DO BOXED WAVEPACKETS BECOME FLAT?

Remarks concerning the delocalization/recurrence paradox

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Introduction. Write

$$\left\{ \tfrac{\hbar^2}{2m}\left(\tfrac{\partial}{\partial x}\right)^2 + i\hbar\tfrac{\partial}{\partial t} \right\}\psi(x,t) = 0 \tag{1}$$

to describe the 1-dimensional quantum motion of a mass point m. Assume $\psi(x,0)$ to have the form

$$\psi(x,0) = \left[\tfrac{1}{\sigma\sqrt{2\pi}} \right]^{\frac{1}{2}} \exp\left\{ -\tfrac{1}{4}\left[\tfrac{x-a}{\sigma} \right]^2 \right\} \tag{2}$$

where a and σ are prescribed constants. Then

$$P(x,0) \equiv |\psi(x,0)|^2 = \tfrac{1}{\sigma\sqrt{2\pi}} \exp\left\{ -\tfrac{1}{2}\left[\tfrac{x-a}{\sigma} \right]^2 \right\} \tag{3}$$

is a normalized Gaussian:

$$\int_{-\infty}^{+\infty} P(x,0)\,dx = 1$$

The evolved wave function can, as is well known,[1] be described

$$\psi(x,t) = \left[\tfrac{1}{\sigma[1+i(t/\tau)]\sqrt{2\pi}} \right]^{\frac{1}{2}} \exp\left\{ -\tfrac{1}{4}\tfrac{(x-a)^2}{\sigma^2[1+i(t/\tau)]} \right\} \tag{4}$$

provided we set the "natural time" parameter

$$\tau = 2m\sigma^2/\hbar \tag{5}$$

This amounts, by the way, to setting $2m = \hbar\tau/\sigma^2$, in which notation the

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[1] See "Gaussian wavepackets" (1998), page 4.

Schrödinger equation (1) assumes the simpler appearance

$$\left\{ \sigma^2 \left(\tfrac{\partial}{\partial x}\right)^2 + i\tau \tfrac{\partial}{\partial t} \right\} \psi(x,t) = 0 \tag{6}$$

Mathematica is quick to verify that (4) does in fact describe a solution of (6). From (6) we obtain

$$P(x,t) \equiv |\psi(x,t)|^2 = \tfrac{1}{\sigma(t)\sqrt{2\pi}} \exp\left\{ -\tfrac{1}{2} \left[\tfrac{x-a}{\sigma(t)}\right]^2 \right\} \tag{7.1}$$

with

$$\sigma(t) \equiv \sigma\sqrt{1 + (t/\tau)^2} \tag{7.2}$$

Equations (7) describe a *dispersing Gaussian*:

$$\left. \begin{array}{c} \langle \mathbf{x} \rangle = a \\[2mm] \Delta x \equiv \sqrt{\langle \mathbf{x}^2 \rangle - \langle \mathbf{x} \rangle^2} = \sigma(t) \end{array} \right\} \quad : \quad t > 0 \tag{8}$$

That we become progressively more and more uncertain where measurement would show the free particle to reside has from the outset be recognized to be one of the most characteristic features of quantum theory. I turn now to discussion intended to underscore the fact that the point at issue retains its validity even after abandonment of the the assumption that $P(x,0)$ is Gaussian.

Free particle eigenfunctions can be described

$$\psi_p(x) \equiv \tfrac{1}{\sqrt{h}} e^{\frac{i}{\hbar}px} \tag{9.1}$$

and to describe the temporal evolution of such a function we have

$$\psi_p(x,t) \equiv \tfrac{1}{\sqrt{h}} e^{\frac{i}{\hbar}[px - (p^2/2m)t]} \tag{9.2}$$

The Gaussian wavepacket (2) can be displayed as a weighted superposition of such eigenfunctions:

$$\left[\tfrac{1}{\sigma\sqrt{2\pi}}\right]^{\frac{1}{2}} \exp\left\{ -\tfrac{1}{4} \left[\tfrac{x-a}{\sigma}\right]^2 \right\} = \int_{-\infty}^{+\infty} \varphi(p) \tfrac{1}{\sqrt{h}} e^{\frac{i}{\hbar}px} \, dp$$

with

$$\varphi(p) = \int_{-\infty}^{+\infty} \left[\tfrac{1}{\sigma\sqrt{2\pi}}\right]^{\frac{1}{2}} \exp\left\{ -\tfrac{1}{4} \left[\tfrac{x-a}{\sigma}\right]^2 \right\} \tfrac{1}{\sqrt{h}} e^{-\frac{i}{\hbar}px} \, dx$$

$$= \left[\tfrac{1}{\lambda\sqrt{2\pi}}\right]^{\frac{1}{2}} \exp\left\{ -\tfrac{1}{4} \left[\tfrac{p}{\lambda}\right]^2 \right\} e^{-\frac{i}{\hbar}ap} \tag{10.1}$$

where

$$\lambda \equiv \hbar/2\sigma$$

The effect of launching such an eigenfunction can be described

$$\int_{-\infty}^{+\infty} \varphi(p) \tfrac{1}{\sqrt{h}} e^{\frac{i}{\hbar}px} \, dp \quad \longmapsto \quad \int_{-\infty}^{+\infty} \varphi(p) \tfrac{1}{\sqrt{h}} e^{\frac{i}{\hbar}[px-(p^2/2m)t]} \, dp \qquad (10.2)$$

and is found by calculation to give back (4).

