WAVEPACKET IN A BOX

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Introduction. I am motivated by difficulties recently encountered in another connection to return here to the playground where many of us began our quantum mechanical education: the problem of a "particle-in-a-box"—otherwise known as the problem of the "infinite square well" or (in Einstein's quaint phrase) the problem of a "ball between walls." I expect to demonstrate that in some respects it *is* a problem, and that the physics of the system, utterly simple though it is standardly represented to be, holds some surprises. To begin at the familiar beginning:

A mass point m is confined by infinite forces to the interior $0 \leqslant x \leqslant a$ of an interval (or "box"), within which it moves freely. The time-independent Schrödinger equation reads

$$\psi''(x) = -k^2\psi(x) \quad \text{with} \quad k \equiv \sqrt{2mE/\hbar^2} \tag{1}$$

and physically acceptable solutions are required

- to be continuous
- to vanish outside the box
- to be normalized.

Immediately

$$\psi_n(x) = \sqrt{\tfrac{2}{a}}\sin k_n x \quad \text{with} \quad k_n \equiv n\,\tfrac{\pi}{a} \quad : \quad n = 1, 2, 3, \ldots \tag{2}$$

and

$$E_n = (\hbar^2/2m)k_n^2 = \mathcal{E}n^2 \quad \text{with} \quad \mathcal{E} \equiv h^2/8ma^2 \tag{3}$$

The eigenfunctions (2) are orthonormal as written

$$\int_0^a \psi_m(x)\psi_n(x)\,dx = \delta_{mn} \tag{4}$$

and well-known to be complete, so we expect any initial state to be expressible

$$\psi(x) = \sum_n c_n\psi_n(x) \tag{5.1}$$

$$c_n = \int_0^a \psi_n(x)\psi(x)\,dx \tag{5.2}$$

Normalization[1] in the sense

$$\int_0^a \psi^*(x)\psi(x)\,dx = 1 \tag{6}$$

entails/requires

$$\sum_n c_n^* c_n = 1 \tag{7}$$

The probability density $|\psi(x)|^2$ is a more complicated object

$$|\psi(x)|^2 = \sum_{m,n} c_m^* c_n \psi_m^*(x)\psi_n(x) \tag{8}$$

"Turning on time" sets the eigenfunctions a-buzz

$$\psi_n(x) \equiv \psi_n(x,0) \quad\longmapsto\quad \psi_n(x,t) = e^{-i\Omega n^2 t}\psi_n(x) \quad : \quad \Omega \equiv \mathcal{E}/\hbar \tag{10}$$

and imparts motion to all linear combinations of eigenfunctions:

$$\psi(x,t) = \sum_n c_n e^{-i\Omega n^2 t}\psi_n(x) \tag{11}$$

So we obtain (here enter the $(m^2 - n^2)$'s that I write about in "Coincident spectral lines" (January 2001))

$$|\psi(x,t)|^2 = \sum_{m,n} c_m^* c_n e^{-i\Omega(m^2-n^2)t}\psi_m^*(x)\psi_n(x) \tag{12}$$

The off-diagonal terms make no contribution to $\int |\psi(x,t)|^2\,dx$, but it is *only* they that contribute to the *motion* of $|\psi(x,t)|^2$.

Notice in connection with (12) that

$$\begin{aligned}\psi_m^*(x)\psi_n(x) &= \tfrac{1}{a}\cos(m-n)\tfrac{\pi}{a}x - \tfrac{1}{a}\cos(m+n)\tfrac{\pi}{a}x \\ &= \text{long wavelength component} \\ &\qquad\qquad - \text{long wavelength component}\end{aligned} \tag{13}$$

Notice also how it comes about that the cosines *in combination* manage to vanish at either end of the box.

My problem: How, in explicit detail, does one, within such a framework, *fabricate and trace the motion of an* *<u>initially localized wavepacket</u>*? How, more particularly, does one demonstrate the *diffusive behavior—the <u>tendency toward flatness</u>*—which on intuitive grounds one expects to be a dominanat feature of the physics?

[1] I install *'s, though it will be a moment before they have work to do.

Fourier-analytic distinction between periodic and clamped formalisms. Abandon the box for a moment. Imagine $\psi(x)$ to range on the entire real line, and let $\Psi(k)$ be its Fourier transform:

$$\psi(x) = \int \Psi(k)e^{ikx}\,dk \tag{14.1}$$

$$\Psi(k) = \tfrac{1}{2\pi}\int \psi(x)e^{-ikx}\,dx \tag{14.2}$$

At (2) we had

$$\psi_n(x) = \sqrt{\tfrac{2}{a}}\,\tfrac{1}{2i}\Big\{e^{ik_nx} - e^{-ik_nx}\Big\} \tag{15.1}$$

which entails

$$\Psi_n(k) = \sqrt{\tfrac{2}{a}}\,\tfrac{1}{2i}\Big\{\delta(k-k_n) - \delta(k+k_n)\Big\} \tag{15.2}$$

The eigenfunction $\psi_n(x)$ was imagined at (2) to extend periodically beyond the physical bounds of the box, and from periodicity follows the spiky structure of $\Psi_n(k)$.

