Concerning the resolution of a

Curious Normalization Problem

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Introduction. Shortly before Einstein's death in 1955, Einstein and Max Born (joined later by Pauli) selected the simple particle-in-a-box problem as a context within which to debate the merits of Einstein's contention that in certain fundamental respects the quantum theory of the time (which remains the quantum theory of this time) is defective/incomplete.[1] An elaborately detailed echo of that debate can be detected in a paper that Born wrote in collabortion with Wolfgang Ludwig in 1958.[2]

For at least fifty years it has been my intuitive conviction that—just as a heat pulse injected into a conductive rod leads ultimately to a quiescent uniform temperature distribution, and an initially non-uniform gas distribution in an enclosure will become ultimately uniform—the probability density of a boxed quantum wavepacket will in asymptotic time become quiescently flat,[3] this though it is unarguable quantum theory predicts periodic recurrence of the initial wavepacket. My problem has been to identify the "missing physical element" that accounts for—that when included would entail—my conjectured asymptotic flatness. Recently I have—with decoherence in mind—been led to use *Mathematica*-based techniques to revisit aspects of the Born-Ludwig argument, and have in the course of that experimental work exposed the "normalization problem" that it is my objective here to describe and resolve.

The problem stated. Let the normalized function $\psi(x,0)$ describe the initial state of a mass point m that moves freely on the unrestricted x-axis. At time t the unitary evolution of $\psi(x,0)$ has sent

$$\psi(x,0) \longrightarrow \psi(x,t) \quad \text{generated by} \quad \mathsf{H} = \tfrac{1}{2m}\,\mathsf{p}^2$$

[1] The debate was conducted by an exchange of letters, which are reproduced (with editorial comments by Born) as letters 105-116 on pages 205-228 of *The Born-Einstein Letters* (1971).

[2] "Zur Quantenmechanik des kräftefreien Teilchens," Zeitschrift für Physik **150**, 106 (1958). Notes from my own close study of that paper can be found on pages 9-32 of my *Feynman Formalism for Polygonal Domains* (1971-1976).

[3] I would expect experimentalists to be hard-pressed to produce evidence that contradicts that expectation.

which is what I will call a "Schrödinger function," meaning that that it is a solution of the (free particle) Schrödinger equation $-(\hbar^2/2m)\partial_{xx}\psi = i\hbar\,\partial_t\psi$. With Born & Ludwig we construct the (unnormalized) odd function

$$\varphi(x,t) = \psi(x,t) - \psi(-x,t)$$

and from $\varphi(x,t)$ we construct the (unnormalized) periodic Schrödinger function

$$\psi_{\text{boxed}}(x,t) = \sum_{n=-\infty}^{\infty} \varphi(x+2a,t) = \psi_{\text{boxed}}(x+2a,t)$$

From $\psi_{\text{boxed}}(x,t) = -\psi_{\text{boxed}}(-x,t)$ we obtain

$$\psi_{\text{boxed}}(0,t) = 0 \quad : \quad \text{all } t$$

while $\psi_{\text{boxed}}(a,t) = -\psi_{\text{boxed}}(-a,t) = -\psi_{\text{boxed}}(-a+2a,t) = -\psi_{\text{boxed}}(a,t)$ gives

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

So $\psi_{\text{boxed}}(x,t)$ is a Schrödinger function that satisfies the familiar "box boundary conditions."

Clearly, the (complex) values assumed by $\psi_{\text{boxed}}(x,t)$ on $[-a,0]$ are the negated mirror images of the values assumed on $[0,a]$, while the (real) values assumed by $P_{\text{boxed}}[x,t] \equiv |\psi_{\text{boxed}}(x,t)|^2$ on $[-a,0]$ are the non-negated mirror images of the values assumed on $[0,a]$. It follows that at any time t

$$\int_{na}^{(n+1)a} P_{\text{boxed}}(x,t) \ \text{ is the same for all } n$$

and therefore that $\psi_{\text{boxed}}(x,t)$ is not normalizable: $\int_{-\infty}^{\infty} P_{\text{boxed}}(x,t)\,dx = \infty$.[4]

