PHASE SPACE FORMULATION OF THE QUANTUM MECHANICAL PARTICLE-IN-A-BOX PROBLEM

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Introduction. The "phase space formulation of quantum mechanics" radiates from a definition

$$P_\psi(x,p) \equiv \tfrac{2}{h}\int \psi^*(x+\xi)\, e^{2\frac{i}{\hbar}p\,\xi}\, \psi(x-\xi)\, d\xi \tag{1}$$

which Wigner[1] was content to introduce as an unmotivated *ad hoc* contrivance, an aid to discussion of the relation of quantum statistical mechanics to its classical counterpart. The "Wigner distribution" is known today to possess a number of elegant and highly useful properties—some of which were known already to its co-inventor (whose acknowledged companion in this instance was Szilard)—but many of those are non-obvious/hidden, while on its face (1) displays some off-putting features. One of those that will concern us is its seeming xp-asymmetry.

By the mid-1940's it had been realized by several people[2] that Wigner's construction arises quite naturally from the (xp-symmetric) theory of the "Weyl transform," which had been sketched by Weyl already in 1927.[3] Specifically,

[1] E. P. Wigner, "On the quantum correction for thermodynamic equilibrium," Phys. Rev. **40**, 749 (1932).

[2] J. H. Groenwold, "On the principles of elementary quantum mechanics," Physica **12**, 405 (1946); J. E. Moyal, "Quantum mechanics as a statistical theory," Proc. Camb. Phil. Soc. **45**, 92 (1949).

[3] The Weyl transform uses generalized Fourier analytic techniques to set up an association ("Weyl correspondence") of the form

$$\text{classical observable } A(x,p) \xleftrightarrow[\text{Weyl}]{\hspace{2cm}} \text{quantum observable } \mathsf{A}$$

For review of the essentials see pages 4–9 of "Weyl transform and the phase space formalism," which is Chapter 2 of ADVANCED QUANTUM TOPICS (2000).

$hP_\psi(x,p)$ was recognized to be the Weyl transform of the pure-state density operator $\boldsymbol{\rho}_\psi$:

$$hP_\psi(x,p) \xleftrightarrow[\text{Weyl}]{} \boldsymbol{\rho}_\psi \equiv |\psi)(\psi|$$

Explicitly

$$hP_\psi(x,p) = \tfrac{1}{h}\iint (\psi|e^{-\frac{i}{\hbar}(\alpha\,\mathbf{p}+\beta\,\mathbf{x})}|\psi)\,e^{\frac{i}{\hbar}(\alpha p+\beta x)}\,d\alpha d\beta \tag{2}$$

which, we note in passing, *is* xp-symmetric. To recover (1) from (2) one might proceed this way:

Look first to

$$(\psi|e^{-\frac{i}{\hbar}(\alpha\,\mathbf{p}+\beta\,\mathbf{x})}|\psi) = \iint (\psi|x)dx(x|e^{-\frac{i}{\hbar}(\alpha\,\mathbf{p}+\beta\,\mathbf{x})}|p)dp(p|\psi)$$

Borrow from Campbell-Baker-Hausdorff theory the identity

$$e^{-\frac{i}{\hbar}(\alpha\,\mathbf{p}+\beta\,\mathbf{x})} = e^{\frac{1}{2}\frac{i}{\hbar}\alpha\beta}e^{-\frac{i}{\hbar}\beta\,\mathbf{x}}e^{-\frac{i}{\hbar}\alpha\,\mathbf{p}}$$

(which is a consequence ultimately of $[\mathbf{x},\mathbf{p}] = i\hbar\,\mathbf{I}$) to obtain

$$(\psi|e^{-\frac{i}{\hbar}(\alpha\,\mathbf{p}+\beta\,\mathbf{x})}|\psi) = e^{\frac{1}{2}\frac{i}{\hbar}\alpha\beta}\iint (\psi|x)\,e^{-\frac{i}{\hbar}\beta x}e^{-\frac{i}{\hbar}\alpha p}(x|p)(p|\psi)\,dxdp \tag{3}$$

But $(x|p) = \frac{1}{\sqrt{h}}e^{\frac{i}{\hbar}px}$ and

$$(p|\psi) = \int (p|x)dx(x|\psi) = \tfrac{1}{\sqrt{h}}\int e^{-\frac{i}{\hbar}px}(x|\psi)\,dx$$

so

$$\begin{aligned}(\psi|e^{-\frac{i}{\hbar}(\alpha\,\mathbf{p}+\beta\,\mathbf{x})}|\psi) &= \tfrac{1}{h}\,e^{\frac{1}{2}\frac{i}{\hbar}\alpha\beta}\iiint (\psi|x)\,e^{-\frac{i}{\hbar}\beta x}e^{-\frac{i}{\hbar}\alpha p}e^{\frac{i}{\hbar}p(x-x)}(x|\psi)\,dxdpdx\\ &= e^{\frac{1}{2}\frac{i}{\hbar}\alpha\beta}\iint (\psi|x)\,e^{-\frac{i}{\hbar}\beta x}\delta(x-x-\alpha)(x|\psi)\,dxdx\\ &= \int (\psi|x)e^{-\frac{i}{\hbar}\beta(x-\frac{1}{2}\alpha)}(x-\alpha|\psi)\,dx\end{aligned}$$

Returning with this information to (2) we have

$$\begin{aligned}hP_\psi(x,p) &= \tfrac{1}{h}\iiint (\psi|x)e^{-\frac{i}{\hbar}\beta(x-\frac{1}{2}\alpha)}\,e^{\frac{i}{\hbar}(\alpha p+\beta x)}(x-\alpha|\psi)\,dxd\alpha d\beta\\ &= \iint (\psi|x)e^{\frac{i}{\hbar}\alpha p}\delta(x-x+\tfrac{1}{2}\alpha)(x-\alpha|\psi)\,dxd\alpha\\ &= \int(\psi|x+\tfrac{1}{2}\alpha)\,e^{\frac{i}{\hbar}\alpha p}(x-\tfrac{1}{2}\alpha|\psi)\,d\alpha\end{aligned} \tag{4.1}$$

which gives back (1) after a trivial change of variables: $\alpha = 2\xi$.

Had we, on the other hand, introduced

$$(\psi|x) = \int (\psi|p)dp(p|x) = \tfrac{1}{\sqrt{h}}\int (\psi|p)e^{+\frac{i}{\hbar}px}\,dp$$

into (3) we would have been led by the same argument to this "momental companion" of (4.1):

$$hP_\psi(x,p) = \int (\psi|p - \tfrac{1}{2}\beta)\, e^{\frac{i}{\hbar}\beta\, x}(p + \tfrac{1}{2}\beta|\psi)\,d\beta \tag{4.2}$$

Equations (4) *collaboratively* restore xp-symmetry to the Wigner formalism, and show how—by installation of a convention—that underlying symmetry comes to *seem* broken.

In the preceding discussion

$$\text{all integrals are to be read } \int_{-\infty}^{+\infty}$$

which is "natural to the physics" of (say) free particles and oscillators, but presents a nest of formal difficulties when one attempts to apply the Wigner formalism to the particle-in-a-box problem. My objective here will be to identify and, if possible, to resolve those difficulties.[4]

Essentials of the particle-in-a-box problem. 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.[5] The time-independent Schrödinger equations reads

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

and physically acceptable solutions are required
- to be continuous
- to vanish outside the box
- to be normalized.

Immediately

$$\psi_n(x) = \sqrt{\tfrac{2}{a}}\sin k_n x \quad \text{with} \quad k_n \equiv n\,\tfrac{\pi}{a} \quad : \quad n = 1, 2, 3, \ldots \tag{5.1}$$

and

$$E_n = (\hbar^2/2m)k_n^2 = \mathcal{E}n^2 \quad \text{with} \quad \mathcal{E} \equiv h^2/8ma^2 \tag{5.2}$$

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[4] The topic is explored on pages 33–45 of Rodney Yoder's "The phase space formulation of quantum mechanics and the problem of negative probabilities," (Reed College thesis, 1992).

[5] I adhere to the conventions adopted in "2-dimensional 'particle-in-a-box' problems in quantum mechanics: Part I. Propagator & eigenfunctions by the method of images" (1997). Yoder, on the other hand, elected to distribute his box boundaries symmetrically about the origin: $-a \leqslant x \leqslant +a$.

Writing

$$E_n = p_n^2/2m$$

we have

$$p_n = \hbar k_n = n(h/2a) \tag{5.3}$$

Classically, such a confined free particle traces a rectangular trajectory in phase space, of

$$\text{phase area}_n = 2p_n \cdot a = nh$$

as required by the "Planck quantization condition."

Calculation supplies the following moment data:

$$\begin{aligned}
\langle x^1\rangle_n &\equiv \int_0^a \psi_n^*(x)\,x^1\psi_n(x)\,dx = \tfrac{1}{2}a \qquad : \qquad \text{all } n\\
\langle x^2\rangle_n &\equiv \int_0^a \psi_n^*(x)\,x^2\psi_n(x)\,dx = \big\{\tfrac{1}{3} - \tfrac{1}{2\pi^2 n^2}\big\}a^2\\
&\qquad\qquad\qquad\qquad\qquad\quad\downarrow\\
&\qquad\qquad\qquad\qquad\qquad = \tfrac{1}{3}a^2 \quad \text{for } n \text{ large}\\
&\qquad\qquad\qquad\qquad\qquad = \text{result from } \textit{flat} \text{ distribution!}
\end{aligned}$$

Therefore (by precisely the calculation that yields $I = \frac{1}{12}m\ell^2$ for the moment of inertial of a uniform rod, pinned at its center)

$$\Delta x = \sqrt{\langle x^2\rangle - \langle x^1\rangle^2} = \begin{cases} 0.18075\,a & : \quad n = 1\\ \frac{1}{\sqrt{12}}a = 0.28867\,a & : \quad \text{for } n \text{ large}\end{cases}$$

The uncertainty principle requires

$$\Delta x\,\Delta p \geqslant \tfrac{1}{2}\hbar$$

so we have

$$\Delta p = \sqrt{\langle p^2\rangle - \langle p^1\rangle^2} \geqslant \begin{cases} 2.76625\,\hbar/a & : \quad n = 1\\ 1.73208\,\hbar/a & : \quad \text{for } n \text{ large}\end{cases}$$

which gets smaller as the box gets larger. On the other hand, if the system is known to be in the n^{th} eigenstate then E_n is known precisely, and p_n is known *to within a sign*; we might expect, therefore, to have

$$\langle p^1\rangle = 0 \quad \text{and} \quad \langle p^2\rangle = 2mE_n = \hbar^2\big(n\,\tfrac{\pi}{a}\big)^2$$

giving $\Delta p = (n\pi)\hbar/a$; this, we note, is consistent with the uncertainty principle even in the case $n = 1$.

Confinement serves to assign a *largest possible* value to Δx, which is evidently achieved in the case $\psi(x) = \sqrt{\frac{1}{2}\delta(x-\epsilon) + \frac{1}{2}\delta(x-a+\epsilon)}$. One then has

$$\Delta x_{\max} = a/2$$

giving

$$\begin{aligned}\Delta p_{\text{min}} &= \hbar/a\\ &= p_{n+2} - p_n \quad ; \quad \text{any } n\end{aligned}$$

One can perfectly well contemplate measuring the instantaneous momentum of a particle in a box, but cannot expect to exceed the accuracy just stated. To phrase the issue another way: the time available for an energy measurement is (if we assume the window to be closed by the next wall collision) given on average by

$$\Delta t \leqslant \tfrac{1}{2}(\text{transit time, one side of box to other with speed } p/m) = ma/2p$$

Then $\Delta E\,\Delta t \geqslant \frac{1}{2}\hbar$ supplies

$$\Delta E \geqslant \hbar p/ma$$

But $E = p^2/2m \Rightarrow \Delta E = 2p\Delta p/2m$ so we have $2p\Delta p/2m \geqslant \hbar p/ma$ from which we recover $\Delta p_{\text{min}} = \hbar/a$.

The state of maximal Δx is a high information/low entropy state: one can expect to find the particle at one or the other boundaries of the box. Least information/highest entropy—maximal uncertainty in a sense more profound than is indicated by Δx—requires that the distribution be flat

$$|\psi_{\text{flat}}(x)|^2 = \begin{cases} 1/a & : \quad 0 < x < a\\ 0 & : \quad \text{elsewhere}\end{cases}$$

which in turn requires that

$$\psi_{\text{flat}}(x) = \tfrac{1}{\sqrt{a}}e^{i\,\varphi(x)} \quad : \quad \varphi(x) \text{ real, otherwise arbitrary}$$

If $f(x)$ is odd with period $2a$ (i.e., if $f(x) = -f(-x)$ and $f(x+2na) = f(x)$) the theory of Fourier series supplies

$$\begin{aligned}f(x) &= \sum_{n=1}^{\infty} b_n \sqrt{\tfrac{2}{a}}\sin n\tfrac{\pi}{a}x\\ b_n &= \int_0^a f(x)\cdot\sqrt{\tfrac{2}{a}}\sin n\tfrac{\pi}{a}x\,dx\end{aligned}$$

so we might expect to have

$$\begin{aligned}|\psi_{\text{flat}}(x)|^2 &= \sum_{n=1}^{\infty} b_n \sqrt{\tfrac{2}{a}}\sin n\tfrac{\pi}{a}x\\ b_n &= \int_0^a \tfrac{1}{a}\cdot\sqrt{\tfrac{2}{a}}\sin n\tfrac{\pi}{a}x\,dx = \frac{\sqrt{2}}{n\pi\sqrt{a}}(1-\cos n\pi)\\ &= \tfrac{4}{\pi a}\Big\{\tfrac{1}{1}\sin 1\tfrac{\pi}{a}x + 0 + \tfrac{1}{3}\sin 3\tfrac{\pi}{a}x + 0 + \tfrac{1}{5}\sin 5\tfrac{\pi}{a}x + \cdots\Big\}\\ &= \tfrac{2}{\pi a}\sum_{n=1}^{\infty}\frac{1-\cos n\pi}{n}\sin n\tfrac{\pi}{a}x \qquad (6.1)\end{aligned}$$

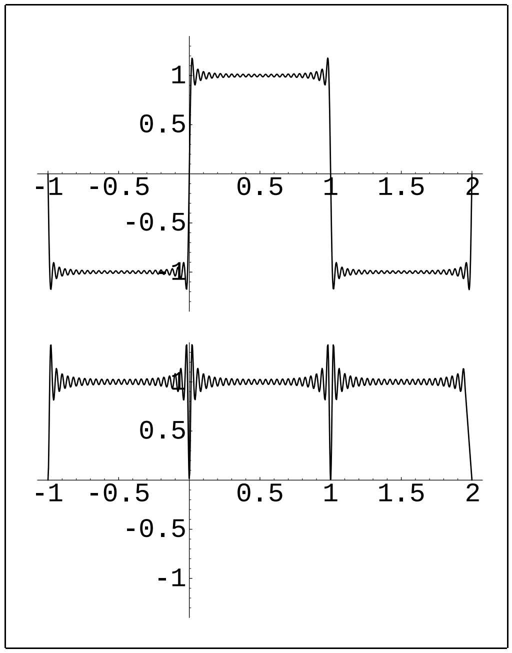

FIGURE 1: *Flat state as superposition of eigenstates. The top figure derives from (6.2), with $a = 1$ and $\varphi(x) \equiv 0$. Terms with $n > 50$ have been abandoned, and Gibbs' phenomenon is evident. The physical box is positioned $0 \leqslant x \leqslant 1$, and $\psi(x)$ is continued as an odd function into the exterior region. The lower figure shows $|\psi(x)|^2$, which is continued as an even function.*

but this does not suffice to nail down $\psi_{\text{flat}}(x)$ itself. Were we to set

$$\psi_{\text{flat}}(x) = \tfrac{2}{\pi\sqrt{a}} \sum_{n=1}^{\infty} \tfrac{1-\cos n\pi}{n} \sin n\,\tfrac{\pi}{a}x \cdot e^{i\,\varphi(x)} \tag{6.2}$$

then $|\psi_{\text{flat}}(x)|^2$ would be flat, but an *even* periodic function—distinct from (6.1). Note that flat wavefunctions with distinct phase factors will have *distinct spectra*. And that some pretty fancy function theory must enter into any explicit demonstration that (interior to the box) $|(6.2)|^2 = (6.1)$.

The functions discussed above continue periodically/non-vanishingly into regions exterior to the box. To achieve extinction in the exterior region we must abandon Fourier series in favor of the Fourier transform, writing

$$\psi(x) = \int_{-\infty}^{+\infty} b(k)\, e^{ikx}\, dk$$

$$b(k) = \tfrac{1}{2\pi} \int_{-\infty}^{+\infty} \psi(x)\, e^{-ikx}\, dx$$

If $\Psi_{\text{flat}}(x)$ is flat in the strong/aperiodic/more physical sense

$$\Psi_{\text{flat}}(x) = \begin{cases} a^{-\frac{1}{2}} & : \quad 0 < x < a \\ 0 & : \quad \text{elsewhere} \end{cases} \tag{7}$$

then

$$b(k) = \tfrac{1}{2\pi}\int_0^a a^{-\frac{1}{2}} e^{-ikx}\,dx = \tfrac{1}{2\pi ik\sqrt{a}}\big(1 - e^{-iak}\big)$$

supplies

$$\begin{aligned}
\Psi_{\text{flat}}(x) &= \int_{-\infty}^{+\infty} \tfrac{1}{2\pi ik\sqrt{a}}\big(1 - e^{-iak}\big)e^{ikx}\,dk \\
&= 2\int_0^\infty (\text{even part of integrand})\,dk \\
&= \tfrac{1}{\pi\sqrt{a}}\int_0^\infty \frac{\sin kx - \sin k(x-a)}{k}\,dk \qquad (8.1) \\
&= \tfrac{1}{\pi\sqrt{a}}\int_0^\infty \left\{\frac{1-\cos ka}{k}\sin kx + \frac{\sin ka}{k}\cos kx\right\}dk
\end{aligned}$$

which by a change of variables $k = \nu\pi/a$ becomes

$$= \tfrac{1}{\pi\sqrt{a}}\int_0^\infty \left\{\frac{1-\cos\nu\pi}{\nu}\sin\nu\tfrac{\pi}{a}x + \frac{\sin\nu\pi}{\nu}\cos\nu\tfrac{\pi}{a}x\right\}d\nu \tag{8.2}$$

The leading term on the right side of the final expression looks (except for a missing 2 and an omitted phase factor) like a continuous analog of (6.2). *Mathematica* confirms that $\Psi_{\text{flat}}(x)$, as described most conveniently by (8.1), does indeed reproduce (7), but we have

$$\Psi_{\text{flat}}(0) = \Psi_{\text{flat}}(a) = \tfrac{1}{\pi\sqrt{a}}\int_0^\infty \frac{\sin ka}{k}\,dk = \tfrac{1}{2}a^{-\frac{1}{2}}$$

This conforms to the general principle according to which the Fourier transform "splits the difference" at jump discontinuities, and since we are dealing here with an idealized situation we have no secure grounds on which to consider such a result physically dubious.

To address the physical issue just raised, let us look to the "clamped energy eigenstates"

$$\Psi_n(x) = \begin{cases} \sqrt{\tfrac{2}{a}}\sin n\tfrac{\pi}{a}x & : \quad 0 \leqslant x \leqslant a \\ 0 & : \quad \text{elsewhere} \end{cases} \tag{9.1}$$

which are *continuous* at the boundaries of the box (where, however, they exhibit undifferentiable kinks). We compute the Fourier transform

$$b_n(k) = \tfrac{1}{2\pi}\int_0^a \Psi_n(x)e^{-ikx}\,dx = \sqrt{\tfrac{a}{2}}\,n\,\frac{1-(-)^n e^{-iak}}{n^2\pi^2 - a^2k^2} \tag{9.2}$$

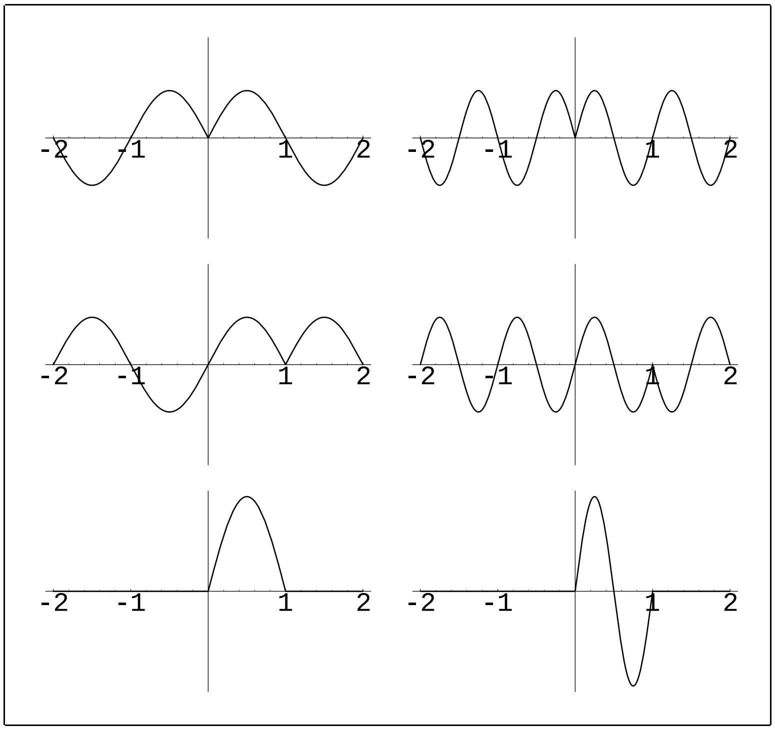

FIGURE 2: *Illustrations of the clever way in which (10) does its work. In the left column $n = 1$, in the right column $n = 2$. Figures in the top row derive from the first term, and figures in the second row from the second term ... on the right side of (10). Addition produces the figures in the bottom row. Simple though it is, I think this—which occurred to* Mathematica *but would never have occurred to me—to be one of the sweetest constructions I have encountered.*

and obtain

$$\begin{aligned}\Psi_n(x) &= \sqrt{\tfrac{a}{2}}\, n\int_{-\infty}^{+\infty} \frac{1}{n^2\pi^2 - a^2k^2}\Big\{e^{ikx} - (-)^n e^{ik(x-a)}\Big\}dk \\ &= \sqrt{2a}\, n\int_0^{\infty} \frac{1}{n^2\pi^2 - a^2k^2}\Big\{\cos kx - (-)^n \cos k(x-a)\Big\}dk\end{aligned}$$

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

$$= \tfrac{1}{\sqrt{2a}}\Big\{\mathrm{Sign}[x]\cdot \sin n\tfrac{\pi}{a}x - (-)^n\,\mathrm{Sign}[x-a]\cdot \sin n\tfrac{\pi}{a}(x-a)\Big\} \qquad (10)$$

Alternatively (though it amounts actually to the same thing), one might appeal

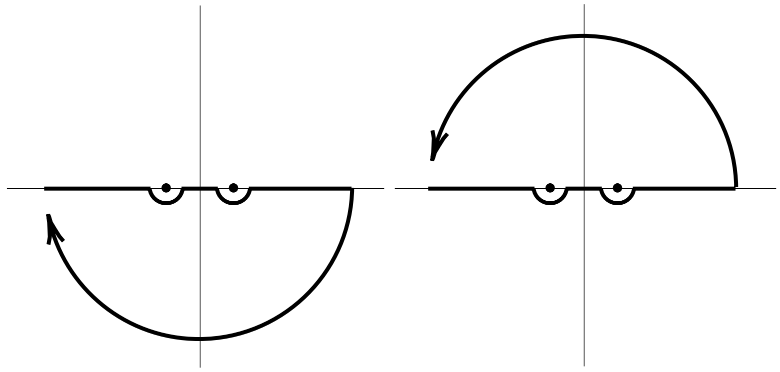

FIGURE 3: *The figure is to be read in reference to (11). Select the left/right contour according as $x \lesseqgtr 0$ to ascribe value to* 1^{st} integral, *and according as $x \lesseqgtr a$ to ascribe value to* 2^{nd} integral.

to the calculus of residues: use

$$\frac{1}{n^2\pi^2 - a^2k^2} = \frac{1}{2\pi na}\Big[\frac{1}{k+n\frac{\pi}{a}} - \frac{1}{k-n\frac{\pi}{a}}\Big]$$

to obtain (after complexification of $k : k \mapsto k + i\ell$)

$$\begin{aligned}\Psi_n(x) = \tfrac{1}{\sqrt{2a}}\Big\{ &\quad \tfrac{1}{2\pi i}\oint i\Big[\frac{1}{k+n\frac{\pi}{a}} - \frac{1}{k-n\frac{\pi}{a}}\Big]e^{ikx}\,dk \\ &- (-)^n\tfrac{1}{2\pi i}\oint i\Big[\frac{1}{k+n\frac{\pi}{a}} - \frac{1}{k-n\frac{\pi}{a}}\Big]e^{ik(x-a)}\,dk\Big\} \\ = 1^{\text{st}} \text{ integral} &- (-)^n\cdot 2^{\text{nd}} \text{ integral}\end{aligned} \tag{11}$$

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 (9.1).