Look now, by way of comparison, to the case[2]

$$\psi(x,0) = \begin{cases} \frac{1}{\sqrt{2b}} & : \quad x^2 < b^2 \\ \\ 0 & : \quad x^2 \geqslant b^2 \end{cases} \qquad (11)$$

In this instance $P(x,0) \equiv |\psi(x,0)|^2$ is *constant* on the interval $-b \leqslant x \leqslant +b$ and vanishes elsewhere. The argument that gave (10.1) now gives

$$\begin{aligned} \varphi(p) &= \int_{-b}^{+b} \tfrac{1}{\sqrt{2bh}} e^{-\frac{i}{\hbar}px} \, dx \\ &= \tfrac{\sqrt{\hbar}}{p\sqrt{\pi b}} \sin \tfrac{bp}{\hbar} \end{aligned} \qquad (12)$$

As a check on the accuracy of this weight function we compute

$$\begin{aligned} \psi(x,0) &= \int_{-\infty}^{+\infty} \tfrac{\sqrt{\hbar}}{p\sqrt{\pi b}} \sin \tfrac{bp}{\hbar} \cdot \tfrac{1}{\sqrt{h}} e^{\frac{i}{\hbar}px} \, dp \\ &= \tfrac{1}{\sqrt{2b}} \cdot \tfrac{1}{2} \Big\{ \varepsilon(x+b) - \varepsilon(x-b) \Big\} \quad \text{where} \quad \varepsilon(x) \equiv \begin{cases} +1 & : \quad x > 0 \\ 0 & : \quad x = 0 \\ -1 & : \quad x < 0 \end{cases} \\ &= \tfrac{1}{\sqrt{2b}} \cdot \Big\{ \theta(x+b) - \theta(x-b) \Big\} \quad \text{where} \quad \theta(x) \equiv \begin{cases} 1 & : \quad x > 0 \\ \frac{1}{2} & : \quad x = 0 \\ 0 & : \quad x < 0 \end{cases} \\ &= \tfrac{1}{\sqrt{2b}} \cdot \theta(b^2 - x^2) \end{aligned}$$

This result[3] is easily seen to be in precise agreement with (11). Looking to the temporal evolution of such a "box packet" we undertake to compute

$$\begin{aligned} \psi(x,t) = \int_{-\infty}^{+\infty} \tfrac{\sqrt{\hbar}}{p\sqrt{\pi b}} \sin \tfrac{bp}{\hbar} \\ \cdot \tfrac{1}{\sqrt{h}} \Big\{ \cos\big[\tfrac{1}{\hbar}\big(px - \tfrac{p^2}{2m}t\big)\big] + i \sin\big[\tfrac{1}{\hbar}\big(px - \tfrac{p^2}{2m}t\big)\big] \Big\} \, dp \end{aligned}$$

Mathematica supplies

$$= F(x,t) + iG(x,t) \qquad (13)$$

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[2] I owe my special interest in this case to a conversation with David Griffiths (August 2003).

[3] The step functions (or "switches") $\varepsilon(x)$ and $\theta(x)$ are known to *Mathematica* as `Sign[x]` and `UnitStep[x]`, respectively. For review of their properties see Chapter 8 in J. Spanier & K. B. Oldham, *An Atlas of Functions* (1987).

where $F(x,t)$ and $G(x,t)$ are sums of "generalized hypergeometric functions" multiplied by algebraic functions and switches (but so complicated that it would serve no useful purpose to write them out). We construct

$$P(x,t) \equiv |\psi(x,t)|^2 = F^2(x,t) + G^2(x,t) \tag{14}$$

and note that, according to *Mathematica*, $F(x,t)$ & $G(x,t)$ are—non-obviously but not surprisingly—both *even* functions of x:

$$F(x,t) = F(-x,t) \quad \text{and} \quad G(x,t) = G(-x,t)$$

So $P(x,t)$ is even, from which it follows immediately that

$$\langle \mathbf{x}^{\text{odd}} \rangle_t = \int_{-\infty}^{+\infty} x^{\text{odd}} P(x,t)\, dx = 0 \quad : \quad \text{all } t$$

From $P(x,0) = \frac{1}{2b}\theta(b^2 - x^2)$ we find that initially

$$\langle \mathbf{x}^{2n} \rangle_0 = \frac{b^{2n}}{n+1} \quad : \quad n = 0, 1, 2, \ldots \tag{15.1}$$

But *Mathematica* seems to be powerless to compute

$$\langle \mathbf{x}^{2n} \rangle_t \equiv 2 \int_0^\infty x^{2n} P(x,t)\, dx \tag{15.2}$$

except numerically, and even with the numerical integration it has to struggle ... for reasons that I will undertake later to explain.

As it happens, there exists an illuminating general line of argument—which I digress now to review—that enables one to circumvent (or at least to reduce the sting of) difficulties of the sort just encountered. I have described elsewhere[4] the sense in which quantum mechanics can be looked upon as a "theory of interactive moments." Within that formalism it becomes the business of the Hamiltonian operator to set the system-specific design of the coupled "moment equations" that lie at the analytic heart of the theory. I have shown in particular that in the case $\mathbf{H} = \frac{1}{2m}\mathbf{p}^2$ one has

$$\left. \begin{aligned} \frac{d}{dt}\langle \mathbf{p} \rangle &= 0 \\ \frac{d}{dt}\langle \mathbf{x} \rangle &= \tfrac{1}{m}\langle \mathbf{p} \rangle \\ \\ \frac{d}{dt}\langle \mathbf{p}^2 \rangle &= 0 \\ \frac{d}{dt}\langle \mathbf{xp} + \mathbf{px} \rangle &= \tfrac{2}{m}\langle \mathbf{p}^2 \rangle \\ \frac{d}{dt}\langle \mathbf{x}^2 \rangle &= \tfrac{1}{m}\langle \mathbf{xp} + \mathbf{px} \rangle \\ &\vdots \end{aligned} \right\} \tag{16}$$

