Aspects of a

Quantum Asymptotics "Problem"

Nicholas Wheeler
May 2013

Introduction. Let the initial gas density $\rho(x, y, z, 0)$ within an isolated enclosure be nonuniform. One expects uniformity (in a sufficiently course-grained sense) to be quickly established, by time-reversible microkinetic processes that can be said to be grossly "diffusive;" significant departures from uniformity are recognized to be inevitable, but are expected to occur with vanishing probability. Similarly...

Let $u(x, y, z, 0)$ describe the initially nonuniform temperature distribution within a thermally isolated lump of thermally conductive material. We expect $u(x, y, z, t)$ to become uniform in the limit $t \to \infty$. Similarly...

Let a classical particle be launched with velocity in the neighborhood $\Delta\boldsymbol{v}$ of $\boldsymbol{v}$ from a point in the neighborhood $\Delta\boldsymbol{x}$ of a point $\boldsymbol{x}$ interior to an enclosure $\mathcal{R}$ with perfectly reflecting walls. With a good deal less confidence we might naively expect it to become—after a sufficiently long time—equally likely that the particle will be found in any neighborhood $\Delta\boldsymbol{x} \in \mathcal{R}$.[1]

Now let $\psi(\boldsymbol{x}, 0)$ describe an initial wavepacket on $\mathcal{R}$, and $P(\boldsymbol{x}, 0)$ the associated probability density. I am informed only by my intuition that information concerning the initial location of the particle must ultimately evaporate, that $P(\boldsymbol{x}, t)$ must become asymptotically flat. My "problem"—note the quotation marks in my title—is that standard quantum theory says no such thing, though by the simplest of arguments[2] it says precisely that for unconfined free particles (boundary $\partial\mathcal{R}$ of $\mathcal{R}$ pushed to infinity).

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[1] This is the upshot of a classical version of the *ergodic hypothesis*. But consult the web re "scars" in papers that treat the relationship of classical to quantum chaos. One such paper is Peter Sarnak, "Arithmetic quantum chaos." See also http://en.wikipedia.org/wiki/Dynamical_Billiards. The literature has has, since about 1980, become vast.

[2] See "A note concerning the evolution of free particle wavepackets," (March 2013.

The issues just touched upon are most easily—if at some hazard—addressed in the one-dimensional case, which is my intention in the present essay. The exercise will afford me opportunities—indeed, will require—that I look more deeply into some familiar topics than is customary, and that I explore some unfamiliar byways. Most notably, the one-dimensional particle-in-a-box (infinite square well) problem is universally considered to be so elementary that the authors of quantum texts[3] often treat it before they have marshaled the resources required to explore its deeper reaches.

A discrete model of asymptotic equilibration. A token moves on an n-point lattice $x_k = \{1, 2, \ldots, n\}$, subject to these statistical rules:

$$\begin{aligned}\text{probability of standing in place} &= r\\ \text{probability of step to right/left adjacent node} &= \tfrac{1}{2}(1-r)\end{aligned}$$

Those probabilities sum to unity: the token is always obligated to do *something*. At the end nodes x_1 and x_n the probability of standing in place is

$$1 - \tfrac{1}{2}(1-r) = \tfrac{1}{2}(1+r)$$

The vector defined

$$\boldsymbol{p}(k) = \begin{pmatrix} p_1(k)\\ p_2(k)\\ \vdots\\ p_j(k)\\ \vdots\\ p_{n-1}(k)\\ p_n(k)\end{pmatrix} \;:\; p_j(k) = \begin{cases}\text{probability of finding the token}\\ \text{on the } j^{\text{th}} \text{ node after } k \text{ steps}\end{cases}$$

provides an instance of a "stochastic vector" (all elements non-negative, and sum to unity). The transition $\boldsymbol{p}(k) \to \boldsymbol{p}(k+1) = \mathbb{T}\cdot\boldsymbol{p}(k)$ is a Markov process, accomplished by the transition matrix

$$\mathbb{T} = \begin{pmatrix} \frac{1}{2}(1+r) & \frac{1}{2}(1-r) & 0 & 0 & \cdots & 0 & 0\\ \frac{1}{2}(1-r) & r & \frac{1}{2}(1-r) & 0 & \cdots & 0 & 0\\ 0 & \frac{1}{2}(1-r) & r & \frac{1}{2}(1-r) & \cdots & 0 & 0\\ 0 & 0 & \frac{1}{2}(1-r) & r & \cdots & 0 & 0\\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots\\ 0 & 0 & 0 & 0 & \cdots & r & \frac{1}{2}(1-r)\\ 0 & 0 & 0 & 0 & \cdots & \frac{1}{2}(1-r) & \frac{1}{2}(1+r)\end{pmatrix}$$

the elements of which are interpretable as "transition probabilities" provided

[3] See, for example, David Griffiths, *Introduction to Quantum Mechanics* (2^{nd} edition, 2005), §2.2, pages 30-40.

$0 \leqslant r \leqslant 1$. The real symmetry of $\mathbb{T}$ by itself implies the reality of the spectrum and orthogonality of the spectrum, but the specialized structure of $\mathbb{T}$ permits those general statements to be sharpened:[4]

- The leading eigenvalue of $\mathbb{T}$ is always (*i.e.*, for all $r \in [0, 1]$) unity.
- The eigenvalues are distinct (except when $r = 0$), and bounded by ± 1.
- All elements of the leading eigenvector are identical; division by their sum produces (in all cases: $r \neq 0$) the "flat" stochastic vector

$$\boldsymbol{e}_1 = \begin{pmatrix} 1/n \\ 1/n \\ \vdots \\ 1/n \end{pmatrix}$$

- All other eigenvectors $\{\boldsymbol{e}_2, \boldsymbol{e}_3, \ldots, \boldsymbol{e}_n\}$ possess elements (of both signs) that sum to zero, so do not possess the structure of stochastic vectors.