That the "periodically continuated" and "clamped" approaches to the particle-in-a-box problem (see Figure 4) are—even though $\psi(x)$ and $\Psi(x)$ appear identical to a "physicist-in-the-box"—both analytically *and physically* distinct becomes strikingly evident when one passes from $(x|\psi)$ to $(p|\psi)$ ... though one point of commonality should be noted at the outset: <u>in neither formalism is it possible to speak of a "momentum eigenstate</u>." For the requisite conditions

$$\tfrac{\hbar}{i}\tfrac{d}{dx}\psi_p(x) = p\,\psi_p(x)\,, \quad \psi_p(0) = \psi_p(a) = 0\,, \quad \int_0^a |\psi_p(x)|^2\,dx = 1$$

cannot hold simultaneously. Common also to both formalisms are the equations

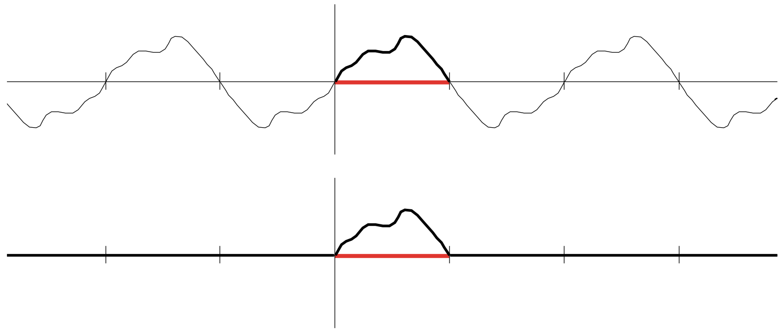

FIGURE 4: *Two distinct ways to conceptualize the "particle-in-a-box" problem. At top one imagines the wave function $\psi(x)$ to have been "periodically continuated" into regions external to the physical box, while at bottom $\psi(x)$ has been "clamped." The former is the approach standard to the textbooks, but the latter adheres more closely to the physical facts of the matter.*

$$\begin{aligned}\psi(x) &= \tfrac{1}{\sqrt{h}}\int e^{\frac{i}{\hbar}p\,x}\varphi(p)\,dp\\ &= \tfrac{1}{2\pi}\int e^{i\,k\,x}\phi(k)\,dk\\ &\qquad\qquad \phi(k) = \int e^{-i\,k\,x}\psi(x)\,dx\end{aligned}$$

In the periodically continuated formalism we therefore have descriptions

$$\psi_n(x) = \sqrt{\tfrac{2}{a}}\sin k_n x \quad\longleftrightarrow\quad \phi_n(k) = \tfrac{\pi}{i}\sqrt{\tfrac{2}{a}}\Big\{\delta(k-k_n) - \delta(k+k_n)\Big\} \tag{12}$$

of the energy eigenstates $|n)$. Notice that $\phi_n(k)$ is so singular that it is senseless to speak of "momentum density" $|\phi_n(k)|^2$, and that to write

$$\int_{-\infty}^{+\infty} |\psi_n(x)|^2\,dx = \int_{-\infty}^{+\infty} |\varphi_n(p)|^2\,dp = 1$$

would in this context be to engage in meaningless frivolity.

Contrast that with the altogether more temperate situation that arises when one adopts the clamped formalism. One then obtains

$$\mathit{\Phi}_n(k) = \int_0^a e^{-i\,k\,x}\Psi_n(x)\,dx = n\pi\sqrt{2a}\,\frac{1-(-)^n e^{-iak}}{n^2\pi^2 - a^2k^2} \tag{13.1}$$

giving

$$|\mathit{\Phi}_n(k)|^2 = 4an^2\pi^2\,\frac{1-(-)^n\cos ak}{(n^2\pi^2 - a^2k^2)^2} \tag{13.2}$$

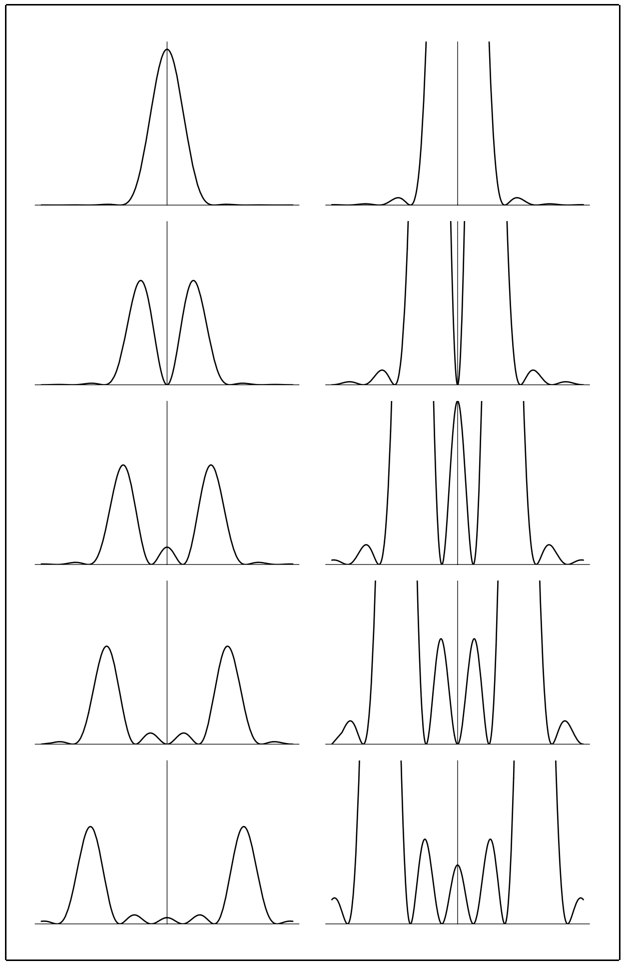

FIGURE 5: *Graphs of the functions* $|\varPhi_n(k)|^2$*, with (reading down the left column)* $n = 1, 2, 3, 4, 5$*. The respective major peaks are positioned at* $k = \pm\, n\pi/a$*. At the right I have stretched the vertical scale to reveal the small amplitude oscillations.*

Here the numerator has contrived to kill the singularities which would otherwise result from the numerator, to produce the non-pathological functions shown above. We have

$$\int_{-\infty}^{+\infty} |\Psi_n(x)|^2\, dx = \tfrac{1}{2\pi}\int_{-\infty}^{+\infty} |\varPhi_n(k)|^2\, dk$$

for which *Mathematica* supplies the remarkable information that (for all a)

$$= -(-)^n\sqrt{\tfrac{1}{2}n}\,\pi^2 J_{\frac{3}{2}}(n\pi) = 1 \quad : \quad n = 1, 2, 3, \ldots$$

Further computation supplies

$$
\begin{aligned}
\langle E\rangle_n &= \tfrac{\hbar^2}{2m}\langle k^2\rangle_n \\
\langle k^2\rangle_n &= \tfrac{1}{2\pi}\int_{-\infty}^{+\infty} |\Phi_n(k)|^2\, k^2\, dk \\
&= \text{linear combination of } J_{\frac{1}{2}}(n\pi) \text{ and } J_{\frac{3}{2}}(n\pi) \\
&= (n\pi/a)^2 \equiv k_n^2
\end{aligned}
$$

Moreover

$$
\begin{aligned}
\langle k^4\rangle_n &= \text{complicated Bessel expression, evaluates to } (n\pi/a)^4 = \langle k^2\rangle_n^2 \\
\langle k^6\rangle_n &= \text{complicated Bessel expression, evaluates to } (n\pi/a)^6 = \langle k^2\rangle_n^3 \\
\langle k^8\rangle_n &= \text{complicated Bessel expression, evaluates to } (n\pi/a)^8 = \langle k^2\rangle_n^4 \\
&\vdots
\end{aligned}
$$

Since $\Psi_n(x)$ refers to an *energy eigenfunction* we <u>expect the energy distribution to be sharp</u>; i.e., we expect all centered moments to vanish:

$$
\big\langle (E-\langle E\rangle_n)^\nu \big\rangle_n = 0 \qquad : \qquad \nu = 1,2,3,\ldots
$$

And indeed

$$
\big\langle (E-\langle E\rangle_n)^\nu \big\rangle_n = \big(\tfrac{\hbar^2}{2m}\big)^\nu \big\langle (k^2-k_n^2)^\nu \big\rangle_n = 0 \tag{14}
$$

by virtue of the equations just established. This striking result is profoundly counterintuitive, for we naively expect sharp E to imply sharp $p = \pm\sqrt{2mE}$.

By entrenched tradition, every author of an introductory quantum text *talks* about the 1-dimensional particle-in-a-box problem, but I am aware of no author who supports that discussion by an appeal to observational data—data which would serve to discriminate between (12) and (13). Nor is it immediately evident how such an experiment could be designed. But it should be possible to obtain relevant data by observation of a "trapped electron/atom" in an acceptable approximation to a cubic box.

Wigner functions for energy eigenstates in the periodic formalism. Feed (5.1) into (1) to obtain

$$
\begin{aligned}
P_n(x,p) &= \tfrac{2}{h}\int_{-\infty}^{+\infty} \tfrac{2}{a}\sin k_n(x+\xi)\, e^{2ik\xi}\sin k_n(x-\xi)\, d\xi \qquad : \qquad k\equiv p/\hbar \\
&= \tfrac{2}{h}\tfrac{1}{a}\int e^{2ik\xi}\Big\{\cos 2k_n\xi - \cos 2k_n x\Big\}\, d\xi \\
&= \tfrac{2}{h}\tfrac{1}{a}\int \Big\{\tfrac{1}{2}e^{2i(k+k_n)\xi} + \tfrac{1}{2}e^{2i(k-k_n)\xi} - e^{2ik\xi}\cdot\cos 2k_n x\Big\}\, d\xi \\
&= \tfrac{2}{h}\tfrac{1}{a}\Big\{\tfrac{\pi}{2}\delta(k+k_n) + \tfrac{\pi}{2}\delta(k-k_n) - \pi\delta(k)\cdot\big[1-2\sin^2 k_n x\big]\Big\} \\
&= \tfrac{1}{2a}\Big\{\delta(p+p_n) + \delta(p-p_n) - 2\delta(p) + 2\delta(p)\cdot a\,|\psi_n(x)|^2\Big\}
\end{aligned} \tag{15}
$$

with $p_n = \hbar k_n = (\hbar\pi/a)n$. As a check on the accuracy of this rather strange result we compute

$$\int_{-\infty}^{+\infty} P_n(x,p)\,dp = \tfrac{1}{2a}\Big\{1+1-2+2a\,|\psi_n(x)|^2\Big\}$$

Then

$$\iint_{\text{entire phase plane}} P_n(x,p)\,dxdp = \int_{-\infty}^{+\infty} |\psi_n(x)|^2\,dx = \infty$$

But the *classical* phase space of the particle-in-a-box consists of a *strip* on the $\{x,p\}$-plane, and when we integrate *over the strip* we obtain

$$\iint_{\text{classical phase strip}} P_n(x,p)\,dxdp = \int_0^a |\psi_n(x)|^2\,dx = 1 \tag{16}$$

According to (15) we have

$$\begin{aligned}
\langle x\rangle_n &= \iint_{\text{classical strip}} P_n(x,p)\,x\,dxdp \\
&= \int_0^a |\psi_n(x)|^2\,x\,dx = \tfrac{1}{2}a && (17.1)\\
\langle p\rangle_n &= \iint_{\text{classical strip}} P_n(x,p)\,p\,dxdp \\
&= \int_0^a \tfrac{1}{2a}\Big\{(-p_n)+(+p_n)-0+0\cdot a\,|\psi_n(x)|^2\Big\}\,dx = 0 && (17.2)\\
\langle E\rangle_n &= \iint_{\text{classical strip}} P_n(x,p)\,\tfrac{1}{2m}p^2\,dxdp \\
&= \tfrac{1}{2m}\int_0^a \tfrac{1}{2a}\Big\{(-p_n)^2+(+p_n)^2-0+0\cdot a\,|\psi_n(x)|^2\Big\}\,dx = \tfrac{1}{2m}p_n^2 && (17.3)
\end{aligned}$$

—all of which make good sense. The marginal distributions implicit in (15)

$$\int_0^a P_n(x,p)\,dx = \tfrac{1}{2}\delta(p+p_n)+\tfrac{1}{2}\delta(p-p_n) \tag{18.1}$$

$$\int_{-\infty}^{+\infty} P_n(x,p)\,dp = |\psi_n(x)|^2 \tag{18.2}$$

are also quite satisfactory (though the former cannot be expressed $|\varphi_n(p)|^2$).

I give now an alternative derivation (which is to say: a radical revision of our former derivation) of (15): The transform $\varphi_n(p)$ of $\psi_n(x)$—in the familiar sense

$$\psi_n(x) \equiv \sqrt{\tfrac{2}{a}}\,\sin k_n x = \tfrac{1}{\sqrt{h}}\int e^{\frac{i}{\hbar}p\,x}\varphi_n(p)\,dp$$

—is given (compare (12)) by

$$\varphi_n(p) = \sqrt{\tfrac{2h}{a}}\,\tfrac{1}{2i}\Big\{\delta(p-p_n)-\delta(p+p_n)\Big\} \tag{19}$$

Feed this information into (4.2) to obtain

$$\begin{aligned}
P_n(x,p) &= \tfrac{1}{a}\int \Big\{\delta(p-p_n-\zeta)-\delta(p+p_n-\zeta)\Big\} \\
&\qquad\qquad \cdot\, e^{2\frac{i}{\hbar}x\zeta}\Big\{\delta(p-p_n+\zeta)-\delta(p+p_n+\zeta)\Big\}\,d\zeta \\
&= \tfrac{1}{2a}\Big\{e^{2\frac{i}{\hbar}x(p-p_n)}\big[\delta(p-p_n)-\delta(p)\big]-e^{2\frac{i}{\hbar}x(p+p_n)}\big[\delta(p)-\delta(p+p_n)\big]\Big\} \\
&= \tfrac{1}{2a}\Big\{\delta(p+p_n)+\delta(p-p_n)-\delta(p)\cdot 2\cos 2k_nx\Big\} \\
&= \tfrac{1}{2a}\Big\{\delta(p+p_n)+\delta(p-p_n)-2\delta(p)+4\delta(p)\sin^2 k_nx\Big\} \\
&= \tfrac{1}{2a}\Big\{\delta(p+p_n)+\delta(p-p_n)-2\delta(p)\Big\}+\delta(p)\cdot|\psi_n(x)|^2
\end{aligned}$$

which is a slight variant of (15). Here we made initial use of

$$\int f(x)\delta(x-a)\delta(x-b)\,dx = f(a)\delta(a-b) \quad : \quad a\neq b$$

and repeated use of $f(x)\delta(x-a)=f(a)\delta(x-a)$; *i.e.*, of $e^{ikx}\delta(x)=\delta(x)$.

Wigner functions for energy eigenstates in the clamped formalism. We might—in principle—proceed along the lines just sketched. Which is to say: we might insert (10) into (4.1); alternatively we might insert its Fourier transform (see again (13.1)) into (4.2). Both procedures lead, however, to integrals which *Mathematica* finds awkward. So we manage "by hand" the effect of the clamps: insert

$$\Psi_n(x)=\sqrt{\tfrac{2}{a}}\sin k_nx$$

into

$$P_\Psi(x,p)\equiv \tfrac{2}{h}\int \Psi^*(x+\xi)\,e^{2\frac{i}{\hbar}p\,\xi}\,\Psi(x-\xi)\,d\xi$$

and notice that the integrand vanishes unless it is simultaneously the case that

$$0\leqslant x+\xi\leqslant a \quad\text{and}\quad 0\leqslant x-\xi\leqslant a$$

From those conditions, as spelled out in Figure 6, we conclude that

$$\begin{aligned}
P_n(x,p) &= \tfrac{4}{ha}\left\{\begin{matrix}\displaystyle\int_{-x}^{+x}\\[1ex] \displaystyle\int_{-(a-x)}^{+(a-x)}\end{matrix}\right\}\sin k_n(x+\xi)e^{2ik\,\xi}\sin k_n(x-\xi)\,d\xi \\
&= \tfrac{2}{ha}\left\{\quad\text{etc.}\quad\right\}e^{2ik\,\xi}\Big\{\cos 2k_n\xi-\cos 2k_nx\Big\}\,d\xi \qquad (20)
\end{aligned}$$

according as $0\leqslant x\leqslant \frac{1}{2}a$ or $\frac{1}{2}a\leqslant x\leqslant a$; *i.e.*, according as $x\in\triangleleft$ or $x\in\triangleright$.

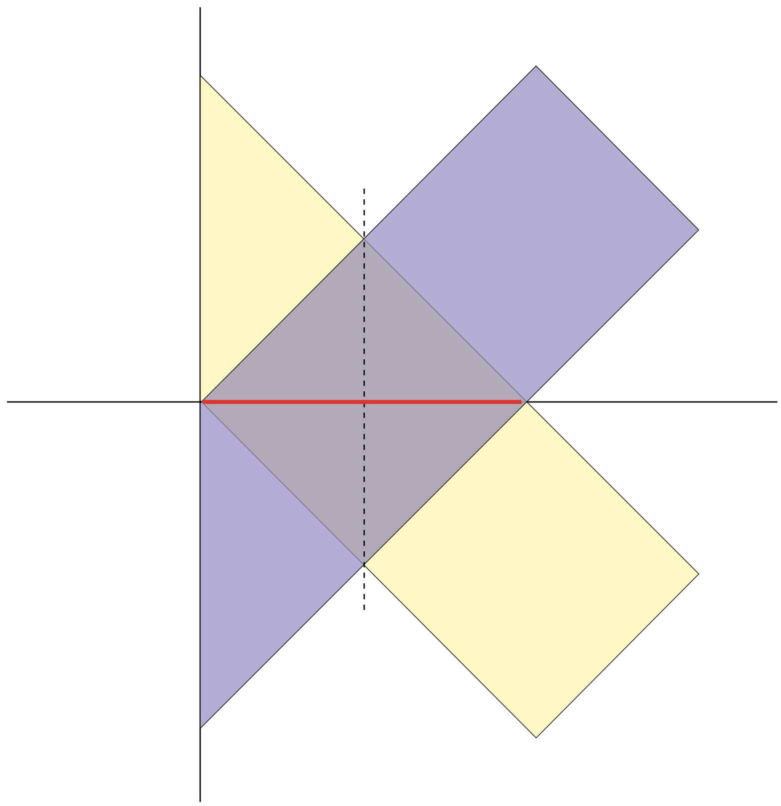

FIGURE 6: *The x-axis runs $\leftrightarrow$, the ξ-axis runs $\updownarrow$. The red segment represents the interior of the box. The downsloping yellow band locates points at which $0 \leqslant x+\xi \leqslant a$, while the upsloping blue band locates points at which $0 \leqslant x-\xi \leqslant a$. The Wigner function $P(x,p)$ arises from an $\int d\xi$ process that ranges on the gray intersect of the two bands, and therefore splits naturally into a $\triangleleft$ fragment and a $\triangleright$ fragment.*

Note that from $\cos 2k_n(a-x) = \cos 2k_n x$ it now follows that $P_n(x,p)$ is *bilaterally symmetric*:

$$P_n(a-x,p) = P_n(x,p) \quad : \quad \text{all } n$$

We therefore have

$$P_n(x,p) = \begin{cases} 0 & : \quad x \leqslant 0 \\ F_n(x,p) & : \quad 0 \leqslant x \leqslant \frac{1}{2}a \\ F_n(a-x,p) & : \quad \frac{1}{2}a \leqslant x \leqslant a \\ 0 & : \quad a \leqslant x \end{cases} \tag{21}$$

with

$$F_n(x,p) \equiv \tfrac{2}{ha}\int_{-x}^{+x} e^{2ik\xi}\Big\{\cos 2k_n\xi - \cos 2k_n x\Big\}\,d\xi$$

Mathematica now supplies[6]

$$\begin{aligned}F_n(x,p) &= \tfrac{2}{\hbar}\Big\{\frac{ak\cos 2k_nx\,\sin 2kx - n\pi\sin 2k_nx\,\cos 2kx}{a^2k^2-n^2\pi^2}\\&\qquad\qquad -\frac{\cos 2k_nx\,\sin 2kx}{ak}\Big\} &(22.1)\\&= \frac{ap\cos 2k_nx\,\sin\frac{2px}{\hbar} - \hbar n\pi\sin 2k_nx\,\cos\frac{2px}{\hbar}}{\pi(a^2p^2-\hbar^2n^2\pi^2)}\\&\qquad\qquad -\frac{\cos 2k_nx\,\sin\frac{2px}{\hbar}}{\pi ap} &(22.2)\end{aligned}$$

by $k\equiv p/\hbar$, and where (as always) $k_n\equiv n\pi/a$. We gain confidence in the accuracy of this result from the computations which—which after major (!) simplifications in the first instance—show the associated marginal distributions to be given by

$$\begin{aligned}\hbar\int_{-\infty}^{+\infty}\big\{\text{right side of (22.1)}\big\}dk &= \tfrac{1}{a}-\tfrac{1}{a}\cos 2k_nx\\&= \tfrac{2}{a}\sin^2 k_nx = |\Psi_n(x)|^2 &(23.1)\\2\int_0^{\frac{1}{2}a}\big\{\text{right side of (22.1)}\big\}dx &= \text{complicated stuff} - \text{complicated stuff}\\&= \tfrac{1}{\hbar}4an^2\pi^2\,\frac{1-\cos n\pi\,\cos ak}{(n^2\pi^2-a^2p^2)^2} &(23.2)\end{aligned}$$

From (23.1) it becomes obvious that the $P_n(x,p)$ which results from feeding (22) into (21) is in fact *normalized*, while (23.2) reproduces the upshot of (13.2), and when compared with (18.1) serves once again to dramatize the profound distinction between the periodic and clamped formalisms. The latter point, however, can hardly be made more vivid than is done by comparing the alternative descriptions (15) and (21/22) of $P_n(x,p)$ itself.