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[4] See *Advanced Quantum Topics* (2000), Chapter 2 ("Weyl Transform & the Phase Space Formalism"), pages 51–60.

from which it follows that

$$
\left.\begin{aligned}
\langle \mathbf{p} \rangle_t &= p_0 \\
\langle \mathbf{x} \rangle_t &= x_0 + \tfrac{1}{m} p_0 t \\[6pt]
\langle \mathbf{p}^2 \rangle_t &= \wp^2 \\
\langle \mathbf{x}\mathbf{p} + \mathbf{p}\mathbf{x} \rangle_t &= s + \tfrac{2}{m}\wp^2 t \\
\langle \mathbf{x}^2 \rangle_t &= \xi^2 + \tfrac{1}{m} s t + \tfrac{1}{m^2}\wp^2 t^2 \\
&\ \ \vdots
\end{aligned}\right\}
\tag{17}
$$

Here p_0, x_0, $\wp^2$, s and ξ^2 are constants of evident physical dimension. From

$$
\left.\begin{aligned}
p_0 &= \langle \mathbf{p} \rangle_0 = \int \psi^*(x,0)\, \mathbf{p}\, \psi(x,0)\, dx \\
x_0 &= \langle \mathbf{x} \rangle_0 = \int \psi^*(x,0)\, \mathbf{x}\, \psi(x,0)\, dx \\
\wp^2 &= \langle \mathbf{p}^2 \rangle_0 = \int \psi^*(x,0)\, \mathbf{p}^2\, \psi(x,0)\, dx \\
s &= \langle \mathbf{x}\mathbf{p} + \mathbf{p}\mathbf{x} \rangle_0 = \int \psi^*(x,0)\, (\mathbf{x}\mathbf{p} + \mathbf{p}\mathbf{x})\, \psi(x,0)\, dx \\
\xi^2 &= \langle \mathbf{x}^2 \rangle_0 = \int \psi^*(x,0)\, \mathbf{x}^2\, \psi(x,0)\, dx
\end{aligned}\right\}
\tag{18}
$$

we see that they can be considered to derive their numerical values from the prescribed structure of $\psi(x,0)$. One has to evaluate only *initial* integrals to evaluate the constants, and can then use (17) to obtain descriptions of the evolved moments: one is thus spared the tedium of trying to evaluate evolved integrals ... which is one of the advantages afforded by the program. Another is that one can use it to draw certain *general* conclusions. Observe, for example, that equations (17) entail

$$
(\Delta x)_t^2 \equiv \langle \mathbf{x}^2 \rangle_t - \langle \mathbf{x} \rangle_t^2 = \alpha + \beta(t - t_0)^2
\tag{19.1}
$$

with

$$
\left.\begin{aligned}
\alpha &= (\xi^2 - x_0^2) - \frac{(s - 2x_0 p_0)^2}{4(\wp^2 - p_0^2)} \\
\beta &= \frac{\wp^2 - p_0^2}{m^2} \\
t_0 &= -\frac{s - 2x_0 p_0}{2(\wp^2 - p_0^2)}
\end{aligned}\right\}
\tag{19.2}
$$

If, in particular, $\psi(x,0)$ is Gaussian, as described by (2), we compute

$$p_0 = 0$$
$$x_0 = a$$
$$\wp^2 = \left(\tfrac{\hbar}{2\sigma}\right)^2$$
$$s = 0$$
$$\xi^2 = a^2 + \sigma^2$$

from which it follows in particular that

$$\alpha = \sigma^2$$
$$\beta = \left(\tfrac{\hbar}{2m\sigma}\right)^2$$
$$t_0 = 0$$

whence

$$(\Delta x)_t^2 = \sigma^2 + \left(\tfrac{\hbar}{2m\sigma}\right)^2 t^2$$
$$= \sigma^2 \left[1 + (t \cdot \hbar/2m\sigma^2)^2\right]$$

We have recovered precisely (7.2), but by an argument which underscores the important fact that the hyperbolic growth of $(\Delta x)_t$ is not special to Gaussians: it pertains to the free-body motion of *all* wavepackets for which the relevant initial moments are well-defined.

Look back again, in this light, to the case (11) of the boxpacket

$$\psi(x,0) = \tfrac{1}{\sqrt{2b}} \cdot \left\{\theta(x+b) - \theta(x-b)\right\}$$

We know already that

$$x_0 \equiv \langle \mathbf{x} \rangle_0 = 0 \qquad \text{and} \qquad \xi^2 \equiv \langle \mathbf{x}^2 \rangle_0 = \tfrac{1}{3}b^2$$

That

$$p_0 \equiv \langle \mathbf{p} \rangle_0 = 0$$

can be argued in several ways: we might write

$$p_0 = \tfrac{1}{2b} \int \left\{\theta(x+b) - \theta(x-b)\right\} \tfrac{\hbar}{i} \tfrac{\partial}{\partial x} \left\{\theta(x+b) - \theta(x-b)\right\} dx$$
$$= \tfrac{1}{2b} \tfrac{\hbar}{i} \int \left\{\theta(x+b) - \theta(x-b)\right\} \left\{\delta(x+b) - \delta(x-b)\right\} dx$$
$$= \tfrac{1}{2b} \tfrac{\hbar}{i} \left\{\theta(0) - \theta(-2b) - \theta(+2b) + \theta(0)\right\}$$
$$= \tfrac{1}{2b} \tfrac{\hbar}{i} \left\{\tfrac{1}{2} - 0 - 1 + \tfrac{1}{2}\right\} = 0$$

though that line of argument seems precariously formal. Alternatively, we might appeal to the general observation that if $\psi(x)$ is real-valued then

$$\int \psi(x) \tfrac{\hbar}{i} \tfrac{\partial}{\partial x} \psi(x) \, dx \quad \left\{\begin{array}{l} \text{is transparently imaginary} \\ \text{but must be real, so vanishes} \end{array}\right.$$