Born & Ludwig appear to suggest that one could use functions of the form

$$\psi_{BL}(x,t) = \begin{cases} 0 & : \quad x < 0 \\ \psi_{\text{boxed}}(x,t) & : \quad 0 \leqslant x \leqslant a \\ 0 & : \quad a < x \end{cases}$$

to develop the quantum dynamics of a boxed particle. Such functions are, after all, Schrödinger functions, and do satisfy the required boundary conditiopns. Numerical computation reveals, however, that $\int_0^a P_{BL}(x,t)\,dx$ is *not constant*, but as the seed wavepacket $\psi(x,t)$ delocalizes (as I shown in an earlier note[5] it will in all cases inevitably do) steadily decreases in value:

$$\lim_{t\uparrow\infty} \int_0^a P_{BL}(x,t)\,dx = 0$$

My problem: how to account for that surprising fact.

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[4] In those respects $\psi_{\text{boxed}}(x,t)$ mimics properties of (say) $\sin(\pi x/a)$.

[5] "Free particle wavepackets" (March 2013).

The problem resolved. The dynamical evolution of the states of isolated quantum systems is unitary

$$|\psi)_0 \longrightarrow |\psi)_t = \mathbf{U}(t)|\psi)_0$$

from which norm-preservation follows as an immediate corrolary:

$$_t(\psi|\psi)_t = {}_0(\psi|\mathbf{U}^+(t)\mathbf{U}(t)|\psi)_0 = {}_0(\psi|\psi)_0 \quad : \quad \text{all t}$$

That elementary argument pertains with equal force to states that are presented as linear combinations of states

$$|\psi)_t = \sum_k c_k|\psi_k)_t \quad : \quad \sum_k |c_k|^2 = 1$$

and, more particuarly, to states that are presented as linear combinations of buzzing eigenstates. Looking to the latter situation in finer detail, if

$$\mathbf{H}|n) = E_n|n) \quad \text{and} \quad (m|n) = \delta_{mn}$$

then

$$|\psi)_t = \sum_k c_k e^{-i\omega_k t}|k) \quad \text{with} \quad \begin{cases} c_k = (k|\psi)_0 \\ \omega_k = E_k/\hbar \end{cases}$$

and

$$\begin{aligned} _t(\psi|\psi)_t &= \sum_{m,n} \bar{c}_m c_n e^{-i\omega_{mn}t}(m|n) \quad \text{where} \quad \omega_{mn} = \omega_m - \omega_n \\ &= \sum_k |c_k|^2 = 1 \quad \text{by orthonormality of the eigenstates} \end{aligned}$$

Passing to the x representation—the representation in which Born & Ludwig elected to work—we have

$$\begin{aligned} P(x,t) &= |\psi(x,t)|^2 \\ &= \sum_{m,n} \bar{c}_m c_n e^{-i\omega_{mn}t}\, \bar{\psi}_m(x)\psi_n(x) \\ &= \sum_k C_k^2 P_k(x) + 2\sum_{m>n} C_m C_n \cos(\omega_{mn}t - \gamma_{mn}) \cdot \psi_m(x)\psi_n(x) \end{aligned}$$

where we have written $c_k = Ce^{i\gamma_k}$, $\gamma_{mn} = \gamma_m - \gamma_n$ and assumed without loss of generality that the eigenfunctions $\psi_n(x) = (x|n)$ are real-valued. The preceding equation describes the temporal "sloshing" of the probability density associated with the evolving wavepacket $\psi(x,t)$, and it is again by orthonormality that it entails probability conservation (norm preservation):

$$\begin{aligned} \int_{\mathcal{R}} P(x,t)\,dx &= \sum_k C_k^2 \int_{\mathcal{R}} \psi_k(x)\psi_k(x)\,dx \\ &\qquad + 2\sum_{m>n} C_m C_n \cos(\omega_{mn}t - \gamma_{mn}) \cdot \int_{\mathcal{R}} \psi_m(x)\psi_n(x)\,dx \\ &= \sum_k C_k^2 + 2\sum_{m>n} C_m C_n \cos(\omega_{mn}t - \gamma_{mn}) \cdot \delta_{mn} \\ &= 1 \end{aligned}$$

