FREE MOTION OF INITIALLY BOX-LIKE WAVEPACKETS

with special reference to the rate at which they disperse

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Introduction. That the initially Gaussian wavefunction

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

when allowed to evolve by action of the free particle Hamiltonian

$$\mathsf{H} = \tfrac{1}{2m}\mathsf{p}^2$$

becomes progressively less compact is a fact of which students of quantum mechanics are very soon made aware.[1] Students are encouraged to think

[1] See, for example, Problems **2.22** & **2.40** which appear on pages 50 & 69 of David Griffiths' *Introduction to Quantum Mechanics* (1995). While Schrödinger himself was certainly well aware of this "characteristic feature of the quantum theory," the evidence is circumstantial, for examination of his early papers (English translations of which can be found in his *Collected Papers on Wave Mechanics*, the augmented 3rd edition of which was published by Chelsea in 1982) reveals that in those papers Schrödinger treated the hydrogen atom, the oscillator, the rotor, the perturbed atom . . . but avoided the free particle—perhaps because it is in some respects pathological (the energy/momentum eigenstates are not normalizable), but more probably because he was anxious to demonstrate that his new theory had things to say about experimental realities, and people tend not to experiment with free particles. However, near the end of his 3rd quantum mechanical paper ("The continuous transition from micro- to macro-mechanics," 1926) he points out how remarkable it is that the Gaussian state (1), when allowed to evolve by action of the oscillator Hamiltonian

$$\mathsf{H} = \tfrac{1}{2m}\mathsf{p}^2 + \tfrac{1}{2}m\omega^2\mathsf{x}^2$$

is periodically recurrent . . . which is to say: does *not* disperse.

that this analytically-neat property of Gaussian wavepackets is typical of wavepackets-in-general . . . and in many respects it is. My objective here will be to discuss an instance and a sense in which it isn't.

More specifically, I will discuss properties of the initially box-like wavepacket

$$\psi(x,0)=\begin{cases}0 & : \quad x<-b\\ \frac{1}{\sqrt{2b}} & : \quad -b<x<+b\\ 0 & : \quad x>+b\end{cases} \tag{2}$$

My interest in such packets derives from the coincidental confluence of two circumstances:

- a conversation with David Griffiths (late August, 2003), whose effort to prepare a 2^{nd} edition of his text[1] had exposed a certain computational difficulty, and
- the realization, while pondering potential thesis topics, that I had yet to establish the sense in which—by my intuition (and Einstein's)—Griffiths' initial state (2) describes the *universal end-state* of all particle-in-a-box systems, whatever might have been the initial state.

The latter issue will be reserved for a companion essay.

1. Gaussian preliminaries. The dynamical evolution of *any* initial wavepacket can, in principle, be described

$$\psi(x,t)=\int K(x,t;y,0)\,\psi(y,0)\,dy \tag{3}$$

where in the case $\mathsf{H}=\frac{1}{2m}\mathsf{p}^2$ the propagator becomes

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

which can be looked upon as the solution of $\big\{(\hbar^2/2m)\partial_x^2+i\hbar\partial_t\big\}K(x,t;\bullet,\bullet)=0$ that evolves in time t from the idealized wavepacket $\delta(x-y)$:

$$\lim_{t\downarrow 0}K(x,t;y,0)=\delta(x-y)$$

Introducing (1) into (3) we compute

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

where

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

The (complex-valued) function (4) goes smoothly over to the (real-valued) function (1) as $t \downarrow 0$, and it supplies

$$P(x,t) \equiv |\psi(x,t)|^2 = \frac{1}{\sigma(t)\sqrt{2\pi}}\,\exp\left\{-\frac{1}{2}\left[\frac{x}{\sigma(t)}\right]^2\right\} \tag{6}$$

$$\sigma(t) \equiv \sigma\sqrt{1+(t/\tau)^2} \tag{7}$$

Looking to the *moving moments* to which the normal distribution (6) gives rise, we note that because $P(x,t)$ is, for all t, and *even* function of x it is immediate that

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

while by calculation

$$\begin{aligned}
\langle \mathsf{x}^0\rangle_t &= 1\\
\langle \mathsf{x}^2\rangle_t &= 1\cdot[\sigma(t)]^2\\
\langle \mathsf{x}^4\rangle_t &= 1\cdot 3\cdot[\sigma(t)]^4\\
\langle \mathsf{x}^6\rangle_t &= 1\cdot 3\cdot 5\cdot[\sigma(t)]^6\\
\langle \mathsf{x}^8\rangle_t &= 1\cdot 3\cdot 5\cdot 7\cdot[\sigma(t)]^8\\
&\vdots
\end{aligned}$$

A standard measure of the instantaneous "width" or "degree of localization" of the moving distribution is provided by the "uncertainty" or "variance" or "rms $\equiv \sqrt{\text{centered second moment}}$"

$$\begin{aligned}
[\Delta x]_t \equiv \sqrt{\langle(\mathsf{x}-\langle\mathsf{x}\rangle_t)^2\rangle_t} &= \sqrt{\langle\mathsf{x}^2\rangle_t - \langle\mathsf{x}\rangle_t^2}\\
&= \sqrt{[\sigma(t)]^2 - 0^2} = \sigma(t)
\end{aligned} \tag{8}$$

In (8) we see the analytical source of the familiar claim that if $\psi(x,0)$ is Gaussian, and refers to the initial state of a *free* particle, then

$$[\Delta x]_t \text{ grows hyperbolically} \quad : \quad [\Delta x]_t = \sigma\sqrt{1+(t/\tau)^2} \tag{9}$$

An identical statement is readily shown to pertain to "launched" Gaussians that are initially centered at points arbitrarily distant from the origin.[2] Less familiar is the claim that (9) pertains also to many/most *non-Gaussian* initial states. Our main concern here will be with a simple initial state that provides, however, a vivid exception to the rule.

[2] *Mathematica* stands ready to verify all the computational details that I have omitted in the preceding discussion. Those and many related details are developed in "Gaussian wavepackets" (1998).

1. Quantum mechanics as a theory of interactive moments. I have described elsewhere[3] 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 (generally infinite) set of coupled "moment equations" that lie at the analytic heart of the theory. I have shown in particular that in the case $\mathsf{H} = \frac{1}{2m}\mathsf{p}^2$ one has

$$\left.\begin{aligned}
\tfrac{d}{dt}\langle \mathsf{p}\rangle &= 0\\
\tfrac{d}{dt}\langle \mathsf{x}\rangle &= \tfrac{1}{m}\langle \mathsf{p}\rangle\\
\\
\tfrac{d}{dt}\langle \mathsf{p}^2\rangle &= 0\\
\tfrac{d}{dt}\langle \mathsf{x}\mathsf{p}+\mathsf{p}\mathsf{x}\rangle &= \tfrac{2}{m}\langle \mathsf{p}^2\rangle\\
\tfrac{d}{dt}\langle \mathsf{x}^2\rangle &= \tfrac{1}{m}\langle \mathsf{x}\mathsf{p}+\mathsf{p}\mathsf{x}\rangle\\
&\vdots
\end{aligned}\right\}\tag{10}$$