On following pages I present a portfolio of figures intended to illustrate the meaning of (21/22). Similar figures can be found on pages 41–45 of Yoder's thesis.[4] Notice, in relation to the bottom figures, that

$$P_n(\tfrac{1}{2}a,p) = -\tfrac{2}{\hbar}\cos n\pi\Big\{\sin ak\Big[\frac{1}{ak}+\frac{ak}{n^2\pi^2-a^2k^2}\Big]\Big\}$$

has zeros at $k=\frac{\pi}{a}\cdot(1,2,3,\ldots,n-1,\bullet,n+1,n+2,\ldots)$, and that its "dominant outlying maximum" occurs near the "missing zero:" $k=k_n\equiv n\frac{\pi}{a}$.

We could now use results already in hand to develop descriptions of

$$\langle x\rangle_n = \iint xP_n(x,p)\,dxdp\,,\quad \langle p\rangle_n\,,\quad \langle\tfrac{1}{2m}p^2\rangle_n\,,\quad\text{etc.}$$

. . . but won't, since the results are totally unsurprising.

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[6] Use `ExpToTrig` to simplify the expressions constructed by *Mathematica*. I have introduced color coding to indicate which terms come from where.

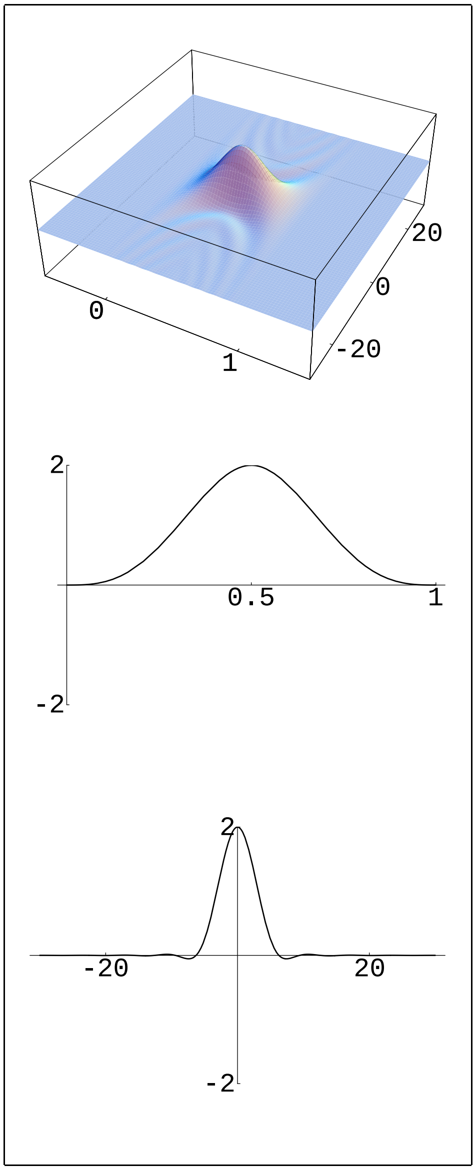


FIGURE 7a: *At the top is a representation of the function* $P_1(x,p)$, *as given by (21/22). In the middle is the central section* $p = 0$, *and at the bottom is the central section* $x = \frac{1}{2}a$. *Notice that for the particle-in-a-box problem <u>even the groundstate of the Wigner function displays regions of negativity</u>. In constructing this and subsequent figures I have set* $a = 1$.

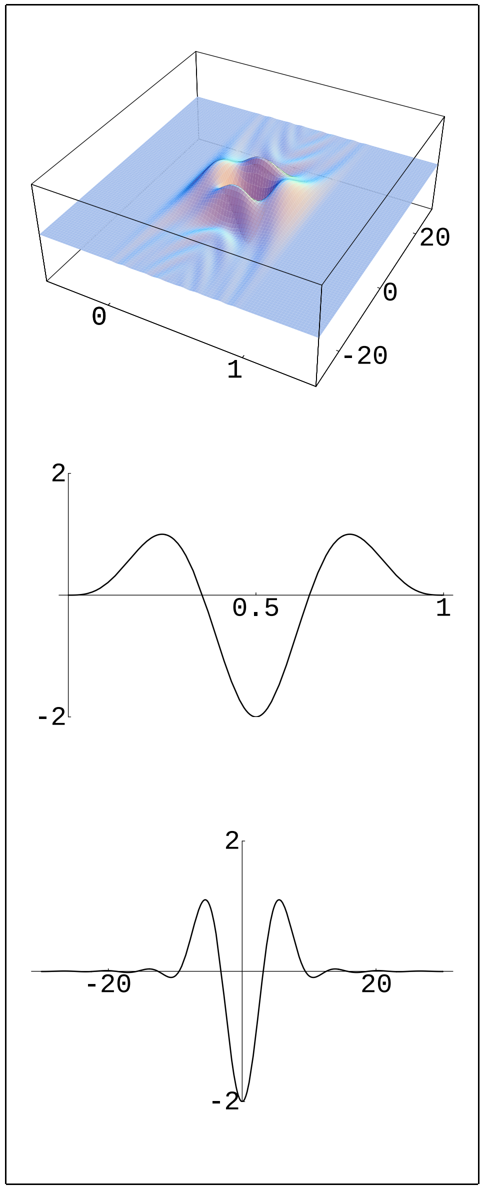


FIGURE 7b: *Representation of the Wigner function* $P_2(x, p)$.

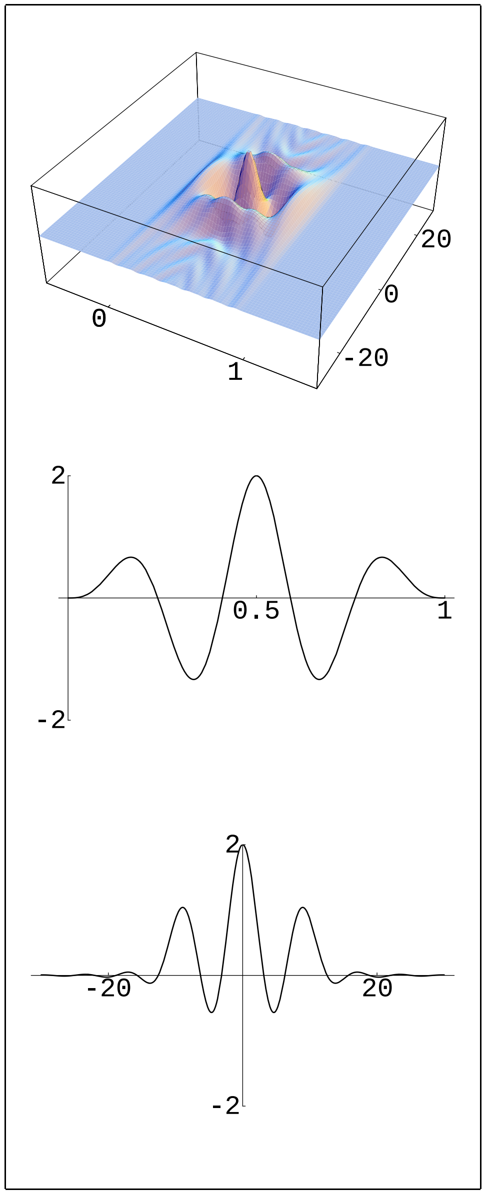


FIGURE 7C: *Representation of the Wigner function* $P_3(x,p)$.

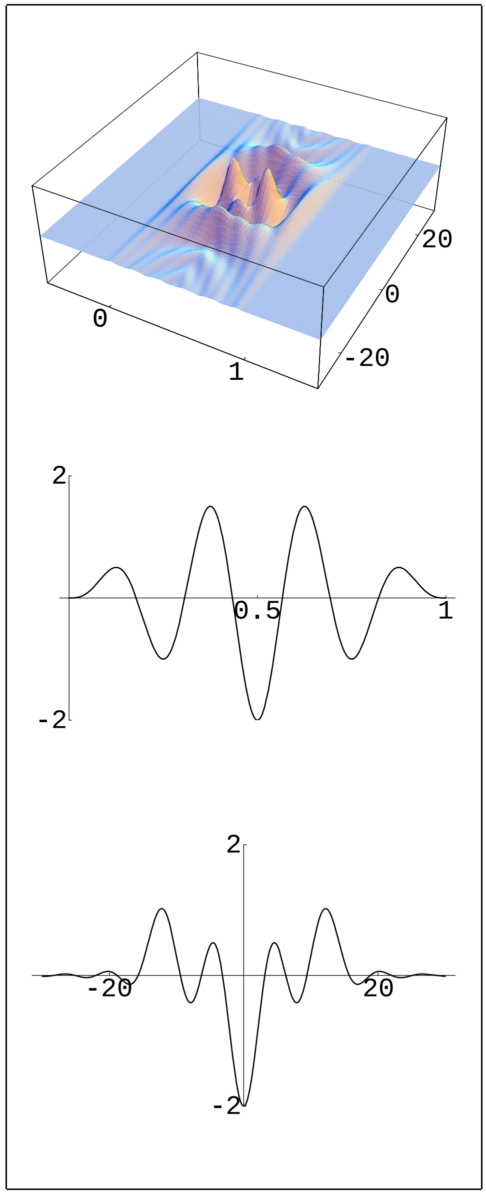


FIGURE 7d: *Representation of the Wigner function $P_4(x,p)$.*

Wigner functions for flat distributions in the clamped formalism. As was remarked already on page 5, the flatness condition

$$|\psi_{\text{flat}}(x)|^2 = \begin{cases} 1/a & : \quad 0 < x < a \\ 0 & : \quad \text{elsewhere} \end{cases}$$

entails

$$\psi_{\text{flat}}(x) = \tfrac{1}{\sqrt{a}} e^{i\,\varphi(x)} \quad : \quad \varphi(x) \text{ real}$$

but leaves $\varphi(x)$ arbitrary/indeterminate. An equivalent indeterminacy attaches therefore to the associated Wigner function

$$P_{\text{flat}}(x,p) \equiv \tfrac{2}{ha}\int e^{2\frac{i}{\hbar}p\,\xi}\, e^{i\left\{\varphi(x-\xi)-\varphi(x+\xi)\right\}}\,d\xi \tag{24}$$

It is important to notice that the (trivial) bilateral symmetry of the marginal distribution

$$|\psi_{\text{flat}}(\tfrac{1}{2}a+y)|^2 = |\psi_{\text{flat}}(\tfrac{1}{2}a-y)|^2$$

does not imply/require bilateral symmetry of the associated wave function:

$$\psi_{\text{flat}}(\tfrac{1}{2}a+y) = \psi_{\text{flat}}(\tfrac{1}{2}a-y) \quad \text{holds only exceptionally}$$

—holds, that is to say, if an only if it happens to be the case that

$$\varphi(\tfrac{1}{2}a+y) = \varphi(\tfrac{1}{2}a-y)$$

which in the present context is equivalent to the condition

$$\varphi(x) = \varphi(a-x) \tag{25}$$

It follows that we must, in general, write

$$P_{\text{flat}}(x,p) = \begin{cases} 0 & : \quad x \leqslant 0 \\ F_{\text{flat}}(x,p) & : \quad 0 \leqslant x \leqslant \frac{1}{2}a \\ G_{\text{flat}}(x,p) & : \quad \frac{1}{2}a \leqslant x \leqslant a \\ 0 & : \quad a \leqslant x \end{cases} \tag{26}$$

with

$$F_{\text{flat}}(x,p) \equiv \tfrac{2}{ha}\int_{-x}^{+x} e^{2\frac{i}{\hbar}p\,\xi}\, e^{i\left\{\varphi(x-\xi)-\varphi(x+\xi)\right\}}\,d\xi \tag{27.1}$$

$$G_{\text{flat}}(x,p) \equiv \tfrac{2}{ha}\int_{-(a-x)}^{+(a-x)} e^{2\frac{i}{\hbar}p\,\xi}\, e^{i\left\{\varphi(x-\xi)-\varphi(x+\xi)\right\}}\,d\xi \tag{27.2}$$

and will have bilateral symmetry of the Wigner function

$$F_{\text{flat}}(x,p) = G_{\text{flat}}(a-x,p)$$

if

$$\varphi(x-\xi)-\varphi(x+\xi) = \varphi(a-x-\xi)-\varphi(a-x+\xi) \tag{28}$$

The point is that (25) and (28) impose *distinct* conditions upon $\varphi(x)$.

Look to the case $\varphi(x) \equiv 0$: trivially, *both* of the bilaterality conditions (25/28) are in this case satisfied. From (26/27) we obtain

$$P_{\text{flat}}(x,p) = \begin{cases} 0 & : \quad x \leqslant 0 \\ F_{\text{flat}}(x,p) & : \quad 0 \leqslant x \leqslant \frac{1}{2}a \\ F_{\text{flat}}(a-x,p) & : \quad \frac{1}{2}a \leqslant x \leqslant a \\ 0 & : \quad a \leqslant x \end{cases} \tag{29}$$

with

$$\begin{aligned} F_{\text{flat}}(x,p) &= \tfrac{2}{ha}\int_{-x}^{+x} e^{2ik\,\xi}\,d\xi \\ &= \frac{2\sin 2kx}{ahk} \end{aligned} \tag{30}$$

Elementary calculation now returns

$$\int P_{\text{flat}}(x,p)\,dp = \begin{cases} a^{-1} & : \quad 0 < x < a \\ 0 & : \quad \text{otherwise} \end{cases} \tag{31.1}$$

and supplies this new information:

$$\int P_{\text{flat}}(x,p)\,dx = \frac{2\,(1-\cos ak)}{ahk^2} \tag{31.2}$$

Either of those marginal distribution formulæ can be used to produce

$$\iint P_{\text{flat}}(x,p)\,dxdp = 1$$

The Wigner function described by (29/30) is shown in Figure 8.

Look next to the example $\varphi(x) \equiv Kx$. The bilaterality condition (28) is satisfied (though (25) is not), so we again have (29), but with $F_{\text{flat}}(x,p)$ given now by

$$\begin{aligned} F_{\text{flat}}(x,p) &= \tfrac{2}{ha}\int_{-x}^{+x} e^{2ik\,\xi} e^{i\left\{K(x-\xi)-K(x+\xi)\right\}}\,d\xi \\ &= \frac{2\sin 2[k-K]x}{ah[k-K]} \end{aligned} \tag{32}$$

which gives back (30) in the case $K=0$: the Wigner function shown in Figure 8 has been *shifted along the p-axis*. The marginal distribution (31.1) remains unchanged, but (31.2) has become

$$\int P_{\text{flat}}(x,p)\,dx = \frac{2\left(1-\cos a[k-K]\right)}{ah[k-K]^2}$$

Look finally to the case $\varphi(x) = (x-\frac{1}{2}a)^2/\sigma^2$. Now it is the bilaterality condition (25) that is satisfied and (28) that is not; we must work therefore from (26), with

$$\begin{aligned} F_{\text{flat}}(x,p) &\equiv \tfrac{2}{ha}\int_{-x}^{+x} e^{2\frac{i}{\hbar}p\,\xi}\, e^{i\left\{2(a-2x)\,\xi/\sigma^2\right\}}\,d\xi \\ &= \tfrac{2}{ha}\frac{\sigma^2\sin[2x(a-2x+k\sigma^2)/\sigma^2]}{(a-2x+k\sigma^2)} \end{aligned} \tag{33.1}$$

$$G_{\text{flat}}(x,p) = \tfrac{2}{ha}\frac{\sigma^2\sin[2(a-x)(a-2x+k\sigma^2)/\sigma^2]}{(a-2x+k\sigma^2)} \tag{33.2}$$

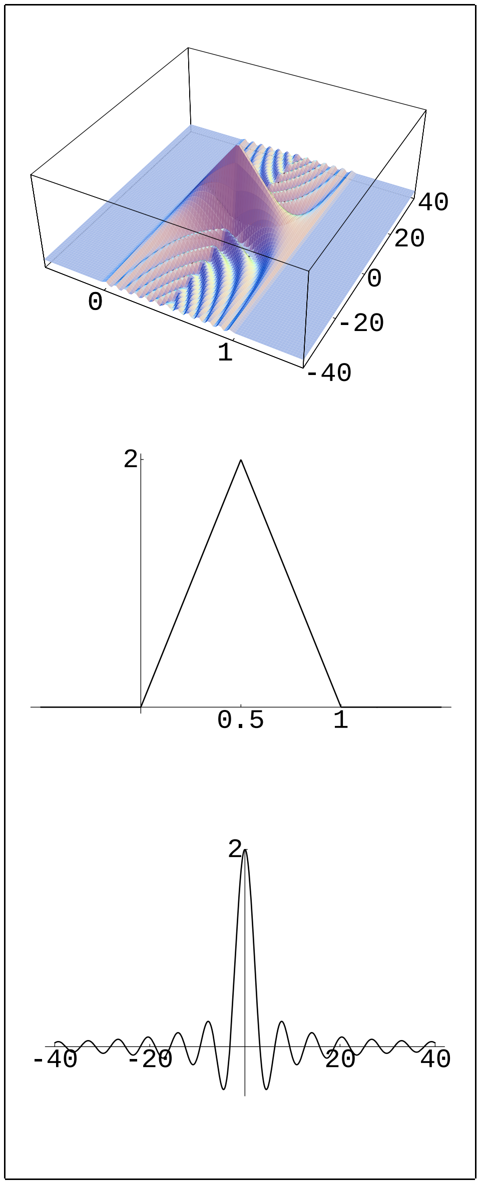


FIGURE 8: *Representation of the $P_{\text{flat}}(x,p)$ encountered at (29/30). Notice that we have automatic continuity at the box boundaries, and these central sections:*

$$P_{\text{flat}}(\ x\ ,0) = \tfrac{2}{h}\cdot\begin{cases} 2x/a & : \quad 0 \leqslant x \leqslant \tfrac{1}{2}a \\ 2(a-x)/a & : \quad \tfrac{1}{2}a \leqslant x \leqslant a \end{cases}$$

$$P_{\text{flat}}(\tfrac{1}{2}a,p) = \tfrac{2}{h}\cdot\frac{\sin ka}{ka}$$

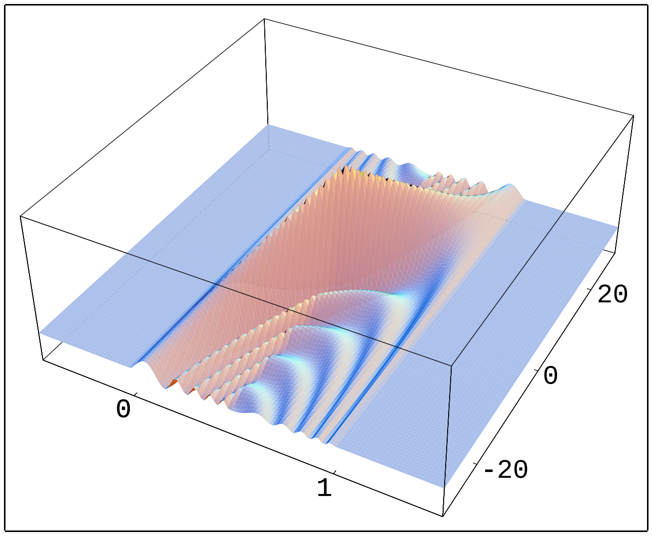


FIGURE 9: *Representation of the bilaterally asymmetric* $P_{\text{flat}}(x,p)$ *encountered at (26/33).*

Mathematica is able, after a bit of a struggle, to reproduce (31.1), but reports that

$$\int P_{\text{flat}}(x,p)\,dx \text{ is borderline intractable}$$

Additional Wigner distributions of the type $P_{\text{flat}}(x,p)$ could be produced in unlimited variety—that is the point of this discussion—but in *most* cases the integrals will be intractable.