Given $\boldsymbol{p}_0 \equiv \boldsymbol{p}(0)$—which might, in particular, have 0-elements except for a solitary 1, signaling that we know the initial location of the token—we have

$$\boldsymbol{p}(k) = \mathbb{T}^k \boldsymbol{p}_0$$

In spectral representation

$$\mathbb{T} = \mathbb{P}_1 + \lambda_2 \mathbb{P}_2 + \lambda_3 \mathbb{P}_3 + \cdots + \lambda_n \mathbb{P}_n$$

where $\mathbb{P}_i$ projects onto the i^{th} eigenspace. From the orthonormality of those matrices ($\mathbb{P}_i \mathbb{P}_j = \delta_{ij} \mathbb{P}_j$) it follows that

$$\mathbb{T}^k = \mathbb{P}_1 + \lambda_2^k \mathbb{P}_2 + \lambda_3^k \mathbb{P}_3 + \cdots + \lambda_n^k \mathbb{P}_n$$

which by $-1 < \lambda_i < +1 : i = 2, 3, \ldots, n$ gives

$$\lim_{k \to \infty} \mathbb{T}^k = \mathbb{P}_1 = \begin{pmatrix} 1/n & 1/n & \cdots & 1/n \\ 1/n & 1/n & \cdots & 1/n \\ \vdots & \vdots & \ddots & \vdots \\ 1/n & 1/n & \cdots & 1/n \end{pmatrix}$$

So we have

$$\lim_{k \to \infty} \boldsymbol{p}(k) = \lim_{k \to \infty} \mathbb{T}^k \boldsymbol{p}_0 = \mathbb{P}_1 \boldsymbol{p}_0 = \boldsymbol{e}_1 \quad : \quad \text{every stochastic } \boldsymbol{p}_0$$

which establishes the sense in which the model "equilibrates."

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[4] The following statements are presented without proof. *Mathematica*-based numerical experimentation will convince readers of their validity.

But we touch here upon a subtlety. It is clear that $\mathbb{P}_1$ is singular, so it is not possible to write $\boldsymbol{p}_0 = \mathbb{P}_1^{-1}\boldsymbol{e}_1$ and thus to proceed from the asymptotic state back to the initial state from which it sprang... which makes sense, since all initial states give rise to the *same* asymptotic state. On the other hand,

- $\mathbb{T}$ is non-singular, except when n is even and $r = 0$

so in non-singular cases it *is* possible to recover the initial state $\boldsymbol{p}_0$ from the evolved state $\boldsymbol{p}(k)$, however finitely large k may be: $\boldsymbol{p}_0 = \mathbb{T}^{-k}\boldsymbol{p}(k)$.

The model serves therefore to illustrate *how irreversibility arises from reversible processes*, and thus to address an ancient conundrum. In the present instance, *information is lost, but only in the asymptotic limit*.

We have learned to associate high information with low entropy, and the loss of information with entropy gain, but the entropy measure—as a single function

$$S(p_1, p_2, p_3, \ldots, p_n) = -\sum_{i=1}^{n} p_i \log p_i$$

of many arguments—is necessarily ambiguous, and can, as I will show in a moment, be profoundly misleading. Concerning the source of that ambiguity: suppose we know the token to sit momentarily on (say) node x_2; then $S(0, 1, 0, \ldots, 0) = 0$. From the news that $S = 0$ we can infer that the token is known to sit on *some* particular node, but cannot say which. Look next to

$$S(k) \equiv S(\mathbb{T}^k \boldsymbol{p}_0) = -\sum_{i=1}^{n} p_i(k) \log p_i(k)$$

Numerical experiments (with $\boldsymbol{p}_0$ selected randomly) demonstrate that

$$S(0) \xrightarrow[\text{monotonic growth}]{} S(\infty) = -\log(\tfrac{1}{n}) = \log n$$

where the monotonic entropy increase surprising the demonstrated fact that the processes is reversible: no initial information is lost, the initial state is precisely recoverable (compromised only by the finite precision of the computation) until one “actually arrives” at $k = \infty$.

I look finally to the continuous limit of the discrete process described above. We proceed from the observation that $\boldsymbol{p}(k+1) - \boldsymbol{p}(k)$ can be written

$$\begin{aligned}
p_1(k+1) - p_1(k) &= \tfrac{1}{2}(1-r)\cdot[p_2(k) - p_1(k)]\\
p_i(k+1) - p_i(k) &= \tfrac{1}{2}(1-r)\cdot[p_{i+1}(k) - 2p_i(k) + p_{i-1}(k)]\\
p_n(k+1) - p_n(k) &= -\tfrac{1}{2}(1-r)\cdot[p_n(k) - p_{n-1}(k)]
\end{aligned}$$

with $i = 2, 3, \ldots, n-1$. Let us now agree that if the k^{th} hop takes place at time t then the $(k+1)^{\text{th}}$ occurs at time $t + \tau$; that if the i^{th} node lives at x then the $(i+1)^{\text{th}}$ lives at $x + \xi$; that node #1 lives at $x = 0$ while node #n lives at $x = n\xi = a$. With those (merely notational) adjustments the preceding equations become

$$\begin{aligned}
p(0,t+\tau)-p(0,t) &= \tfrac{1}{2}(1-r)\cdot[p(0+\xi,t)-p(0,t)]\\
p(x,t+\tau)-p(x,t) &= \tfrac{1}{2}(1-r)\cdot[p(x+\xi,t)-2p(x,t)+p(x-\xi,t)]\\
p(a,t+\tau)-p(a,t) &= -\tfrac{1}{2}(1-r)\cdot[p(a,t)-p(a-\xi,t)]
\end{aligned}$$

which can be written

$$\begin{aligned}
\frac{p(0,t+\tau)-p(0,t)}{\tau} &= \tfrac{1}{2}(1-r)(\xi/\tau)\cdot\frac{p(\xi,t)-p(0,t)}{\xi}\\
\frac{p(x,t+\tau)-p(x,t)}{\tau} &= \tfrac{1}{2}(1-r)(\xi^2/\tau)\cdot\frac{p(x+\xi,t)-2p(x,t)+p(x-\xi,t)}{\xi^2}\\
\frac{p(a,t+\tau)-p(a,t)}{\tau} &= -\tfrac{1}{2}(1-r)(\xi/\tau)\cdot\frac{p(a,t)-p(a-\xi,t)}{\xi}
\end{aligned}$$

Let τ and $\xi\downarrow 0$ in such a way as to preserve the finite value of the ratio $R\equiv\xi^2/\tau$, and $n\uparrow\infty$ in such a way as to preserve the finite value of $a=n\xi$. The second of the preceding equations then becomes

$$\partial_t p(x,t)=\tfrac{1}{2}(1-r)R\cdot\partial_{xx}p(x,t) \tag{1}$$

while the first and third of those equations become

$$\left.\begin{aligned}
\partial_t p(0,t) &= +\infty\cdot p_x(0,t)\\
\partial_t p(a,t) &= -\infty\cdot p_x(a,t)
\end{aligned}\right\}\quad:\quad\text{here } p_x(x,t)\equiv\partial_x p(x,t)$$

which are absurd unless we set

$$\partial_x p(x,t)=0 \quad:\quad x=0 \text{ and } x=a \quad (\text{all } t) \tag{2}$$

in which case the first and third equations become simply indeterminate.