These equations are readily integrated, and give

$$\left.\begin{aligned}
\langle \mathsf{p}\rangle_t &= \langle \mathsf{p}\rangle_0\\
\langle \mathsf{x}\rangle_t &= \langle \mathsf{x}\rangle_0 + \tfrac{1}{m}\langle \mathsf{p}\rangle_0 t\\
\\
\langle \mathsf{p}^2\rangle_t &= \langle \mathsf{p}^2\rangle_0\\
\langle \mathsf{x}\mathsf{p}+\mathsf{p}\mathsf{x}\rangle_t &= \langle \mathsf{x}\mathsf{p}+\mathsf{p}\mathsf{x}\rangle_0 + \tfrac{2}{m}\langle \mathsf{p}^2\rangle_0 t\\
\langle \mathsf{x}^2\rangle_t &= \langle \mathsf{x}^2\rangle_0 + \tfrac{1}{m}\langle \mathsf{x}\mathsf{p}+\mathsf{p}\mathsf{x}\rangle_0 t + \tfrac{1}{m^2}\langle \mathsf{p}^2\rangle_0 t^2\\
&\vdots
\end{aligned}\right\}\tag{11}$$

from which it follows in particular that

$$[\Delta x]_t^2 = \big[\langle \mathsf{x}^2\rangle_0 + \tfrac{1}{m}\langle \mathsf{x}\mathsf{p}+\mathsf{p}\mathsf{x}\rangle_0 t + \tfrac{1}{m^2}\langle \mathsf{p}^2\rangle_0 t^2\big] - \big[\langle \mathsf{x}\rangle_0 + \tfrac{1}{m}\langle \mathsf{p}\rangle_0 t\big]^2$$

is *always* a quadratic function of t, can *always* be written

$$= \sigma_0^2\Big[1 + \big(\tfrac{t-t_0}{\tau}\big)^2\Big]\tag{12.1}$$

with

$$\left.\begin{aligned}
\sigma_0^2 &= \big[\langle \mathsf{x}^2\rangle_0 - \langle \mathsf{x}\rangle_0^2\big] - \frac{\big[\langle \mathsf{x}\mathsf{p}+\mathsf{p}\mathsf{x}\rangle_0 - 2\langle \mathsf{x}\rangle_0\langle \mathsf{p}\rangle_0\big]^2}{4\big[\langle \mathsf{p}^2\rangle_0 - \langle \mathsf{p}\rangle_0^2\big]}\\
\sigma_0^2/\tau^2 &= \frac{\langle \mathsf{p}^2\rangle_0 - \langle \mathsf{p}\rangle_0^2}{m^2}\\
t_0 &= \frac{2\langle \mathsf{x}\rangle_0\langle \mathsf{p}\rangle_0 - \langle \mathsf{x}\mathsf{p}+\mathsf{p}\mathsf{x}\rangle_0}{2\big[\langle \mathsf{p}^2\rangle_0 - \langle \mathsf{p}\rangle_0^2\big]}
\end{aligned}\right\}\tag{12.2}$$

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

To make use of this information we must possess evaluations of the initial moments $\langle \mathsf{x}\rangle_0$, $\langle \mathsf{x}^2\rangle_0$, $\langle \mathsf{p}\rangle_0$, $\langle \mathsf{x}\mathsf{p}+\mathsf{p}\mathsf{x}\rangle_0$ and $\langle \mathsf{p}^2\rangle_0$.[4] We have already remarked that if $\psi(x,0)$ is even (symmetric about the point $x=0$) then transparently

$$\langle \mathsf{x}^{\text{odd}}\rangle_0 = 0$$

Equally transparent is the fact that if $\psi(x,0)$ is real-valued—as are both the initial Gaussian (1) and the initial box packet (2)—then[5]

$$\langle \mathsf{p}^{\text{odd}}\rangle_0 = 0$$

Real-valuedness, by that same argument, entails

$$\langle \mathsf{x}\mathsf{p}+\mathsf{p}\mathsf{x}\rangle_0 = 0$$

The implication is that if $\psi(x,0)$ is simultaneously even *and* real-valued then (11) simplifies radically: under such circumstances we have

$$\left.\begin{aligned} \sigma_0^2 &= \langle \mathsf{x}^2\rangle_0 \\ \sigma_0^2/\tau^2 &= \frac{\langle \mathsf{p}^2\rangle_0}{m^2} \implies \tau = \sqrt{m^2\langle \mathsf{x}^2\rangle_0/\langle \mathsf{p}^2\rangle_0} \\ t_0 &= \quad 0 \end{aligned}\right\}$$

giving

$$[\Delta x]_t^2 = \langle \mathsf{x}^2\rangle_0 \left\{ 1 + \frac{t^2}{m^2\langle \mathsf{x}^2\rangle_0/\langle \mathsf{p}^2\rangle_0} \right\} \tag{13}$$

[4] The full-blown "theory of interactive moments" identifies the higher-order companions of the mixed construction $\frac{1}{2}(\mathsf{x}\mathsf{p}+\mathsf{p}\mathsf{x})$, but in those we have no immediate interest.

[5] To establish the point it is sufficient to write

$$\langle \mathsf{p}^{\text{odd}}\rangle_0 = \int \psi(x,0)\big(\tfrac{\hbar}{i}\tfrac{\partial}{\partial x}\big)^{\text{odd}}\psi(x,0)\,dx$$

and to observe that the expression on the left is, by self-adjointness, necessarily real, while the expression on the right is manifestly imaginary. If follows, by the way, that if we would "launch" $\psi(x,0)$ with velocity $v \equiv p/m$ then we must *complexify* the wavefunction: specifically, we must send

$$\psi(x,0) \longmapsto \psi_{\text{launched}}(x,0) \equiv e^{\frac{i}{\hbar}px}\cdot \psi(x,0)$$

That done, we by quick argument obtain

$$\langle \mathsf{p}^{\text{odd}}\rangle_0 = (mv)^{\text{odd}}$$

See again Griffiths' Problem **2.40**. An elaborate discussion can be found in §5 of "Gaussian wavepackets" (1998).

Look back again, in the light of this result, to the Gaussian case (1). We have already established that $\langle \mathsf{x}^2\rangle_0 = \sigma^2$, and by calculation have

$$\langle \mathsf{p}^2\rangle_0 = (\hbar/2\sigma)^2$$

so in instance of (13) obtain

$$\begin{aligned}[\Delta x]_t^2 &= \sigma^2\Big\{1 + (t/\tau)^2\Big\}\\ &\qquad\tau = \sqrt{m^2\sigma^2/(\hbar/2\sigma)^2} = 2m\sigma^2/\hbar\end{aligned}$$

This is precisely the statement encountered already at (9), but obtained now as the Gaussian instance of a much more general "law of hyperbolic dispersal."

2. Theory of interactive moments applied to the box-packet. Working from (2) we find

$$\langle \mathsf{x}^n\rangle_0 = \frac{b^n + (-b)^n}{2(n+1)} = \begin{cases} 0 & : \quad n = 1, 3, 5, \ldots \\[2ex] \frac{1}{n+1}b^n & : \quad n = 0, 2, 4, \ldots \end{cases}$$

so by (13)

$$[\Delta x]_t^2 = \tfrac{1}{3}b^2\left\{1 + \frac{t^2}{\frac{1}{3}m^2b^2}\langle \mathsf{p}^2\rangle_0\right\} \tag{14}$$

and we confront the problem of evaluating $\langle \mathsf{p}^2\rangle_0$. This might be attempted by the following line of argument:

Let (2) be notated

$$\psi(x, 0) = \tfrac{1}{\sqrt{2b}}\big\{\theta(x+b) - \theta(x-b)\big\} \tag{15}$$

where $\theta(x)$ refers to the Heaviside step function:

$$\theta(x) \equiv \int_{-\infty}^{x} \delta(y)\,dy = \begin{cases} 0 & : \quad x < 0 \\ \frac{1}{2} & : \quad x = 0 \\ 1 & : \quad x > 0 \end{cases}$$

We note in passing that $\psi(x, 0)$, thus described, is manifestly real (with consequences spelled out on the preceding page) and that its evenness follows from the identity $\theta(-x) = 1 - \theta(x)$. From (15) we are led to write

$$\begin{aligned}\langle \mathsf{p}^2\rangle_0 &= \tfrac{1}{2b}\big(\tfrac{\hbar}{i}\big)^2\int \big\{\theta(x+b) - \theta(x-b)\big\}\big\{\theta''(x+b) - \theta''(x-b)\big\}\,dx\\ &= -\tfrac{1}{2b}\hbar^2\int \big\{\theta(x+b) - \theta(x-b)\big\}\big\{\delta'(x+b) - \delta'(x-b)\big\}\,dx\end{aligned}$$

which after an integration-by-parts becomes

$$\begin{aligned}&= +\tfrac{1}{2b}\hbar^2\int \big\{\delta(x+b) - \delta(x-b)\big\}\big\{\delta(x+b) - \delta(x-b)\big\}\,dx\\ &= +\tfrac{1}{2b}\hbar^2\big\{\delta(0) - \delta(-2b) - \delta(2b) + \delta(0)\big\}\\ &= +\tfrac{1}{2b}\hbar^2\big\{\infty - 0 - 0 + \infty\big\}\\ &= \infty\end{aligned} \tag{16}$$