Suppose, however, that in the name of physical realism we were to install the requirement that the wave function should *vanish* beyond the bounds of the box (since there is, by assumption, no possibility that the particle will ever be found there):

$$\psi_n(x) = \begin{cases} \sqrt{\tfrac{2}{a}}\sin k_nx & : \quad 0 \leqslant x \leqslant a \\ \\ 0 & : \quad \text{elsewhere} \end{cases} \tag{16.1}$$

From (14.2) we then obtain

$$\Psi_n(k) = \sqrt{\tfrac{a}{2}}\,n\,\frac{1-(-)^n e^{-iak}}{n^2\pi^2 - a^2k^2} \tag{16.2}$$

where

$$\frac{1}{n^2\pi^2 - a^2k^2} = \frac{1}{2\pi na}\left\{\frac{1}{k+k_n} - \frac{1}{k-k_n}\right\} \tag{17}$$

shows the expression on the right side of (16.2) to possess simple poles at $k = \pm k_n$, and in that respect to resemble (15.2), but to differ markedly from (15.2) in that it is non-zero at other values of k: *clamping brings additional Fourier components into play.*

Those additional Fouier components notwithstanding, the $\psi_n(x)$ defined at (16.1) clearly satisfies the Schrödinger equation (1) at *all*[2] points x, and is normalized in the strong sense that $\int_{-\infty}^{\infty}|\psi_n(x)|^2\,dx = 1$.

[2] At the endpoints of the box one must distinguish left derivatives from right derivatives.

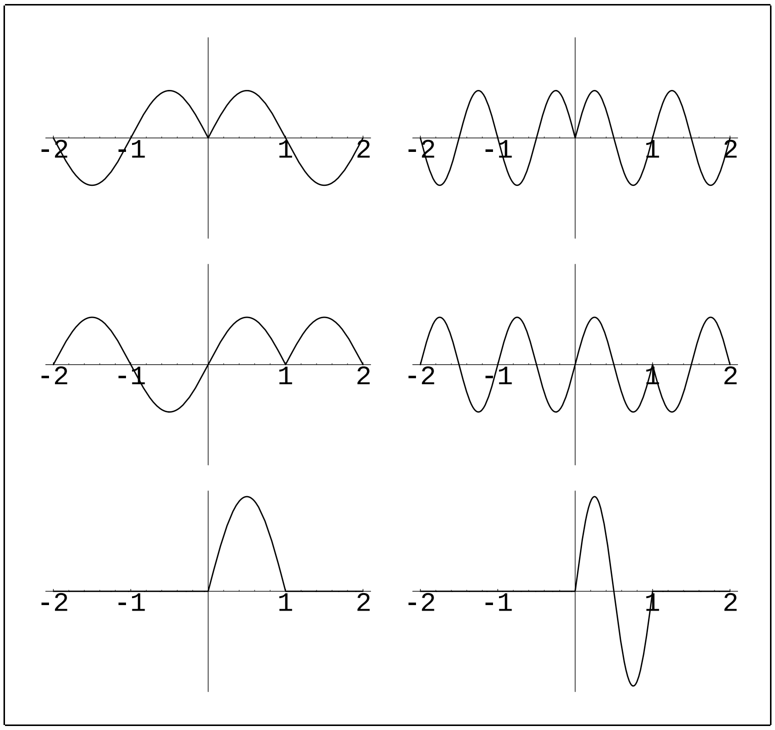

FIGURE 1: *Illustrations of the clever way in which (19) does its work. In the left column $n = 1$, in the right column $n = 2$. Figures in the top row derive from the first term, and figures in the second row from the second term . . . on the right side of (19). Addition produces the figures in the bottom row.*

Returning to (14.1) with (16.2) we obtain

$$\psi_n(x) = \sqrt{\tfrac{a}{2}}\, n\int_{-\infty}^{+\infty} \frac{1}{n^2\pi^2 - a^2k^2}\Big\{e^{ikx} - (-)^n e^{ik(x-a)}\Big\}dk \tag{18.1}$$

$$= \sqrt{2a}\, n\int_{0}^{\infty} \frac{1}{n^2\pi^2 - a^2k^2}\Big\{\cos kx - (-)^n \cos k(x-a)\Big\}dk \tag{18.2}$$

Though the integrand becomes singular at $k = \pm n\pi/a$, the integral yields to *Mathematica*'s `PrincipalValue`→`True` option, which supplies

$$= \tfrac{1}{\sqrt{2a}}\Big\{\text{Sign}[x]\cdot\sin n\frac{\pi}{a}x - (-)^n\, \text{Sign}[x-a]\cdot\sin n\frac{\pi}{a}(x-a)\Big\} \tag{19}$$

The preceding figure shows how (19) accomplishes its mission.[3] Alternatively

[3] Simple though it is, I think this—which occurred to *Mathematica*, but would never have occurred to me—to be one of the sweetest little constructions I have encountered!

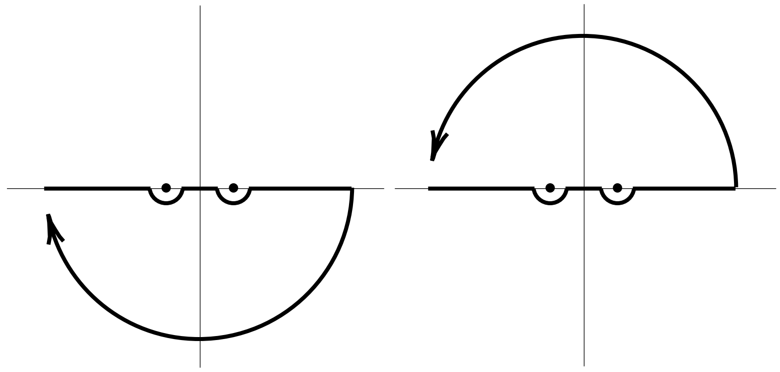

FIGURE 2: *The figure is to be read in reference to (20). Select the left/right contour according as* $x \lesseqgtr 0$ *to ascribe value to* 1^{st} integral, *and according as* $x \lesseqgtr a$ *to ascribe value to* 2^{nd} integral.