Equation (1) can be written

$$\partial_{xx}p(x,t)=D\,\partial_t p(x,t) \tag{3}$$

which is the one-dimensional *diffusion equation*, otherwise known as the *heat equation*. On the basis of our experience with its discrete analog we expect spatially bounded solutions of (3) to become asymptotically flat; we expect the scent of perfume in a room to become uniform.[5]

Thermal equilibration of a heated rod. Let $u(x,t)$ describe the temperature distribution (at time t) along a thin rod of unit length, and let $q(x,t)$ describe the linear thermal energy density. Assuming the rod to have constant cross

[5] The image sprang to mind when—moments ago—I passed Lois Hobbs in a hallway of the physics building.

section, and to be materially homogeneous, one expects to have

$$q(x,t) = Ku(x,t)$$

where K is a constant implicit in the cross sectional geometry of the rod and the intrinsic specific heat of the material from which it has been fabricated. One expects also to have

$$\text{energy flux} = -C\partial_x u(x,t)$$

and—in the absence of radiative/conductive loss mechanisms—to have the continuity equation

$$\partial_x(\text{energy flux}) + \partial_t q(x,t) = 0$$

as an expression of local energy conservation. We are led thus to the heat equation $-C\partial_{xx}u + K\partial_t u = 0$, which is an instance of (3) with $D = K/C$ and in a suitably rescaled time becomes

$$\partial_{xx}u = \partial_t u \tag{4.1}$$

If, as we insist, thermal energy is neither injected nor extracted at the boundary points then we must impose upon solutions of (4.1) the boundary conditions

$$\partial_x u(x,t) = 0 \quad : \quad x = 0 \text{ and } x = 1 \quad (\text{all } t) \tag{4.2}$$

Separation of variables supplies

$$u(x,t) = \phi(x)\cdot e^{-\lambda t} \quad \text{with} \quad \partial_{xx}\phi(x) = -\lambda\phi(x)$$

and to achieve compliance with (4.2) we are obliged to set

$$\phi(x) \sim \cos(\pi n x),\ \ \lambda_n = \pi^2 n^2 \quad : \quad n = 0, 1, 2, \ldots$$

We are led thus to introduce functions

$$\phi_n(x) = \begin{cases} 1 & : \quad n = 0 \\ \sqrt{2}\cos(\pi n x) & : \quad n = 1, 2, 3, \ldots \end{cases} \tag{5}$$

which comprise an orthonormal basis in $\mathcal{H}^\star$. Arbitrary elements of $\mathcal{H}^\star$ can be developed

$$u(x,t) = \sum_{n=0}^{\infty} \phi_n(x)\, e^{-\pi^2 n^2 t} c_n \quad \text{with} \quad c_n = \int_0^1 \phi_n(y)u(y,0)\,dy \tag{6}$$

$$= \int_0^1 \mathcal{G}(x,y,t)u(y,0)\,dy \tag{7.1}$$

$$\mathcal{G}(x,y,t) = \sum_{n=0}^{\infty} \phi_n(x)\, e^{-\pi^2 n^2 t}\phi_n(y) \tag{7.2}$$

From (6) it follows that in all cases $u(x,t)$ becomes *asymptotically flat*:

$$\lim_{t\to\infty} u(x,t) = c_0 = \int_0^1 u(x,t)\,dx = \text{mean temperature}$$
$$= \frac{\text{total energy}}{K}$$

Which, of course, conforms to intuition and experience (though we have relatively little direct experience with hot bodies for which radiative/conductive cooling is not an option): initial temperature irregularities diffuse away, the temperature becomes uniform and static.

The **theory of Jacobi theta functions**[6] permits one to construct some elegant —and very informative—alternative descriptions of the thermal Green function. Working from (7.2), we have

$$\begin{aligned}\mathcal{G}(x,y,t) &= 1 + 2\sum_{n=1}^{\infty} e^{-\pi^2 n^2 t}\cos(\pi n x)\cos(\pi n y)\\ &= 1 + \sum_{n=1}^{\infty} e^{-\pi^2 n^2 t}\big\{\cos[\pi n(x+y)] + \cos[\pi n(x-y)]\big\}\end{aligned}$$

The Jacobi function $\vartheta_3(v,\tau)$ is defined

$$\vartheta_3(v,\tau) = \sum_{n=-\infty}^{\infty} e^{i\pi[\tau n^2 - 2vn]} = 1 + 2\sum_{k=1}^{\infty} e^{i\pi\tau k^2}\cos(2\pi k v) \tag{8}$$

and permits one to write

$$\mathcal{G}(x,y,t) = \tfrac{1}{2}\vartheta_3\Big[\frac{x+y}{2}, i\pi t\Big] + \tfrac{1}{2}\vartheta_3\Big[\frac{x-y}{2}, i\pi t\Big] \tag{9}$$

Central to the theory of ϑ-functions are variants of the wonderful identity

$$\vartheta_3(v,\tau) = A\cdot\vartheta_3\big(\tfrac{v}{\tau}, -\tfrac{1}{\tau}\big) \quad \text{with} \quad A = \sqrt{i/\tau}\,e^{-i\pi v^2/\tau} \tag{10}$$

concerning which Bellman[8] remarks that it

> *has amazing ramifications in the fields of algebra, number theory, geometry, and other parts of mathematics* [*also physics*!]. *In fact, it is not easy to find another identity of comparable significance.*

and devotes much of his slim classic to demonstrating the force of that claim. Remarkably, τ—which lives "upstairs" on the left side of (10)—lives "downstairs" on the right side; the "Jacobi transformation" (10) is evidently akin to the various "inversive" transformations that are encountered elsewhere in geometry, analysis and potential theory (think Möbius, Appell, Kelvin). Returning with (10) to the definion (8), we have

$$\begin{aligned}\vartheta_3(v,\tau) &= \sum_{n=-\infty}^{\infty} e^{i\pi[\tau n^2 - 2vn]}\\ &= \sqrt{i/\tau}\,e^{-i\pi v^2/\tau}\cdot e^{-i\pi[n^2+2vn]/\tau}\\ &\Downarrow\\ \vartheta_3(v,i\pi t) &= \frac{1}{\sqrt{\pi t}}\sum_{n=-\infty}^{\infty} e^{-(v+n)^2/t}\end{aligned}$$

[6] See, for example, Richard Bellman, *A Brief Introduction to Theta Functions* (1961); Whittaker & Watson, *A Course of Modern Analysis* (4^{th} edition 1927, reprinted 2002), Chapter 21, pages 462-490; Magnus & Oberhettinger, *Formulas & Theorems for the Functions of Mathematical Physics* (1954), pages 98-100; Abramowitz & Stegun, *Handbook of Mathematical Functions* (1964), Chapter 16, pages 576-579. It was Jacobi's study of the theory of elliptic functions that led him to develop the foundations of this subject (1829), some aspects of which had been anticipated by Fourier.

which we use to cast (9) into the form

$$\mathcal{G}(x,y,t)=\frac{1}{\sqrt{4\pi t}}\sum_{n=-\infty}^{\infty}\Big\{\exp\Big[-\frac{(y+x+2n)^2}{4t}\Big]+\exp\Big[-\frac{(y-x+2n)^2}{4t}\Big]\Big\} \tag{11}$$

This description of the thermal Green function was (so far as I am aware) first obtained by Sommerfeld,[7] by an argument reproduced in Chapter III of his *Partial Differential Equations of Physics* (1949), and admits of a pretty interpretation.