But is this result for real? Can we have confidence in conclusions drawn form an argument that culminates in naked δ-functions (δ-functions unprotected by the shade of an $\int$-sign), that asks us to regard the Dirac distribution as function? Perhaps not ... but evidence that (16) is nevertheless correct as it stands is provided by the fact that several alternative lines of argument lead to the same conclusion. Most simply:

By Fourier transformation

$$\begin{aligned}\psi(x,0) \;\longmapsto\; \varphi(p,0) &= \tfrac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{+\infty}\psi(x,0)\,e^{-\frac{i}{\hbar}px}\,dx\\ &= \tfrac{1}{\sqrt{2\pi\hbar}}\int_{-b}^{+b}e^{-\frac{i}{\hbar}px}\,dx\\ &= \frac{\sqrt{\hbar/\pi b}\,\sin\frac{bp}{\hbar}}{p}\end{aligned} \tag{17}$$

obtain the *momentum representation* of the box packet (2), which is the case $b=\hbar=1$ is displayed in Figure 1b. From the obvious facts that $\varphi(p,0)$ is real-valued and even (symmetric about $p=0$) we recover

$$\langle \mathbf{p}^{\text{odd}}\rangle_0 = \lim_{q\uparrow\infty}\int_{-q}^{+q}\varphi(p,0)\,p^{\text{odd}}\,\varphi(p,0)\,dp = 0$$

while by calculation[6]

$$\langle \mathbf{p}^2\rangle_0 = \lim_{q\uparrow\infty}\int_{-q}^{+q}\varphi(p,0)\,p^2\,\varphi(p,0)\,dp = \lim_{q\uparrow\infty}\tfrac{\hbar}{\pi b}\Big\{q-\tfrac{\hbar}{2b}\sin\tfrac{2bq}{\hbar}\Big\} = \infty$$

... which is (16) again.

Equation (14) has now become

$$[\Delta x]_t^2 = \begin{cases}\frac{1}{3}b^2 & : \quad t=0\\ \infty & : \quad t>0\end{cases} \tag{18}$$

[6] More generally one finds

$$\langle \mathbf{p}^n\rangle_0 = \lim_{q\uparrow\infty}\int_{-q}^{+q}\varphi(p,0)\,p^n\,\varphi(p,0)\,dp = \infty \quad : \quad n=2,4,6,\ldots$$

but *Mathematica* seems to find it difficult to establish that

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

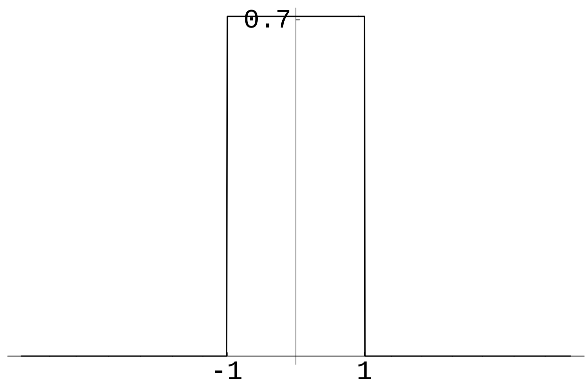

FIGURE 1a: *Graph, based upon* (15), *of the initial boxpacket* $\psi(x, 0)$, *in the case* $b = 1$.

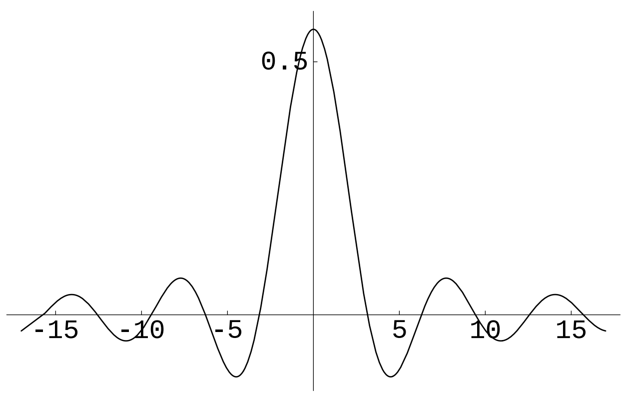

FIGURE 1b: *Fourier transform* $\varphi(p, 0)$ *of the wavepacket shown above, taken from* (17) *with* $b = \hbar = 1$

which is, I now argue, . . .

3. Strange . . . but by no means impossible. For the phenomenon encountered at (18) is precisely reproduced by the following simple model. 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:[7]

$$\begin{aligned} G(x;\sigma) &= \tfrac{1}{\sigma\sqrt{2\pi}}e^{-\frac{1}{2}(x/\sigma)^2} \\ L(x;a) &= \tfrac{1}{a\pi}\tfrac{1}{1+(x/a)^2} \end{aligned}$$

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

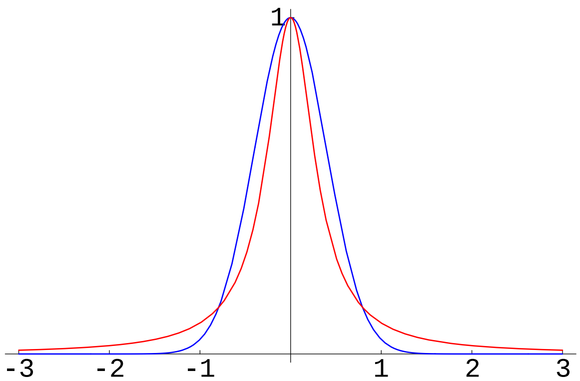

FIGURE 2: *Comparative display of the Gaussian distribution* $G(x;\sigma)$ *and the Lorentzian distribution* $L(x;a)$. *To facilitate the comparison I have set* $\sigma = \frac{1}{\sqrt{2\pi}}$ *and* $a = \frac{1}{\pi}$ *so as to achieve* $G_{\max} = L_{\max} = 1$. *The Lorentzian distribution is seen to have a relatively sharp central peak but relatively broad shoulders—shoulders so broad that the integrals* $\langle x^{\text{even}} \rangle$ *do not converge.*

Both distribution 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

$$\langle x^n \rangle_{\text{Lorentz}} \equiv \lim_{k\uparrow 0} \int_{-k}^{+k} x^n L(x;a)\,dx \quad : \quad n \text{ even}$$

we find

$$= \begin{cases} 1 & : \quad n = 0 \\ \infty & : \quad n = 2, 4, 6, \ldots \end{cases}$$

—this even though graphs of the two distributions (Figure 2) 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 second moment of that distribution. It is evident from preceding remarks that (and why!)

$$\langle x^2 \rangle_\epsilon \equiv \lim_{k\uparrow 0} \int_{-k}^{+k} x^2 W(x;\sigma,a;\epsilon)\,dx = \begin{cases} 1 & : \quad \epsilon = 0 \\ \infty & : \quad \epsilon > 0 \end{cases}$$

The lesson to be drawn is not that something bizarre happens to the distribution as the control parameter ϵ increases from zero to values greater than zero, but that $\langle x^2 \rangle$ abruptly becomes unserviceable as a measure of the "width" of the distribution: we must look to some other quantifier of that intuitive notion. We might in this instance be tempted to adopt as our quantifier the distance between the points at which the distribution falls to half of its maximal value; *i.e.*, where

$$W(x\,;\sigma,a\,;\epsilon) = \tfrac{1}{2}W(0\,;\sigma,a\,;\epsilon)$$

The problem is that, while those points would be easy to locate on a graph, they are not easy to describe analytically. The short of it: there appears to be *no* universally available natural descriptor of "distribution width."