where $\mathcal{R}$ refers to the "hermiticity domain"—the domain on which the hermiticity of H acquires it meaning, on which the eigenfunctions of H live, and with respect to which it becomes possible (by hermiticity) to write

$$(\psi_m, \psi_n) \equiv \int_{\mathcal{R}} \bar{\psi}_m(x)\psi_n(x)\,dx = \delta_{mn}$$

Born & Ludwig, however, take as their starting point an infinite set of free particle wavepackets $\{\psi(x + 2na, t), \psi(-x + 2na, t)\}$ for which the hermiticity domain $\mathcal{R}$ includes the entire real line $-\infty < x < +\infty$, and which are, moreover, not eigenfunctions of $\mathsf{H}_{\text{free}} = \frac{1}{2m}\mathsf{p}^2$. From those they excise fragments, which in terms of the box function

$$\text{box}(x, a) \equiv \theta(x) - \theta(x - a) = \begin{cases} 0 & : \quad x < 0 \\ 1 & : \quad 0 \leqslant x \leqslant a \\ 0 & : \quad a < x \end{cases}$$

can be described

$$\psi_n^{\pm}(x, t) = \text{box}(x, a) \cdot \psi(\pm x + 2na, t) \tag{1.1}$$

Those functions are indeed Schrödinger functions, in the sense that at points interior to the interval $[0, a]$ they do satisfy the local condition

$$-(\hbar^2/2m)\partial_{xx}\psi = i\hbar\,\partial_t\psi$$

But they are not eigenfunctions of H_{free}, and they are not orthonormal:

$$\int_0^a \bar{\psi}_m^{\text{eithersign}}(x, t)\,\psi_n^{\text{eithersign}}(x, t)\,dx \neq \delta_{mn}$$

We are therefore deprived of grounds on which to assert that the norm of

$$\psi_{BL}(x, t) = \sum_{n=-\infty}^{\infty} \big\{\psi_n^{+}(x, t) - \psi_n^{-}(x, t)\big\} \tag{1.2}$$

is time-independent.

Gaussian models. Gaussian wavepackets have tails that prevent their being fitted into boxes, except approximately (narrow Gaussians, centrally positioned, may have tails that are negligibly small at the box boundaries. . . but under free evolution they do not forever remain negligibly small). One way to circumvent this problem is to replace the initial Gaussian

$$\psi(x, 0) = \sqrt{\text{Gaussian}(x; \mu, \sigma)} \quad : \quad 0 \ll \mu \ll a$$

with the root $\sqrt{a^{-1}\beta(x/a; p, q)}$ of a beta distribution, since such distributions vanish automatically at $x = 0$ and $x = a$ and for some values of $\{p, q\}$ provide excellent approximations to normal distributions.[6] Born & Ludwig describe what on its face might appear to be an attractive alternative procedure: they would have us take as our "seed" the "launched Gaussian" wavepacket[7]

$$G(x,t) = \Big[\tfrac{1}{\sigma[1+i(t/\tau)]\sqrt{2\pi}}\Big]^{\frac{1}{2}} \cdot \exp\Big\{\tfrac{1}{1+i(t/\tau)}\Big[-\tfrac{x^2}{4\sigma^2} + i\tfrac{1}{\hbar}\big(mvx - \tfrac{1}{2}mv^2t\big)\Big]\Big\} \tag{2.1}$$

and work from (1). Defining

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

and using $\sigma[1+i(t/\tau)] = \sigma(t)e^{i\arctan(t/\tau)}$, $[1+i(t/\tau)]^{-1} = [1+(t/\tau)^2]^{-1}[1-i(t/\tau)]$ we find that (2.1) can be brought to the polar form