We have proceeded thus far in this discussion of (clamped) flat distributions without reference to the (clamped) energy eigenstates $\Psi_n(x)$ from which such states—in all their variety—can be considered to be assembled. Generally, if

$$\Psi(x) = \sum_n c_n \Psi_n(x)$$

then

$$P_\Psi(x,p) = \sum_m \sum_n c_m^* P_{mn}(x,p) c_n \tag{34.1}$$

$$P_{mn}(x,p) \equiv \tfrac{2}{h}\int \Psi_m^*(x+\xi)\, e^{2\frac{i}{\hbar}p\,\xi}\, \Psi_n(x-\xi)\,d\xi \tag{34.2}$$

We note that the matrix $\mathbb{P}(x,p) \equiv \|P_{mn}(x,p)\|$ is hermitian, so can be written

$$\begin{aligned}\mathbb{P}(x,p) &= (\text{real symmetric}) + i(\text{real antisymmetric})\\ &\equiv \mathbb{S}(x,p) + i\,\mathbb{A}(x,p)\end{aligned} \tag{35}$$

At (6.2) we learned to write

$$\Psi_{\text{flat}}(x) = \sum_n c_n \Psi_n(x)\cdot e^{i\,\varphi(x)}$$
$$c_n = \tfrac{\sqrt{2}}{\pi}\,\tfrac{1-\cos n\pi}{n}$$

which is, as it stands, an imperfect/incomplete expansion, for the $e^{i\,\varphi(x)}$-factor remains to be absorbed into redefined coefficients c_n. Let us, for the purposes of this discussion, agree to skirt that problem by setting $\varphi(x)\equiv 0$. We are led then to

$$P_{\text{flat}}(x,p) = \tfrac{2}{\pi^2}\sum\sum_{m,n \text{ both odd}} \tfrac{4}{mn} P_{mn}(x,p) \tag{36}$$

Back up now and notice that (34.1) can be notated

$$\begin{aligned}
P_\Psi(x,p) &= \boldsymbol{c}^{\mathsf{t}}\,\mathbb{P}\,(x,p)\,\boldsymbol{c}\\
&= \boldsymbol{c}^{\mathsf{t}}\,\mathbb{S}\,(x,p)\,\boldsymbol{c} + i\,\boldsymbol{c}^{\mathsf{t}}\,\mathbb{A}\,(x,p)\,\boldsymbol{c}\\
&\downarrow\\
&= \boldsymbol{c}^{\mathsf{t}}\,\mathbb{S}\,(x,p)\,\boldsymbol{c}\quad\text{when }\boldsymbol{c}\text{ is real (or imaginary)}
\end{aligned}$$

so in the present context—as distinguished from an important context that lies ahead—we need not actually concern ourselves with the construction of $\mathbb{A}\,(x,p)$. But will (and will also discuss cases in which m and n are not both odd)... in anticipation of that future need. We have

$$\begin{aligned}
S_{mn}(x,p) &\equiv \tfrac{4}{ha}\int \sin\big[m\tfrac{\pi}{a}(x+\xi)\big]\sin\big[n\,\tfrac{\pi}{a}(x-\xi)\big]\cdot\cos 2k\xi\,d\xi\\
A_{mn}(x,p) &\equiv \tfrac{4}{ha}\int \sin\big[m\tfrac{\pi}{a}(x+\xi)\big]\sin\big[n\,\tfrac{\pi}{a}(x-\xi)\big]\cdot\sin 2k\xi\,d\xi
\end{aligned}$$

where the $\int$ means $\int_{-x}^{+x}$ if $0\leqslant x\leqslant \frac{1}{2}a$, and $\int_{-(a-x)}^{+(a-x)}$ if $\frac{1}{2}a\leqslant x\leqslant a$. By extension of notation introduced at (26), I will write

$$SF_{mn}(x,p) = \tfrac{4}{ha}\int_{-x}^{+x}\text{etc}\cdot\cos 2k\xi\,d\xi \tag{37.1}$$

$$SG_{mn}(x,p) = \tfrac{4}{ha}\int_{-(a-x)}^{+(a-x)}\text{etc}\cdot\cos 2k\xi\,d\xi \tag{37.2}$$

$$AF_{mn}(x,p) = \tfrac{4}{ha}\int_{-x}^{+x}\text{etc}\cdot\sin 2k\xi\,d\xi \tag{37.3}$$

$$AG_{mn}(x,p) = \tfrac{4}{ha}\int_{-(a-x)}^{+(a-x)}\text{etc}\cdot\sin 2k\xi\,d\xi \tag{37.4}$$

Mathematica can do the integrals, but (especially in cases of type G) produces lengthy, difficult-to-simplify output; it was by graphical experimentation that I was led to the following list of symmetry properties (some of which are more nearly obvious than others, and for none of which will I offer analytical proof):

$$\begin{aligned} SF_{mn}(x,p) &= +SF_{nm}(x,p) \qquad & AF_{mn}(x,p) &= -AF_{nm}(x,p) \\ SG_{mn}(x,p) &= +SG_{nm}(x,p) \qquad & AG_{mn}(x,p) &= -AG_{nm}(x,p) \end{aligned} \tag{38.1}$$

$$\begin{aligned} SF_{mn}(x,p) &= +SF_{mn}(x,-p) \qquad & AF_{mn}(x,p) &= -AF_{mn}(x,-p) \\ SG_{mn}(x,p) &= +SG_{mn}(x,-p) \qquad & AG_{mn}(x,p) &= -AG_{mn}(x,-p) \end{aligned} \tag{38.2}$$

$$\begin{aligned} SF_{mn}(a-x,p) &= \quad (-)^{m+n}SG_{mn}(x,p) \\ AF_{mn}(a-x,p) &= -(-)^{m+n}AG_{mn}(x,p) \end{aligned} \tag{38.3}$$

From (38.1) it follows, of course, that $AF_{mm}(x,p) = AG_{mm}(x,p) = 0$ for all values of x and p. At $p = 0$ we have the bilateral antisymmetry conditions

$$\left.\begin{aligned} SF_{mn}(a-x,0) &= -SF_{mn}(x,0) \\ SG_{mn}(a-x,0) &= -SG_{mn}(x,0) \end{aligned}\right\} \quad \text{provided } m \neq n$$

which, however, do not persist when $p \neq 0$. The A-analogs of the preceding statements are trivial, since from (38.2) it follows that

$$AF_{mn}(x,0) = AG_{mn}(x,0) = 0$$

We are in position now to write

$$\begin{aligned} S_{mn}(x,p) &= \begin{cases} SF_{mn}(x,p) & : \quad 0 \leqslant x \leqslant \tfrac{1}{2}a \\ (-)^{m+n}SF_{mn}(a-x,p) & : \quad \tfrac{1}{2}a \leqslant x \leqslant a \end{cases} \\ A_{mn}(x,p) &= \begin{cases} AF_{mn}(x,p) & : \quad 0 \leqslant x \leqslant \tfrac{1}{2}a \\ -(-)^{m+n}AF_{mn}(a-x,p) & : \quad \tfrac{1}{2}a \leqslant x \leqslant a \end{cases} \end{aligned} \tag{39}$$

and to observe that

$$S_{mn}(x,p) \text{ is bilaterally} \begin{Bmatrix} \text{symmetric} \\ \text{antisymmetric} \end{Bmatrix} \text{according as } m,\, n \text{ have} \begin{Bmatrix} \text{same} \\ \text{opposite} \end{Bmatrix} \text{parity}$$

$$A_{mn}(x,p) \text{ is bilaterally} \begin{Bmatrix} \text{symmetric} \\ \text{antisymmetric} \end{Bmatrix} \text{according as } m,\, n \text{ have} \begin{Bmatrix} \text{opposite} \\ \text{same} \end{Bmatrix} \text{parity}$$

Note—in anticipation of things soon to come—that in all off-diagonal cases an element of bilateral asymmetry is introduced *by one or the other* of the functions $S_{mn}(x,p)$ and $A_{mn}(x,p)$.

Mathematica now supplies

$$\begin{aligned} SF_{mn}(x,p) = \tfrac{2}{h}\Big[&-\cos\big[(m+n)\pi\tfrac{x}{a}\big]\Big\{ \frac{\sin\big[\{2ka-(m-n)\pi\}\tfrac{x}{a}\big]}{2ka-(m-n)\pi} \\ &\qquad\qquad + \frac{\sin\big[\{2ka+(m-n)\pi\}\tfrac{x}{a}\big]}{2ka+(m-n)\pi}\Big\} \\ &+\cos\big[(m-n)\pi\tfrac{x}{a}\big]\Big\{ \frac{\sin\big[\{2ka-(m+n)\pi\}\tfrac{x}{a}\big]}{2ka-(m+n)\pi} \\ &\qquad\qquad + \frac{\sin\big[\{2ka+(m+n)\pi\}\tfrac{x}{a}\big]}{2ka+(m+n)\pi}\Big\}\Big] \end{aligned} \tag{40.1}$$

$$
\begin{aligned}
AF_{mn}(x,p) = \tfrac{2}{\hbar}\Big[&+\sin\big[(m+n)\pi\tfrac{x}{a}\big]\bigg\{ \frac{\sin\big[\{2ka-(m-n)\pi\}\frac{x}{a}\big]}{2ka-(m-n)\pi} \\
&\qquad\qquad\qquad - \frac{\sin\big[\{2ka+(m-n)\pi\}\frac{x}{a}\big]}{2ka+(m-n)\pi}\bigg\} \\
&-\sin\big[(m-n)\pi\tfrac{x}{a}\big]\bigg\{ \frac{\sin\big[\{2ka-(m+n)\pi\}\frac{x}{a}\big]}{2ka-(m+n)\pi} \\
&\qquad\qquad\qquad - \frac{\sin\big[\{2ka+(m+n)\pi\}\frac{x}{a}\big]}{2ka+(m+n)\pi}\bigg\}\Big]
\end{aligned} \tag{40.2}
$$

The expressions on the right can, of course, be written in a large number of alternative ways; I have chosen designs that make transparent the important fact that the zeros in the denominators are in every case tempered by associated zeros in the numerators: $\lim_{\kappa\downarrow 0}\frac{\sin\kappa x}{\kappa} = x$.

Return now to (36), which has become

$$
P_{\text{flat}}(x,p) = \tfrac{2}{\pi^2}\sum_{m,n\text{ both odd}}\sum \tfrac{4}{mn}S_{mn}(x,p)
$$

which we see already to be bilaterally symmetric, and an even function of p. *Mathematica* responds to an initial

$$
\sum_{m\text{ odd}}
$$

with yards of hypergeometric output; simplification sufficient to permit closed evaluation of

$$
\sum_{n\text{ odd}}
$$

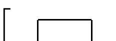
seems out of the question. So I try a simpler problem: *Mathematica* supplies the gratifying information that

$$
\hbar\int_{-\infty}^{+\infty} S_{mn}\,dk = \tfrac{2}{a}\sin m\pi\tfrac{x}{a}\sin n\pi\tfrac{x}{a} = \Psi_m(x)\Psi_n(x)
$$

so we have

$$
\begin{aligned}
\int P_{\text{flat}}(x,p)\,dp &= \tfrac{2}{\pi^2}\tfrac{2}{a}\bigg\{\sum_{m\text{ odd}}\tfrac{2}{m}\sin m\pi\tfrac{x}{a}\bigg\}\bigg\{\sum_{n\text{ odd}}\tfrac{2}{n}\sin n\pi\tfrac{x}{a}\bigg\} \\
&= \bigg[\tfrac{4}{\pi\sqrt{a}}\sum_{n\text{ odd}}\tfrac{1}{n}\sin n\pi\tfrac{x}{a}\bigg]^2
\end{aligned}
$$

which we saw at (6.1) has the meaning

$= \Big[$  function of base a, height $\sqrt{a}\,\Big]^2$ (41)

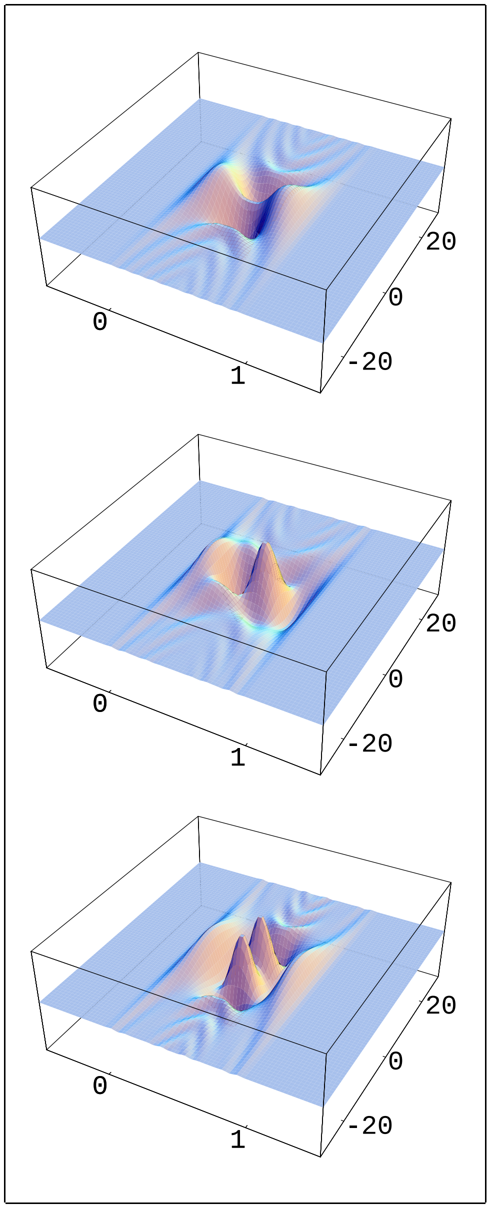


FIGURE 10: *Representations of* $S_{mn}(x,p)$ *based upon (39/40.1). The box size is* $a = 1$*, and—reading from top to bottom—*

$$\{m,n\} = \begin{cases} \{1,3\} & : \textit{ odd-odd, so bilaterally symmetric} \\ \{1,4\} & : \textit{ odd-even, so bilaterally antisymmetric} \\ \{2,2\} & : \textit{ even-even, so bilaterally symmetric} \end{cases}$$

All such functions are even in p*.*

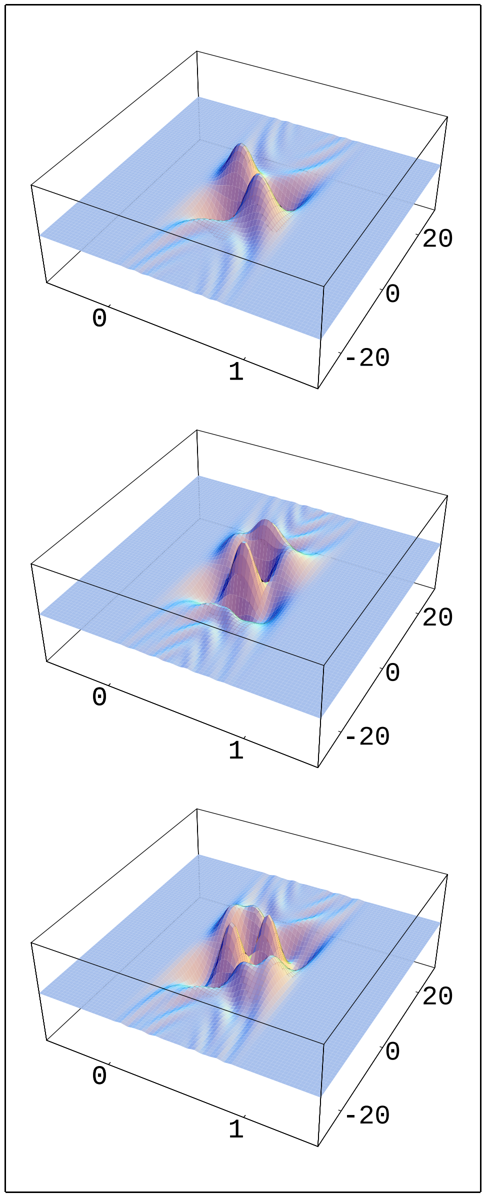


FIGURE 11: *Representations of* $A_{mn}(x,p)$ *based upon (39/40.2). The box size is* $a = 1$*, and—reading from top to bottom—*

$$\{m,n\} = \begin{cases} \{1,3\} & : \textit{ odd-odd, so bilaterally antisymmetric} \\ \{1,4\} & : \textit{ odd-even, so bilaterally symmetric} \\ \{2,2\} & : \textit{ even-even, so bilaterally antisymmetric} \end{cases}$$

All such functions are odd in p.

This is, so far as it goes, a pretty enough result. But I have failed in my effort to reproduce (29/30).

Clamped formulation of quantum dynamics in a box. Quite generally, it is when one turns from statics to dynamics that the energy eigenbasis displays its special virtue: one "turns on time" and obtains

$$\begin{aligned}\Psi(x,0) &= \sum_n c_n\Psi_n(x)\\ &\downarrow\\ \Psi(x,t) &= \sum_n e^{-i\omega_n t}c_n\Psi_n(x) \quad\text{with}\quad \omega_n\equiv E_n/\hbar\end{aligned}\tag{42}$$

For the box problem we found at (5.2) that $E_n=\mathcal{E}n^2$ so

$$\omega_n=\Omega n^2 \quad\text{with}\quad \Omega\equiv\mathcal{E}/\hbar = h\pi/4ma^2\tag{43}$$

The implied motion of the Wigner function becomes

$$\begin{aligned}P_\Psi(x,p;0) &= \boldsymbol{c}^{\mathsf{t}}\,\mathbb{P}\,(x,p)\,\boldsymbol{c}\\ &\downarrow\\ P_\Psi(x,p;t) &= \boldsymbol{c}^{\mathsf{t}}(t)\,\mathbb{P}\,(x,p)\,\boldsymbol{c}(t)\\ &= \sum_{m,n} c_m^* P_{mn}(x,p)\,c_n\cdot e^{i(\omega_m-\omega_n)t}\end{aligned}\tag{44}$$

Clearly, *terms on the diagonal do not move*: it is in precisely this sense that "quantum dynamics is an interference effect."

From (42) we obtain

$$|\Psi(x)|^2=\sum_{m,n}c_m^*\Psi_m^*(x)\Psi_n(x)\,c_n\cdot e^{i(\omega_m-\omega_n)t}\tag{45}$$

to which a similar remark pertains. Notice that the preceding equation can be obtained by *sacrificing some of the information written into* (44)—as a description of the motion of the *marginal* distribution $P_\Psi(x,t)\equiv\int P_\Psi(x,p;t)\,dp$. An identical statement pertains to the motion of $P_\Psi(p,t)\equiv\int P_\Psi(x,p;t)\,dx$; this, however, I refrain from notating

$$|\Phi(p)|^2=\sum_{m,n}c_m^*\Phi_m^*(p)\Phi_n(p)\,c_n\cdot e^{i(\omega_m-\omega_n)t}$$

for what can be the meaning of $\Phi_n(p)\equiv(p|n)$ if, as in the present context, eigenstates $|p)$ of $\mathbf{p}$ do not exist?

Look now to what these general propositions have to say about particle motion in a box. Let us, in the interests of simplicity, suppose the c's to be real. Writing $\theta_{mn} \equiv (\omega_m - \omega_n)t$ we then have

$$\begin{aligned} P_\Psi(x,p;t) &= \sum_n c_n P_{nn} c_n + \sum_{m>n} c_m \big[P_{mn}e^{i\theta_{mn}} + P_{nm}e^{-i\theta_{mn}}\big]c_n \\ &= \sum_n c_n S_{nn} c_n + \sum_{m>n} c_m \big[\quad S_{mn}\big(e^{i\theta_{mn}} + e^{-i\theta_{mn}}\big) \\ &\qquad\qquad\qquad\qquad + iA_{mn}\big(e^{i\theta_{mn}} - e^{-i\theta_{mn}}\big)\big]c_n \\ &= \sum_n c_n S_{nn} c_n + 2\sum_{m>n} c_m \big[S_{mn}\cos\theta_{mn} - A_{mn}\sin\theta_{mn}\big]c_n \qquad (46) \end{aligned}$$

which in the limit $t \downarrow 0$ gives back

$$= \sum_n c_n S_{nn} c_n + 2\sum_{m>n} c_m S_{mn} c_n = \sum_{m,n} c_m S_{mn} c_n$$

Explicit descriptions of S_{mn} and A_{mn} are obtained from (39/40). In particular, $A_{mn}(x,p)$ was found at (38.2) to be an *odd* function of p, so

$$\int A_{mn}(x,p)\,dp = 0$$

while the argument that gave (41) supplied

$$\begin{aligned} \int S_{mn}(x,p)\,dp &= \tfrac{2}{a}\sin m\pi\tfrac{x}{a}\sin n\pi\tfrac{x}{a} \qquad (47) \\ &= \Psi_m(x)\Psi_n(x) \end{aligned}$$

It follows therefore from (46)—as also (directly) from (42)—that the motion of the marginal distribution

$$P_\Psi(x,t) \equiv \int P_\Psi(x,p;t)\,dp = |\Psi(x,t)|^2$$

can be described

$$\begin{aligned} |\Psi(x,t)|^2 &= \sum_n c_n c_n |\Psi_n(x)|^2 + 2\sum_{m>n} c_m c_n \Psi_m(x)\Psi_n(x)\cos\theta_{mn} \\ &= \tfrac{2}{a}\Big\{\sum_n c_n c_n \sin^2 n\pi\tfrac{x}{a} + 2\sum_{m>n} c_m c_n \sin m\pi\tfrac{x}{a}\sin n\pi\tfrac{x}{a}\cdot\cos\theta_{mn}\Big\} \\ &= \Big\{\text{sum of static terms, bilaterally symmetric in all cases}\Big\} \qquad (48) \\ &\quad + \left\{\begin{array}{l}\text{sum of dynamic terms, bilaterally symmetric/antisymmetric} \\ \text{and therefore “blink” or “slosh” according as } m \text{ and } n \text{ have the} \\ \text{same or opposite parity: } i.e., \text{ according as } m+n \text{ is even/odd}\end{array}\right\} \end{aligned}$$

The descriptive text here follows from the elemantary observation that $\Psi_n(x)$ is bilaterally symmetric/asymmetric according as n is odd/even. Notice that from the orthonormality of the $\Psi_n(x)$ it follows that

$$\int |\Psi_n(x)|^2\,dx = \sum_n c_n c_n + \Big\{\text{no contribution from dynamic terms}\Big\} = 1$$