A physical problem has led us—at (18)—to a situation in which the most common "width descriptor" happens to fail. Such a development is, in the light of the preceding discussion, hardly an occasion for surprise, and certainly not an occasion for distress.

4. Motion of the probability density: first approach. The "theory of interactive moments" to which I have alluded,[3] and of which we have in fact been making use, proceeds from and lends weight to the proposition that *if one were in position to describe the motion of a certain infinite set of moments then one would in effect possess all the physical information latent in the moving wave function* $\psi(x,t)$. We, however, are in position to describe the motion of only a small handfull of low-order moments, which collectively are but a pale shadow of—and cast only a dim light upon—the motion of the wave function that evolves from the $\psi_{\text{box}}(x,0)$ described at (2), and again at (15). It was to discuss computational problems latent in the construction of $\psi_{\text{box}}(x,t)$ that Griffiths sought me out, and it is to consideration of those that I now turn.

In design $\mathsf{H} = \frac{1}{2m}\mathsf{p}^2$ of the free particle Hamiltonian is so exceptionally simple that in the momentum representation the time-dependent Schrödinger equation becomes

$$\tfrac{1}{2m}p^2\varphi(p,t) = i\hbar\partial_t\varphi(p,t)$$

which is an *ordinary* differential equation, of only first order. Its solution is immediate[8]

$$\varphi(p,t) = \varphi(p,0)\cdot e^{-\frac{i}{\hbar}(p^2/2m)t} \tag{19}$$

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[8] From this result it follows, by the way, that the function $Q(p,t) \equiv |\varphi(p,t)|^2$ that describes probability density in momentum space is *constant*

$$Q(p,t) = Q(p,0)$$

and therefore that

$$\langle \mathsf{p}^n\rangle_t = \langle \mathsf{p}^n\rangle_0 \quad : \quad \text{all } n, \text{ all } t$$

It follows more particularly that

$$\langle \text{energy}\rangle_t = \langle \text{energy}\rangle_0 = \infty$$

and on this basis we can dismiss the initial boxpacket (2) as a reference to a <u>profoundly unphysical situation</u>. I am tempted to argue that "If it ain't physical it's *entitled* to some absurdities!

and gives

$$\begin{aligned}\psi(x,t) &= \tfrac{1}{\sqrt{2\pi\hbar}}\int \varphi(p,t)\,e^{\frac{i}{\hbar}px}\,dp\\ &= \tfrac{1}{\sqrt{2\pi\hbar}}\int \varphi(p,0)\,e^{\frac{i}{\hbar}[px-(p^2/2m)t]}\,dp \end{aligned}\tag{19}$$

In principle, we have "only" to introduce the $\varphi_{\text{box}}(p,0)$ of (17) into (19) and evaluate the integral to obtain a description of $\psi_{\text{box}}(x,t)$.

For (what is revealed to be, after some exploratory tinkering) the convenience of *Mathematica*, we resolve $\psi_{\text{box}}(x,t)$ into its real and imaginary parts

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

and discover that the integrals

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

are—in fact, and to my surprise—intelligible to *Mathematica*. At $t=0$ we are informed that

$$\left.\begin{aligned}F(x,0) &= \tfrac{1}{\sqrt{2b}}\big\{\theta(x+b)-\theta(x-b)\big\}\\ G(x,0) &= 0\end{aligned}\right\}\tag{20}$$

—which, gratifyingly, are in precise agreement with the statement (15) that was our point of departure. At this point I

- set $b=\hbar=m=1$ and
- invite (urge!) my reader to fire up *Mathematica* and to follow along, for we are about to encounter expressions of such complexity that, while they reside contentedly enough within *Mathematica*'s memory, it would stupifyingly pointless to commit to the TEXed page. That done, my reader will confirm that . . .

At times $t>0$ we (according to *Mathematica*) have

$$\begin{aligned}&F(x,t)\\ &\quad= \tfrac{1}{12\sqrt{2\pi}\,t^{3/2}}\Big[6t\sqrt{1-x^2}\,\varepsilon(1-x)\text{HypergeometricPFQ}\big(\tfrac{3}{4},\big\{\tfrac{1}{2},\tfrac{5}{4}\big\},-\tfrac{(1-x)^4}{16t^2}\big)\\ &\qquad\qquad + \text{three roughly similar terms}\Big]\end{aligned}\tag{21.1}$$

$$\begin{aligned}&G(x,t)\\ &\quad= \tfrac{1}{12\sqrt{2\pi}\,t^{3/2}}\Big[\text{ similar mess }\Big]\end{aligned}\tag{21.2}$$

where

$$\varepsilon(x) \equiv 2[\theta(x)-1] = \begin{cases}+1 & : \quad x>0\\ 0 & : \quad x=0\\ -1 & : \quad x<0\end{cases}$$

is sometimes written $\text{sgn}(x)$ and is known to *Mathematica* as `Sign[x]`.

One might expect $F(x,t) + i\,G(x,t)$ to give back (20) at $t = 0$, but *Mathematica* refuses to do so, claiming that it has encountered "indeterminate expressions and complex singularities." Look again to where t appears on the right side of (21) and such complaints will not seem implausible.

Our primary interest attaches not to $F(x,t)$ and $G(x,t)$ themselves, but to the probability density

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

constructed from them, with the aid of which we propose to study

$$\langle \mathsf{x}^2 \rangle_t = \int x^2 P(x,t)\,dx$$

Mathematica appears not to mind that $P(x,t)$ is a horrible (!) mess when written out in detail, but again declines to speak of $P(x,0)$... for reasons upon

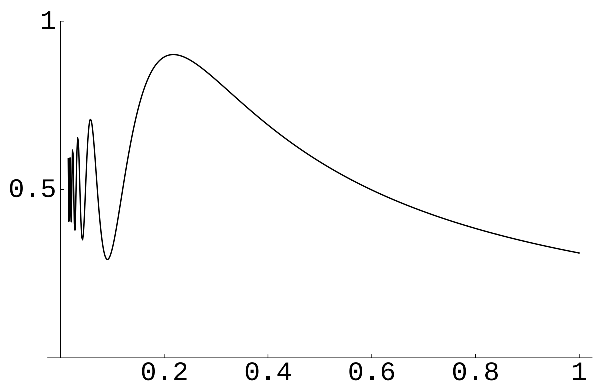

FIGURE 3: *Graph—derived from* (21)*—of* $P(0,t)$ *at short times. As* $t \downarrow 0$ *the oscillations become faster and faster. The figure suggests—but* Mathematica *refuses to state in plain words—that* $P(0,0) = \frac{1}{2}$, *which we know from* (15) *to be the case. At times* $t > 0.25$ *the central value* $P(0,t)$ *of the distribution drops smoothly* (*exponentially*?) *to zero.*

which the preceding figure casts some light.

At times t that are greater than (and not too near to) zero, *Mathematica* is happy to plot $P(x,t)$ but all such figures are—for some obscure reason—marked by symmetrically placed[9] pairs of noisy spikes (see Figure 4b). The spikes are found to recede as t increases, but within each pair the separation appears (Figure 5) always to remain roughly equal to the width of the initial boxpacket. Why is that? The question will soon lose its interest.

[9] The symmetry, at least, is no mystery: $P(x,t)$ is demonstrably an *even* function of x. I exploit this labor-saving fact in the production of all subsequent graphs.