Or we could elect to work in the momentum representation, from (12):

$$\varphi(p) = \frac{\sqrt{\hbar}}{p\sqrt{\pi b}} \sin \frac{bp}{\hbar}, \quad \text{which is an } even \; real\text{-}valued \text{ function of } p$$

Direct calculation confirms that

$$\int_{-\infty}^{+\infty} \varphi(p) \, p^0 \varphi(p) \, dp = 1$$

and that

$$p_0 = \int_{-\infty}^{+\infty} \varphi(p) \, p^1 \varphi(p) \, dp = 0$$

But when we look by this means to $\wp^2 \equiv \langle \mathbf{p}^2 \rangle_0$ we are informed that

$$\wp^2 = \int_{-\infty}^{+\infty} \varphi(p) \, p^2 \varphi(p) \, dp = \infty \quad \text{(does not converge)}$$

Argument in the x-representation is more formal

$$\wp^2 = -\tfrac{\hbar^2}{2b} \int \left\{ \theta(x+b) - \theta(x-b) \right\} \left\{ \delta'(x+b) - \delta'(x-b) \right\} dx$$

$$= +\tfrac{\hbar^2}{2b} \int \left\{ \delta(x+b) - \delta(x-b) \right\} \left\{ \delta(x+b) - \delta(x-b) \right\} dx$$

$$= +\tfrac{\hbar^2}{2b} \left\{ \delta(0) - \delta(-2b) - \delta(+2b) + \delta(0) \right\}$$

$$= +\tfrac{\hbar^2}{2b} \left\{ \infty - 0 - 0 + \infty \right\} \; : \; \text{undefined}$$

and therefore less convincing, but appears to lead to the same conclusion. Look finally to the value of $s \equiv \langle \mathbf{xp} + \mathbf{px} \rangle_0 = \langle 2\mathbf{px} + i\hbar\mathbf{I} \rangle_0 = 2\langle \mathbf{px} \rangle_0 + i\hbar$. Working in the momentum representation we have

$$s = i\hbar + 2 \int_{-\infty}^{+\infty} \varphi(p) \, p\left(-\tfrac{\hbar}{i} \tfrac{\partial}{\partial p} \right) \varphi(p) \, dp = i\hbar - i\hbar = 0$$

which—arguing as before—we might consider to have been forced by the reality of $\varphi(p)$. Returning with the information now in hand to (19.2) we find

$$\alpha = \left(\tfrac{1}{3}b^2 - 0^2 \right) - \frac{(0 - 2 \cdot 0 \cdot 0)^2}{4(\infty - 0^2)} = \tfrac{1}{3}b^2$$

$$\beta = \frac{\infty - 0^2}{m^2} = \infty$$

$$t_0 = -\frac{0 - 2 \cdot 0 \cdot 0}{2(\infty - 0^2)} = 0$$

from which it would appear (by (19.1)) to follow

$$(\Delta x)_t^2 = \tfrac{1}{3}b^2 + \infty \cdot t^2 = \left\{ \begin{array}{lll} \tfrac{1}{3}b^2 & : & t = 0 \\ \infty & : & t > 0 \end{array} \right. \tag{20}$$
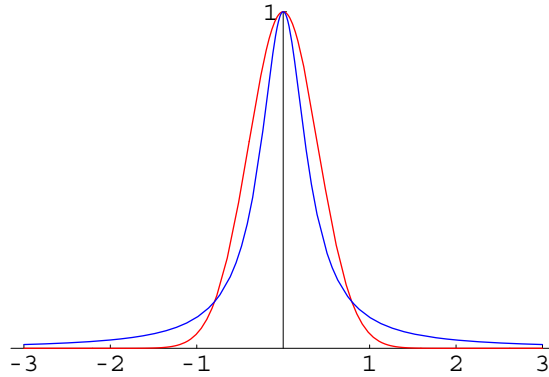
FIGURE 1: *Comparative display of the Gaussian distribution $G(x, \sigma)$ and the Lorentzian distribution $L(x, a)$. To facilitate the comparison I have set $\sigma = 1/\sqrt{\pi}$ and $a = 1/\pi$ so as to achieve $G_{\max} = L_{\max} = 1$. The Lorentzian distribution is seen to have a relatively sharp central peak but relatively broad shoulders. It is, in Richard Crandall's despairing opinion, "too fat"—so fat that $\langle x^2 \rangle = \infty$.*
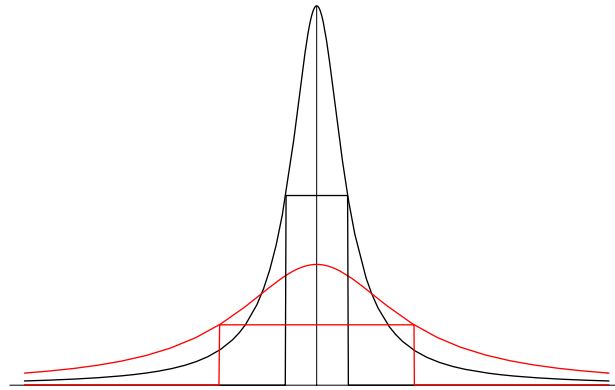