(though it amounts actually to the same thing), one might appeal to the calculus of residues: use (17) to obtain (after complexification of $k : k \mapsto k + i\ell$)

$$\begin{aligned} \psi_n(x) = \tfrac{1}{\sqrt{2a}}\Big\{ &\quad \tfrac{1}{2\pi i}\oint i\Big[\frac{1}{k+n\frac{\pi}{a}} - \frac{1}{k-n\frac{\pi}{a}}\Big]e^{ikx}\,dk \\ &- (-)^n \tfrac{1}{2\pi i}\oint i\Big[\frac{1}{k+n\frac{\pi}{a}} - \frac{1}{k-n\frac{\pi}{a}}\Big]e^{ik(x-a)}\,dk\Big\} \\ = 1^{\text{st}} \text{ integral} - (-)^n \cdot 2^{\text{nd}} \text{ integral} \end{aligned} \tag{20}$$

Selecting contours as indicated in the preceding figure, one obtains

$$1^{\text{st}} \text{ integral} = \begin{cases} 0 & : \quad x < 0 \\ \sqrt{\frac{2}{a}}\sin n\frac{\pi}{a}x & : \quad 0 < x \end{cases}$$

$$2^{\text{nd}} \text{ integral} = \begin{cases} 0 & : \quad x < a \\ (-)^{2n}\sqrt{\frac{2}{a}}\sin n\frac{\pi}{a}x & : \quad a < x \end{cases}$$

—whence the desired result (16.1). And working from (20) one can use this corollary

$$\tfrac{d^2}{dx^2}\Big\{\tfrac{1}{2\pi i}\oint \tfrac{1}{k-k_n}e^{ikx}\,dk\Big\} = \tfrac{1}{2\pi i}\oint \tfrac{-k^2}{k-k_n}e^{ikx}\,dk = -k_n^2 \cdot \tfrac{1}{2\pi i}\oint \tfrac{1}{k-k_n}e^{ikx}\,dk$$

of Cauchy's principle

$$\tfrac{1}{2\pi i}\oint \tfrac{1}{z-a}f(z)\,dz = f(a)\cdot \tfrac{1}{2\pi i}\oint \tfrac{1}{z-a}\,dz$$

to construct an alternative direct demonstration that the clamped functions $\psi_n(x)$ do in fact satisfy the Schrödinger equation:

$$\psi_n''(x) = -k_n^2\psi_n(x) \tag{21}$$

This last remark provides the resolution of what otherwise might seem a mystery: How can a function that according to this notational variant of (18)

$$\psi_n(x) = -\sqrt{\tfrac{a}{2}}\,n\frac{1}{a^2}\int_{-\infty}^{+\infty}\frac{1}{k^2-k_n^2}\Big\{1-(-)^n e^{-ika}\Big\}e^{ikx}dk \tag{22}$$

appears to contain Fourier components additional to $e^{\pm ik_n x}$ be nevertheless a solution of (21)? The answer appears to be that the intrusive components are ghostly spectators—not really present.

How are we to launch such an eigenfunction into dynamical motion? Our instinct is to write

$$\psi_n(x) \;\longmapsto\; \psi_n(x,t) \equiv \psi_n(x)\cdot e^{-i\omega_n t}$$
$$\omega_n \equiv E_n/\hbar = \mathcal{E}n^2/\hbar = \Omega n^2 = \tfrac{\hbar}{2m}k_n^2$$

as was done already at (10). But the right side of (22) reminds us that the time-dependent free particle Schrödinger equation

$$-\tfrac{\hbar^2}{2m}\psi_{xx} = i\hbar\psi_t \tag{23}$$

is satisfied by *every* complex exponential $e^{i(px-Et)/\hbar}$ subject to the dispersion relation $E = p^2/2m$; is satisfied, that is to say, by every $e^{i(kx-\omega t)}$ subject to $\omega = (\hbar/2m)k^2$. It becomes natural in this light to write

$$\psi_n(x,t) = -\sqrt{\tfrac{a}{2}}\,n\frac{1}{a^2}\int_{-\infty}^{+\infty}\frac{1}{k^2-k_n^2}\Big\{1-(-)^n e^{-ika}\Big\}e^{i(kx-\omega t)}dk \tag{24}$$

Such a $\psi(x,t)$, by the argument recent rehearsed, will satisfy (23) if

$$\omega(k) = (\hbar/2m)k^2$$

(and will on that assumption also vanish at and beyond the boundaries of the box) and appears to present a continuum of frequencies. But the frequencies $\omega \neq \omega_n$ are, I argue, ghostly silent hummers.

Our success in the preceding discussion has been seen to hinge on correct management of the singularities present in the integrands of (18/20/22/24).