Having equal claim to out attention—but rather more interesting in some technical respects—is the marginal distribution

$$P_\Psi(p,t) \equiv \int P_\Psi(x,p;t)\,dx \quad : \quad \text{not expressible } |\varPhi(p,t)|^2$$

Bilateral symmetry serves to kill many of the integrals now presented by the right side of (46): from (39) it follows that

$$\int S_{mn}(x,p)\,dx = \begin{cases} 2\int_0^{\frac{1}{2}a} SF_{mn}(x,p)\,dx & : \quad m \text{ and } n \text{ have same parity} \\ \\ 0 & : \quad m \text{ and } n \text{ have opposite parity} \end{cases}$$
$$\int A_{mn}(x,p)\,dx = \begin{cases} 0 & : \quad m \text{ and } n \text{ have same parity} \\ \\ 2\int_0^{\frac{1}{2}a} AF_{mn}(x,p)\,dx & : \quad m \text{ and } n \text{ have opposite parity} \end{cases}$$

So we have

$$\begin{aligned} P_\Psi(p,t) = \sum_n c_n c_n &\Big\{2\int_0^{\frac{1}{2}a} SF_{nn}(x,p)\,dx\Big\} \\ &+ 2\sum_{\substack{m>n \\ \text{same parity}}} c_m c_n \Big\{2\int_0^{\frac{1}{2}a} SF_{mn}(x,p)\,dx\Big\}\cos\theta_{mn} \\ &- 2\sum_{\substack{m>n \\ \text{opposite parity}}} c_m c_n \Big\{2\int_0^{\frac{1}{2}a} AF_{mn}(x,p)\,dx\Big\}\sin\theta_{mn} \end{aligned} \tag{49}$$

At (38.2) it is reported that the S-terms are p-even in all cases, and that the A-terms are p-odd. We therefore have

$$\begin{aligned} &= \Big\{\text{sum of static terms, } p\text{-even in all cases}\Big\} \\ &\quad + \Big\{\text{sum of } p\text{-even blinkers: } m \text{ and } n \text{ of same parity}\Big\} \\ &\quad + \Big\{\text{sum of } p\text{-odd sloshers: } m \text{ and } n \text{ of opposite parity}\Big\} \end{aligned} \tag{50}$$

Mathematica declines to provide *general* descriptions of the $\int$'s in braces, but has no difficulty when m and n are assigned any specific integral values. We find, for example, that

$$
\begin{aligned}
\int_0^{\frac{1}{2}a} SF_{11}(x,p)\,dx &= \tfrac{2}{h}a\frac{\pi^2\big[1+\cos ak\big]}{(ak-\pi)^2(ak+\pi)^2}\\
\int_0^{\frac{1}{2}a} SF_{22}(x,p)\,dx &= \tfrac{2}{h}a\frac{(2\pi)^2\big[1-\cos ak\big]}{(ak-2\pi)^2(ak+2\pi)^2}\\
\int_0^{\frac{1}{2}a} SF_{33}(x,p)\,dx &= \tfrac{2}{h}a\frac{(9\pi)^2\big[1+\cos ak\big]}{(ak-3\pi)^2(ak+3\pi)^2}\\
&\vdots\\
\int_0^{\frac{1}{2}a} SF_{nn}(x,p)\,dx &= \tfrac{2}{h}a\frac{(n\pi)^2\big[1-(-)^n\cos ak\big]}{(ak-n\pi)^2(ak+n\pi)^2}
\end{aligned}
\tag{51.1}
$$

and, provided m and n have the <u>same</u> parity,[7]

$$
\begin{aligned}
&\int_0^{\frac{1}{2}a} SF_{mn}(x,p)\,dx\\
&\qquad = \tfrac{2}{h}a\frac{\mu mn\pi^2\big[1-(-)^{mn}\cos ak\big]}{(ak-m\pi)(ak-n\pi\pi)(ak+n\pi)(ak+m\pi)}
\end{aligned}
\tag{51.2}
$$

where the multiplier

$$
\mu \equiv \tfrac{3}{2}-(-)^{mn}\tfrac{1}{2} = \begin{cases} 2 & \text{if } m \text{ and } n \text{ are both odd}\\ 1 & \text{if } m \text{ and } n \text{ are both even}\end{cases}
$$

Finally, if $m>n$ have <u>opposite</u> parity[8] then

$$
\begin{aligned}
&\int_0^{\frac{1}{2}a} AF_{mn}(x,p)\,dx\\
&\qquad = (-)^n\tfrac{2}{h}a\frac{mn\pi^2\sin ak}{(ak-m\pi)(ak-n\pi\pi)(ak+n\pi)(ak+m\pi)}
\end{aligned}
\tag{51.3}
$$

and the sign is reversed if $m<n$. I must emphasize that the general propositions (51) have not been properly "derived," but have been inferred from specific instances. I have high confidence, however, in their validity. Note that they make manifest the p-evenness/oddness of $\int S_{mn}(x,p)\,dx$ and $\int A_{mn}(x,p)\,dx$. Graphical analysis of (51)—see below—indicates that the zeros in the denominators always coincide with zeros in the numerators, and so never give rise to singularities.

---

[7] Happily we have no present need of the formula appropriate to cases in which m and n have the opposite parity, which is much more complicated, and grows ever more complicated as m and n become larger.

[8] If $m>n$ have the same parity then one encounters again the situation described in the preceding footnote.

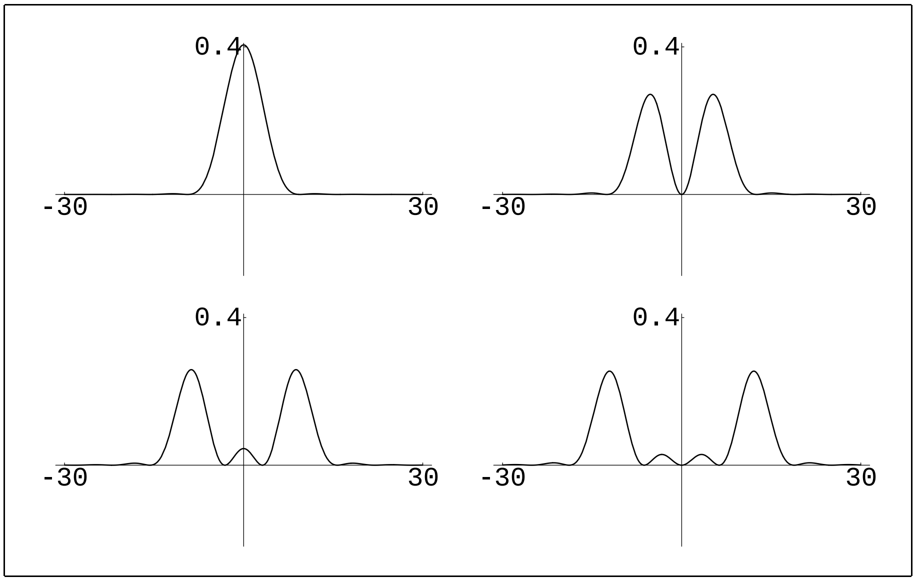


FIGURE 12: *Graphs of functions of diagonal type* $\int S_{nn}(x,p)\,dx$*, taken from (50.1) with* $a = h = 1$*. They are presented in the array*

$$\begin{array}{cc} \{1,1\} & \{2,2\} \\ \{3,3\} & \{4,4\} \end{array}$$

Note the p*-evenness, non-negativity and absence of singularities.*

Introduction of (51) into (49) yields a result too complicated to comprehend except—in particular instances—graphically. It should, however, be possible to establish that $\int P_\Psi(p,t)\,dp = 1$, which would test (weakly) the accuracy of the complicated formula in question. To that end, we notice that it follows already from the p-oddness of $\int A_{mn}(x,p)\,dx$ that

$$\iint A_{mn}(x,p)\,dxdp = 0 \quad : \quad m > n \text{ have opposite parity}$$

Computation[9] leads, moreover, to the conclusion that

$$\iint S_{mn}(x,p)\,dxdp = 0 \quad : \quad m > n \text{ have the same parity}$$

[9] *Mathematica* tends to trip on the seeming singularities, and needs delicate coaxing.

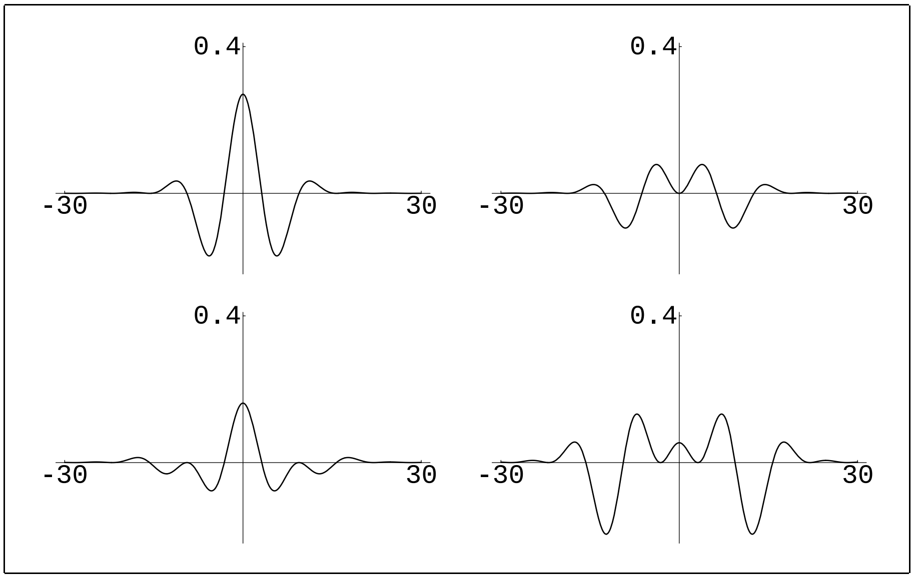


FIGURE 13: *Graphs of functions of the off-diagonal type* $\int S_{mn}(x,p)\,dx$*, taken from (50.2). They are presented in the array*

$$\begin{matrix}\{3,1\} & \{4,2\}\\ \{5,1\} & \{5,3\}\end{matrix}$$

Note here again the p-evenness and absence of singularities. Non-negativity has, however, been lost: the area under each such curve is zero.

and in cases on the diagonal supplies (see again page 11)

$$\begin{aligned}\iint S_{mn}(x,p)\,dxdp &= \int_{-\infty}^{+\infty} \tfrac{2}{h}a\frac{(n\pi)^2\big[1-(-)^n\cos ak\big]}{(ak-n\pi)^2(ak+n\pi)^2}\hbar dk\\ &= \tfrac{2}{h}\hbar\big[-(-)^n\sqrt{n/2}\,\pi^2 J_{\frac{3}{2}}(n\pi)\big]\\ &= 1 \quad : \quad n = 1,2,3,\ldots\end{aligned}$$

So from (49) we are in fact led to the anticipated result

$$\int P_\Psi(p,t)\,dp = \sum_n c_n c_n + \Big\{\text{no contribution from dynamic terms}\Big\} = 1$$

To clarify the situation as it has developed, let us suppose $\Psi(x)$ has the especially simple—but otherwise fairly representative—design

$$\Psi(x) = c_2\Psi_2(x) + c_3\Psi_3(x) + c_4\Psi_4(x) \tag{52.0}$$

where the real c's satisfy $c_2^2+c_3^2+c_4^2 = 1$ but are otherwise arbitrary. From (46)

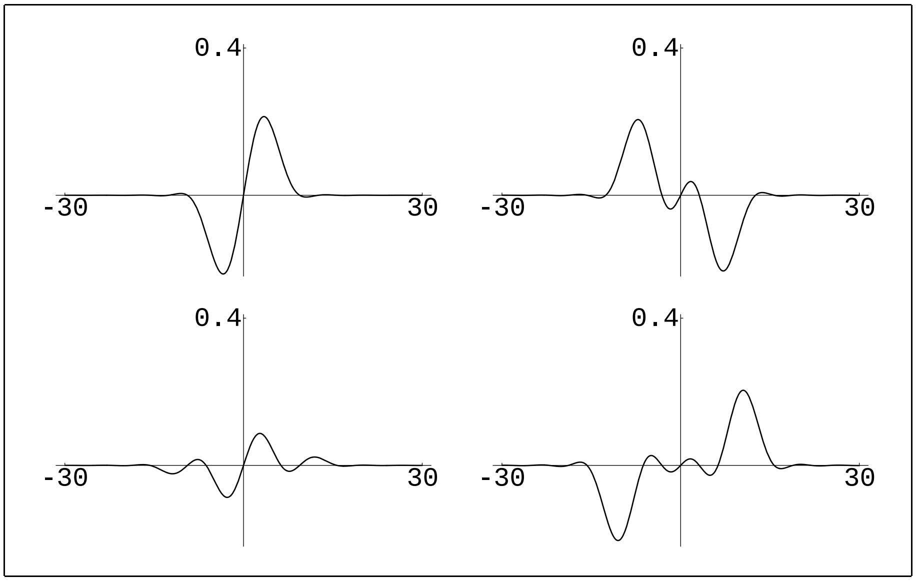


FIGURE 14: *Graphs of functions of the off-diagonal type* $\int A_{mn}(x,p)\,dx$, *taken from (50.3). They are presented in the array*

$$\begin{matrix} \{2,1\} & \{3,2\} \\ \{4,1\} & \{4,3\} \end{matrix}$$

Note again the absence of singularities. Also that p-evenness has become now p-oddness: non-positivity is therefore automatic, and the vanishing of the integrated area has become manifest.

we then have

$$\begin{aligned} P_\Psi(x,p;t) = c_2^2 S_{22} + c_3^2 S_{33} + c_4^2 S_{44} \qquad\qquad & \\ + 2\,c_3c_2\big[S_{32}\cos\theta_{32} - A_{32}\sin\theta_{32}\big] & \\ + 2\,c_4c_2\big[S_{42}\cos\theta_{42} - A_{42}\sin\theta_{42}\big] & \\ + 2\,c_4c_3\big[S_{43}\cos\theta_{43} - A_{43}\sin\theta_{43}\big] & \end{aligned} \tag{52.1}$$

where the $S_{mn}(x,p)$ and $A_{mn}(x,p)$ are supplied by (39/40) and where

$$\begin{aligned} \theta_{mn} \equiv (\omega_m - \omega_n)\,t = (m^2 - n^2)\cdot\Omega\,t & \\ \Omega \equiv \mathcal{E}/\hbar = h\pi/4ma^2 & \end{aligned}$$

Integration on p supplies, according to (48), the moving marginal distribution

$$\begin{aligned}\int P_\Psi(x,p;t)\,dp = \tfrac{2}{a}\Big\{c_2^2\sin^2 2\pi\tfrac{x}{a} + c_3^2\sin^2 3\pi\tfrac{x}{a} + c_4^2\sin^2 4\pi\tfrac{x}{a} \\ + 2\,c_3c_2\sin 3\pi\tfrac{x}{a}\sin 2\pi\tfrac{x}{a}\cdot\cos\theta_{32} \\ + 2\,c_4c_2\sin 4\pi\tfrac{x}{a}\sin 2\pi\tfrac{x}{a}\cdot\cos\theta_{42} \\ + 2\,c_4c_3\sin 4\pi\tfrac{x}{a}\sin 3\pi\tfrac{x}{a}\cdot\cos\theta_{43}\Big\}\end{aligned} \tag{52.2}$$

Integration on x leads, on the other hand, to the complementary moving marginal distribution, which according to (49/51) is given by

$$\begin{aligned}&\int P_\Psi(x,p;t)\,dx \\ &= \tfrac{2a}{h}\Big\{c_2^2\frac{(2\pi)^2(1-\cos ak)}{(ak-2\pi)^2(ak+2\pi)^2} + c_3^2\frac{(3\pi)^2(1+\cos ak)}{(ak-3\pi)^2(ak+3\pi)^2} \\ &\qquad + c_4^2\frac{(4\pi)^2(1-\cos ak)}{(ak-4\pi)^2(ak+4\pi)^2} \\ &\quad + 2\,c_4c_2 2\frac{4\cdot 2\pi^2(1-\cos ak)}{(ak-4\pi)(ak-2\pi)(ak+2\pi)(ak+4\pi)}\cos\theta_{42} \\ &\quad - 2\,c_3c_2 2\frac{3\cdot 2\pi^2\sin ak}{(ak-3\pi)(ak-2\pi)(ak+2\pi)(ak+3\pi)}\sin\theta_{32} \\ &\quad + 2\,c_4c_3 2\frac{4\cdot 3\pi^2\sin ak}{(ak-4\pi)(ak-3\pi)(ak+3\pi)(ak+4\pi)}\sin\theta_{43}\Big\}\end{aligned} \tag{52.3}$$

In both (52.2) and (52.3) we expect the c_{42}-term to be a "blinker," and the c_{32} and c_{43}-terms to be "sloshers." Finally we have

$$\begin{aligned}\theta_{32} &= \ \ 5\cdot\Omega t \\ \theta_{42} &= 12\cdot\Omega t \\ \theta_{43} &= \ \ 7\cdot\Omega t\end{aligned}$$

Computer animation is clearly the method of choice if one's objective is to gain a vivid sense of what equations (52) are trying to tell us. As first steps toward that objective one might

- set $a = h = 1$, $\Omega = 2\pi$
- assign interesting specific values to c_{32}, c_{42} and c_{43}

but would still confront the questions *how large to set the increment* Δt? *how many frames* N *to include in the filmstrip*? One wants also to make the mesh size small enough to capture relevant spatial detail (it was that consideration that led me to assign *small* values to m and n), and must approach these interrelated issues with an eye to (i) what they imply about total computation time and (especially) (ii) the demand they impose upon available memory. It is such practical considerations that motivate the following remarks:

The *period* of oscillation in the mn-mode is given by

$$\tau_{mn} = \frac{2\pi}{(m^2 - n^2)\Omega}$$

so the times "natural" to the circumstances at hand are

$$\tau_{42} = \frac{2\pi}{12\Omega} \quad < \quad \tau_{43} = \frac{2\pi}{7\Omega} \quad < \quad \tau_{32} = \frac{2\pi}{5\Omega}$$

It is evident that at time

$$t = 12\,\tau_{42} = 7\,\tau_{43} = 5\,\tau_{32} = 2\pi/\Omega$$

- the 42-mode will have completed 12 cycles
- the 43-mode will have completed 7 cycles
- the 32-mode will have completed 5 cycles

and the trio will be back in synchrony. Acceptable temporal resolution would be achieved if we set

$$\Delta t = \frac{\text{briefest natural time}}{10} = \frac{2\pi}{120\Omega}$$

and drew film frames at times

$$t_j = 0 + j\Delta t \quad : \quad j = 0, 1, 2, \ldots, 119$$

. . . which makes for a long, memory-intensive movie. The briefest 3-state movie (80 frames) arises from

$$t = 8\,\tau_{31} = 5\,\tau_{32} = 3\,\tau_{21} = 2\pi/\Omega$$

The situation becomes rapidly worse as the number of states increases, for while the sequence

$$(n+2)^2 - n^2 \quad \text{proceeds} \quad 8, 12, 16, 20, 24, \ldots$$

we upon inclusion of progressively more states encounter

$$(n+3)^2 - n^2 \quad \text{proceeds} \quad 15, 21, 27, 33, 39, \ldots$$

$$(n+4)^2 - n^2 \quad \text{proceeds} \quad 24, 32, 40, 48, 56, \ldots$$

and it becomes worse still if the participating states are not contiguously indexed (a circumstance which would introduce extra "spread" into the value of $m^2 - n^2$).

Thus are we led to look more seriously to 2-state superpositions, for which

$$(n+1)^2 - n^2 \quad \text{proceeds} \quad 3, 5, 7, 9, 11, 13, \ldots$$

and which—since "it takes two to interfere"—are *simplest possible* from a quantum dynamical point of view. Relevant formulæ can be obtained from (52) by setting c_2 else c_3 else c_4 equal to zero. Such systems possess a *single* "natural time," and the "synchrony problem" is absent.

The real solutions of $c_2^2 + c_3^2 + c_4^2 = 1$ associate naturally with points on the "unit sphere in 3-dimensional $\boldsymbol{c}$-space," and therefore can be neatly identified/distinguished by specification of a pair of "spherical mixing angles," which I will (on the principle "odd man out") take to be defined in such a way

$$\begin{aligned} c_2 &= \cos\alpha\cos\beta \\ c_3 &= \sin\alpha \\ c_4 &= \cos\alpha\,\sin\beta \end{aligned}$$

that c_3 vanishes "on the equator."

In a set of *Mathematica* notebooks attached as appendices to these notes[10] I present 2-state and 3-state animations based upon (52). Much shown there conforms to expectation: we find, for example that the x-marginal and p-marginal distributions that arise from superpositions of (mixed-parity) types

$$\begin{pmatrix} c_2 \\ c_3 \\ 0 \end{pmatrix} \quad \text{else} \quad \begin{pmatrix} 0 \\ c_3 \\ c_4 \end{pmatrix} \quad \text{both "slosh"}$$

while those that arise from superpositions of the (same-parity) equatorial type

$$\begin{pmatrix} c_2 \\ 0 \\ c_4 \end{pmatrix} \quad \text{both "blink"}$$

And we find that the x-marginal distributions are in all cases *everywhere non-negative* (as proper distributions are supposed to be). We find, moreover, that in *all* cases $P_\Psi(x, p; t)$ exhibits a chirality of the $\circlearrowright$ sense associated with the *classical* physics of a particle-in-a-box. But we encounter also a major surprise:

We find that p-marginal distributions sometimes assume negative values, and so properly are not "distributions" at all. This curious development can be understood as a ramification of the celebrated fact that the Wigner function is itself not positive-semidefinite—a circumstance which we would be protected if it were possible to write

$$\int P_\Psi(x, p; t)\,dx = |\varPhi(p, t)|^2$$

but, as I have several times remarked, the clamped formulation of the particle-in-a-box problem provides no such $\varPhi(p, t)$.

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[10] The notebooks bear titles which are variants of "Box Animations.nb"

A further surprise: We find that the time-averaged p-marginal distributions *are* everywhere non-negative, *are* proper distributions. The analytical proof that this is so—an effort motivated in this instance by graphic analysis—is fussy, and will be omitted.