FIGURE 2: *A Lorentzian distribution falls to half of its maximal value $1/a\pi$ at $x = \pm a$ ... which the superimposed boxes are intended to illustrate: each box stands half as high as its associated curve.*

That (20) describes a situation which is not so bizarre as it might at first appear is readily established by example. Let $G(x; \sigma)$ be Gaussian (or "normal") and let $L(x, a)$ describe what physicists call a Lorentzian (and mathematicians

call a Cauchy) distribution:[5]

$$G(x, \sigma) = \frac{1}{\sigma\sqrt{\pi}} e^{-(x/\sigma)^2}$$
$$L(x; a) = \frac{1}{a\pi} \frac{1}{1 + (x/a)^2}$$

Both distributions functions are even, so in both cases $\langle x^{\text{odd}} \rangle = 0$. The normal distribution is well known to possess even moments of all orders, while if we look to

$$\langle x^{\text{odd}} \rangle_{\text{Lorentz}} \equiv \lim_{k \uparrow \infty} \int_{-k}^{+k} x^{\text{even}} L(x; a) \, dx$$

we discover that the even-order moments of the Lorentz distribution are (except for the moment of order zero) all infinite—this even though graphs the two distributions (Figure 1) appear to have pretty much the same shape. Now construct the distribution

$$W(x; \sigma, a; \epsilon) \equiv (1 - \epsilon)G(x, \sigma) + \epsilon L(x; a)$$

and look in particular to the 2nd moment of that distribution:

$$\langle x^2 \rangle_\epsilon \equiv \lim_{k \uparrow \infty} \int_{-k}^{+k} x^2 W(x; \sigma, a; \epsilon) \, dx$$

It is evident from preceding remarks that

$$\langle x^2 \rangle_\epsilon = \begin{cases} \frac{1}{2}a & : & \epsilon = 0 \\ \infty & : & \epsilon \neq 0 \end{cases}$$

which provides a simple instance of the phenomenon encountered at (20). When $\langle x^2 \rangle$ is not available—as, even in simple situations, it sometimes isn't!—one must look to some other device to describe the "width" of a distribution. In the Lorentzian case it is natural to look to (say) the distance between the points at which $L(x, a) = \frac{1}{2}(\text{maximal value})$, which (by easy calculation: see Figure 2) would be to take

$$\text{Lorentzian ``width"} = 2a$$

We are, however, destined to confront a case in which those "half-max points" are not easily located, and can readily imagine cases in which there are more than two of them ... or none. There appears to be no universally available natural descriptor of "distribution width."

We encountered at (20) a situation that, if not "bizarre," is nevertheless unprecedented in my experience, and is the fruit of a non-standard line of argument. Can it be illuminated by *direct* analysis of $\langle \mathsf{x}^2 \rangle$? I have described at

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[5] For review of the basic properties of Lorentzian distribution functions, see pages 415–417 in Chapter 7 of PRINCIPLES OF CLASSICAL ELECTRODYNAMICS (2001/2002).

the construction of functions $F(x,t;b,m,\hbar)$ and $G(x,t;b,m,\hbar)$ from which, at (14), was assembled the distribution $P(x,t;b,m,\hbar)$ that in time t evolves from an initially box-like wavepacket:
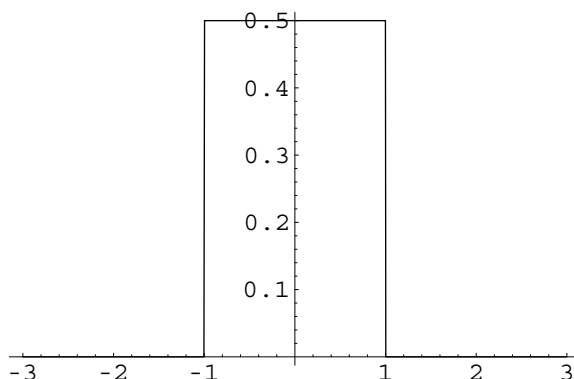

FIGURE 3: *Initial probability distribution* $P_{\mathrm{box}}(x,0) = |\psi_{\mathrm{box}}(x,0)|^2$ *in the case* $b = 1$.

Confining our explicit attention henceforth to the illustrative case

$$b = m = \hbar = 1$$

we find[6] that $P_{\mathrm{box}}(x,t)$, thus constructed, has the complicated structure

$$P(x,t) = \tfrac{1}{288t^3}\Big[-6t\sqrt{(1-x)^2}\,\varepsilon(1-x)\mathrm{HypergeometricPFQ}\big(\big\{\tfrac{3}{4}\big\},\big\{\tfrac{1}{2},\tfrac{5}{4}\big\},-\tfrac{(1-x)^4}{16t^2}\big)$$

$$+ \text{three similar terms}\,\Big]^2 + \Big[\, \text{similar mess}\,\Big]^2 \tag{21}$$

One might suppose that a graph of $P(x,0)$ would reproduce Figure 3, but *Mathematica* refuses to draw such a graph, claiming that it has encountered indeterminate expressions and complex singularities. That it has a hard time at small times is clear from Figure 4. By $t = 0.005$ *Mathematica* is willing—if given enough time—to draw (Figure 5) at least the central part of $P(x,0.005)$, but at about $x \approx 0.4$ begins to encounter wild fluctuations and to bog down. As t becomes progressively larger *Mathematica* finds it progressively easier to plot $P(x,t)$, but—see Figures 6, 7 & 8—always displays, on left and right, twin regions of wild fluctuation. The twins become progressively more remote, but appear to be invariably separated by the length of the initial box. I have made no attempt to account theoretically for those experimental observations, partly because such an effort would require one to dig deeply into the intricacies of (21) but mainly because a separate line of argument (see below) suggests that the twinned fluctuations in question are spurious—an artifact created by *Mathematica* itself.