Imagine the unit interval to be bounded by mirrors. The points $x_n^{\text{even}}=x+2n$ then mark the location of "images" of the point x which are "even" in this sense: let (y,t_0) and (x_n^{even},t) mark points on a spacetime diagram,[8] The line $(y,t_0)\longrightarrow(x_n^{\text{even}},t)$ passes through an even number of partitions; *i.e.*, it experiences an even number of reflections. The points $x_n^{\text{odd}}=-x+2n$ are "odd" in a similar sense. Now borrow from classical mechanics[9] the notion of a "two-point thermal action function"

$$\mathcal{S}(x_1,t_1;x_0,t_0)=\frac{1}{4}\frac{(x_1-x_0)^2}{t_1-t_0}$$

which satisfies the "thermal Hamilton-Jacobi equations"

$$\big(\tfrac{\partial\mathcal{S}}{\partial x_1}\big)^2+\tfrac{\partial\mathcal{S}}{\partial t_1}=0 \quad:\quad \big(\tfrac{\partial\mathcal{S}}{\partial x_0}\big)^2-\tfrac{\partial\mathcal{S}}{\partial t_0}=0$$

and posseses the additional property that

$$\mathcal{D}\equiv\big|\tfrac{\partial^2\mathcal{S}}{\partial x_1\partial x_0}\big|=\tfrac{1}{2(t_1-t_0)}$$

In this notation (11) becomes

$$\mathcal{G}(x,y,t)=\sqrt{\tfrac{1}{2\pi}\mathcal{D}}\sum_{n=-\infty}^{\infty}\Big\{\exp\big[-\mathcal{S}_n^{\text{even}}(x,y,t)\big]+\exp\big[-\mathcal{S}_n^{\text{odd}}(x,y,t)\big]\Big\} \tag{12}$$

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[7] Math. Ann. **45**, 263 (1894); Proc. Lond. Math. Soc. **28**, 395 (1897).

[8] We assume both x and $y\in[0,1]$, and find it convenient to assume moreover that $0<t_0<t$.

[9] From the free particle Lagrangian $L(\dot x)=\frac{1}{2}m\dot x^2$ we are led to dynamical trajectories of the form

$$(x_0,t_0)\longrightarrow(x_1,t_1)\quad:\quad x(t)=x_0+\frac{x_1-x_0}{t_1-t_0}(t-t_0)$$

of which the two-point action function is

$$S(x_1,t_1;x_0,t_0)=\int_{t_0}^{t_1}L(\dot x(t))\,dt=\frac{m}{2}\frac{(x_1-x_0)^2}{t_1-t_0}$$

which satisfies the Hamilton-Jacobi equations

$$\tfrac{1}{2m}\big(\tfrac{\partial S}{\partial x_1}\big)^2+\tfrac{\partial S}{\partial t_1}=0 \quad:\quad \tfrac{1}{2m}\big(\tfrac{\partial S}{\partial x_0}\big)^2-\tfrac{\partial S}{\partial t_0}=0$$

Figure 1 goes here

FIGURE 1: *Image points associated with Sommerfeld's construction of the thermal Green function for heat flow on a uniform rod of finite length. The same figure—differently interpreted—illustrates Feynman's construction of the quantum propagator for a particle confined to the interior of a box (infinite potential well).*

where (setting $t_0 = 0$)

$$\begin{aligned}\mathcal{S}_n^{\text{even}}(x, y, t) &= \mathcal{S}(2n + x, t; y, 0)\\ \mathcal{S}_n^{\text{odd}}(x, y, t) &= \mathcal{S}(2n - x, t; y, 0)\end{aligned}$$

and now $\mathcal{D} = |\partial^2 \mathcal{S}/\partial x \partial y| = 1/2t$. The sum in (12) might be notated

$$\sum_{\text{images of } x}$$

References to the "thermal method of images" (a terminology introduced by Sommerfeld) can be found on the web, and on pages 273-281 of Carslaw & Jaeger's classic *Conduction of Heat in Solids* (2^{nd} edition 1959), but not in Widder's *The Heat Equation* (1975). Readers familiar with the Feynman's quantum mechanical sum-over-paths formalism might be tempted to write

$$\sum_{\text{paths}}$$

But the theory of heat provides no conceptual basis on which to regard the line segment $(x_0, t_0) \longrightarrow (x_1, t_1)$ as the "trajectory" of something, and in this respect differs markedly from classical mechanics, the source of the imagery that Feynman would have us believe underlies quantum mechanics.[10]

Formal unification of the theory of heat and quantum mechanics. The free particle Schrödinger equation

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

is formally (see again (3)) a diffusion equation with imaginary diffusion constant.

[10] This formal development raises a too-seldom-asked question: On what grounds might one argue that Feynmans's imagery is more than a picturesque fiction?

Setting $\hbar = 2m = 1$ (else absorbing the $2m/\hbar$ into a rescaled time parameter), we look to the α-parameterized class of theories that follow the equation

$$e^{i\alpha}\partial_{xx}\psi = \partial_t\psi \quad : \quad \begin{cases} \text{heat equation at } \alpha = 0 \text{ mod } 2\pi \\ \text{Schrödinger equation at } \alpha = \frac{1}{2}\pi \text{ mod } 2\pi \end{cases} \tag{13.1}$$

which written

$$\partial_x(-e^{i\alpha}\partial_x\psi) + \partial_t\psi = 0 \tag{13.2}$$

assumes the form of a continuity equation with

$$\begin{aligned} \psi &= \text{complex density} \\ -e^{i\alpha}\partial_x\psi &= \text{complex flux} \end{aligned}$$