Periodic aspects of the classical/quantum box problem. Classically, a particle in a box is effectively a clock, going "tick . . . tock . . . tick . . . tock . . . tick . . . " with period

$$\tau = \frac{2a}{\text{speed}} = \frac{2a}{\sqrt{2E/m}}$$

and angular frequency

$$\omega = 2\pi/\tau = 2\pi\sqrt{\frac{E}{2ma^2}}$$

The appearance of E on the right informs us that such "box oscillators" are anharmonic.

A pair of such systems, if started at the same time, will speak

$$\begin{array}{lcl} \tau_1 & : & \text{tick} \ldots \text{tock} \ldots \text{tick} \ldots \text{tock} \ldots \text{tick} \ldots \\ \tau_2 & : & \text{tick} \ldots\ldots \text{tock} \ldots\ldots \text{tick} \ldots\ldots \text{tock}\,.\,. \end{array}$$

with occasional coincidence if an only if there exist least integers n_1 and n_2 such that

$$\tau_{\text{coincidence}} \equiv n_1\tau_1 = n_2\tau_2$$

but this requires that τ_1/τ_2 be rational, which in classical physics would be an unnatural state of affairs.

Suppose, however, we assign to E the values borrowed from quantum mechanics: $E_n = \mathcal{E}n^2$. We then have

$$\omega_n = 2\pi\sqrt{\frac{m\mathcal{E}}{2a^2}}\cdot n = \frac{\pi h}{2ma^2}\cdot n$$

and find that the coincidence condition is *always* satisfied.

Quantum mechanics ascribes to such a system an angular frequency which is, on the other hand, given by

$$\omega_n = (\mathcal{E}/\hbar)\cdot n^2$$

That, however, refers not to "motion" but to an unphysical "buzz;" quantum motion is, as I have repeatedly stressed, an interference effect, evident only when the quantum state Ψ has been assembled by superposition of (at least) two energy eigenstates—call them Ψ_m and Ψ_n; it is then only the frequency *difference*

$$\Delta\omega = (\mathcal{E}/\hbar)\cdot(m^2 - n^2)$$

that has observable consequences. Suppose $m = n + 1$. Then

$$\begin{aligned}\Delta\omega &= (\mathcal{E}/\hbar)\cdot(2n+1) \sim (2\mathcal{E}/\hbar)\cdot n \quad \text{if } n \text{ is large}\\ &= \frac{\pi h}{2ma^2}\cdot n\end{aligned}$$

Thus does the n^2-dependence characteristic of the quantum theory go over into the linear n-dependence characteristic of the classical theory. Note, however, the importance of the assumption that Ψ_m and Ψ_n are *proximate* states; if there were more remote neighbors $m = n + \nu$ we would have obtained

$$\Delta\omega \sim \nu\cdot\left[\frac{\pi h}{2ma^2}\cdot n\right] \sim \nu\cdot\left[\frac{\pi h}{2ma^2}\cdot\frac{(n+\nu)+n}{2}\right]$$

which describes integral multiples (harmonics) of the (mean) classical frequency that become progressively higher as the neighbors become more remote.

But if $\nu = 2$ (or is even) then $\Delta\omega$ refers not to sloshing but to a "blinking" that has no classical counterpart. One of the animations makes this point very clearly.

Wavepackets in a box. Equations (52), and the animations based upon them, allude to the *very low energy* quantum physics of a particle in a box, to events deep within the quantum realm—events which, remarkably, are found nevertheless to prefigure events (most notably: rectangular $\circlearrowright$-circulation in phase space) most characteristic of the classical physics of such systems. Of greater interest to me, however, is the high energy quantum physics, the more pronouncedly "semi-classical" physics that presumably follows from (46) when the c's are assigned values that become predominant in the vicinity of some large n (see the following figure) . . . but at present I lack the computer resouces required to penetrate such a regime. My effort here, therefore, will to to attempt to construct an analytical end-run around that difficulty. I have incidental interest also in discovering whether certain fairly standard devices survive the imposition of clamping (extinction of $\psi(x)$ outside of the box), and in trying to clarify the "evolution of flatness."

Let $f(x)$ be a continuous function defined on the entire real line and endowed with whatever modestly nice properties may be required to make the following manipulations work. Construct

$$\begin{aligned}f_{\text{odd}}(x) &\equiv f(x) - f(-x)\\ &= 2\big\{\text{odd part of } f(x)\big\}\end{aligned}$$

Clearly $f_{\text{odd}}(0) = 0.$[11] Construct

$$g(x) \equiv \sum_{j=-\infty}^{+\infty} f_{\text{odd}}(x + 2ja) \quad : \quad \text{convergence assumed}$$

[11] $f_{\text{odd}}(x)$ would vanish *identically* if $f(x)$ were even, which we will assume not to be the case.

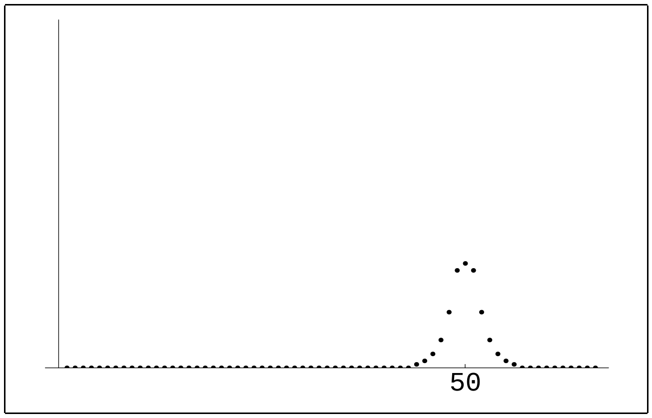

FIGURE 15: *A c_n-assignment that would presumably give rise to more distinctly "semi-classical" quantum physics, but that lies well beyond my present means to explore numerically.*

which is manifestly periodic

$$g(x+2a) = g(x) \quad : \quad \text{all } x$$

and therefore vanishes at $\ldots, -4a, -2a, 0, +2a, +4a, \ldots$ From

$$\begin{aligned} g(a) &= -g(-a) \quad \text{because } g(x) \text{ is odd} \\ g(a) &= +g(-a) \quad \text{because } g(x) \text{ is periodic, with period } 2a \end{aligned}$$

we see that $g(x)$, if continuous, must vanish also at the midpoints of those intervals; in short,

$$g(ja) = 0 \quad : \quad j = 0, \pm1, \pm2, \ldots$$

so in particular we have nodes $g(0) = g(a) = 0$ at the ends of the "physical interval" or "box" $0 \leqslant x \leqslant a$. All of which is entirely familiar from the elementary physics of strings: if $f(x - vt)$ describes a pulse or wavepacket gliding to the right along an infinite string, then

$$g(x,t) \equiv \sum_{j=-\infty}^{\infty} \Big\{ f(x + 2ja - vt) - f(-x + 2ja - vt) \Big\} \tag{55}$$

describes countermoving periodic trains of such pulses, and within the box looks like a single pulse bouncing back and forth, reversing sign with each pulse. The idea is animated in an appendix. Multiplication by the "box function"

$$B(x) \equiv \begin{cases} 1 & : \quad 0 \leqslant x \leqslant a \\ 0 & : \quad \text{elsewhere} \end{cases} \tag{56}$$

extinguishes the wave outside the bounds of the box

$$g(x,t) \longmapsto G(x,t) \equiv B(x)\cdot g(x,t) \tag{57}$$

and thus achieves passage from the "periodically continuated formalism" to the "clamped formalism."

Look to the Fourier analytic aspects of the preceding discussion. Starting from

$$f(x) = \int_{-\infty}^{+\infty} \phi(k)\, e^{ik\,x}\, dk$$

we extract

$$\begin{aligned} f_{\text{odd}}(x) &= \int_{-\infty}^{+\infty} \phi_{\text{odd}}(k)\, e^{ik\,x}\, dk \quad \text{with} \quad \phi_{\text{odd}}(k) \equiv \phi(k) - \phi(-k) \\ &= \int_{-\infty}^{+\infty} \phi(k)\, 2i\sin kx\, dk \end{aligned}$$

We then construct $g(x)$, the established periodicity properties of which permit us to write

$$g(x) = \sum_{n=1}^{\infty} g_n \sin n\pi\tfrac{x}{a} = \int_{-\infty}^{+\infty} \gamma(k)\, e^{ik\,x}\, dk \tag{58.1}$$

$$\gamma(k) = \sum_{n=1}^{\infty} g_n\, \tfrac{1}{2i}\Big\{\delta(k - n\tfrac{\pi}{a}) - \delta(k + n\tfrac{\pi}{a})\Big\}$$

But

$$\begin{aligned} g_n &= \tfrac{1}{a}\int_0^{2a} g(x)\sin n\pi\tfrac{x}{a}\, dx \\ &= \tfrac{1}{a}\int_{-\infty}^{+\infty} f_{\text{odd}}(x)\sin n\pi\tfrac{x}{a}\, dx \\ &= \tfrac{1}{2\pi a}\iint_{-\infty}^{+\infty} \phi_{\text{odd}}(k)\, \frac{e^{i(k+n\pi/a)\,x} - e^{i(k-n\pi/a)\,x}}{2i}\, dxdk \\ &= \tfrac{1}{2i\,a}\int_{-\infty}^{+\infty} \phi_{\text{odd}}(k)\Big\{\delta(k + n\tfrac{\pi}{a}) - \delta(k - n\tfrac{\pi}{a})\Big\}dk \\ &= \tfrac{1}{2i\,a}\Big\{\phi_{\text{odd}}(-n\tfrac{\pi}{a}) - \phi_{\text{odd}}(n\tfrac{\pi}{a})\Big\} \\ &= \tfrac{i}{a}\,\phi_{\text{odd}}(n\tfrac{\pi}{a}) \end{aligned}$$

so

$$\gamma(k) = \tfrac{1}{2a}\sum_{n=1}^{\infty} \phi_{\text{odd}}(n\tfrac{\pi}{a})\,\Big\{\delta(k - n\tfrac{\pi}{a}) - \delta(k + n\tfrac{\pi}{a})\Big\} \tag{58.2}$$

The transformation $f(x) \longmapsto g(x)$ has by Fourier transformation assumed a form $\phi(k) \longmapsto \gamma(k)$ in which only certain specific wave numbers survive.

Clamping, which was achieved by multiplication in x space, will be achieved by convolution in k space: we have

$$g(x) = \int \gamma(k)\, e^{ikx}\, dk$$

and (formally)[12]

$$B(x) = \vartheta(x) - \vartheta(x-a) = \tfrac{1}{2\pi i}\int \frac{1-e^{-ika}}{k}\, e^{ikx}\, dk \equiv \int \beta(k)\, e^{ikx}\, dk$$

so

$$G(x) \equiv B(x)g(x) = \int \varGamma(k) e^{ikx}\, dk \tag{59.1}$$

where

$$\begin{aligned}
\varGamma(k) &= \int \beta(\ell)\gamma(k-\ell)\, d\ell \\
&= \tfrac{1}{2\pi i}\tfrac{1}{2a}\sum_{n=1}^{\infty}\phi_{\text{odd}}(n\tfrac{\pi}{a})\int \frac{1-e^{-i\ell a}}{\ell}\Big\{\delta(k-\ell-n\tfrac{\pi}{a}) - \delta(k-\ell+n\tfrac{\pi}{a})\Big\}\, d\ell \\
&= \tfrac{1}{2\pi i}\tfrac{1}{2}\sum_{n=1}^{\infty}\phi_{\text{odd}}(n\tfrac{\pi}{a})\bigg\{\frac{1-e^{-i(ka-n\pi)}}{ka-n\pi} - \frac{1-e^{-i(ka+n\pi)}}{ka+n\pi}\bigg\}
\end{aligned} \tag{59.2}$$

The important points to notice are that

- k-discreteness has evaporated—a casualty of clamping;
- the singularities on the right (situated at the formerly prefered k values, were δ-spikes used to stand) are illusory—have in fact become zeros.

When, in my introduction to this section, I expressed an "incidental interest . . . in . . . certain fairly standard devices" I had in mind the fact that some of the preceding arguments (those up to the point of clamping, at the top of this page) are close variants of those which give rise to the Poisson Summation Formula, which I digress now to review.[13] From $F(x)$ construct the periodic function

$$\begin{aligned}
G(x) &\equiv \sum_{j=-\infty}^{\infty} F(x+ja) \quad : \quad \text{period } a \\
&= \sum_{k=-\infty}^{\infty} G_k\, e^{i\,2\pi k\frac{x}{a}}
\end{aligned}$$

[12] In the following equation $\vartheta(x)$ is the Heaviside step function:

$$\vartheta(x) \equiv \int_{-\infty}^{x} \delta(x)\, dx = \begin{cases} 0 & : \quad x<0 \\ 1 & : \quad x>0 \end{cases}$$

[13] I follow R. Courant & D. Hilbert, *Methods of Mathematical Physics: Volume I* (1953), pages 76–77, which I have modified so as to achieve direct contact with the result quoted in *Encyclopedic Dictionary of Mathematics* (2nd edition 1993), §**192-C**.

Use

$$\begin{aligned} G_k &= \tfrac{1}{a}\int_0^a e^{-i\,2\pi k\frac{x}{a}}G(x)\,dx \\ &= \tfrac{1}{a}\int_{-\infty}^{+\infty} e^{-i\,2\pi k\frac{x}{a}}F(x)\,dx \quad : \quad \text{this is the essential trick} \end{aligned}$$

to obtain

$$\begin{aligned} \sum_{j=-\infty}^{\infty} F(x+ja) &= \tfrac{1}{a}\sum_{k=-\infty}^{\infty} e^{i\,2\pi k\frac{x}{a}}\int_{-\infty}^{+\infty} F(x)e^{-i\,2\pi k\frac{x}{a}}\,dx \\ &= \tfrac{\sqrt{2\pi}}{a}\sum_{k=-\infty}^{\infty} e^{i\,2\pi k\frac{x}{a}}\,\Phi(bk) \\ &\qquad\qquad b \equiv \tfrac{2\pi}{a} \end{aligned}$$

where $\Phi(k) = \frac{1}{\sqrt{2\pi}}\int F(x)e^{-ikx}\,dx$ is the Fourier transform of $F(x)$. Finally set $x = 0$ to obtain the "Poisson summation formula"

$$\sqrt{a}\sum_{j=-\infty}^{\infty} F(ja) = \sqrt{b}\sum_{k=-\infty}^{\infty}\Phi(kb) \quad : \quad ab = 2\pi \tag{60}$$

Since a great many interpretations can be assigned to $F(x)$ this provides a very powerful tool for converting one series into another. The new series may converge more rapidly or offer other analytical advantages.

Let us see what the results now in hand have to say in an illustrative concrete case—specifically: the case of a Gaussian wavepacket. In order to underscore certain key distinctions I look first to the classical motion of a Gaussian pulse on a string, then to the quantum dynamics of a Gaussian wavepacket.

To describe the initial shape of the classical pulse we write

$$f(x,0) = \tfrac{1}{\sigma\sqrt{2\pi}}\,e^{-\frac{1}{2}\left[\frac{x}{\sigma}\right]^2} \quad : \quad \text{normalized initial Gaussian pulse} \tag{61.1}$$

To launch the wavepacket into motion along a string of infinite length we form

$$f(x,t) = \tfrac{1}{\sigma\sqrt{2\pi}}\,e^{-\frac{1}{2}\left[\frac{x-ct}{\sigma}\right]^2} \quad : \quad \text{launched Gaussian pulse} \tag{61.2}$$

which is a solution of the wave equation: $f_{xx} - c^{-2}f_{tt} = 0$. To model our presumption that the pulse lives on a string of finite length $0 \leqslant x \leqslant a$ we construct countermoving periodic trains of such pulses:

$$g(x,t) \equiv \sum_{j=-\infty}^{\infty}\tfrac{1}{\sigma\sqrt{2\pi}}\left\{e^{-\frac{1}{2}\left[\frac{x+2ja-ct}{\sigma}\right]^2} - e^{-\frac{1}{2}\left[\frac{-x+2ja-ct}{\sigma}\right]^2}\right\} \tag{61.3}$$

Manifestly, $x = 0$ and $x = a$ are persistent nodes:

$$g(0,t) = g(a,t) = 0 \quad : \quad \text{all } t$$

... but notice:

$$g(x,0) = 0 \quad \text{for } \textit{all } x$$

and this situation recurs whenever $ct/2a$ is an integer. At such moments none of the energy resident in the string is energy of deformation—all is kinetic (which, physically, is an entirely acceptable state of affairs). Finally we clamp the wave (discard the the periodic replications of the physics that live only in the mind, beyond the ends of the physical string): we form

$$G(x,t) = B(x)\cdot g(x,t) = \begin{cases} g(x,t) & : \quad 0 \leqslant x \leqslant a \\ 0 & : \quad \text{elsewhere} \end{cases}$$

Turn now to the *quantum* dynamics of a mass m that moves freely and (as we shall initially assume) unrestrictedly in one dimension. To describe a "standing Gaussian wavepacket" in such a context we might write[14]

$$\psi(x,t) = \Big[\tfrac{1}{\sigma[1+i(t/\tau)]\sqrt{2\pi}}\Big]^{\frac{1}{2}} \exp\Big\{-\tfrac{1}{4}\frac{(x-x_0)^2}{\sigma^2[1+i(t/\tau)]}\Big\} \tag{62.1}$$

where σ is a positive real constant, $\tau = 2m\sigma^2/\hbar$ is an associated "natural time" and x_0 marks the "mean point of departure." The wave function just described satisfies the Schrödinger equation $-(\hbar/2m)\psi_{xx} = i\hbar\psi_t$ and produces a Gaussian distribution

$$|\psi(x,t)|^2 = \tfrac{1}{\sigma(t)\sqrt{2\pi}} \exp\Big\{-\tfrac{1}{2}\big[\tfrac{x-x_0}{\sigma(t)}\big]^2\Big\} \tag{62.2}$$

of growing dispersion

$$\sigma(t) \equiv \sigma\sqrt{1+(t/\tau)^2} \tag{63}$$

Were we to "launch" such a wavepacket we would obtain[15]

$$\begin{aligned} \psi(x,t) = \Big[\tfrac{1}{\sigma[1+i(t/\tau)]\sqrt{2\pi}}\Big]^{\frac{1}{2}} \exp\Big\{&-\tfrac{1}{4}\frac{(x-x_0)^2}{\sigma^2[1+i(t/\tau)]} \\ &+ \tfrac{i}{\hbar}\tfrac{1}{1+i(t/\tau)}\big[\wp(x-x_0) - \mathcal{E}\,t\big]\Big\} \end{aligned} \tag{64.1}$$

giving

$$|\psi(x,t)|^2 = \tfrac{1}{\sigma(t)\sqrt{2\pi}} \exp\Big\{-\tfrac{1}{2}\Big[\frac{(x-x_0)-vt}{\sigma(t)}\Big]^2\Big\} \tag{64.2}$$

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[14] See, for example, §2 of my "Gaussian wavepackets" (1998).

[15] See §5 in the note just cited for elaborate discussion of the surprisingly intricate details. Launching a Gaussian quantum wavepacket is not so easy as launching a Gaussian pulse down a string: the former moves dispersively, the latter rigidly; the former can be accomplished by Galilean transformation, but the entails what is effectively a Lorentz transformation.

Here $\wp \equiv mv$ where v is the prescribed drift velocity of the wavepacket, and $\mathcal{E} \equiv \wp^2/2m$. To create persistent nodes at the boundaries of the box we must first seek protection from the possibility that $\psi(x,t)$ ever becomes even in x, for in that case the ensuing formalism collapses into empty triviality: we would then be led to a clamped $\Psi(x,t)$ that vanishes *everywhere*, which is quantum mechanically disallowed. Evenness is seen to require that it be simultaneously the case that

$$(x - x_0)^2 = (-x - x_0)^2 \quad \text{and} \quad \wp(x - x_0) = \wp(-x - x_0)$$

We are led thus to require that $x_0 \neq 0$, which upon construction of the odd periodic function

$$g(x,t) \equiv \sum_{j=-\infty}^{\infty} \Big\{ \psi(x + 2ja, t) - \psi(-x + 2ja, t) \Big\} \tag{65}$$

becomes the requirement that $0 < x_0 < a$: the particle cannot be launched from either *end* of the box.[16] Our plan now is to install the clamps

$$g(x,t) \longmapsto G(x,t) \equiv B(x) \cdot g(x,t)$$

and then to normalize:

$$\begin{aligned} G(x,t) \longmapsto \Psi(x,t) &= A(t) \cdot G(x,t) \\ A(t) &\equiv \left[\int_0^a |G(x,t)|^2 \, dx \right]^{-\frac{1}{2}} \end{aligned} \tag{66}$$

Which is more easily said than done, even when $\psi(x,t)$ has been endowed with the nice properties of a Gaussian. Before I turn to the oppressive details I digress to interject some historical remarks:

In 1953 Einstein submitted an essay for publication in *Scientific Papers presented to Max Born on his retirement from the Tait Chair of Natural Philosophy in the University of Edinburgh* in which he argues that "in the limiting case of macroscopic dimensions the quantum mechanical solution [of the problem of a "ball bouncing between two walls"] does not become the classical motion." There followed an exchange of letters, which are reproduced (with Born's annotations) as

105:	Born to Einstein	26 November 1953
106:	Einstein to Born	3 December 1953
107:	Born to Einstein	22 December 1953
108:	Einstein to Born	1 January 1954
109:	Born to Einstein	2 January 1954
110:	Einstein to Born	12 January 1954
111:	Born to Einstein	20 January 1954
112:	Pauli to Born	3 March 1954
115:	Pauli to Born	31 March 1954
116:	Pauli to Born	15 April 1954

[16] This restriction arises simply from the symmetry of our chosen wavepacket, and would evaporate if we adopted an asymmetric $\psi(x,t)$. The point, therefore, is technical/incidental, not deeply physical.

in *The Born–Einstein Letters* (1971: Forward by Bertrand Russell, Introduction by Werner Heisenberg) and deserve to be more widely known. In **105** Born claims that Einstein failed to recover classical motion because he chose the "wrong quantum state" (an energy eigenstate); claims Einstein should have watched the quantum motion of a wavepacket of initially small Δx and Δp and made $m \to \infty$ to arrest the growth of uncertainty (beyond that expected already classically if Δx and Δp are—though small—non-zero) ... and announces his intention to "carry out a thorough calculation ... with my collaborator (which is not easy to do formally)."[17] But in an editorial remark he observes that in responding thus he missed Einstein's main point ... which Einstein restates in **106**. One *should not have to specialize the state* according to Einstein, else one would be forced to the conclusion that classical mechanics "cannot claim to describe, even approximately, most of the [macro-events that are quantum mechanically conceivable]" ... and should "be very surprised if a star, or a fly, seen for the first time, appeared even to be quasi-localized."[18]

In **107** Born reports that he has completed the promised "thorough calculation"—*without* the help of his assistant (though "it is not at all easy, and I really had to rack my brain")—that all worked out exactly as he had asserted it would, and that he is preparing to submit the paper for publication in *Proceedings of the Royal Society* with instructions that the editor is to accept whatever remarks Einstein might care to add. But in **108** Einstein states that "Your concept is completely untenable" and that "I do not want to take part in any further discussion, such as you seem to envisage. I content myself with having expressed my opinion clearly." Born's MS was eventually published elsewhere,[19] and Einstein did not immediately honor his own stated intention ... perhaps because Born had been in contact with Pauli, who was then at the Institute for Advanced Studies and began himself to discuss these matters with Einstein, face to face. In commentary on three letters in which Pauli reports the upshot of those conversations, Born quotes from an (unpublished) letter, dated 11 December 1955, in which Pauli acknowledges receipt of a copy of the

[17] That effort resulted finally in M. Born & W. Ludwig, "Zur Quantenmechanik des kräftefreien Teilchens," Zeitschrift für Physik **150**, 106 (1956), but it had to await the injection of certain technical ideas by Pauli, and did not appear in print until after Einstein had died (18 April 1955). That paper has been my own principal source: see pages 9–32 in APPLICATIONS OF THE FEYNMAN FORMALISM TO FREE PARTICLE SYSTEMS 1971–1976.