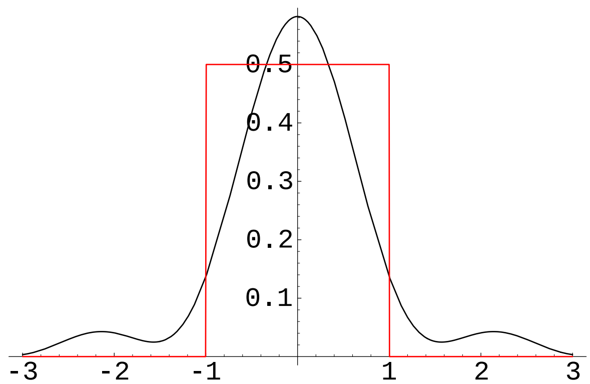

FIGURE 4a: *Central portion of the evolved distribution $P(x, 0.5)$, superimposed upon a graph of the initial distribution $P(x, 0)$.*

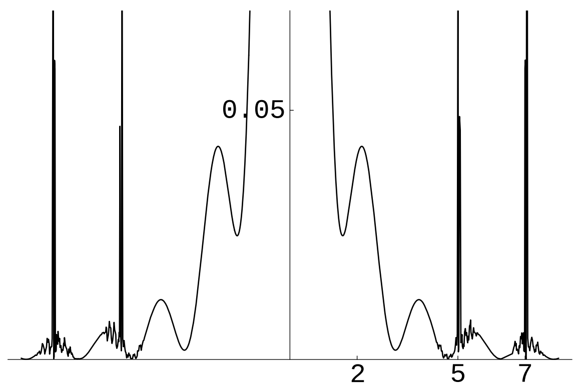

FIGURE 4b: *Extended (and much magnified) version of the preceding figure, showing complications in the neighborhoods of $x = \pm 5$ and $x = \pm 7$. Note that*

$$7 - 5 = 2 = \textit{width of the initial boxpacket}$$

For x greater than about 8 (less than about minus 8) the chaotic oscillations settle down, and the curve becomes gently undulatory again. Details on the left are redundant with those on the right, and will henceforth be omitted.

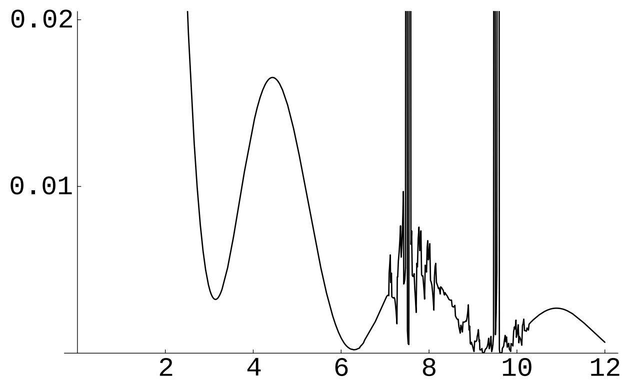

FIGURE 5: *Right half of a graph of $P(x,t)$ drawn at the later time $t = 1.0$. Note the high magnification, and that while the spikes have shifted to the right during the last half timeunit they retain their former separation. I cannot—have not really attempted—to account analytically for the fact that these trends appear, on numerical/graphical evidence, to be persistent.*

5. Motion of the probability density: alternative approach. Introduction if (2) into (3) leads to the conclusion that the propagated boxpacket should be describable

$$\psi_{\text{box}}(x,t) = \tfrac{1}{\sqrt{2b}}\int_{-b}^{+b}\sqrt{\frac{m}{i\,2\pi\hbar\, t}}\exp\Big\{\frac{i}{\hbar}\frac{(x-y)^2}{t}\Big\}\,dy$$

$$\Big\downarrow \text{ specialize to the case } b{=}\hbar{=}m{=}1$$

$$= \tfrac{1}{\sqrt{4\pi i t}}\int_{-1}^{+1}\exp\Big\{i\,\tfrac{(x-y)^2}{t}\Big\}\,dy \tag{22}$$

which is to say: by an integral quite different from the

$$\psi_{\text{box}}(x,t) = \tfrac{1}{\pi\sqrt{2}}\int_{-\infty}^{+\infty}\tfrac{1}{p}\sin p\cdot\exp\Big\{i\big[px-\tfrac{1}{2}p^2t\big]\Big\}\,dp$$

encountered at (19). *Mathematica*, when asked about (22), supplies[10]

$$= i\tfrac{1}{2\sqrt{2}}\Big\{\text{erfi}\Big[\frac{(-)^{\frac{1}{4}}(x-1)}{\sqrt{2t}}\Big] - \text{erfi}\Big[\frac{(-)^{\frac{1}{4}}(x+1)}{\sqrt{2t}}\Big]\Big\}$$

[10] Here

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

Note also that $(-)^{\frac{1}{4}} = e^{i\frac{\pi}{4}} = \frac{1}{\sqrt{2}}(1+i)$.

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

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

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

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 (21) on page 11, but wear tildes to emphasize that they have been assembled now not from `HypergeometricPFQ` functions but from the real and imaginary parts of the so-called "imaginary error function."

Finally we ask *Mathematica* to construct (and to retain in its memory)

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

Possibly Euler himself, if presented with TEX'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 (say) Figure 4a one finds—see Figure 6—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 7, which *Mathematica* refused to draw when asked to work with $P(x,t)$.

Experimental calculations such as the one that produced Figure 8 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. It must be possible to account for such artifacts, to explain *why* graphs of $P(x,t)$ display spurious details, but as the explanation is unlikely to involve any point of *physical* principle I will not pursue the matter.

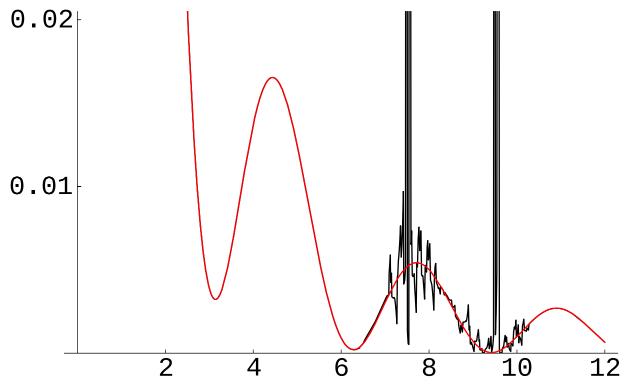

FIGURE 6: *Graph of* $\tilde{P}(x, 1.0)$*, superimposed upon the graph of* $P(x, 1.0)$ *that appears in* FIGURE 5*. The superimposed curve shows none of the wild fluctation to which* $P(x, 1.0)$ *is prone on the interval* $7 \lessapprox x \lessapprox 11$*, and which I am on this evidence inclined to dismiss as a* <u>*computational artifact*</u>*. At points remote from the chaotic region the agreement is so precise that the graph of* $\tilde{P}(x, 1.0)$ *masks the graph of* $P(x, 1.0)$*.*

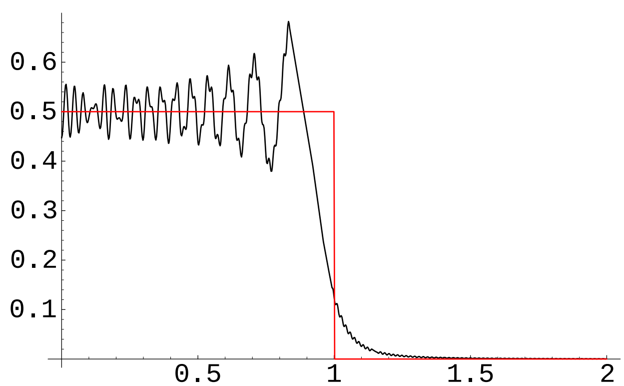

FIGURE 7: *Extended graph of* $\tilde{P}(x, .005)$*, superimposed upon a graph of the initial distribution* $P_{\text{box}}(x, 0)$*. Mathematica was unable to produce such a figure when asked to work with* $P(x, .005)$*. The figure provides an informative and convincing account of the initial evolution of the boxpacket.*

6. Direct approach to the description of $\langle \mathsf{x}^2 \rangle_t$. It was by application of the "theory of interactive moments" that we were led—at (18)—to the conclusion that Δx grows "explosively." We stand now in position to reproduce that somewhat surprising property of boxpackets by *direct* analysis, by an argument that proceeds without reference to the unfamiliar formalism just mentioned.