To achieve conservation of $Q = \int_0^1 \psi\, dx$ we require that the flux vanish at the boundaries of the unit box ($\partial_x\psi = 0$ at $x = 0$ and $x = 1$), and are led back again to the functions $\phi_n(x) : n = 0, 1, 2, \ldots$ defined at (5). By temporal evolution those functions become

$$\phi_n(x,t) = \exp\left\{e^{i\alpha}\partial_{xx}\right\}\phi_n(x) = e^{-e^{i\alpha}\pi^2 n^2 t}\,\phi_n(x) \tag{14}$$

We have, in effect, simply complexified the time parameter: writing

$$\mathcal{T} = e^{i\alpha}t = t\cos\alpha + i\,t\sin\alpha$$

we have

$$\phi_n(x,t) = e^{-\pi^2 n^2 \mathcal{T}}\,\phi_n(x)$$

which is persistently real-valued only when $\sin\alpha = 0$; *i.e.*, when (13) reduces to the forward/backward heat equation. The functions

$$\psi(x,t) = \sum_{n=0}^{\infty} c_n\phi_n(x,t) \in \mathcal{H}^\star \tag{15}$$

must be assumed therefore (except in the thermal case $\sin\alpha = 0$) to be complex-valued.

Complex-valued densities and fluxes (currents) are notions to which—however uncommon they may be—we can take no objection in principle, but they are in the present context not very interesting: working from (14) and (15) one is led in all cases to the globally conserved quantity

$$Q = \int_0^1 \psi(x,t)\,dx = c_0$$

It was, so far as I am aware, Born who first noticed that a continuity equation involving real-valued density and flux is implicit in the Schrödinger equation and its conjugate

$$\begin{aligned} -i\partial_{xx}\psi + \partial_t\psi &= 0 \\ +i\partial_{xx}\bar\psi + \partial_t\bar\psi &= 0 \end{aligned}$$

Multiplying the former by $\bar\psi$, the latter by ψ and adding, we obtain

$$\partial_x(i\{\psi\partial_x\bar\psi - \bar\psi\partial_x\psi\}) + \partial_t(\bar\psi\psi) = 0$$

with (by Born's interpretation)

$$\left.\begin{aligned} \bar\psi\psi &= \text{probability density} \\ i\{\psi\partial_x\bar\psi - \bar\psi\partial_x\psi\} &= \text{probability flux} \end{aligned}\right\} \tag{16}$$

Were we to proceed similarly from the generalized equation (13.2) we would obtain

$$\partial_x\big\{-e^{-i\alpha}\psi\,\partial_x\bar\psi - e^{i\alpha}\bar\psi\,\partial_x\psi\big\} + 2\cos\alpha\cdot\partial_x\bar\psi\cdot\partial_x\psi + \partial_t(\bar\psi\psi) = 0$$

which assumes the form of a continuity equation only in the case $\cos\alpha = 0$. In that case $\alpha = \pm\frac{1}{2}\pi \bmod 2\pi$ so $e^{\pm i\alpha} = \pm i$ and we recover Born's familiar result, which is seen to be peculiar to the quantum instance of the unified formalism. Note particularly that, if we assign to α its thermal value $\alpha = 0 \bmod 2\pi$ and take into account the fact that the thermal field $u(x,t)$ is real-valued, the preceding equation becomes

$$\partial_x(-2u\,\partial_x u) + 2(\partial_x u)^2 + \partial_t(u^2) = 0$$

which does not possess the structure of a continuity equation, and which shows why the quadratic construction u^2 does not acquire in thermal physics the importance that is assigned to $\bar\psi\psi$ in quantum physics.

We look finally to the antihermiticity of $e^{i\alpha}\partial_{xx}$, which is required if the exponentiation of that operator is to be unitary. A double integration-by-parts supplies

$$(a, e^{i\alpha}\partial_{xx}b) = e^{i\alpha}\Big\{a\cdot\partial_x b\Big|_0^1 - \partial_x a\cdot b\Big|_0^1 + (\partial_{xx}a, b)\Big\}$$

The boundary terms vanish if $a(x)$ and $b(x)$ are both elements of either

- $\mathcal{H}$, the space of functions that vanish at the boundary points, or
- $\mathcal{H}^\star$, the space of functions with derivatives that vanish at the boundaries

but we then have antihermiticity

$$= (-e^{-i\alpha}\partial_{xx}a, b)$$

if and only if $e^{i\alpha} = -e^{-i\alpha}$, which entails $\alpha = \frac{1}{2}\pi$ and again serves to distinguish the quantum instance of the unified formalism. In all cases we have conservation of $Q = \int_0^1 \psi\,dx = c_0$, but only in quantum theory do we also have conservation of $P = \int_0^1 \bar\psi\psi\,dx = 1$.

Standard quantum theory of a boxed particle. A mass m moves freely on the interval $x \in [0,a]$. The theory of this simplest of all quantum systems[11] proceeds from

$$\partial_t\psi = i\tfrac{\hbar}{2m}\partial_{xx}\psi \tag{17.1}$$

---

[11] Which is, however, not too simple to have served by Born and Einstein as a context within which to debate issues that lie at the foundations of quantum theory (and, more particularly, that concern the relationship of quantum to classical mechanics). See M. Born, *The Born-Einstein Letters* (pages 205-228) for the text and commentary of letters exchanged among Born, Einstein and Pauli (November 1953-April 1954).

with the specification of initial/boundary conditions, the latter of which in what I call the "standard theory" (the theory presented in textbooks[12]) is invariably taken to have the form $\psi \in \mathcal{H}$. The assumption that

$$\psi(0,t) = \psi(a,t) = 0 \quad : \quad \text{all } t \tag{17.2}$$

is standardly based upon a continuity argument, the underlying observation being that to avoid "sources/sinks of probability" the probability flux

$$J(x,t) = i\{\psi\partial_x\bar{\psi} - \bar{\psi}\partial_x\psi\}$$

must at all points and times be *continuous*. It is pointed out that for potential square wells of finite depth one can achieve continuity of $J(x,t)$ by requiring that *both* ψ and $\partial_x\psi$ be continuous at both boundaries of the well, but that as the well depth becomes infinite it becomes impossible to maintain that requirement, for it would force $\psi(x)$ to *vanish* inside the well (because it vanishes outside). Looking to graphs of $\psi(x)$ for wells of progressively increased depth (see Ballentine's Figure 4.2) one is led to read (17.2) as the natural limiting form of the statement

$$\psi_{\text{inside}}(x) = \psi_{\text{outside}}(x) \quad : \quad x \text{ either boundary point}$$

even though purchased at this cost: $\partial_x\psi_{\text{inside}}(x) \neq \partial_x\psi_{\text{outside}}(x)$. I will argue later that that reasoning is circular, that we confront a situation in which

$$\text{the physics of the limit} \neq \text{the limit of the physics}$$

But we agree to proceed at present with the standard boundary conditions (17.2).