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[6] I urge my reader to turn on *Mathematica* and prepare actually to *do* the calculations to which I allude in the text.
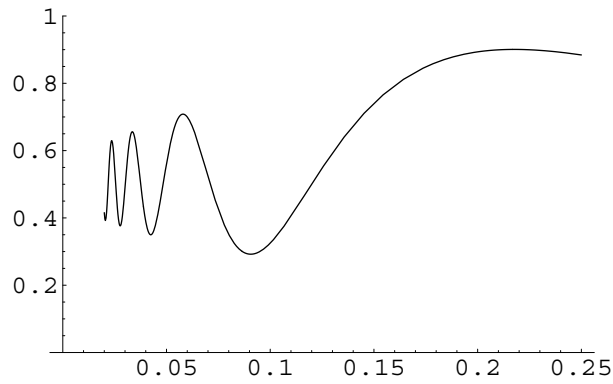
FIGURE 4: *Graph—derived from* (21)*—of* $P(0,t)$ *at short times. As* $t \downarrow 0$ *the oscillations become faster and faster. At times* $t > 0.25$ *the central value* $P(0,t)$ *of the distribution drops "exponentially" to zero.*
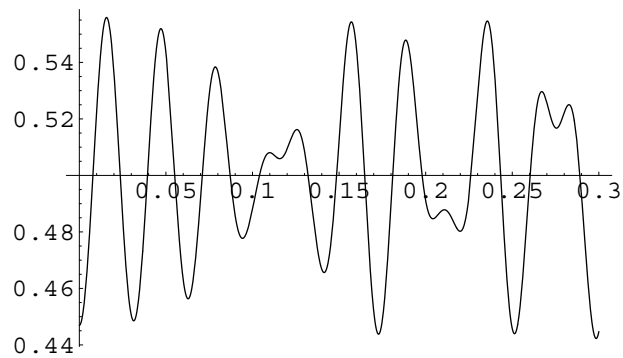

FIGURE 5: *Central portion of* $P(x,t)$ *at time* $t = 0.005$. *The curve is seen to dither about its initial value* $P(x,0) = \frac{1}{2}$. *If extended to slightly larger values of* x *the graph would show wild fluctuations. One the interval* $-0.3 \leqslant x \leqslant 0$ *one encounters the mirror image of the curve shown.*
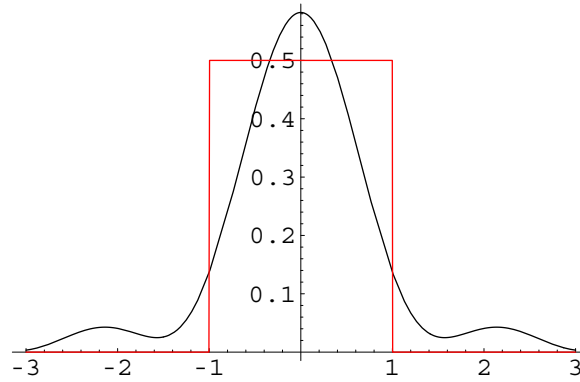
FIGURE 6: *Central portion of the evolved distribution $P(x, 0.5)$, superimposed upon a graph of the original distribution $P(x, 0)$.*
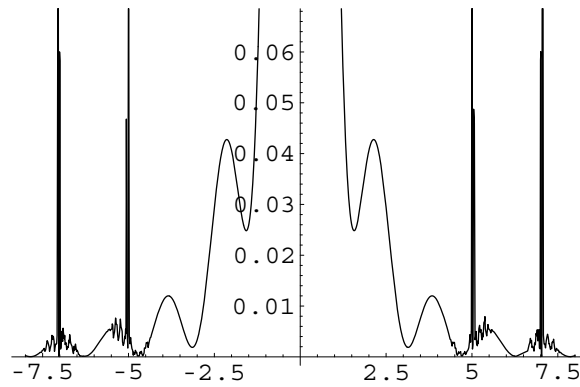

FIGURE 7: *Extended (and much magnified) version of the preceding figure, showing complications in the neighborhoods of $x = \pm 5$ and $x = \pm 7$. Note that $7 - 5 = 2$, the width of the original packet. For $x > 8$ the chaotic oscillations settle down, and the curve becomes gently undulatory again.*
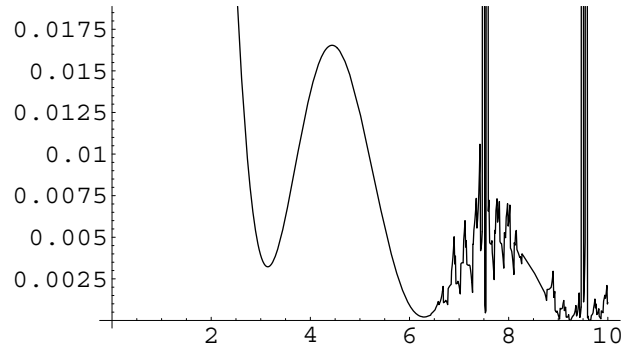
FIGURE 8: *Right half of a graph of $P(x,t)$ drawn at the later time $t = 1.0$. Note the high magnification, and that while the spikes have shifted to the right during the last half second they retain their former separation. I cannot—have not really attempted— to account analytically for the fact that these trends appear, on numerical/graphical evidence, to be persistent.*