[18] Einstein goes on to observe that—setting aside that problem—for Born's position to make sense ψ must refer to an ensemble (Born agrees) and that quantum mechanics must for that reason be held to be "incomplete" (Born disagrees, thinks that Einstein was handicapped by "inadequate knowledge of quantum mechanics").

[19] It appears under the title "Continuity, determinism and reality" as a contribution to a collection of papers honoring Niels Bohr's 70$^{\text{th}}$ birthday: Kong. Dansk. Videnskabernes Selskab, Mathematiskfysiske Meddelelser **30**, 1 (1955).

Bohr festschrift, reports the death of Hermann Weyl, and remarks that "I had used the mathematics of the example of the mass point between two walls, and of the wavepackets which belong to it, in my lectures in such a way that the transformation formula of the theta-functions comes into play. But that is a mere detail."[20] Born comments that "It was more than a detail. It shows that Pauli had long been familiar with all that I had to say . . . His remark about the theta-function made me take up this example again." It was thus that Born & Ludwig[16] came to be written. Regarding the essential use made there of the "Jacobi theta transformation" (which Born/Ludwig use to pass smoothly from the "wave representation" to the "particle representation"), Born remarks that he learned of the technique from Paul Ewald.[21, 22]

Born concludes his editorial remarks with the observation that "Although this problem deals with a case which is physically trivial and unimportant in practice, it gives a clear insight into the connection between classical and quantum mechanics, and seems to me to be more useful than any philosophizing about the question. It should be brought into, and discussed in, every elementary lecture about quantum mechanics." I agree (though *every* elementary lecture may be a few too many), but my deepest motivation has closer kinship with Einstein's question than with Born's somewhat pat response: *Given that the world is quantum mechanical, how does it happen that the world*

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[20] See *Pauli Lectures on Physics 6: Selected Topics in Field Quantization* (1950–51), page 172.

[21] Born/Ludwig cite Ann. Phys. **64**, 253 (1921). Ewald (1888–1985) began as a student of chemistry at Cambridge in 1905, but in quest of greater formal rigor went in 1906/7 to Göttingen to study mathematics with Hilbert, and in 1907 to Munich to study physics under Sommerfeld. It was Sommerfeld who introduced him to the research area (interaction of radiation with crystals) in which he established his reputation. Collaboration with Max von Laue in 1912 contributed to the early development of X-ray crystalography. Ewald—whose wife was Jewish, and who was himself part Jewish—left Germany in 1937 to teach successively at Cambridge, Belfast (where J. S. Bell was among his students, and much influenced by him) and the Brooklyn Polytechnic Institute, from which he retired in 1959. His last years were spent in Ithaca, New York, where Hans Bethe—his former thesis student, now son-in-law—was professor of physics, and where also Peter Debye (1884–1966) then lived.

[22] Neither Pauli nor Born acknowledge indebtedness to Arnold Sommerfeld, though the mathematical essence of their work—spelled out as it relates not to the quantum mechanical particle-in-a-box problem but to heat conduction on a uniform bar—can be found in his *Lectures on Theoretical Physics 6: Partial Differential Equations in Physics* (1949); see §16 in Chapter 3, where the "method of images" leads to theta functions, and to an application of "Jacobi's theta transformation," concerning which Sommerfeld remarks that "For us it constitutes the passage from Fourier's method to the method of heat poles. In quantum theory [it] is of importance for the rotational energy of diatomic molecules and for the calculation of their specific heat at low temperature."

of gross experience manages—not by contrivance, but spontaneously—to seem classical?

Now to the "oppressive details," which even Born found "not at all easy" ...let us, in an effort to reduce notational clutter, assume initially that $\wp = 0$. And let us look initially only to the first of the terms that appear on the right side of (65):

$$\begin{aligned}\sum_{n=-\infty}^{\infty}\psi(x+2na,t) &= \Big[\tfrac{1}{\sigma u(t)\sqrt{2\pi}}\Big]^{\frac{1}{2}}\sum_{n=-\infty}^{\infty}\exp\Big\{-\tfrac{1}{4\sigma^2 u(t)}(x-x_0+2na)^2\Big\}\\ &= \Big[\tfrac{1}{\sigma u(t)\sqrt{2\pi}}\Big]^{\frac{1}{2}}\sum_{n=-\infty}^{\infty}\exp\Big\{-\tfrac{a^2}{\sigma^2 u(t)}\big(\tfrac{x-x_0}{2a}+n\big)^2\Big\}\\ &= \Big[\tfrac{(\sigma/a)^2}{\sigma\sqrt{2/\pi}}\Big]^{\frac{1}{2}}\cdot\sqrt{\tfrac{i}{\tau}}\sum_{n=-\infty}^{\infty}\exp\Big\{-\frac{i\pi}{\tau}\Big(\frac{z}{\pi}+n\Big)^2\Big\}\\ &= \Big[\tfrac{(\sigma/a)^2}{\sigma\sqrt{2/\pi}}\Big]^{\frac{1}{2}}\cdot\vartheta(z,\tau)\end{aligned}$$

where

$$\begin{aligned}u(t)&\equiv[1+i(t/\tau)]\\ z&\equiv\tfrac{\pi}{2}\tfrac{x-x_0}{a}\\ \tau&\equiv i\pi(\sigma/a)^2u(t)\end{aligned}$$

are notations introduced to enable us to establish explicit contact with the theory of theta functions.[23] Returning with this information to (65) we have

$$g(x,t)=\Big[\tfrac{(\sigma/a)^2}{\sigma\sqrt{2/\pi}}\Big]^{\frac{1}{2}}\cdot\Big\{\vartheta\big(\tfrac{\pi}{2}\tfrac{x-x_0}{a},\tau\big)-\vartheta\big(\tfrac{\pi}{2}\tfrac{-x-x_0}{a},\tau\big)\Big\} \tag{67}$$

The expression on the right is manifestly odd in x, so vanishes persistently at the origin. The ϑ-literature[24] supplies $\vartheta_3(z+\pi,\tau)=\vartheta_3(z,\tau)$ from which it follows that $g(x+2a,t)=g(x,t)$, so it is also persistently the case that $g(a,t)=0$.

The Poisson summation formula supplies Jacobi's celebrated identity[25]

$$\vartheta(z,\tau)=A\cdot\vartheta\Big(\tfrac{z}{\tau},-\tfrac{1}{\tau}\Big)\quad:\quad A\equiv\sqrt{i/\tau}\,e^{z^2/i\pi\tau} \tag{68}$$

[23] See "2-dimensional 'particle-in-a-box' problems in quantum mechanics, Part I: Propagator & eigenfunctions by the method of images" (1997), page 4. What I call $\vartheta(z,\tau)$ is more properly written $\vartheta_3(z,\tau)$.

[24] See R. Bellman, *A Brief Introduction to Theta Functions* (1961), page 4.

[25] Concerning which Bellman remarks that "it is not easy to find another identity of comparable significance" and dedicates his elegant little book to support of that claim.

which we can use to obtain this variant of (67):

$$
\begin{aligned}
g(x,t) &= \Big[\tfrac{(\sigma/a)^2}{\sigma\sqrt{2/\pi}}\Big]^{\frac{1}{2}}\cdot\sum_{n=-\infty}^{\infty}\Big\{\quad\exp\Big[i\big(\pi\tau n^2-2n\tfrac{\pi}{2}\tfrac{+x-x_0}{a}\big)\Big]\\
&\qquad\qquad\qquad\qquad -\exp\Big[i\big(\pi\tau n^2-2n\tfrac{\pi}{2}\tfrac{-x-x_0}{a}\big)\Big]\Big\}\\
&= \Big[\tfrac{(\sigma/a)^2}{\sigma\sqrt{2/\pi}}\Big]^{\frac{1}{2}}\cdot\sum_{n=-\infty}^{\infty}e^{i\pi\tau n^2}\Big\{\quad\exp\big[-in\frac{\pi}{a}(x-x_0)\big]\\
&\qquad\qquad\qquad\qquad -\exp\big[+in\frac{\pi}{a}(x+x_0)\big]\Big\}\\
&= \Big[\tfrac{(\sigma/a)^2}{\sigma\sqrt{2/\pi}}\Big]^{\frac{1}{2}}\cdot\sum_{n=-\infty}^{\infty}e^{i\pi\tau n^2}(2/i)\sin n\frac{\pi}{a}x\cdot\exp\big[in\frac{\pi}{a}x_0\big]\\
&= \Big[\tfrac{(\sigma/a)^2}{\sigma\sqrt{2/\pi}}\Big]^{\frac{1}{2}}\cdot\sum_{n=1}^{\infty}e^{i\pi\tau n^2}4\sin n\frac{\pi}{a}x\cdot\sin n\frac{\pi}{a}x_0\\
&= \sum_{n=1}^{\infty}g_n(t)\Psi_n(x) &&(69.1)\\
g_n(t) &= \sqrt{2\sigma\sqrt{2\pi}}\,e^{-\pi^2(\sigma/a)^2[1+i(t/\tau)]n^2}\cdot\Psi_n(x_0) &&(69.2)
\end{aligned}
$$

It is gratifying to discover that $\psi(x,t)$ does in fact satisfy the time-dependent Schrödinger equation, as follows from the observations that

$$g_n(t) = g_n(0)\cdot e^{-\frac{i}{\hbar}\big\{\hbar\pi^2(\sigma/a)^2n^2/\tau\big\}t}$$

and that $\big\{\text{etc.}\big\} = h^2n^2/8ma^2 = \mathcal{E}n^2 = E_n$. Writing

$$g(x,t) = \sum_{n=1}^{\infty}c_ne^{-\frac{i}{\hbar}E_nt}\Psi_n(x)\Psi_n(x_0) \tag{70.1}$$

we notice that $g(x,t)$ *would become precisely the Green's function if it were the case that all the c's were unity* ... but in fact we have

$$c_n = \sqrt{2\sigma\sqrt{2\pi}}\,e^{-\pi^2(\sigma/a)^2n^2} \tag{70.2}$$

The expression on the right side of (67) provides what Born & Ludwig call the "particle representation" of $g(x,t)$, while (70) provides what they call the "wave representation." The latter renders transparent the properties discussed at the end of the preceding paragraph.

We install the clamps and, as a final step toward the construction (66) of our "boxed Gaussian wavepacket," concern ourselves with the evaluation of the normalization factor

$$\begin{aligned}
A(t) &\equiv \left[\int_0^a |G(x,t)|^2\,dx\right]^{-\frac{1}{2}}\\
&= \left[\sum_{n=1}^\infty |g_n(0)|^2\right]^{-\frac{1}{2}}\\
&= \left[\sum_{n=1}^\infty c_n^2\Psi_n^2(x_0)\right]^{-\frac{1}{2}}
\end{aligned}$$

which by $\Psi_n^2(x_0) = \frac{2}{a}\sin^2 n\frac{\pi}{a}x_0 = \frac{1}{a}\big[1-\cos 2n\frac{\pi}{a}x_0\big]$ becomes

$$= \left[2(\sigma/a)\sqrt{2\pi}\sum_{n=1}^\infty e^{-2\pi^2(\sigma/a)^2n^2}\cdot\big[1-\cos 2n\tfrac{\pi}{a}x_0\big]\right]^{-\frac{1}{2}}$$

and which, we notice, is in fact t-independent. Notice also that $\big[\text{etc.}\big]^{-\frac{1}{2}}$ vanishes (normalization becomes impossible) if x_0 is placed at either *end* of the box. Now write[26]

$$\begin{aligned}
\sum_{n=1}^\infty e^{-2\pi^2(\sigma/a)^2n^2}&\cdot\big[1-\cos 2n\tfrac{\pi}{a}x_0\big]\\
&= \tfrac{1}{2}\sum_{n=-\infty}^\infty e^{-2\pi^2\beta^2n^2}\big[1-e^{i(2\pi x_0/a)n}\big] &(71.1)\\
&\equiv \tfrac{1}{2}\sum_{-\infty}^\infty e^{i\pi\tau n^2} - \tfrac{1}{2}\sum_{-\infty}^\infty e^{i(\pi\tau n^2-2zn)}\\
&= \tfrac{1}{2}\Big\{\vartheta(0,\tau)-\vartheta(z,\tau)\Big\}\\
&= \tfrac{1}{2}\sqrt{i/\tau}\Big\{\vartheta\big(0,-\tfrac{1}{\tau}\big)-e^{z^2/i\pi\tau}\vartheta\big(\tfrac{z}{\tau},-\tfrac{1}{\tau}\big)\Big\}\\
&= \tfrac{1}{2}\sqrt{i/\tau}\sum_{-\infty}^\infty\left[\exp\Big\{-\frac{i\pi}{\tau}n^2\Big\}-\exp\Big\{-\frac{i\pi}{\tau}\Big(\frac{z}{\pi}+n\Big)^2\Big\}\right]\\
&= \tfrac{1}{2}\tfrac{1}{\beta\sqrt{2\pi}}\sum_{-\infty}^\infty\Big[\quad\exp\Big\{-\tfrac{1}{2\beta^2}n^2\Big\} &(71.2)\\
&\qquad\qquad -\exp\Big\{-\tfrac{1}{2\beta^2}\Big(\frac{x_0}{a}+n\Big)^2\Big\}\Big]
\end{aligned}$$

with $\beta\equiv\sigma/a$. We have physical interest in the situation $\sigma\ll a$ (*i.e.*, $\beta\ll 0$), but want ultimately to be in position to trace the quantum motion until

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

[26] The pattern of these manipulations was adapted from a source already cited.[23]

signals that the distribution has become nearly flat. When β is small the sum on the right side of (71.1) converges very slowly, but the sum (71.2) converges very, very (!!) rapidly: give the partial sums a name

$$f(\sqrt{2}\beta, N) \equiv \sum_{-N}^{+N} \Big[\exp\Big\{-\tfrac{1}{2\beta^2}n^2\Big\} - \exp\Big\{-\tfrac{1}{2\beta^2}(\xi+n)^2\Big\}\Big]$$

and observe, for example, that

$$\begin{aligned}
f(\tfrac{1}{101},0) &= 1 - e^{-\frac{1}{10201}\xi^2}\\
f(\tfrac{1}{101},1) &= f(\tfrac{1}{101},0) + 2e^{-\frac{1}{10201}} \;\;- e^{-\frac{1}{10201}(-1+\xi)^2} - e^{-\frac{1}{10201}(+1+\xi)^2}\\
f(\tfrac{1}{101},2) &= f(\tfrac{1}{101},1) + 2e^{-\frac{1}{10201}4} - e^{-\frac{1}{10201}(-2+\xi)^2} - e^{-\frac{1}{10201}(+2+\xi)^2}\\
f(\tfrac{1}{101},3) &= f(\tfrac{1}{101},2) + 2e^{-\frac{1}{10201}9} - e^{-\frac{1}{10201}(-3+\xi)^2} - e^{-\frac{1}{10201}(+3+\xi)^2}\\
&\;\;\vdots
\end{aligned}$$

The pretty implication is that we have (for all t, and all $0 < \xi \equiv x_0/a < 1$)

$$A = \Big[2\beta\sqrt{2\pi}\cdot\tfrac{1}{2\beta\sqrt{2\pi}}f(\sqrt{2}\beta,\infty)\Big]^{-\frac{1}{2}} \approx 1 \quad \text{for } \beta \ll 1$$

and that the approximation is extremely good.[27] signals that the distribution has become nearly flat. When β is small the sum on the right side of (71.1) converges very slowly, but the sum (71.2) converges very, very (!!) rapidly: give the partial sums a name

$$f(\sqrt{2}\beta, N) \equiv \sum_{-N}^{+N} \Big[\exp\Big\{-\tfrac{1}{2\beta^2}n^2\Big\} - \exp\Big\{-\tfrac{1}{2\beta^2}(\xi+n)^2\Big\}\Big]$$

[27] Continuing this discussion a bit, *Mathematica* supplies

$$\sum_{-\infty}^{\infty} e^{-n^2} = 1.772637$$

At the point $\sqrt{2}\beta = 1$ which serves to separate $\beta \ll 1$ from $\beta \gg 1$ we compute, as ξ ranges on the unit interval,

$$f(1,\infty) \approx f(1,6) = \begin{cases} 0.000000 & \text{at } \xi = 0.0 \text{ and } \xi = 1.0\\ 0.000035 & \text{at } \xi = 0.1 \text{ and } \xi = 0.9\\ 0.000126 & \text{at } \xi = 0.2 \text{ and } \xi = 0.8\\ 0.000240 & \text{at } \xi = 0.3 \text{ and } \xi = 0.7\\ 0.000331 & \text{at } \xi = 0.4 \text{ and } \xi = 0.6\\ 0.000366 & \text{at } \xi = 0.5 \end{cases}$$

which when plotted look roughly Gaussian. For $\beta \ll 1$ the ξ-dependence, though always present, is preceeded by many more 0's.

and observe, for example, that

$$\begin{aligned}
f(\tfrac{1}{101},0) &= 1 - e^{-\frac{1}{10201}\xi^2}\\
f(\tfrac{1}{101},1) &= f(\tfrac{1}{101},0) + 2\,e^{-\frac{1}{10201}} \;\; - e^{-\frac{1}{10201}(-1+\xi)^2} - e^{-\frac{1}{10201}(+1+\xi)^2}\\
f(\tfrac{1}{101},2) &= f(\tfrac{1}{101},1) + 2\,e^{-\frac{1}{10201}4} - e^{-\frac{1}{10201}(-2+\xi)^2} - e^{-\frac{1}{10201}(+2+\xi)^2}\\
f(\tfrac{1}{101},3) &= f(\tfrac{1}{101},2) + 2\,e^{-\frac{1}{10201}9} - e^{-\frac{1}{10201}(-3+\xi)^2} - e^{-\frac{1}{10201}(+3+\xi)^2}\\
&\;\;\vdots
\end{aligned}$$

The pretty implication is that we have (for all t, and all $0 < \xi \equiv x_0/a < 1$)

$$A = \Big[2\beta\sqrt{2\pi}\cdot \tfrac{1}{2\beta\sqrt{2\pi}} f(\sqrt{2}\beta,\infty)\Big]^{-\frac{1}{2}} \approx 1 \quad \text{for } \beta \ll 1 \tag{72}$$

and that the approximation is extremely good.[28]

Return now with (72) to (66/70) and obtain

$$\Psi(x,t) = B(x)\cdot\sum_{n=1}^{\infty} g_n(0)\, e^{-\frac{i}{\hbar}\mathcal{E}n^2 t}\,\Psi_n(x) \tag{73.1}$$

$$g_n(0) = \sqrt{4\beta\sqrt{2\pi}}e^{-\pi^2\beta^2 n^2}\sin n\pi\xi_0 \tag{73.2}$$

[28] Continuing this discussion a bit, *Mathematica* supplies

$$\sum_{-\infty}^{\infty} e^{-n^2} = 1.772637$$

At the point $\sqrt{2}\beta = 1$ which serves to separate $\beta \ll 1$ from $\beta \gg 1$ we compute, as ξ ranges on the unit interval,

$$f(1,\infty) \approx f(1,6) = \begin{cases} 0.000000 & \text{at } \xi = 0.0 \text{ and } \xi = 1.0\\ 0.000035 & \text{at } \xi = 0.1 \text{ and } \xi = 0.9\\ 0.000126 & \text{at } \xi = 0.2 \text{ and } \xi = 0.8\\ 0.000240 & \text{at } \xi = 0.3 \text{ and } \xi = 0.7\\ 0.000331 & \text{at } \xi = 0.4 \text{ and } \xi = 0.6\\ 0.000366 & \text{at } \xi = 0.5 \end{cases}$$

which when plotted look roughly Gaussian. For $\beta \ll 1$ the ξ-dependence is announced after a much longer string of 0's.