Working as heretofore in the configuration representation, our problem, as standardly posed, is to describe the solutions $\psi(x,t)$ of

$$\mathsf{H}\psi = i\hbar\partial_t\psi \quad \text{with} \quad \psi(0,t) = \psi(a,t) = 0 \ : \ \text{all } t$$

where $\mathsf{H} = \frac{1}{2m}\mathsf{p}^2 = -\frac{\hbar^2}{2m}\partial_{xx}$ and $\psi(x,0)$ is given. Separation of variables leads to normalized solutions of the form

$$\psi_n(x,t) = \psi_n(x)\cdot e^{-i\omega_n t} \tag{18.1}$$

where $\omega_n = (\pi^2\hbar/2ma^2)n^2 \ : \ n = 1,2,3,\dots$ and $\psi_n(x) = \sqrt{2/a}\,\sin(n\pi x/a)$. We agree at the outset to set $\hbar = 2m = a = 1$, so the Schrödinger equation reads

$$\partial_{xx}\psi + i\,\partial_t\psi = 0$$

[12] See, for example, Griffiths[3], pages 31 & 72; Mark Beck, *Quantum Mechanics Theory & Experiment* (2012), page 257; L. E. Ballentine, *Quantum Mechanics* (1990), §4.5.

and the harmonically buzzing eigensolutions become (18) with

$$\omega_n = \pi^2 n^2 \tag{18.2}$$

$$\psi_n(x) = \sqrt{2}\sin(n\pi x) \tag{18.3}$$

The energy eigenfunctions (18.3) are orthonormal in the sense

$$\int_0^1 \psi_m(x)\psi_n(x)\,dx = \delta_{mn}$$

and are considered to span the space $\mathcal{H}$ of admissible wavepackets, which is to say: every such initial wavepacket $\psi(x,0)$ can be developed

$$\psi(x,0) = \sum_{n=1}^{\infty} c_n\psi_n(x) \quad \text{with} \quad c_n = \int_0^1 \psi_n(y)\psi(y)\,dy \tag{19}$$

and one has

$$\int_0^1 |\psi(x)|^2 dx = 1 \quad \Longleftrightarrow \quad \sum_{n=1}^{\infty} |c_n|^2 = 1 \tag{20}$$

All of which could have been taken from any introductory quantum text.

Bringing (18) to (19), we have

$$\begin{aligned}\psi(x,t) &= \sum_{n=1}^{\infty} \psi_n(x,t)\,c_n \\ &= \sum_{n=1}^{\infty} \psi_n(x)e^{-i\pi^2 n^2 t}\int_0^1 \psi_n(y)\psi(y,0)\,dy \\ &= \int_0^1 G(x,y,t)\psi(y,0)\,dy \end{aligned} \tag{21}$$

where (compare (7.2))

$$G(x,y,t) = \sum_{n=1}^{\infty} \psi_n(x)e^{-i\pi^2 n^2 t}\psi_n(y) \tag{22}$$

is the spectral representation of the relevant "quantum Green function" or "propagator."[13] Drawing upon (18.3), we have

$$\begin{aligned}G(x,y,t) &= 2\sum_{n=1}^{\infty} e^{-i\pi^2 n^2 t}\sin(\pi nx)\sin(\pi ny) \\ &= \sum_{n=1}^{\infty} e^{-i\pi^2 n^2 t}\big\{\cos[\pi n(x-y)] - \cos[\pi n(x+y)]\big\}\end{aligned}$$

[13] The construct $G(x,y,0) = \sum_n \psi_n(x)\psi_n(y) = \delta_{\text{boxed}}(x,y)$ serves to describe the "boxed delta function," which lives—in at least the familiar formal sense—within $\mathcal{H}$.

Recalling the definition (8) of the Jacobi theta function $\vartheta_3(v,\tau)$, we have

$$G(x,y,t) = \tfrac{1}{2}\vartheta_3\Big[\frac{x-y}{2}, -\pi t\Big] - \tfrac{1}{2}\vartheta_3\Big[\frac{x+y}{2}, -\pi t\Big]$$

which by Jacobi's transformation (10) becomes

$$\begin{aligned} G(x,y,t) = & \quad \frac{1}{\sqrt{4\pi i t}}\exp\Big\{i\frac{(x-y)^2}{4t}\Big\}\cdot\vartheta_3\Big[-\frac{x-y}{2\pi t},\frac{1}{\pi t}\Big] \\ & - \frac{1}{\sqrt{4\pi i t}}\exp\Big\{i\frac{(x+y)^2}{4t}\Big\}\cdot\vartheta_3\Big[-\frac{x+y}{2\pi t},\frac{1}{\pi t}\Big] \\ & = \frac{1}{\sqrt{4\pi i t}}\sum_{n=-\infty}^{\infty}\Big\{\exp\Big[i\frac{(y-x+2n)^2}{4t}\Big] - \exp\Big[i\frac{(y+x+2n)^2}{4t}\Big]\Big\} \end{aligned} \tag{23}$$

As has already been remarked,[9] the two-point action function associated with the classical trajectory $(y,0) \longrightarrow (x,t)$ reads $S(x,y,t) = \frac{m}{2t}(x-y)^2$, which when $2m=1$ becomes $S(x,y,t) = \frac{1}{4t}(x-y)^2$. For the classical trajectory that experiences an even/odd number of reflections while proceeding (in time t) from $y \longrightarrow x$; *i.e.*, that—in the sense of FIGURE 1—proceeds from y to an even/odd-ordered *image* of x, we have

$$\begin{aligned} S_n^{\text{even}}(x,y,t) &= \tfrac{1}{4t}(y-x+2n)^2 \\ S_n^{\text{odd}}(x,y,t) &= \tfrac{1}{4t}(y+x+2n)^2 \end{aligned}$$

and (23) becomes[14]

$$G(x,y,t) = \sqrt{\tfrac{m}{iht}}\Big\{\sum_{n=-\infty}^{\infty}\exp\big\{\tfrac{i}{\hbar}S_n^{\text{even}}(x,y,t)\big\} - \sum_{n=-\infty}^{\infty}\exp\big\{\tfrac{i}{\hbar}S_n^{\text{odd}}(x,y,t)\big\}\Big\}$$

Comparing (23) with (11), we see that the transition from the thermal problem to its (standardly interpreted) quantum counterpart entails $t \longrightarrow it$ and a sign reversal. The source of the latter is elementary—compare

$$\begin{aligned} 2\cos a\cos b &= \cos(a-b) + \cos(a-b) \\ 2\sin a\sin b &= \cos(a-b) - \cos(a-b) \end{aligned}$$

—but admits of an interesting physical interpretation, as will emerge near the end of the next section.