We work in a context where (because the packet was assumed to have been initially centered at the origin) $\langle \mathsf{x} \rangle_t = 0$, so we have $[\Delta x]_t = \sqrt{\langle \mathsf{x}^2 \rangle_t}$ and it is to the moving second moment

$$\langle \mathsf{x}^2 \rangle_t = 2 \cdot \begin{cases} \displaystyle\int_0^\infty x^2 P(x,t)\,dx, \text{ alternatively} \\ \displaystyle\int_0^\infty x^2 \tilde{P}(x,t)\,dx \end{cases}$$

that we direct our computational attention. The distributions $P(x,t)$ and $\tilde{P}(x,t)$ are so complicated that the integration must be done numerically ... which requires that we temper the ∞ upper limit: we study

$$\lim_{\xi\uparrow\infty} \begin{cases} \displaystyle\int_0^\xi x^2 P(x,t)\,dx, \text{ alternatively} \\ \displaystyle\int_0^\xi x^2 \tilde{P}(x,t)\,dx \end{cases}$$

but discover that if ξ lies on the far side of the spikes then numerical evaluation of the first of those integrals is not feasible. Subsequent work will proceed, therefore, from the statement

$$\langle \mathsf{x}^2 \rangle_t = 2 \cdot \lim_{\xi\uparrow\infty} \texttt{NIntegrate[}\,x^2 \tilde{P}(x,t)\texttt{,}\ \big\{x,\,0,\,\xi\,\big\}\texttt{]} \ :\ t \text{ given \& fixed}$$

where $\tilde{P}(x,t)$ is the tempered (spike-free) variant of $P(x,t)$.

We remind ourselves that, on graphical evidence (Figures 8 & 9), $\tilde{P}(x,t)$ is (for every $t > 0$) a function that oscillates to a rapid death. How rapid? The evidence of Figures 10 strongly suggests that $\tilde{P}(x,t)$ dies like x^{-2}, that

$x^2\tilde{P}(x,t)$ oscillates with asymptotically constant amplitude and period

The structure of

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

becomes in this light qualitatively obvious (see Figure 11), and we acquire fresh insight into why it is that

$$\langle \mathsf{x}^2 \rangle_t = 2 \cdot \lim_{\xi\uparrow\infty} w(\xi) = \infty \tag{23}$$

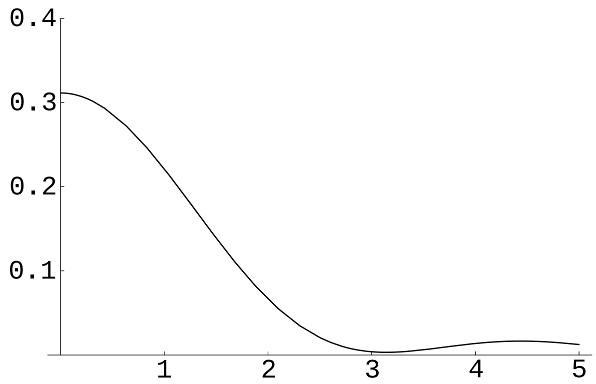

FIGURE 8a: *Graph of* $\tilde{P}(x,1)$.

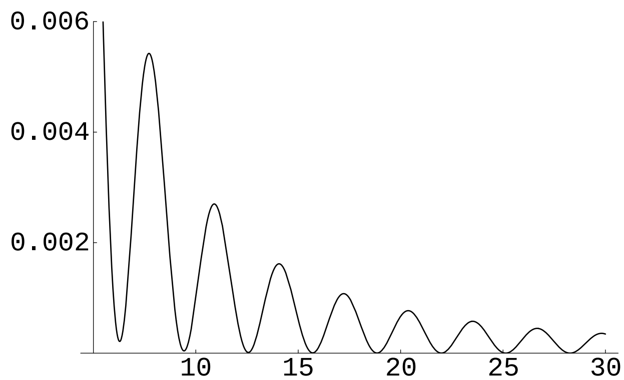

FIGURE 8b: *Graph of* $\tilde{P}(x,1)$ *on an extended base.*

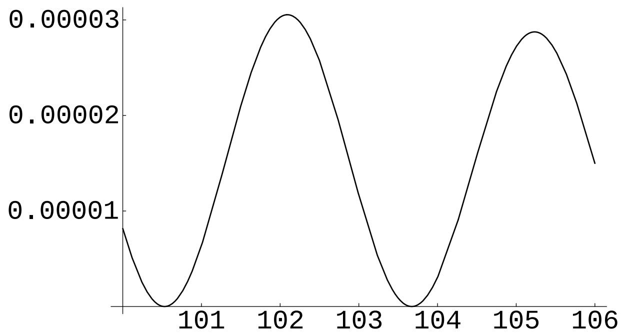

FIGURE 8c: *Highly magnified graph of $\tilde{P}(x,1)$ at large x-values.*

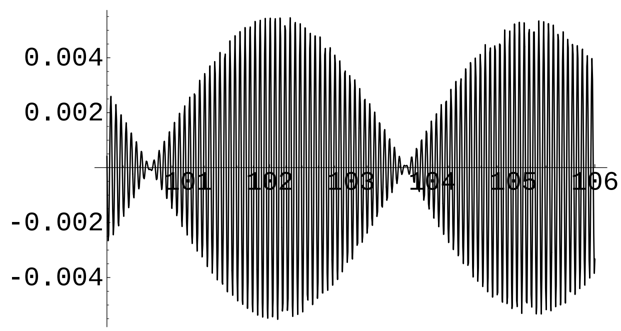

FIGURE 9a: *Graph of $\tilde{F}(x,1)$, the real part of $\psi_{\text{box}}(x,1)$, for that same set of x-values.*

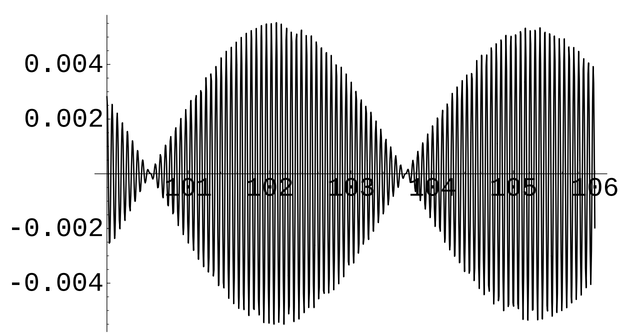

FIGURE 9b: *Graph of $\tilde{G}(x,1)$, the imaginary part of $\psi_{\text{box}}(x,1)$. It may seem remarkable that $\tilde{P}(x,1) = \tilde{F}^2(x,1) + \tilde{G}^2(x,1)$ has the simple form shown in* FIGURE 8c.

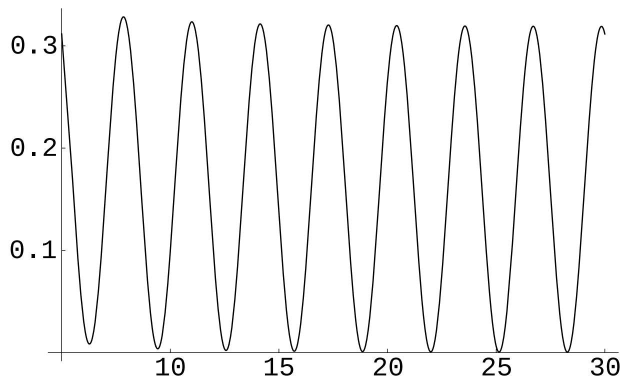

FIGURE 10a: *Graph of $x^2\tilde{P}(x,1)$ and small values of x.*

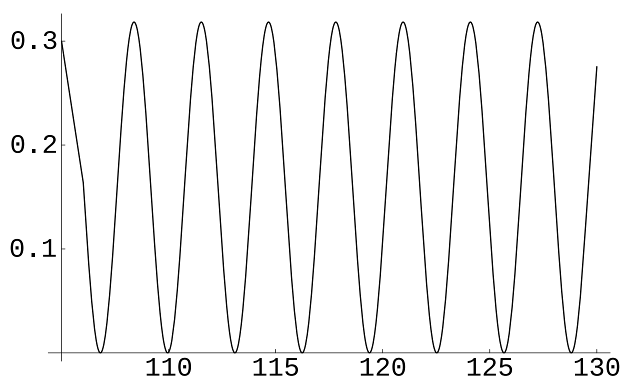

FIGURE 10b: *Graph of $x^2\tilde{P}(x,1)$ and much larger values of x.*

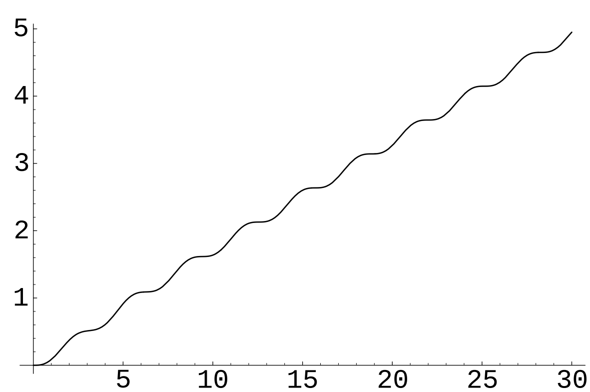

FIGURE 11: *Rippled linear growth of the function $\int_0^\xi x^2\tilde{P}(x,1)\,dx$.*