$$\begin{aligned} &= \Big[\tfrac{1}{\sigma(t)\sqrt{2\pi}}\Big]^{\frac{1}{2}} \exp\Big\{\tfrac{1}{1+(t/\tau)^2}\Big[-\tfrac{x^2}{4\sigma^2} + \tfrac{t/\tau}{\hbar}\big(mvx - \tfrac{1}{2}mv^2t\big)\Big]\Big\} \\ &\qquad \cdot \exp\Big\{i\Big(\tfrac{1}{1+(t/\tau)^2}\Big[(t/\tau)\tfrac{x^2}{4\sigma^2} + \tfrac{1}{\hbar}\big(mvx - \tfrac{1}{2}mv^2t\big)\Big] \\ &\qquad\qquad - \tfrac{1}{2}\arctan(t/\tau)\Big)\Big\} \qquad (2.2) \\ &= g(x,t)\cdot e^{if(x,t)} \end{aligned}$$

which is more useful for the purposes at hand. With *Mathematica*'s assistance we establish that for all v and b (which is intended to mark a point $b \in [0,a]$)

$$\big\{\tfrac{\hbar^2}{2m}\partial_{xx} + i\hbar\partial_t\big\}G(\pm x + b, t) = 0 \quad \text{iff} \quad \tau = 2m\sigma^2/\hbar$$

and that the latter condition permits $g(x,t)$ to be written

$$g(x,t) = \Big[\tfrac{1}{\sigma(t)\sqrt{2\pi}}\Big]^{\frac{1}{2}} \exp\Big\{-\tfrac{1}{4}\Big[\tfrac{x - v\,t}{\sigma(t)}\Big]^2\Big\}$$

We are led thus to the normally distributed probability density

$$P_G(x-b,t) = |G(x-b,t)|^2 = \tfrac{1}{\sigma(t)\sqrt{2\pi}}\cdot\exp\Big\{-\tfrac{1}{2}\Big[\tfrac{x-b-vt}{\sigma(t)}\Big]^2\Big\}$$

of which the

$$\text{mean} = b + vt$$

translates with uniform velocity v while the variance $\sigma^2(t)$ grows hyperbolically and the rate of growth of the uncertainty is asymptotically linear

$$\text{uncertainty} = \sigma(t) \approx t/\tau \text{ for } t \gg \tau$$

and inversely proportional to m.

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[6] This was the procedure adopted by Cimarron Wortham in his Reed College thesis, "Motion of launched wavepackets in the infinite square well," (2004).

[7] See my "Gaussian wavepackets" (1998), equation (22) on page 9.

Proceeding now in immitation of the line of argument introduced at (1), we construct

$$\psi_{BL}(x,t) = \text{box}(x,a)\cdot\sum_{n=-\infty}^{\infty} H_n(x,t)$$

where

$$\begin{aligned} H_n(x,t) &= G(c_n+x,t) - G(c_n-x,t) \quad \text{with} \quad c_n = 2na - b - vt \\ &= g(c_n+x,t)\cdot e^{if(c_n+x,t)} - g(c_n-x,t)\cdot e^{if(c_n-x,t)} \end{aligned}$$

In this notation we have

$$\begin{aligned} |\psi_{BL}(x,t)|^2 &= \text{box}(x,a)\cdot\sum_{m,n=-\infty}^{\infty}\bar{H}_m(x,t)H_n(x,t) \\ &= \text{box}(x,a)\cdot\Big\{\sum_k \bar{H}_k H_k + \sum_{m>n}\big[\bar{H}_m H_n + \bar{H}_n H_m\big]\Big\} \end{aligned}$$

$$\text{positive real} = \textstyle\sum \text{reals}$$

The function $\psi_{BL}(x,t)$ satisfies the free particle Schrödinger equation and the box boundary conditions $\psi_{BL}(0,t) = \psi_{BL}(a,t) = 0$ but is—as will emerge—not normalized; the "normalization constant" is in fact t-dependent

$$N(t) = \int_0^a |\psi_{BL}(x,t)|^2\,dx \neq 1$$

On the other hand, the normalized function

$$\Psi_{BL}(x,t) = N^{-\frac{1}{2}}(t)\cdot\psi_{BL}(x,t)$$

satisfies the box boundary conditions but not the Schrödinger equation:

$$\begin{aligned} \big\{(\hbar^2/2m)\,\partial_{xx} + i\hbar\partial_t\big\}\Psi_{BL}(x,t) &= \tfrac{1}{2}i\hbar\,\Psi_{BL}(x,t)\cdot\partial_t\log N(t) \\ &\neq 0 \end{aligned}$$