Flat wavefunctions. Wavefunctions of the form

$$\psi(x) = \tfrac{1}{\sqrt{a}}\,e^{i\varphi(x)} \quad : \quad \varphi(x) \text{ arbitrary} \tag{25}$$

give probability distributions

$$|\psi(x)|^2 = \tfrac{1}{a} \tag{26}$$

which are constant in the interior of the box. They are susceptible to the criticism that they *fail to vanish at the box boundaries*, but the force of that criticism is blunted by the observation that the requirement $\psi(0) = \psi(a) = 0$ derives from the deeper/weaker requirement that the "probability current"

$$J(x,t) \equiv \tfrac{i\hbar}{2m}\big(\psi\psi_x^* - \psi_x\psi^*\big) \tag{27}$$

vanish (all t) at the boundaries. For wavefunctions of the flat design (25) we have

$$J(x) = \tfrac{\hbar}{ma}\varphi_x(x)$$

so it is physically sufficient to stipulate that

$$\varphi_x(0) = \varphi_x(a) = 0 \tag{28}$$

Which would, of course, be satisfied were we to set $\varphi(x) \equiv$ constant (call it 0). In that case (which will be shown in a moment to be the *only* admissible case) we can use (5) to obtain

$$\begin{aligned}
\psi_{\text{flat}}(x) \equiv \tfrac{1}{\sqrt{a}} = \sum_n c_n\psi_n(x)& \\
c_n &= \int_0^a \tfrac{1}{\sqrt{a}}\cdot\sqrt{\tfrac{2}{a}}\sin n\tfrac{\pi}{a}x\,dx \\
&= \tfrac{\sqrt{2}}{\pi}\frac{1-\cos n\pi}{n} \\
= \tfrac{1}{\sqrt{a}}\cdot\sum_n \tfrac{2}{\pi}\frac{1-\cos n\pi}{n}\sin n\tfrac{\pi}{a}x& \qquad (29.1)\\
= \tfrac{1}{\sqrt{a}}\cdot\tfrac{4}{\pi}\Big\{\tfrac{1}{1}\sin 1\tfrac{\pi}{a}x + \tfrac{1}{3}\sin 3\tfrac{\pi}{a}x + \tfrac{1}{5}\sin 5\tfrac{\pi}{a}x + \cdots\Big\}& \qquad (29.2)
\end{aligned}$$

Our interest in (29) is restricted to the interior of the box: $0 \leqslant x \leqslant a$. But if we take the larger view then the expressions to the right of the $\cdot$ describe what is familiar to engineers as a "square wave"—an odd periodic function that alternates between the values ± 1 and that crosses the axis (vanishes) at the points $x = \pm na$. Squaring yields a "rectified square wave"—a function that continues to touch (but not cross) the axis at the nodal points $x = \pm na$, but that struggles elsewhere to be constantly $(\pm 1)^2 = 1$. From

$$\sin m\tfrac{\pi}{a}x \cdot \sin n\tfrac{\pi}{a}x = \tfrac{1}{2}\Big\{\cos(m-n)\tfrac{\pi}{a}x - \cos(m+n)\tfrac{\pi}{a}x\Big\}$$

we conclude that

$$\begin{aligned}
&\Big[\tfrac{4}{\pi}\Big\{\tfrac{1}{1}\sin 1\tfrac{\pi}{a}x + \tfrac{1}{3}\sin 3\tfrac{\pi}{a}x + \tfrac{1}{5}\sin 5\tfrac{\pi}{a}x + \cdots\Big\}\Big]^2 \\
&\qquad = \big(\tfrac{4}{\pi}\big)^2\tfrac{1}{2}\Big\{c_0 + c_2\cos 2\tfrac{\pi}{a}x + c_4\cos 4\tfrac{\pi}{a}x + c_6\cos 6\tfrac{\pi}{a}x + \cdots\Big\}
\end{aligned}$$