7. Asymptotic properties of the tempered probability density. Let the results reported on page 15 be abbreviated

$$\tilde{F}(x,t) = -\tfrac{1}{2\sqrt{2}}\Big\{\texttt{Im}\Big(H(x-1)\Big) - \texttt{Im}\Big(H(x+1)\Big)\Big\}$$

$$\tilde{G}(x,t) = \quad \tfrac{1}{2\sqrt{2}}\Big\{\texttt{Re}\Big(H(x-1)\Big) - \texttt{Re}\Big(H(x+1)\Big)\Big\}$$

where[11]

$$H(x) \equiv \text{erfi}\Big[\frac{(1+i)\,x}{2\sqrt{t}}\Big] \quad \text{with} \quad \text{erfi}(z) \equiv \tfrac{2}{\sqrt{\pi}}\int_0^z e^{y^2}\,dy$$

The command `Series[Erfi[x],{x,∞,2}]` supplies $\text{erfi}(z) \sim \frac{1}{\sqrt{\pi}\,z}e^{z^2}$, and if we assume that result can be extended onto relevant sectors of the complex plane we find (with the assistance of `ComplexExpand`) that

$$H(x) \sim \sqrt{t/\pi}\left\{\frac{\sin\frac{x^2}{2t} + \cos\frac{x^2}{2t}}{x} + i\,\frac{\sin\frac{x^2}{2t} - \cos\frac{x^2}{2t}}{x}\right\} \quad : \quad x^2/t \gg 1$$

giving

$$\tilde{F}(x,t) \sim -\sqrt{\tfrac{1}{8\pi}t}\left\{\frac{\sin\frac{(x-1)^2}{2t} - \cos\frac{(x-1)^2}{2t}}{x-1} - \frac{\sin\frac{(x+1)^2}{2t} - \cos\frac{(x+1)^2}{2t}}{x+1}\right\}$$

$$\tilde{G}(x,t) \sim \quad \sqrt{\tfrac{1}{8\pi}t}\left\{\frac{\sin\frac{(x-1)^2}{2t} + \cos\frac{(x-1)^2}{2t}}{x-1} - \frac{\sin\frac{(x+1)^2}{2t} + \cos\frac{(x+1)^2}{2t}}{x+1}\right\}$$

Looking with the assistance of *Mathematica* to the evaluation of

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

we `Simplify`, then use $1+\cos 2z = 2\cos^2 z$ and $1-\cos 2z = 2\sin^2 z$ to obtain

$$\sim \tfrac{1}{\pi}\,t\,\frac{\cos^2(x/t) + x^2\sin^2(x/t)}{(x^2-1)^2}$$

$$\sim \tfrac{1}{\pi}\,t\,\frac{\sin^2(x/t)}{x^2} \tag{24}$$

Upon relaxation of the assumptions $b = \hbar = m = 1$ we therefore expect (on dimensional grounds) to have

$$\tilde{P}(x,t) \sim \tfrac{1}{\pi}\tfrac{\hbar}{mb}\,t\,\frac{\sin^2(mbx/\hbar t)}{x^2} \quad : \quad x^2/t \gg \hbar/m \tag{25}$$

---

[11] See again the preceding footnote. I have, by the way, found it natural to adopt *Mathematica*'s conventions, which agree with those of Abramowitz & Stegun, *Handbook of Mathematical Functions* (1964), page 297 but differ by a factor by those encountered in Erdélyi, *Higher Transcendental Functions* (1953), §**9.9**, Volume 2, page 147.

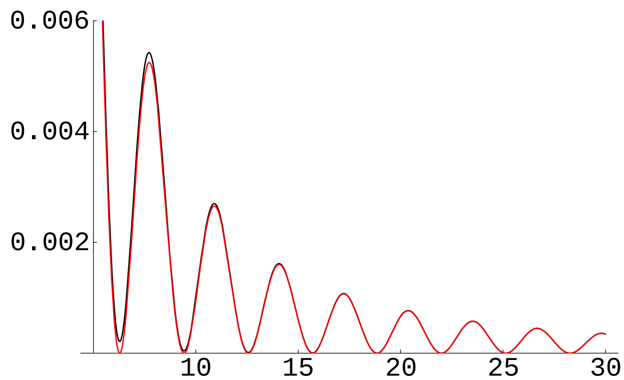

FIGURE 12: *Here superimposed are the graph of* $\tilde{P}(x,1)$ *that was previously presented as* FIGURE 8b *and the graph of its asymptotic approximant* (24). *The agreement is seen to be very good already for* $x \approx 10$.

That this analytical result conforms nicely to our graphics-based expectations is evident in the preceding figure.

It is interesting to note—and more than we might have hoped for—that the approximation procedure that led us at (25) from $\tilde{P}(x,t)$ to the function

$$\tilde{P}_{\text{asymptotic}}(x,t) \equiv \tfrac{1}{\pi}\tfrac{\hbar}{mb}\,t\,\frac{\sin^2(mbx/\hbar t)}{x^2}$$

led us to a function that is itself a distribution: one has $\tilde{P}_{\text{asymptotic}}(x,t) \geqslant 0$ (all x) and

$$\int_{-\infty}^{+\infty} \tilde{P}_{\text{asymptotic}}(x,t) = 1 \quad : \quad \text{all } t \geqslant 0$$

Restoring the assumptions $b = \hbar = m = 1$, we compute

$$\int_0^\xi x^2 \tilde{P}_{\text{asymptotic}}(x,t)\,dx = \tfrac{t}{2\pi}\big[\xi - \tfrac{1}{2}\sin\tfrac{2\xi}{t}\big]$$

which, when plotted at $t = 1$, reproduces Figure 11 to high accuracy and makes clear why it is that the integral blows up in the limit $\xi \uparrow \infty$, thus clinching the analytical demonstration of (23).

We note belatedly that the quantum system in hand comes to us endowed with a

$$\text{natural length} = b$$

so it possesses also a

$$\begin{aligned}\text{natural momentum} &= \hbar/b\\ \text{natural velocity} &= \hbar/mb\\ \text{natural energy} &= \hbar^2/mb^2\\ \text{natural time} &= mb^2/\hbar\end{aligned}$$

The statements

$$\begin{aligned}(\text{natural length})\cdot(\text{natural momentum})&\\ &=(\text{natural energy})\cdot(\text{natural time})\\ &=\hbar\end{aligned}$$

are pretty but convey no real information: they are corollaries of the preceding *definitions*. It is, however, curious that a "natural energy" should attach to a system that in point of idealized physical fact[8] has *infinite* energy.

7. Things learned from <u>and about</u> *Mathematica*. The work summarized here could not have been accomplished without the major assistance of *Mathematica*, which in the instance meant *Mathematica* 4 running on my 400 MHz PowerBook (Mac OS 9.1). But the work also taught me some things <u>about</u> *Mathematica* ... and, more particularly, about some of the differences between *Mathematica* 4 and *Mathematica* 5. For as the work neared completion I was fortunate enough to acquire a PowerMac G5 (running OS 10.2 at 1.6 GHz), on which I undertook to repeat some of my calculations, with curious —and ultimately quite informative—results.