Nonstandard quantum theory of a boxed particle. Unarguably, probability flux $J(x,t)$ must be continuous at the boundaries of a potential well of finite depth, but the argument that formerly led us from that fact to the assertion that

[14] Notice in this connection that $\frac{m}{iht} = \frac{i}{2\pi\hbar}\frac{\partial^2 S}{\partial x\partial y}$ becomes $\frac{1}{4\pi it}$ when $\hbar = 2m = 1$.

necessarily

$$\psi_{\text{inside}}(x) = \psi_{\text{outside}}(x) \quad : \quad x \text{ either boundary point}$$

loses its force when the well depth becomes infinite, because (I assert) exterior physics becomes then *detached from/irrelevant to* interior physics. All one can require in the limiting case is that

$$J(x,t) = 0 \quad \text{at both boundary points (all } t\text{)}$$

which can be achieved in several alternative ways:

$$\begin{aligned}
&i) &\psi(0,t) &= \psi(a,t) = 0\\
&ii) &\psi_x(0,t) &= \psi_x(a,t) = 0\\
&iii) &\psi(0,t) &= \psi_x(a,t) = 0\\
&iv) &\psi_x(0,t) &= \psi(a,t) = 0
\end{aligned}$$

The first option is standard, while the second gives rise to what I call the "nonstandard quantum theory of a boxed particle" (sketched below); the final pair of options will be dismissed because, though possible in one dimension,[15] they do not pertain in a natural way to the quantum mechanics of a particle constrained to move freely within a higher-dimensional enclosure of arbitrary (non-rectangular) shape.[16] In the nonstandard theory the spectrum of the Hamiltonian $\mathsf{H} = -\partial_{xx}$ is unchanged but for the addition of a lowered ground state:

$$\{\omega_n = \pi^2 n^2 \ : \ n = 1, 2, \ldots\} \longrightarrow \{\omega_n = \pi^2 n^2 \ : \ n = 0, 1, 2, \ldots\}$$

Wavepackets $\phi(x,t)$ live now not in $\mathcal{H}$ but in $\mathcal{H}^\star$, which is spanned by the orthonormal eigenbasis $\{\phi_n(x) : n = 0, 1, 2, \ldots\}$ that was defined at (5). When set abuzz those become

$$\phi_n(x,t) = \phi_n(x) e^{-i\pi^2 n^2 t}$$

and for arbitrary normalized wavepackets $\phi(x,t)$ we have (compare (19) and (20))

$$\phi(x,t) = \sum_{n=0}^{\infty} c_n^\star \phi_n(x,t) \quad \text{with} \quad c_n^\star = \int_0^1 \phi_n(y)\phi(y,0)\,dy \tag{24}$$

$$\int_0^1 |\phi(x,t)|^2 dx = 1 \quad \Longleftrightarrow \quad \sum_{n=1}^{\infty} |c_n^\star|^2 = 1 \tag{25}$$

---

[15] Think of the vibration of a string with one clamped end. For a relevant animation, see the "Miscellaneous Essays & Notebooks" file within the "Classical Mechanics" file on my website. The movie was created to illustrate a purported solution of the "Feynman spaghetti problem," the subject of Oren Elrad's Reed College thesis (2006).

[16] Think, however of the vibration of a partially clamped membrane.

In the nonstandard theory the propagator (by arguments that need not be repeated) becomes

$$G^\star(x,y,t) = \sum_{n=0}^{\infty} \phi_n(x) e^{-i\pi^2 n^2 t}\phi_n(y) \tag{26}$$

$$= \frac{1}{\sqrt{4\pi i t}} \sum_{n=-\infty}^{\infty} \Big\{ \exp\Big[i\frac{(y-x+2n)^2}{4t}\Big] + \exp\Big[i\frac{(y+x+2n)^2}{4t}\Big]\Big\} \tag{27}$$

$$= \sqrt{\tfrac{m}{iht}}\Big\{ \sum_{n=-\infty}^{\infty} \exp\big\{\tfrac{i}{\hbar}S_n^{\text{even}}(x,y,t)\big\} + \sum_{n=-\infty}^{\infty} \exp\big\{\tfrac{i}{\hbar}S_n^{\text{odd}}(x,y,t)\big\}\Big\}$$

of which the former differs from its thermal counterpart (7.2) by $t \longrightarrow it$, and the latter from its standard quantum counterpart (23) by a sign reversal.

The fact that the $\mathcal{H} \longleftrightarrow \mathcal{H}^\star$ entails a sign reversal if can be understood if we posit that at reflection points the classical action does/doesn't acquire an additive term according as the boundary is "clamped" (ψ vanishes) or "unclamped" ($\partial_x\psi$ vanishes):

$$S \xrightarrow[\text{reflection from a clamped boundary}]{} S + \tfrac{1}{2}h$$
$$S \xrightarrow[\text{reflection from a unclamped boundary}]{} S$$

Such a principle would render Feynman's formulation of quantum mechanics consonant with the reflection of waves from the clamped/unclamped end of a string[15] and with the reflection of light when it encounters a region where the index of refraction abruptly increases/decreases.[17] And it would permit one to construct a unified description

$$G(x,y,t) = \sqrt{\tfrac{m}{iht}} \sum_{\text{paths}} e^{\frac{i}{\hbar}S[\text{path: }(y,0)\to(x,t)]} \tag{28}$$

of the propagator.[18]

Interlude: Parabolic wavepackets and the "frailty of hermiticity". In some earlier work[19] I was motivated to look to the normalized wavepacket

$$\Psi(x) = \sqrt{30}\,x(1-x) \tag{29}$$

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[17] It becomes in this light plausible that one might use a beam of particles to construct a quantum analog of "Newton's rings," an experimental arrangement for which several useful applications come to mind.

[18] Feynman would have us sum over *all conceivable* paths $(y,0) \longrightarrow (x,t)$, but the sum in (28) ranges only over the classical paths that proceed reflectively from $(y,0)$ to (x,t); *i.e.*, from y to one or another of the images of x. That the conceivable but classically unrealized paths make no net contribution can be attributed to the circumstance that the free Hamiltonian falls within the class of Hamiltonian operators that depend at most quadratically upon $\mathbf{x}$ and $\mathbf{p}$.