with

$$c_0 = \sum_{k=0}^{\infty}\frac{1}{(2k+1)^2} = \tfrac{\pi^2}{8}$$

Evidently

$$\big[\text{etc.}\big]^2 = 1 + (\text{terms struggling to become zero})$$

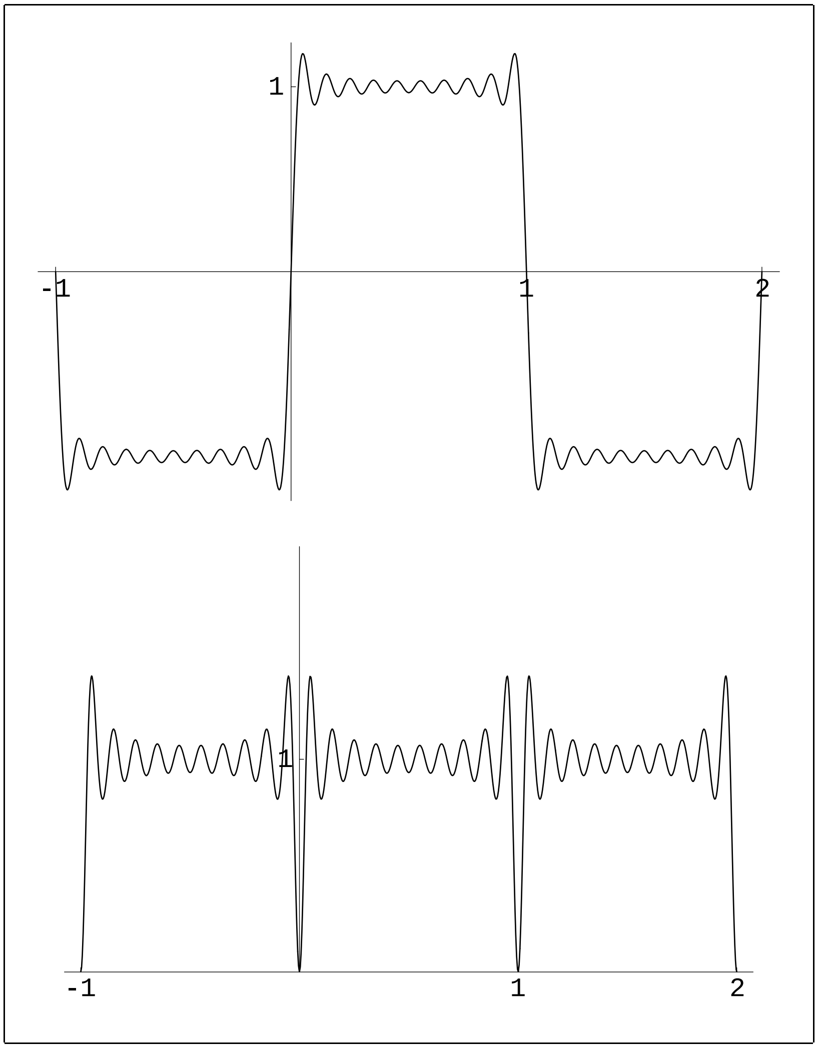

FIGURE 3: *Shown above: the square wave obtained from (29) by setting $a = 1$ and discarding terms with $n > 19$. Shown below: the square of that function. Gibbs' phenomenon is clearly evident in both cases.*

It will be worth our while to look into the details of that struggle (though getting the argument down on the page is itself a bit of a struggle). With columns labeled m and rows labeled n make DIFFERENCE and SUM tables showing the values assumed respectively by $m - n$ and $m + n$. The entries in the former are $0, \pm 2, \pm 4, \ldots$ (but since $\cos \xi$ is even we can abandon the $-$ signs at cost of multiplying our results by 2), while the entries in the SUM table are $2, 4, 6, \ldots$

We observe that $\cos 2\frac{\pi}{a}x$ terms arise from entries

$$\{m,n\} = \begin{cases} \{1,1\} & \text{on the SUM table} \\ \\ \{3,1\} \text{ also } \{1,3\} & \\ \{5,3\} \text{ also } \{3,5\} & \text{on the DIFFERENCE table} \\ \{7,5\} \text{ also } \{5,7\} & \\ \quad\vdots & \end{cases}$$

The implication is that

$$c_2 = \tfrac{1}{2}\Big\{\underbrace{2\Big[\tfrac{1}{1\cdot 3}+\tfrac{1}{3\cdot 5}+\tfrac{1}{5\cdot 7}+\cdots\Big]}_{2} - \tfrac{1}{1\cdot 1}\Big\} = 0$$

Similarly, $\cos 4\frac{\pi}{a}x$ terms arise from entries

$$\{m,n\} = \begin{cases} \{1,3\} & \text{on the SUM table} \\ \{3,1\} & \\ \\ \{5,1\} \text{ also } \{1,5\} & \\ \{7,3\} \text{ also } \{3,7\} & \text{on the DIFFERENCE table} \\ \{9,5\} \text{ also } \{5,9\} & \\ \quad\vdots & \end{cases}$$

So we have

$$c_4 = \tfrac{1}{2}\Big\{\underbrace{2\Big[\tfrac{1}{1\cdot 5}+\tfrac{1}{3\cdot 7}+\tfrac{1}{5\cdot 9}+\cdots\Big]}_{2/3} - \Big[\tfrac{1}{1\cdot 3}+\tfrac{1}{3\cdot 1}\Big]\Big\} = 0$$

In next higher order we encounter

$$c_6 = \tfrac{1}{2}\Big\{\underbrace{2\Big[\tfrac{1}{1\cdot 7}+\tfrac{1}{3\cdot 9}+\tfrac{1}{5\cdot 11}+\cdots\Big]}_{23/45} - \Big[\tfrac{1}{1\cdot 5}+\tfrac{1}{3\cdot 3}+\tfrac{1}{5\cdot 1}\Big]\Big\} = 0$$

and in the general case

$$c_{2p} = \tfrac{1}{2}\Big\{\underbrace{2\sum_{k=0}^{\infty}\tfrac{1}{(2k+1)(2k+1+2p)}}_{f(p)} - \underbrace{\sum_{k=0}^{p-1}\tfrac{1}{(2k+1)(2p-2k-1)}}_{g(p)}\Big\} = 0$$

which vanishes because, according to *Mathematica*,

$$\begin{array}{llll} f(1)=g(1)=1 & & f(6)=g(6) = \frac{3254}{10395} & = 0.313035 \\ f(2)=g(2)=\frac{2}{3} & = 0.666667 & f(7)=g(7) = \frac{88069}{315315} & = 0.279305 \\ f(3)=g(3)=\frac{23}{45} & = 0.511111 & f(8)=g(8) = \frac{11384}{45045} & = 0.252725 \\ f(4)=g(4)=\frac{44}{105} & = 0.419048 & f(9)=g(9) = \frac{1593269}{6891885} & = 0.231180 \\ f(5)=g(5)=\frac{563}{1575} & = 0.357460 & f(10)=g(10) = \frac{15518938}{72747675} & = 0.213326 \\ & & \vdots & \end{array}$$