It was a *Mathematica*l quirk—still unexplained—that had originally sent Griffiths into my office: when he had attempted to evaluate the integral (19) he had been informed by *Mathematica* 5 (*Mathematica* 4 concurs) that

$$\tfrac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty}\frac{\sin p}{p}\,e^{i[px-(p^2/2)t]}\,dp = \frac{i\big\{-\log[-i(x-1)]+\log[i(x-1)]+\log[-i(x+1)]-\log[i(x+1)]\big\}}{2\sqrt{2\pi}}$$

which—absurdly—is t-independent, and which upon simplification is found to be also x-independent, to vanish identically! But when I resolved the complex exponential into its real and imaginary parts I was promptly led, at (21), to the complicated functions $F(x,t)$ and $G(x,t)$ upon which the early part of this work is based.

Reconstruction of those functions was the very first calculation attempted on my fancy new computer, with its improved software. I was distressed to discover that *Mathematica* 5 <u>refused to do the integrals</u>. I brought this disappointing development to the attention of Richard Crandall, Stan Wagon and (at Wagon's suggestion) Michael Trott.[12] Crandall made inquiries of Wolfram Research, and learned that "they do indeed have software problems not

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[12] Crandall (www.perfsci.com/) is the author of *Mathematica for the Sciences* (1991) and of a great many other *Mathematica*-based publications. Wagon (www.stanwagon.com/) is the author of *Mathematica in Action* (2nd edition 1991) and regularly conducts *Mathematica* workshops. Michael Trott, a physicist turned computer graphics specialist at Wolfram Research, is well-established as a leading expert in the field.

yet ironed out," and speculated that I had run afoul of one of those. Wagon was able to replicate both my success and my failure, and to satisfy himself that the results (21) reported by *Mathematica* 4 are indeed correct.[13] He attributed my problem to "subtle changes in some of the algorithms [necessitated by the fact that] some integrals and sums [as done] in version 4 were based on algorithms that were not entirely correct in the generality they were used." Wagon reported on the basis of his own direct experience that the adjustments made in version 5 have had "an impact on some sums" and speculated that they may have had an impact also on some symbolic integrals.

Wagon's take on the situation conformed to my discovery (of which he was unaware) that the results (21) supplied by version 4 appear to be susceptible to numerical instabilities (see again the spikes and underbrush in Figures 4b & 5).

Trott, while granting that the situation I had encountered was "not nice," considered that "such situations are basically unavoidable in developing complex software with millions of lines of code." He reports that the people at Wolfram Research "run thousands of tests every night to make sure that no capabilities or features are lost" but emphasizes that "the process is not foolproof." He interprets my experience to mean that I "found an example that did indeed get lost," and reports that he has "sent your example to the Integrate Developer, [who will] try to restore it for the next version." I am left to wonder (in view of the above-mentioned instability problem) whether the Integrate Developer will report back to Trott that "We dropped that integral intentionally, because it was faulty."

It is Crandall's hunch (mine also: see again page 15) that the "instability problem" should be attributed not to a defect in the claimed functional forms of the integrals in question, but to *Mathematica* 4's default management of the numerical analysis . . . and that it would disappear if one arranged to work in higher precision. Figure 13 provides (weak) evidence that Crandall's intuition may be well founded.

Trott took the trouble to inform me that, while the $F(x,t)$-generating command

```
Integrate[(Sin[p]*Cos[p-(p^2/2)])/p,{p,0,∞}]
```

produces no result[14] in version 5, "you can recover the integral in version 5 by using [the following command:]"

```
Integrate[#,{p,0,∞}, GenerateConditions→False]&/@
Expand[TrigReduce[(Sin[p]*Cos[p-(p^2/2)])/p]
```

and in this he is quite correct! True, the result thus produced is not displayed in quite the familiar way, but if (working necessarily in version 4) one subtracts

[13] This he did by verifying that the symbolic integral agreed with the result of numerical integration at $x = t = 5$.

[14] Not quite: it produces a notification that "The integral does not converge."

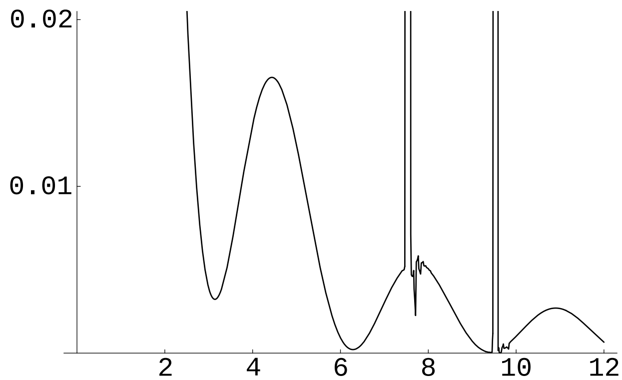

FIGURE 13: *The function* $P(x,1)$ *was a creation of* Mathematica 4, *but has been plotted here by* Mathematica 5. *Comparison with* FIGURE 5 (*which was drawn by* Mathematica 4) *shows a great reduction of "underbrush," which—on the presumption that the newer version has improved numerical analysis capabilities—might be interpreted as evidence that, as Richard Crandall has suggested,* Mathematica 4 *manages the integral correctly, but stumbles on the numerical interpretation of its own symbolic result. Note, however, that the spikes persist.*

the result of Trott's command from the result of the original command and `Simplify`s one does get `0`. The integral $G(x,t)$ can be recovered similarly. At present I do not understand *how* Trott's command manages to persuade *Mathematica* 5 to do what it had declared to be impossible.

Wagon remarks that the command `FunctionExpand`, when applied to the strings of decorated hypergeometric functions that at (21) served to describe $F(x,t)$ and $G(x,t)$, produces <u>strings of decorated Fresnel integrals</u> (plus a couple of dangling hypergeometrics). The essence of the situation is captured by the following statements:

$$\texttt{FunctionCommand[HypergeometricPFQ[}\{\tfrac{1}{4}\},\{\tfrac{1}{2},\tfrac{5}{4}\},-z^4\texttt{]]} = \frac{\sqrt{\pi}\,\texttt{FresnelC[}2z/\sqrt{\pi}\texttt{]}}{2z}$$

$$\texttt{FunctionCommand[HypergeometricPFQ[}\{\tfrac{3}{4}\},\{\tfrac{3}{2},\tfrac{7}{4}\},-z^4\texttt{]]} = \frac{3\sqrt{\pi}\,\texttt{FresnelS[}2z/\sqrt{\pi}\texttt{]}}{4z^3}$$

where

$$\texttt{FresnelC[}z\texttt{]} \equiv \int_0^z \cos\left[\tfrac{\pi}{2}t^2\right]dt \text{ is usually denoted } C(z)$$

$$\texttt{FresnelS[}z\texttt{]} \equiv \int_0^z \sin\left[\tfrac{\pi}{2}t^2\right]dt \text{ is usually denoted } S(z)$$

The Fresnel integrals are well known[15] to be closely related to confluent hypergeometric functions on the one hand, and to the error function on the other, so—fine details aside!—we should perhaps not be surprised to find that functions which by one line of argument came on page 11 to be described in terms of hypergeometric functions have on page 15 come, by a different line of argument, to be described in terms of error functions. But the devil lives in the details. . . for which at the moment I have no stomach.

One final remark: Marianne Colgrove, who serves at the office of Computing & Information Services as the college's *Mathematica* contact person, has approached Wolfram Research on my behalf, and has been informed—this in response to my observation that version 5, even though running on a faster machine, sometimes takes *longer* than version 4 to compute symbolic integrals[16] —that *Mathematica* 5 presently exploits only a fraction of the G5's resources. A 64-bit version is under development, but it is not yet possible to estimate when it will be ready for distribution.

[15] See Abramowitz & Stegun's Chapter 7, especially §**7.3**.

[16] Trott writes that, while my observation is accurate, it is easily explained: version 5 routinely "tries many more transformations than version 4 did, and returns much more exhaustive convergence conditions."