The $\psi(x,t)$ that evolves from $\psi(x,0)$ can, in principle, be described

$$\psi(x,t) = \int_{-\infty}^{+\infty} K(x,t;y,0)\,\psi(y,0)\,dy$$

where $K(x,t;y,0)$ is the propagator … which, as is well known, is in the present instance given by

$$K(x,t;y,0) = \sqrt{\tfrac{m}{i\,2\pi\hbar t}}\,\exp\left\{\tfrac{i}{\hbar}\tfrac{(x-y)^2}{t}\right\}$$

We expect therefore to have

$$\psi_{\text{box}}(x,t) = \int_{-\infty}^{+\infty} K(x,t;y,0)\,\psi_{\text{box}}(y,0)\,dy$$

$$= \sqrt{\tfrac{m}{i\,2\pi\hbar t}\tfrac{1}{2b}}\int_{-b}^{+b}\exp\left\{\tfrac{i}{\hbar}\tfrac{(x-y)^2}{t}\right\}dy$$

Again (at this point, rather than later) setting $b = m = \hbar = 1$, we present the integral to *Mathematica*, who (with some coaxing) supplies

$$= i\tfrac{1}{2\sqrt{2}}\left\{\quad \texttt{Erfi}\left[\frac{(-)^{\frac{1}{4}}(x-1)}{\sqrt{2t}}\right]\right.$$

$$\left. - \texttt{Erfi}\left[\frac{(-)^{\frac{1}{4}}(x+1)}{\sqrt{2t}}\right]\right\} \tag{22}$$

We now use the command `ComplexExpand[%]` to resolve this result into its real and imaginary parts. After assuring *Mathematica* that we understand t to be a positive real number we obtain

$$\psi_{\text{box}}(x,t) = \tilde{F}(x,t) + i\tilde{G}(x,t)$$

where

$$\tilde{F}(x,t) = -\tfrac{1}{2\sqrt{2}}\left\{ \text{Im}\left(\text{Erfi}\left[\frac{(-)^{\frac{1}{4}}(x-1)}{\sqrt{2t}} \right] \right) - \text{Im}\left(\text{Erfi}\left[\frac{(-)^{\frac{1}{4}}(x+1)}{\sqrt{2t}} \right] \right) \right\}$$

$$\tilde{G}(x,t) = \tfrac{1}{2\sqrt{2}}\left\{ \text{Re}\left(\text{Erfi}\left[\frac{(-)^{\frac{1}{4}}(x-1)}{\sqrt{2t}} \right] \right) - \text{Re}\left(\text{Erfi}\left[\frac{(-)^{\frac{1}{4}}(x+1)}{\sqrt{2t}} \right] \right) \right\}$$

may look to us like paraphrases of the question, but are evidently understood by *Mathematica* to be answers. The functions $\tilde{F}$ and $\tilde{G}$ should be identical to the F and G encountered at (13) on page 3, but wear tildes to emphasize that they have been assembled now not from `HypergeometricPFQ` functions but from the so-called "imaginary error function"

$$\text{erfi}(z) \equiv \frac{\text{erf}(iz)}{i} \qquad \text{where} \qquad \text{erf}(z) \equiv \tfrac{2}{\sqrt{\pi}} \int_0^z e^{-t^2}\, dt$$

Finally we ask *Mathematica* to construct

$$\tilde{P}(x,t) = \tilde{F}^2(x,t) + \tilde{G}^2(x,t)$$

which is a sum of six terms that it would serve no useful purpose to write out in detail. Possibly Euler, if presented with T_EX'd renditions of $P(x,t)$ and $\tilde{P}(x,t)$, would recognize that they provide alternative descriptions of the same function, but I do not know off hand how to establish the point . . . except to remark that if one uses $\tilde{P}(x,t)$ to reconstruct the information displayed in Figure 5 one finds—see Figure 9—that the agreement is precise. The important point is that . . .

Mathematica appears to find it *easier* to work with $\tilde{P}(x,t)$: see Figure 10, which *Mathematica* refused to draw when asked to work with $P(x,t)$.

Experimental calculations such as the one that produced Figure 11 lead me to think that $\tilde{P}(x,t)$ is "easier" to work with because *computationally more stable*, and that the "regions of wild fluctuation" that have been seen to bedevil work based upon $P(x,t)$ are *computational artifacts*—not real.

So complicated is the evolved box packet that integrals of the form

$$\langle \mathsf{x}^2 \rangle_t = \int_{-\infty}^{+\infty} x^2 P(x,t)\, dx$$

must be done numerically, and if—which it is my purpose to demonstrate—it is indeed the case that $\langle \mathsf{x}^2 \rangle_t = \infty$ then they cannot be done at all: one must be
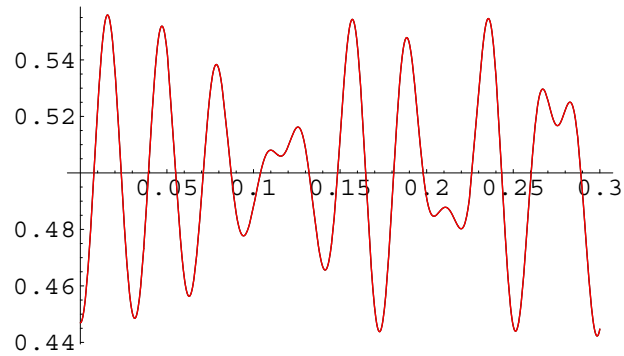
FIGURE 9: *Graph of* $\tilde{P}(x, .005)$, *superimposed upon the graph of* $P(x, .005)$ *that was presented as Figure 5. The agreement is so precise that the underlying graph cannot be seen.*
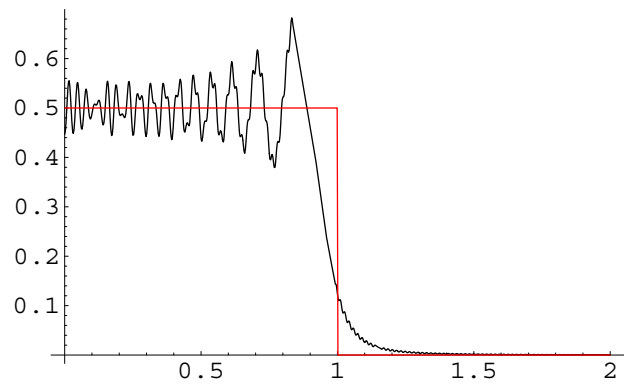