Notice that if we had truncated (29.2) after (say) five terms, squared, and abandoned all but the leading five terms we would have obtained quite a different result:

$$\begin{aligned}\tfrac{1}{a}\tfrac{8}{\pi^2}\Big\{1.183860 &- 0.111111\cos 2\tfrac{\pi}{a}x\\ &- 0.126984\cos 4\tfrac{\pi}{a}x\\ &- 0.151323\cos 6\tfrac{\pi}{a}x\\ &- 0.196825\cos 8\tfrac{\pi}{a}x + \cdots\Big\}\end{aligned}$$

The point is that no matter how large m and n may individually be, if their difference is small (*i.e.*, if $\{m,n\}$ lies close to the diagonal) they will contribute to the long-wavelength design of the squared function; in this respect, squaring a Fourier series is quite unlike squaring a power series. Truncation—though often unavoidable—can lead to deceptive conclusions.

Clearly, any function of the form $\psi(x,t) = (\text{constant})e^{i(\text{constant})}$ satisfies the Schrödinger equation (23), and therefore (or by direct inspection) satisfies also the continuity equation[4]

$$P_t + J_x = 0 \tag{30}$$

Look more generally to

$$\psi(x,t) = (\text{constant})\cdot e^{i\varphi(x,t)}$$

and agree to dismiss the formal difficulties that arise if at isolated points the "constant" abruptly reverses sign or drops to zero. The Schrödinger equation requires $\frac{\hbar^2}{2m}(\varphi_x)^2 - i\frac{\hbar^2}{2m}\varphi_{xx} = -\hbar\varphi_t$ which (separating the real and imaginary parts) can be written

$$\tfrac{1}{2m}(\hbar\varphi_x)^2 + (\hbar\varphi)_t = 0 \quad\text{and}\quad \varphi_{xx} = 0$$

The latter assures local conservation of probability since (30) has become

$$J_x = 0 \quad\text{with}\quad J = (\text{constant})^2\cdot\tfrac{\hbar}{m}\varphi_x$$

while the former can be read as a requirement that $\hbar\varphi$ be a solution of the free particle Hamilton-Jacobi equation. From $\varphi_{xx} = 0$ we obtain

$$\varphi(x,t) = \alpha(t) + \beta(t)x$$

The boundary conditions (28) enforce $\beta(t)\equiv 0$, so the H-J condition reduces to $\alpha_t = 0$, requiring $\alpha(t)$ to be in fact constant. We are brought thus to the conclusion that

$$\psi_{\text{flat}}(x,t) = \tfrac{1}{\sqrt{a}}e^{i\,\alpha} \tag{31}$$

[4] Here $P(x,t)\equiv|\psi(x,t)|^2$ while $J(x,t)$ was defined already at (27).

describes what is in fact (within the context provided by the particle-in-a-box problem) the *most general* admissible flat wavefunction.

In the clamped formalism this result becomes

$$\psi_{\text{flat}}(x) = \int \Psi_{\text{flat}}(k)e^{ikx}\,dk \tag{32.1}$$

$$\begin{aligned}\Psi_{\text{flat}}(k) &= \tfrac{1}{2\pi}\tfrac{1}{\sqrt{a}}e^{i\,\alpha}\int_0^a e^{-ikx}\,dx\\ &= \tfrac{1}{2\pi}\tfrac{1}{\sqrt{a}}e^{i\,\alpha}\,\frac{1-e^{-ika}}{ik}\end{aligned} \tag{32.2}$$

Insert (32.2) back into (32.1) and turn on the `PrincipalValue→True` option: *Mathematica* supplies

$$\psi_{\text{flat}}(x) = \tfrac{1}{\sqrt{a}}e^{i\,\alpha}\left\{\frac{\text{Sign}[x]+\text{Sign}[a-x]}{2}\right\} \tag{33}$$

which does its work by the elegant principle illustrated already in Figure 1. The improper integral yields to also to a slight variant of the $\oint$ technique previously described.

Now "turn on time" (and watch everything come unstuck!). From (29) we obtain

$$\begin{aligned}\psi_{\text{flat}}(x,t) &= \tfrac{1}{\sqrt{a}}\cdot\sum_n \tfrac{2}{\pi}\tfrac{1-\cos n\pi}{n}\,e^{-i\,\Omega n^2 t}\sin n\tfrac{\pi}{a}x\\ &= \tfrac{1}{\sqrt{a}}\cdot\tfrac{4}{\pi}\Big\{\tfrac{1}{1}e^{-i\,\Omega t}\sin 1\tfrac{\pi}{a}x + \tfrac{1}{3}e^{-i\,9\Omega t}\sin 3\tfrac{\pi}{a}x\\ &\qquad\qquad + \tfrac{1}{5}e^{-i\,25\Omega t}\sin 5\tfrac{\pi}{a}x+\cdots\Big\}\end{aligned} \tag{34}$$

