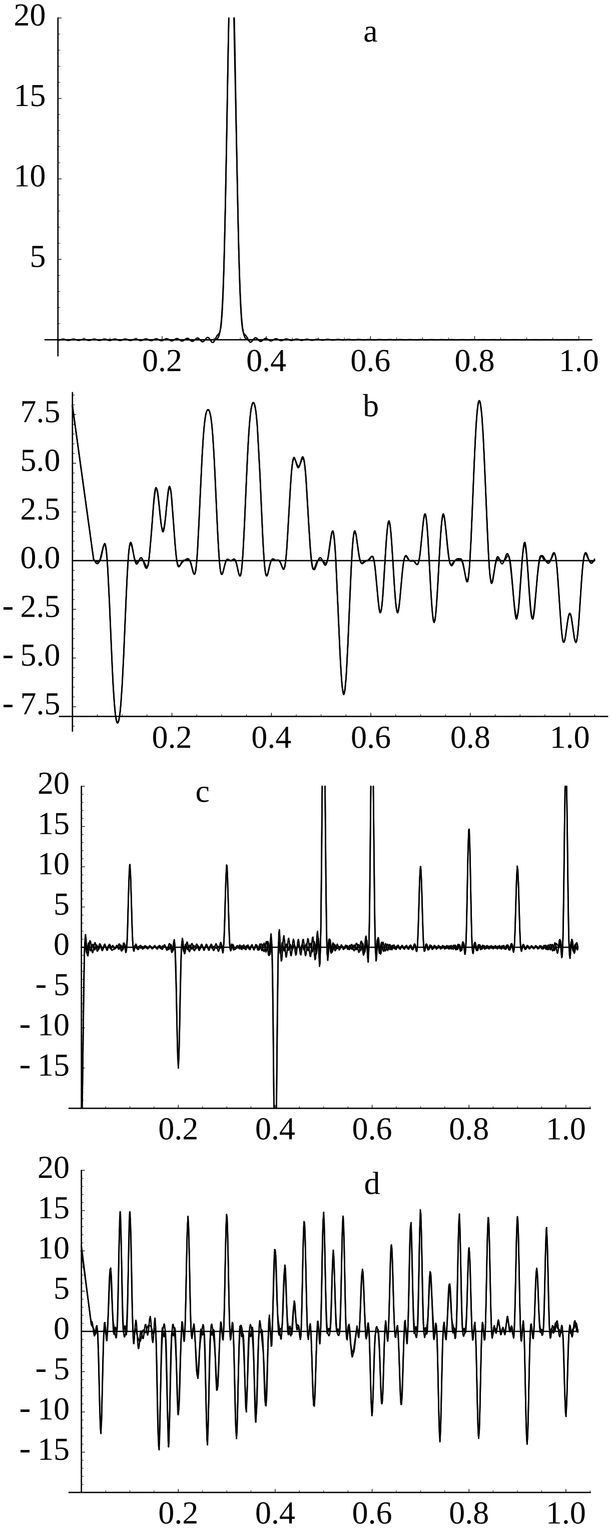

FIG. 2: Re $U(t - i\epsilon, x, 0)$ as function of x. (a) $t = 1/3$, $\epsilon = 0.0001$ ($n_{\max} = k_{\max} = 100$). (b) $t = 1/\pi$, $\epsilon = 0.0001$ ($n_{\max} = k_{\max} = 100$). (c) $t = 0.85$ ($q = 20$), $\epsilon = 0.00001$ ($n_{\max} = k_{\max} = 200$). (d) $t = 0.87$ ($q = 100$), $\epsilon = 0.00001$ ($n_{\max} = k_{\max} = 200$).

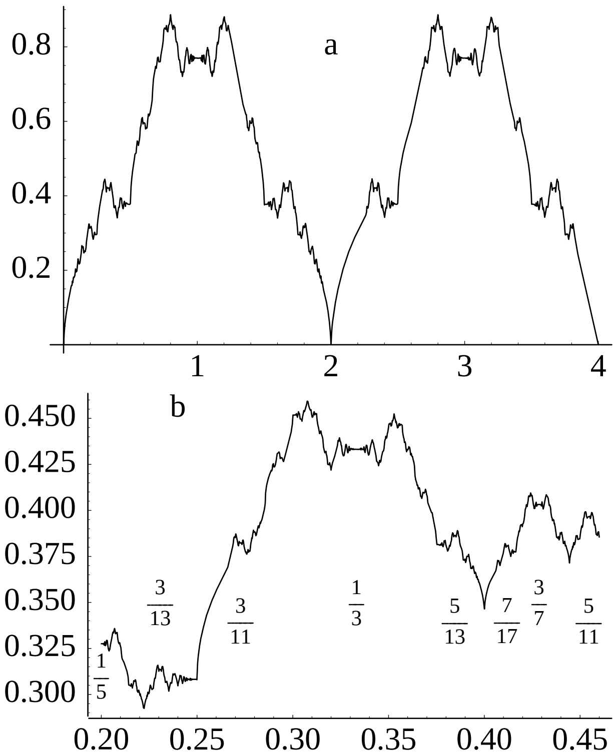

FIG. 3: (a) Two periods of $\mathrm{Re}\,P(t,0)$ ($k_{\mathrm{max}} = 20$). (b) Closeup of $\mathrm{Re}\,P(t,0)$ near $t = 1/3$ ($k_{\mathrm{max}} = 100$). A distinctive pattern is reproduced near the totally odd fractions, which are related to $t = 1$ by the symmetries of Theorem 1. Cusps develop at the fractions with even parts, which are related to $t = 0$ by the symmetries.

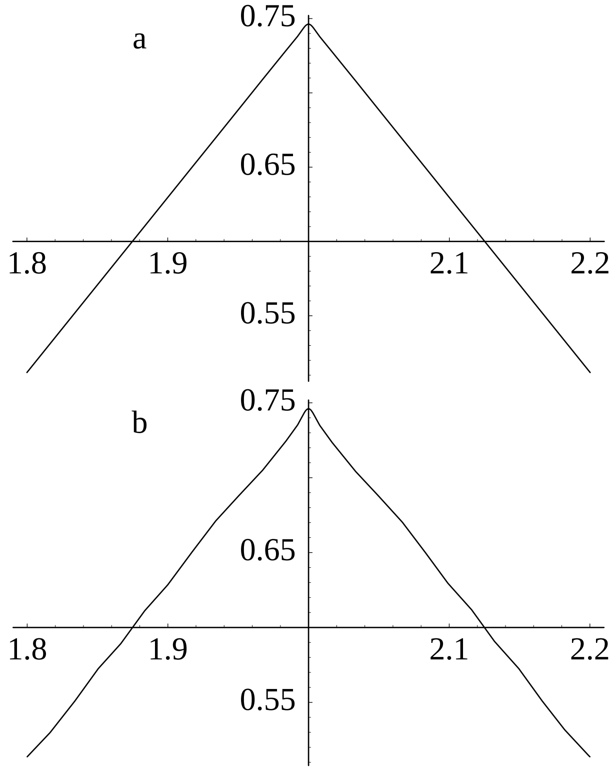

FIG. 4: (a) $\mathrm{Re}\, P(t,x)$ at $t = 7/8 = 0.875$, for x near 1 ($k_{\max} = 200$). The plot is almost exactly piecewise linear, representing a term proportional to $\delta(x-1)$ in its second derivative. (b) The same at a randomly chosen nearby time, $t = 0.8761234$.