This (within the Gaussian context in which we are working) marks the point at which the Born-Ludwig scheme fails.

Looking now to the finer details, we (after some *Mathematica*-assisted computation) have

$$\begin{aligned} \bar{H}_m H_n + \bar{H}_n H_m = &\quad 2\,g(c_m+x)g(c_n+x)\cos\big[f(c_m+x) - f(c_n+x)\big] \\ &- 2\,g(c_m+x)g(c_n-x)\cos\big[f(c_m+x) - f(c_n-x)\big] \\ &- 2\,g(c_m-x)g(c_n+x)\cos\big[f(c_m-x) - f(c_n+x)\big] \\ &+ 2\,g(c_m-x)g(c_n-x)\cos\big[f(c_m-x) - f(c_n-x)\big] \end{aligned}$$

whence

$$\begin{aligned} \bar{H}_k H_k = g^2(c_k+x) + g^2(c_k-x) \\ - 2\,g(c_k+x)g(c_k-x)\cos\big[f(c_k+x - f(c_k-x))\big] \end{aligned}$$

where I have surpressed all t arguments. The cosine factors (which are bounded by ± 1) are multiplied here by factors of the form $g(x-\alpha)\,g(x-\beta)$ which (by a completion of squares argument) can be developed[8]

$$\begin{aligned} g(x-\alpha)\,g(x-\beta) &= \big[\tfrac{1}{(\sigma\sqrt{2})\cdot\sqrt{2\pi}}\big]^{\frac{1}{2}} \exp\Big\{-\tfrac{1}{4}\big[\tfrac{\alpha-\beta}{\sqrt{2}\,\sigma}\big]^2\Big\}\cdot \\ &\qquad \big[\tfrac{1}{(\sigma/\sqrt{2})\cdot\sqrt{2\pi}}\big]^{\frac{1}{2}} \exp\Big\{-\tfrac{1}{4}\big[\tfrac{1}{\sigma/\sqrt{2}}\big(x-\tfrac{\alpha-\beta}{2}\big)\big]^2\Big\} \\ &= \sqrt{G\big(\alpha-\beta;\sigma\sqrt{2}\,\big)}\cdot\sqrt{G\big(x-\tfrac{\alpha+\beta}{2};\sigma/\sqrt{2}\,\big)} \end{aligned}$$

where again, the t-dependence of α, β and σ has been surpressed.

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[8] This is a special case of the general Gaussian product formula (see my *Thermal Physics* (2003), Chapter 3, pages 111-114)

$$\begin{aligned} &G(x-m';\sigma')\cdot G(x-m'';\sigma'') \\ &\qquad = G\big(m'-m'';\sqrt{\sigma'^2+\sigma''^2}\,\big)\cdot G(x-m;\sigma) \end{aligned}$$

where now $G(x-m;\sigma) = [\sigma\sqrt{2\pi}]^{-1/2}\exp\big\{-\frac{1}{2}\big[\frac{x-m}{\sigma}\big]^2\big\}$ is normal, and

$$\begin{aligned} m &= \frac{m'\sigma''^2+m''\sigma'^2}{\sigma'^2+\sigma''^2} \\ \sigma &= \sqrt{\frac{\sigma'^2\sigma''^2}{\sigma'^2+\sigma''^2}} \iff \frac{1}{\sigma^2} = \frac{1}{\sigma'^2}+\frac{1}{\sigma''^2} \end{aligned}$$