The right side of (34) presents a sum of boundary-condition-respecting periodic solutions of the time-dependent Schrödinger equation (23). But at times $t>0$ neither the real nor the imaginary part of the function thus described is flat: factors of the forms $\cos\Omega n^2 t$ and $\sin\Omega n^2 t$ have messed up the coefficients. Neither—for that same reason—is $|\psi_{\text{flat}}(x,t)|^2$ flat. In the latter connection we have

$$\begin{aligned}|\psi_{\text{flat}}(x,t)|^2 &= \big(\tfrac{1}{\sqrt{a}}\tfrac{4}{\pi}\big)^2\Big\{\sum_{n\text{ odd}}\tfrac{1}{n^2}\sin^2 n\tfrac{\pi}{a}x\\ &\qquad + 2\sum_{\substack{m,n\text{ odd}\\ m>n}}\tfrac{1}{mn}\cos\Omega(m^2-n^2)t\cdot\sin m\tfrac{\pi}{a}x\,\sin n\tfrac{\pi}{a}x\Big\}\\ &= \tfrac{1}{a}+\underbrace{\tfrac{1}{a}\cdot\tfrac{8}{\pi^2}\sum_{n\text{ odd}}\tfrac{1}{n^2}\cos 2n\tfrac{\pi}{a}x}_{\text{sawtooth}} + \text{oscillating terms}\end{aligned} \tag{35}$$

where the sawtooth ramps between $\pm\frac{\pi^2}{8}$ with period a: at $t=0$ the oscillating terms kill it, but never again. A typical oscillating term can be described

$$\begin{aligned}&\tfrac{2}{mn}\cos\Omega(m^2-n^2)t\cdot\sin m\tfrac{\pi}{a}x\cdot\sin n\tfrac{\pi}{a}x\\&\qquad=\tfrac{1}{mn}\cos\Omega(m^2-n^2)t\cdot\Big\{\cos(m-n)\tfrac{\pi}{a}x-\cos(m+n)\tfrac{\pi}{a}x\Big\}\end{aligned}$$

The oscillation becomes faster when $\{m,n\}$ lies farther from the diagonal, and oscillations at any given frequency have both a longwavelength and a short-wavelength component.

Time-averaging serves to kill the oscillatory part of (35), but does not kill the sawtooth. One is left with an averaged distribution

$$\overline{|\psi_{\text{flat}}(x,t)|^2}\equiv\lim_{T\to\infty}\tfrac{1}{T}\int_0^T|\psi_{\text{flat}}(x,t)|^2\,dt=\text{displaced sawtooth}$$

of the form shown below:

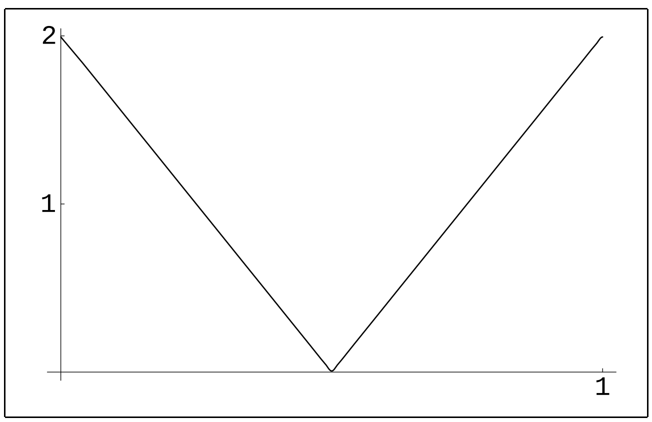

FIGURE 4: *Graph of the first two terms on the right side of (35); i.e., of the "displaced sawtooth" that results when the oscillating terms are abandoned. I have set $a=1$ and summed on the first thirty odd integers. Note that the curve never becomes negative, and that the area under the curve is unity: it describes, in other words, a proper distribution.*

To summarize: the contrived flatness of $|\psi_{\text{flat}}(x,0)|^2$ is *dynamically unstable*, and its time-average has a surprising shape. The question arises: Can one design wavefunctions $\psi(x,0)$ such that $\overline{|\psi(x,t)|^2}$ *is* flat? I will return to this question.

Were we, within the clamped formalism, to attempt to launch (32) into motion, writing

$$\psi_{\text{flat}}(x,t)=\tfrac{1}{\sqrt{a}}e^{i\,\alpha}\cdot\tfrac{1}{2\pi}\int\frac{1-e^{-ika}}{ik}e^{i[kx-\omega(k)t]}\,dk \tag{36}$$

with $\omega(k) \equiv E(k)/\hbar = \frac{\hbar}{2m}k^2 \equiv k\,u(k)$ [5] ...we would encounter two difficulties, the lesser of which is that the integral appears (owing to the exponentiated k^2) to be intractable. The greater problem is that the initial <u>confinement does not persist</u>: what the right side of (36) actually describes is the dispersive motion of an unconfined free-particle wavepacket that was initially $\sqcap$-shaped! To *preserve* confinement we should set a-buzz the securely clamped eigenstates described at (16.1) and described again at (18), writing something like

$$\psi_{\text{flat}}(x,t) = \sum_{n \text{ odd}} \tfrac{1}{n} e^{-\Omega n^2 t} \sqrt{\tfrac{a}{2}}\, n \int_{-\infty}^{+\infty} \frac{1}{n^2\pi^2 - a^2k^2} \Big\{ e^{ikx} - (-)^n e^{ik(x-a)} \Big\} dk$$

But clamping provides no avenue for escape from the dynamical instability of $|\psi_{\text{flat}}(x,t)|^2$, which flops as dizzily as before (though its gyrations are confined now to the interior of the box). Nor does time-averaging help: we produce a "saw with only one tooth."