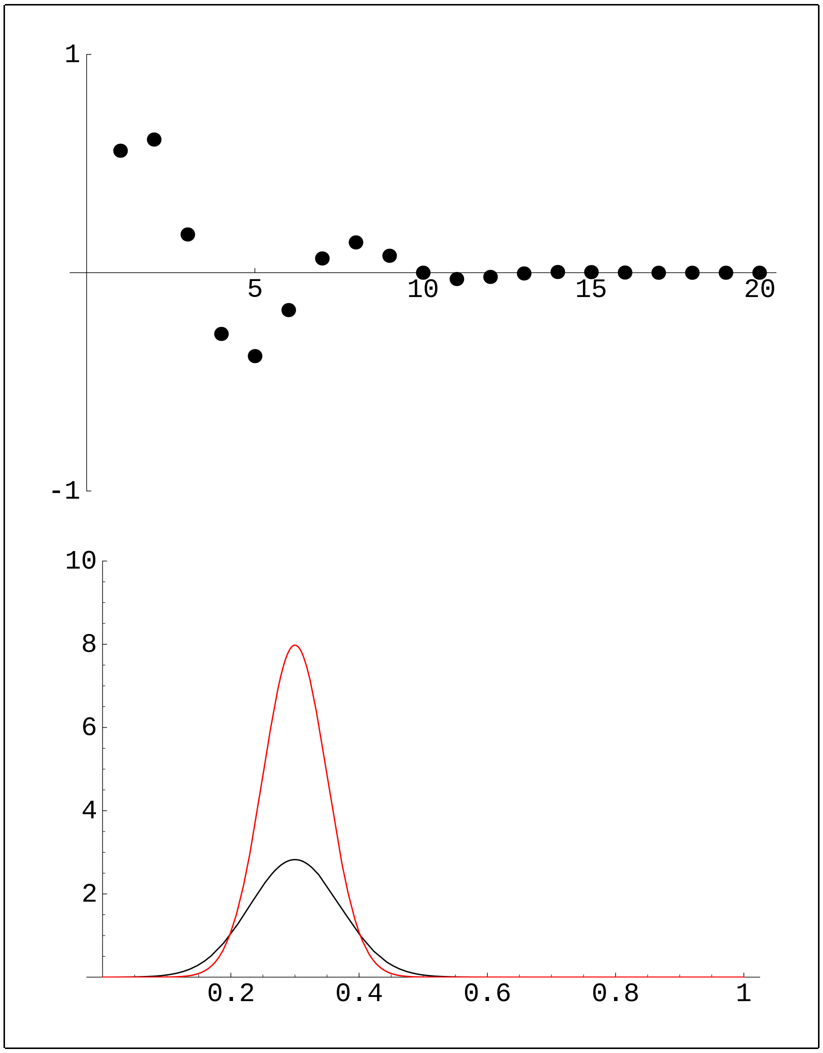

FIGURE 16: *Working from (73), I have set* $a = 1$, $\beta = \frac{1}{20}$ *and* $\xi_0 = \frac{3}{10}$. *From the coefficients* $g_n(0)$ *plotted in the top figure we see there is no reason to carry* n *beyond about* $20 = 1/\beta$. *The series (73.1)—thus truncated—produces the acceptably "Gaussian"* $\Psi(x, 0)$ *shown below in black;* $|\Psi(x, 0)|^2$ *is shown in red.*

Evidently we need keep only those coefficients $g_n(0)$ with

$$\begin{aligned} 1 \leqslant n &< \text{few times } n_{\text{characteristic}} \\ n_{\text{characteristic}} &\equiv \tfrac{1}{\pi\beta} = \tfrac{1}{\pi}\tfrac{\text{box size}}{\text{packet width}} \end{aligned} \tag{74}$$

where on the evidence of the preceding figure we might take "few" $\sim \pi$.

Phenomenologically we expect σ to grow , therefore β to grow

$$\beta \mapsto \beta(t) \equiv \sigma(t)/a = \beta\sqrt{1+(t/\tau)^2}$$

which by (74) entails extinction of the high harmonics: $n_{\text{characteristic}}$ to becomes ever smaller. Such a development is absurd, and points to a defect in (73): if we are to achieve the anticipated evolution toward flatness we must witness an

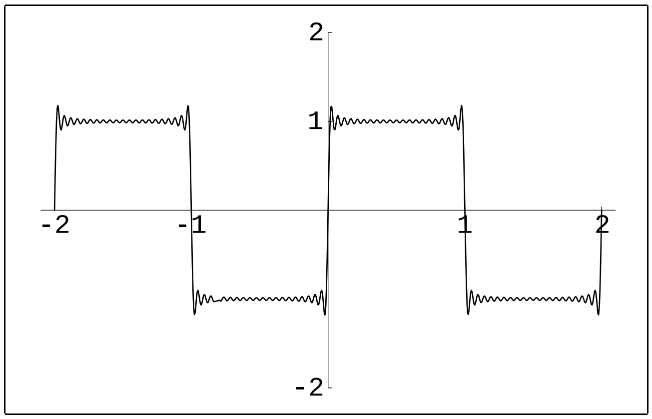

FIGURE 17: *Fourier construction of a square wave*

$$F(x) = \tfrac{4}{\pi}\sum_{k=0}^{\infty}\tfrac{1}{2k+1}\sin\big[(2k+1)\pi x\big]$$

necessarily brings high harmonics into play.

onset of high harmonics. The evidence of Figure 18 serves to associate this development with a loss of normalization as β becomes large.[29] And that can be attributed to our use of an approximation which at (72) was declared to be valid only for $\beta \ll 1$.

[29] On the other hand, normalization rapidly becomes good and stays good as β becomes smaller. Numerical integration supplies

$$\int_0^1 |\Psi(x,0)|^2\,dx = \begin{cases} 0.988891003438855 & \text{at } \beta = \frac{1}{10} \\ 0.999999984770040 & \text{at } \beta = \frac{1}{20} \\ 1.000000000001499 & \text{at } \beta = \frac{1}{30} \\ 0.999999999992603 & \text{at } \beta = \frac{1}{40} \\ 1.000000000000009 & \text{at } \beta = \frac{1}{50} \end{cases}$$

I have assigned a and ξ_0 the values described in the caption to Figure 18, and carried all sums to $n = 150$.

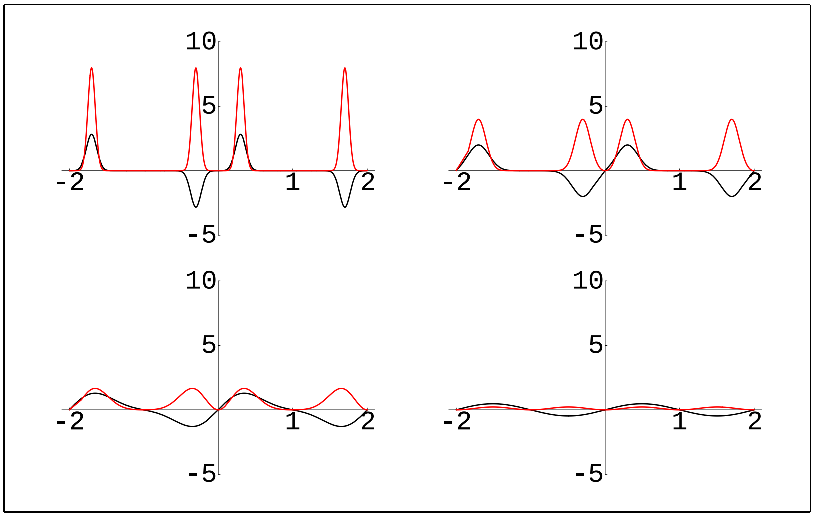

FIGURE 18: *Graphs of the unclamped variant of (73) at* $t = 0$ *with* $a = 1$ *and* $\xi_0 = \frac{3}{10}$. $\Psi(x, 0)$ *is shown in black,* $|\Psi(x, 0)|^2$ *in red. The values assigned successively to* β *are* $\frac{1}{20}, \frac{2}{20}, \frac{4}{20}$ *and* $\frac{8}{20}$. *Numerical integration supplies*

$$\int_0^1 |\Psi(x,0)|^2\,dx = \begin{cases} 1.000000 \\ 0.988891 \\ 0.673167 \\ 0.111571 \end{cases} \quad \textit{respectively}$$

Two related points: First, if we enter into *Mathematica* the definition

$$\Psi(x, t; a, \xi_0, \beta, F, m) \\ := \Big| \sum_{n=1}^{m} \sqrt{4\beta\sqrt{2\pi}}e^{-\pi^2\beta^2 n^2} \sin n\pi\xi_0\, e^{-i2\pi F n^2 t} \sin n\pi\frac{x}{a}\Big|^2 \tag{75}$$

then we can run *animations* based upon (73). Notice that the truncated expression on the right presents a constant term plus oscillating terms with a total of $\frac{1}{2}m(m-1)$ characteristic frequencies[30] (those are given by $F(n_1^2 - n_2^2)$

[30] Some of which may be coincident: the smallest examples are

$$\begin{aligned} 4^2 - 1^2 &= \ \ 8^2 - \ \ 7^2 = 15 = (4-1)(4+1) = (8-7)(8+7) \\ 5^2 - 2^2 &= 11^2 - 10^2 = 21 = (5-2)(5+2) = (11-10)(11+10) \\ 5^2 - 1^2 &= \ \ 7^2 - \ \ 5^2 = 24 = (5-1)(5+1) = (7-5)(7+5) \end{aligned}$$

but there are infinitely many others: see §2 in Daniel W. Wyss & Walter Wyss, "Coincident spectral lines for the hydrogen atom," Foundations of Physics **23**, 465, (1993). Here's a triple coincidence: $120 = 11^2 - 1^2 = 13^2 - 7^2 = 17^2 - 13^2$.

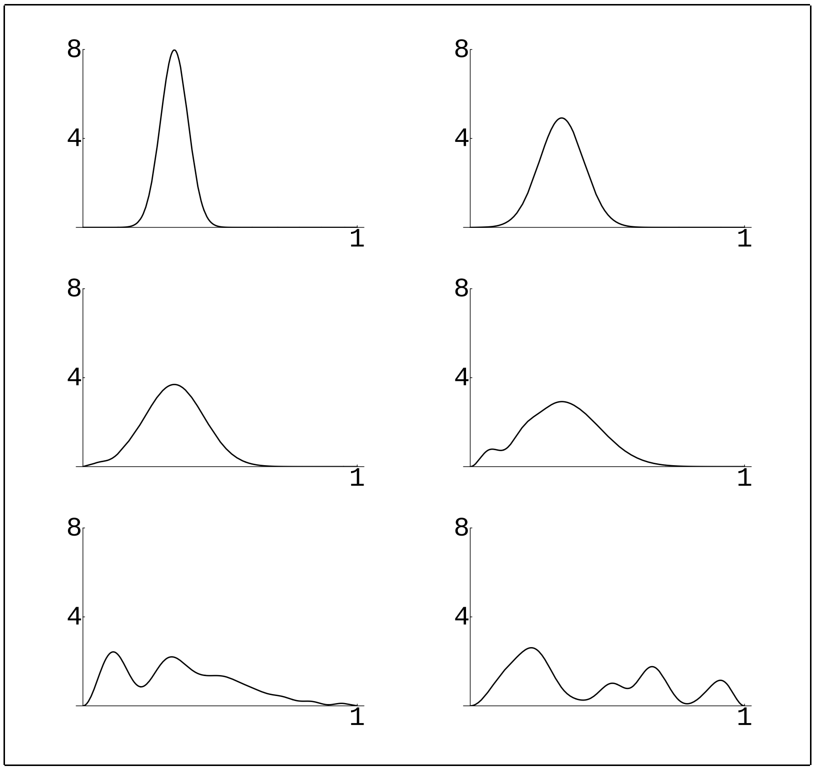

FIGURE 19: *Frames #0, 24, 36, 48, 84 & 168 of a filmstrip based upon (75). Control parameters are those described in a footnote.*[30]

and range from $3F$ to $(m^2-1)F$) and that it repeats itself when $Ft = 1$. No such multiply-periodic expression can describe unending dispersion, a tendency toward flatness. When we watch such animations[31] we observe that

- the Gaussian wavepacket does initially "diffuse," but . . .
- when the leading edge hits the wall it reflects back . . .
- setting up complicated oscillations . . .
- which are found by numerical integration to be norm-preserving.

What we do *not* see is the anticipated

approach to constancy, modulated by dying ripples

Animations do show the expected behavior *briefly* (*i.e.*, while dominated by high frequency components), but begin to "slosh" as soon as lower frequency

[31] When preparing those which can be found in an appendix I have again set $a = 1$, $\beta = \frac{1}{20}$ and $m = 20$. Additionally, I have set $F = 1$ and looked to the representative cases $\xi_0 = \frac{1}{3}$ else $\frac{1}{2}$. To achieve 12-frame resolution of the fastest oscillation I have set $t = k\frac{1}{4788}$ (because $12\cdot 399 = 4788$) and stepped k through the integers. The film then recycles at frame #4788.

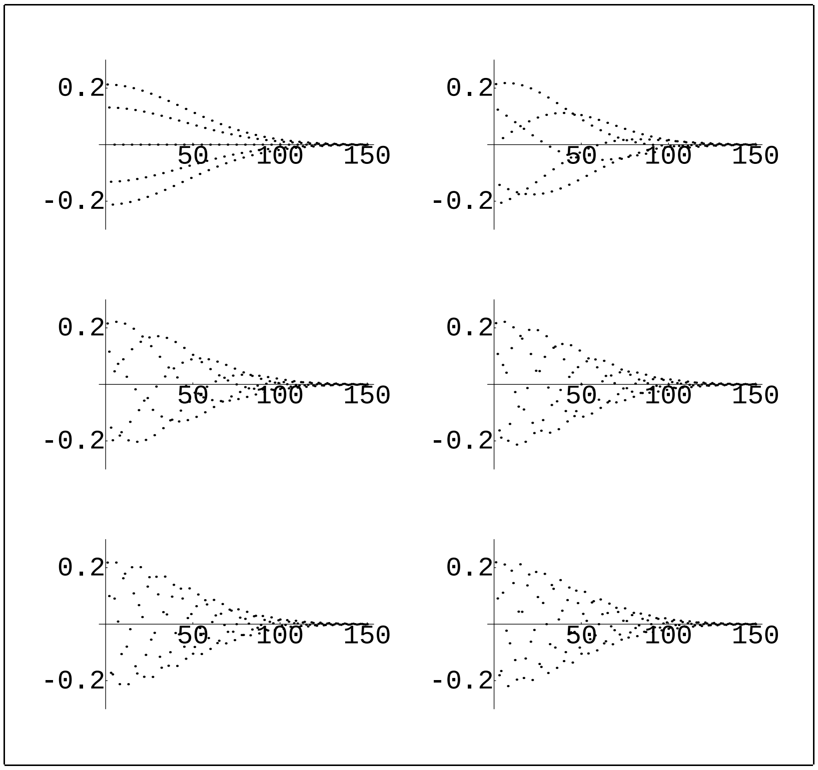

FIGURE 20: *Plots of Fourier coefficients* $g_n(0)$ *taken from (73.2) with* $\beta = \frac{1}{200}$*, showing rapid variation as* ξ_0 *ranges through the values (top left to bottom right)* $\frac{60}{150}, \frac{61}{150}, \frac{62}{150}, \frac{63}{150}, \frac{64}{150}, \frac{65}{150}$*. High frequencies would be needed to describe such variation if it were imagined to take place in time, even though* $\frac{d}{dt}\xi_0$ *itself is small.*

components have had time to express themselves. Selected frames from such a film are presented as Figure 19.

Second related point: It follows from (73.2) that slight/slow adjustments of ξ_0 (such as we might expect to associate with "launched" wavepackets) generate radical/rapid variations of the Fourier coefficients $g_n(0)$. The point is illustrated in Figure 20.

And a reminder: We on page 50 set $\wp = 0$. Were we to relax that assumption (*i.e.*, if we were to "launch" the wavepacket) then details would change, but our general conclusions would remain intact.

We have been working in working in what Born/Ludwig (see again page 51) call the "wave representation," which is commonly supposed to provide the representation of choice when t is large, but which we have found gives rise (at least in every finite approximation) to conclusions which are most reliable/ informative when t is small, and become *misleading* when t is large. It is in an attempt to wiggle around this problem that we revert to the "particle representation." As a preparatory step, let (64.1) be written

$$\psi(x,t) = \left[\tfrac{1}{\sigma[1+i(t/\tau)]\sqrt{2\pi}}\right]^{\frac{1}{2}} \exp\Big\{-\tfrac{1}{4}\frac{(x-x_0)^2}{\sigma^2(t)}[1-i(t/\tau)]\Big\}$$

where the simplifying assumption $\wp = 0$ has been retained. Then (65) acquires the explicit description

$$\begin{aligned} g(x,t) \equiv \left[\tfrac{1}{\sigma[1+i(t/\tau)]\sqrt{2\pi}}\right]^{\frac{1}{2}} \sum_{j=-\infty}^{\infty} \Big\{ &\quad\exp\Big\{-\tfrac{1}{4}\frac{(\ \ x+2ja-x_0)^2}{\sigma^2(t)}[1-i(t/\tau)]\Big\} \\ &-\exp\Big\{-\tfrac{1}{4}\frac{(-x+2ja-x_0)^2}{\sigma^2(t)}[1-i(t/\tau)]\Big\}\Big\} \end{aligned}$$

which in the familiar dimensionless variables (to the list of which we now add $\mathfrak{T} \equiv t/\tau$) becomes

$$\begin{aligned} g(x,t) \equiv \left[\tfrac{1}{\sigma[1+i\,\mathfrak{T}]\sqrt{2\pi}}\right]^{\frac{1}{2}} \sum_{j=-\infty}^{\infty} \Big\{ &\quad\exp\Big\{-\tfrac{1}{4}\frac{(\ \ \xi-\xi_0+2j)^2}{\beta^2(\mathfrak{T})}[1-i\,\mathfrak{T}]\Big\} \\ &-\exp\Big\{-\tfrac{1}{4}\frac{(-\xi-\xi_0+2j)^2}{\beta^2(\mathfrak{T})}[1-i\,\mathfrak{T}]\Big\}\Big\} \end{aligned}$$

which we will abbreviate

$$\begin{aligned} g(x,t) \equiv \left[\tfrac{1}{\sigma[1+i\,\mathfrak{T}]\sqrt{2\pi}}\right]^{\frac{1}{2}} \sum_{j=-\infty}^{\infty} \Big\{ &\quad\exp\Big\{-\frac{X_j^2}{\beta^2(\mathfrak{T})}[1-i\,\mathfrak{T}]\Big\} \\ &-\exp\Big\{-\frac{Y_j^2}{\beta^2(\mathfrak{T})}[1-i\,\mathfrak{T}]\Big\}\Big\} \end{aligned}$$

or again—still more compactly—

$$g(x,t) \equiv \left[\tfrac{1}{\sigma[1+i\,\mathfrak{T}]\sqrt{2\pi}}\right]^{\frac{1}{2}} \sum_{j=-\infty}^{\infty} \Big\{e^{-\mathfrak{X}_j}e^{i\,\mathfrak{X}_j\mathfrak{T}} - e^{-\mathfrak{Y}_j}e^{i\,\mathfrak{Y}_j\mathfrak{T}}\Big\}$$

Therefore

$$\begin{aligned} |g(x,t)|^2 &= \tfrac{1}{a}\cdot\tfrac{1}{\beta^2(\mathfrak{T})\sqrt{2\pi}} \sum_{j,k=-\infty}^{\infty} \Big\{e^{-\mathfrak{X}_j}e^{i\,\mathfrak{X}_j\mathfrak{T}} - e^{-\mathfrak{Y}_j}e^{i\,\mathfrak{Y}_j\mathfrak{T}}\Big\} \\ &\qquad\qquad\qquad\qquad\times\Big\{e^{-\mathfrak{X}_k}e^{-i\,\mathfrak{X}_k\mathfrak{T}} - e^{-\mathfrak{Y}_k}e^{-i\,\mathfrak{Y}_k\mathfrak{T}}\Big\} \\ &= \sum_j (\text{diagonal terms})_j + \sum_{j>k} (\text{off-diagonal terms})_{jk} \end{aligned}$$

Evidently (it is evident at any rate to *Mathematica*)

$$(\text{diagonal term})_j \sim e^{-2\mathcal{X}_j} - 2e^{-(\mathcal{X}_j+\mathcal{Y}_j)}\cos(\mathcal{Y}_j-\mathcal{X}_j)\mathcal{T} + e^{-2\mathcal{Y}_j}$$

while

$$\begin{aligned}(\text{off-diagonal term})_{jk} \sim 2\,e^{-(\mathcal{X}_j+\mathcal{Y}_j+\mathcal{X}_k+\mathcal{Y}_k)}\Big\{\;& e^{(\mathcal{Y}_j+\mathcal{Y}_k)}\cos(\mathcal{X}_j-\mathcal{X}_k)\mathcal{T}\\ &- e^{(\mathcal{X}_j+\mathcal{Y}_k)}\cos(\mathcal{Y}_j-\mathcal{X}_k)\mathcal{T}\\ &- e^{(\mathcal{Y}_j+\mathcal{X}_k)}\cos(\mathcal{X}_j-\mathcal{Y}_k)\mathcal{T}\\ &+ e^{(\mathcal{X}_j+\mathcal{X}_k)}\cos(\mathcal{Y}_j-\mathcal{Y}_k)\mathcal{T}\Big\}\end{aligned}$$

But

$$\begin{aligned}\mathcal{X}_j &\equiv \frac{(x-x_0+2ja)^2}{4\sigma^2}\frac{1}{1+(t/\tau)^2} \sim \frac{1}{\beta^2}j^2(\tau/t)^2\big[1-(\tau/t)^2+\cdots\big]\\ \mathcal{Y}_j &\equiv \frac{(-x-x_0+2ja)^2}{4\sigma^2}\frac{1}{1+(t/\tau)^2} \sim \text{ditto}\end{aligned}$$

shows that

- all such expressions die when $t \gg \tau$
- larger j entails slower death.

So asymptotically[32] we have

$$\begin{aligned}(\text{off-diagonal term})_{jk} &\sim 16\,e^{-(\mathcal{Z}_j+\mathcal{Z}_k)}\cos\Big\{(\mathcal{Z}_j-\mathcal{Z}_j)\mathcal{T}\Big\}\\ &= 16\,\exp\Big\{-\tfrac{1}{\beta^2}(j^2-k^2)(\tau/t)^2\Big\}\cos\Big\{\tfrac{1}{\beta^2}(j^2-k^2)(\tau/t)^1\Big\}\end{aligned}$$

⋮

Here I interrupt this work. It has become clear to me that the wavepacket-in-a-box problem is a tail that has begun to wag the dog. My intention had been to develop that topic elsewhere, and resume this work (i.e., to discuss the translation into phase space formalism) after those results were in hand. But by page 14 of "Wavepacket in a box" (January 2001) it had become clear to me that the result I sought—universal dispersion to flattness—is not to be had, is not in the physics until some new idea is imported into orthodox quantum mechanics.

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[32] Asymptotically $\mathcal{X}_j$ and $\mathcal{Y}_j$ differ insignificantly, so I adopt the generic notation $\mathcal{Z}_j$.