FIGURE 10: *Extended graph of* $\tilde{P}(x, .005)$, *superimposed upon a graph of the initial* $P_{\text{box}}(x, 0)$. *Mathematica was unable to produce such a figure when asked to work with* $P(x, .005)$. *The figure provides an informative and convincing account of the initial deformation of the evolving wavepacket.*
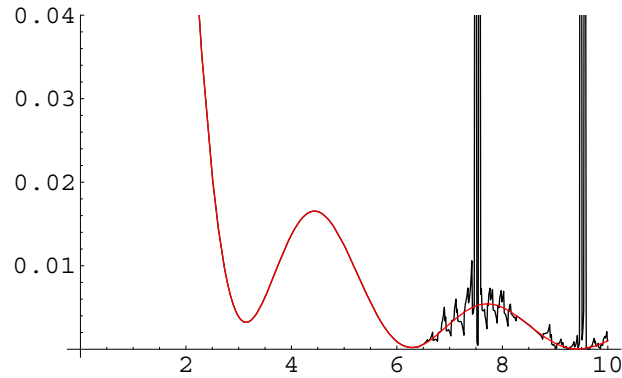
FIGURE 11: *Graph of $\tilde{P}(x,1)$, superimposed upon the graph of $P(x,1)$ that was presented as Figure 8. The superimposed curve shows none of the wild fluctuation to which $P(x,1)$ has been seen to be prone, and which I am on this evidence inclined to dismiss as a computational artifact. At points remote from the chaotic regions the agreement is precise.*

content to gather evidence that, for every $t > 0$,

$$W(k,t) \equiv \int_{-k}^{+k} x^2 P(x,t)\, dx = 2\int_0^k x^2 P(x,t)\, dx$$

increases without bound: $\lim_{k\uparrow\infty} W(k,t) = \infty$. The integral is, however, difficult or impossible to evaluate if k lies on the far side of a "chaotic region." I propose, therefore, to study the better-behaved function

$$\tilde{W}(k,t) \equiv 2\int_0^k x^2 \tilde{P}(x,t)\, dx$$

with the objective of answering this question:

> Is it true that, for all $t > 0$, $\tilde{W}(k,t)$
> grows without bound as $k \uparrow \infty$?   (23)

The simple command

```
Plot[Evaluate[NIntegrate[x^2 P̃(x,1), {x,0,k}], {k,0,30}]];
```

carries with it an enormous computational burden, but *Mathematica*, laboring uncomplainingly for several hours on my 400 MHz PowerMac G3, did at last manage to produce Figure 12, which I interpret to comprise soft evidence that (23) is (at least in the case $t = 1$) to be answered in the affirmative. Numerical methods are, however, incapable-in-principle of supplying compelling evidence, for

• one cannot carry k "all the way to ∞"
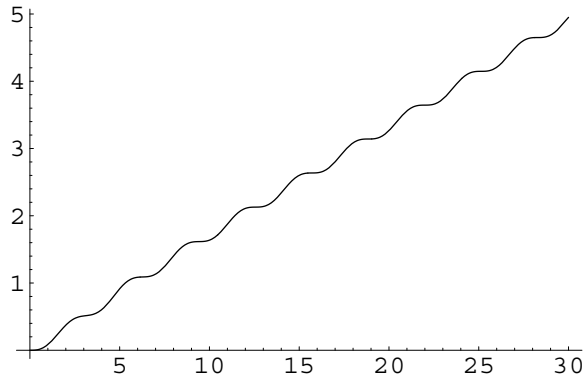
• one cannot consider *all* values of t.

FIGURE 12: *Graph of $\frac{1}{2}\tilde{W}(k,1)$ on the interval $0 \leqslant k \leqslant 30$, produced by laborious numerical intergration. It becomes plausible on this evidence to conjecture that $\lim_{k\uparrow\infty}\tilde{W}(k,1) = \infty$.*

We have no option but to dig deep enough into the function theory to develop the asymptotics of $\tilde{P}(x,t)$.

Bringing $(-)^{\frac{1}{4}} = \frac{1}{\sqrt{2}}(1+i)$ to the definitions of $\tilde{F}$ and $\tilde{G}$ that appear on page 14 we have

$$\tilde{F}(x,t) = -\tfrac{1}{2\sqrt{2}}\left\{ \mathtt{Im}\Big(\mathtt{Erfi}\big[u+iu\big]\Big) - \mathtt{Im}\Big(\mathtt{Erfi}\big[v+iv\big]\Big) \right\}$$

$$\tilde{G}(x,t) = \quad \tfrac{1}{2\sqrt{2}}\left\{ \mathtt{Re}\Big(\mathtt{Erfi}\big[u+iu\big]\Big) - \mathtt{Re}\Big(\mathtt{Erfi}\big[v+iv\big]\Big) \right\}$$

with

$$u \equiv \frac{x-1}{2\sqrt{t}} \qquad \text{and} \qquad v \equiv \frac{x+1}{2\sqrt{t}}$$