I have been concerned in this discussion with the end-state to which—naive intuition informs us—*all* initial wavepackets should asymptotically evolve:

$$\psi_{\text{wavepacket}}(x,0) \xrightarrow[\text{diffusive dynamical evolution}]{} \psi_{\text{flat}}(x,t) \tag{37}$$

We have exposed two problems. The first is that $\psi_{\text{flat}}(x,t)$ is in fact *not flat* in the dynamically stable sense our intuition leads us to anticipate/demand. The second—barely touched upon, as yet—is that quantum mechanics, without the importation of extrinsic ideas, provides *no evolution mechanism*, no way for a wavefunction to become anything other than was written into its genes at the moment of birth.

Dynamical evolution of an arbitrary boxed state. If initially we have

$$\psi(x,0) = \sum_n c_n \sqrt{\tfrac{2}{a}} \sin n\frac{\pi}{a}x \tag{38.1}$$

then at time t we have

$$\psi(x,t) = \sum_n c_n e^{-i\Omega n^2 t} \sqrt{\tfrac{2}{a}} \sin n\frac{\pi}{a}x \tag{38.2}$$

and

$$\begin{aligned} |\psi(x,t)|^2 = \sum_n |c_n|^2 \tfrac{2}{a} \sin^2 n\frac{\pi}{a}x \\ + \sum_{m>n} \Big\{ c_m^* c_n e^{i\Omega(m^2-n^2)t} + c_m c_n^* e^{-i\Omega(m^2-n^2)t} \Big\} \\ \cdot \sin m\frac{\pi}{a}x \sin n\frac{\pi}{a}x \end{aligned}$$

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[5] It is the k-dependence of the wave speed $u(k) = \hbar k/2m$ that causes free particle quantum physics to be "dispersive."

If (as I will assume) the c's are real we obtain therefore the simpler result

$$|\psi(x,t)|^2 = \sum_n c_n^2 \tfrac{2}{a}\sin^2 n\tfrac{\pi}{a}x \tag{38.3}$$
$$+\,2\sum_{m>n} c_m c_n \cos\Omega(m^2-n^2)t\cdot \sin m\tfrac{\pi}{a}x\,\sin n\tfrac{\pi}{a}x$$

Immediately

$$\int_0^a |\psi(x,t)|^2\,dx = \sum_n c_n^2 = 1 \tag{39}$$

while time-averaging supplies

$$\overline{|\psi(x,t)|^2} = \sum_n c_n^2\tfrac{2}{a}\sin^2 n\tfrac{\pi}{a}x = \tfrac{1}{a}\sum_n c_n^2\Big\{1-\cos 2n\tfrac{\pi}{a}x\Big\}$$
$$= \tfrac{1}{a} - \tfrac{1}{a}\sum_n c_n^2 \cos 2n\tfrac{\pi}{a}x \tag{40}$$

If the intuition expressed at (37) is physically sound, then we must provide an answer to this question: What extra-dynamical mechanism serves to kill the second term on the right? Since the c's are at present subject only to the contraint $\sum c_n^2 = 1$, any strategy designed to do so must kill the $\cos 2n\frac{\pi}{a}x$'s *individually*, and that seems a very tall order.

I took up this project when, at page 61 in "Phase space formulation of the quantum mechanical particle-in-a-box problem" (December 2000), I found the tail wagging the dog; I decided to develop within ordinary quantum mechanics the details relating to an imagined "universal dispersive flattening" of confined wavepackets, and to return to my original discussion with those details fresh in hand. What has emerged is that they are details not to be had, details not present in the physics! What has emerged that Born & Ludwig did not understand the lesson of own mathematics when they imagined that served to answer Einstein's criticism; their conclusions were actually drawn from classical imagery which they plausibly/glibly/wrongly supposed their mathematics supported. I will sketch the outlines of a few topics that I had imagined to lie downstream, but the wind has been taken from my sails.

Addenda. ☐ It is established at (73.3) in "Phase space formulation . . . " that to describe a boxed Gaussian wavepacket (centered at x_0, with variance σ) we should set

$$c_n = \sqrt{2\sigma\sqrt{2\pi}}e^{-\pi^2(\sigma/a)^2n^2}\sqrt{2/a}\,\sin n\tfrac{\pi}{a}x_0$$

Returning with this information to (39) and (40) we expect to have

$$1 = 2\sigma\sqrt{2\pi}(2/a)\sum_{n=1}^\infty e^{-2\pi^2(\sigma/a)^2n^2}\sin^2 n\tfrac{\pi}{a}x_0 \tag{41.1}$$

and

$$\overline{|\psi(x,t)|^2} = 2\sigma\sqrt{2\pi}(2/a)\sum_{n=1}^\infty e^{-2\pi^2(\sigma/a)^2n^2}\sin^2 n\tfrac{\pi}{a}x_0\cdot\sin^2 n\tfrac{\pi}{a}x \tag{41.2}$$

Figures 16 and 20 illustrate the high sensitive dependence of c_n upon the value assigned to x_0. *Mathematica* has trouble with the sums, but numerical summation in illustrative concrete cases does tend to confirm (41.1). And (41.2), when plotted in those illustrative cases, is certainly not flat.

□ The Gaussian c_n's discussed above were obtained by Born/Ludwig's method of images. I had planned to illustrate the method in some non-Gaussian cases, but will save that for another occasion.