[19] "Momentum operators for particle-in-a-box problems," February 2010.

which clearly vanishes at the boundaries of the unit interval, and appears on its face to be an unexceptionable element of $\mathcal{H}$. It leads, however, to paradox. From $\mathsf{H} = -\partial_{xx}$ we obtain

$$\langle \mathsf{H} \rangle = 2\sqrt{30}$$
$$\langle \mathsf{H}^2 \rangle = 0$$

giving
$$\Delta E = \sqrt{\langle \mathsf{H}^2 \rangle - \langle \mathsf{H} \rangle^2} = i\sqrt{120}$$

which is nonsense. Moreover,

$$\Psi(x,t) = e^{-i\,\mathsf{H}\,t} = \Psi(x) - i\,2\sqrt{30}\,t = \sqrt{30}\,\big\{x(1-x) - i\,2\,t\big\}$$
$$\Downarrow$$
$$|\Psi(x,t)|^2 = 30x^2 - 60x^3 + 30x^4 + 120\,t^2$$
$$\Downarrow$$
$$\int_0^1 |\Psi(x,t)|^2\,dx = 1 + 120\,t^2$$

so the evolution $\Psi(x,0) \longrightarrow \Psi(x,t)$ is not unitary. These facts become still more surprising when (see FIGURE 2) it is realized that the parabolic wavepacket so closely resembles (see FIGURE 2) the ground state $\psi_1(x) \in \mathcal{H}$,

Figure 2 goes here

FIGURE 2: *Superimposed graphs of the parabolic wavepacket* $\Psi(x)$ *(red) and the ground state* $\psi_1(x)$ *(blue).*

which displays no such anomalies: $\{(\psi_1|\mathsf{H}|\psi_1)=\pi^2, (\psi_1|\mathsf{H}^2|\psi_1)=\pi^4\} \Rightarrow \Delta E=0$ while $\psi_1(x,0) \longrightarrow \psi_1(x,t) = e^{-i\pi^2 t}$ is manifestly unitary.[20] When, on separate occasions, I mentioned my "parabolic state problem" to David Griffiths and Darrell Schroeter who—promptly and identically—responded "Something must have compromised hermiticity," and David loaned me his copy of a brilliant

[20] In those respects, $\psi_1(x)$ exhibits properties universally expected of *all* eigenstates.

undergraduate thesis by one Sarang Gopallakrishnan.[21] I was interested to discover that, in a section entitled "The frailty of hermiticity," Gopallakrishnan treats precisely the "parabolic state problem" and—following Bonneau *et al*—attributes its anomalous features to the fact that, while $\Psi(x) \in \mathcal{H}$,

$$b(x) \equiv (-\partial_{xx})\Psi(x) = 2\sqrt{30} \in \mathcal{H}^\star \quad (\textit{not}\ \mathcal{H})$$

which, as we saw on page 11 (set $\alpha = \pi$ and assume $a(x) \in \mathcal{H}$), gives

$$(a, -\partial_{xx}b) = 0 + \partial_x a \cdot b\Big|_0^1 + (-\partial_{xx}a, b) \neq (-\partial_{xx}a, b)$$

and thus serves to compromise hermiticity.

All problems evaporate when one displays the parabolic wavepacket as a linear combination of basis functions in $\mathcal{H}$. In the energy eigenbasis $\{\psi_n(x)\}$ one has

$$\Psi(x) \longmapsto \tilde{\Psi}(x) = \sum_{n=1}^{\infty} c_n \psi_n(x)$$

where *Mathematica* supplies[22]

$$c_n = \begin{cases} 0 & : \quad n \text{ even} \\ \frac{8\sqrt{15}}{n^3\pi^3} & : \quad n \text{ odd} \end{cases} \tag{30}$$

and confirms that

$$\sum_{n=1}^{\infty} |c_n|^2 = \left(\tfrac{8\sqrt{15}}{\pi^3}\right)^2 \sum_{k=0}^{\infty} \frac{1}{(2k+1)^6} = 1$$

The expected values of H and H^2 now become

$$\langle \mathsf{H} \rangle = \sum_{n=1}^{\infty} |c_n|^2 \omega_n = \left(\tfrac{8\sqrt{15}}{\pi^3}\right)^2 \sum_{k=0}^{\infty} \frac{\pi^2}{(2k+1)^4} = 10 \tag{31.1}$$

$$\langle \mathsf{H}^2 \rangle = \sum_{n=1}^{\infty} |c_n|^2 \omega_n^2 = \left(\tfrac{8\sqrt{15}}{\pi^3}\right)^2 \sum_{k=0}^{\infty} \frac{\pi^4}{(2k+1)^2} = 120 \tag{31.2}$$

---

[21] "Self-adjointness and the renormalization of singular potentials," Amherst College (2006). Gopallakrishnan attributes the example to G. Bonneau, J. Faraut & G. Valent, "Self-adjoint extensions of operators and the teaching of quantum mechanics," AJP **68**, 322 (2001), where in §2 ("The infinite potential well: paradoxes") it in fact plays a central role.

[22] Griffiths[3] considers the parabolic wavepacket in this **Examples 2.2/3**. He supplies computational details, but does not mention the respects in which such wavepackets are problematic. Notice that $c_n \sim n^{-3}$, so one need not keep many terms in the $\sum_n$ to obtain quite good approximate results. From (30) we obtain

$$\Psi(x) = 0.999277\psi_1(x) + 0.037010\psi_3(x) + 0.007994\psi_5(x) + \cdots$$

which accounts for the close agreement of the curves shown in FIGURE 2.

which give $\Delta E = \sqrt{20}$, where formerly we had $\Delta E = i\sqrt{120}$: the anomaly has been healed.

The source of the parabolic anomaly was seen to lie in the circumstance that $(-\partial_{xx})\Psi(x) = 2\sqrt{30}$ is a constant; *i.e.*, that

$$U(x) \equiv \tfrac{1}{2\sqrt{30}}(-\partial_{xx})\Psi(x) = \text{unit function}$$

We are led to look therefore to the function

$$\begin{aligned}\tilde{U}(x) \equiv \tfrac{1}{2\sqrt{30}}(-\partial_{xx})\tilde{\Psi}(x) &= \tfrac{2\sqrt{2}}{\pi}\sum_{k=0}^{\infty}\frac{1}{2k+1}\psi_{2k+1}(x)\\ &= \tfrac{4}{\pi}\sum_{k=0}^{\infty}\frac{1}{2k+1}\sin[\pi(2k+1)x]\end{aligned} \tag{32}$$

which is plotted in the following figure:

Figure 3 goes here

FIGURE 2: *Superimposed graphs of the unit function (red) and its representation in $\mathcal{H}$. Because the coefficients in (32) fall off only as $(2k+1)^{-1}$ one must go to relatively high order to obtain reliable approximations; in the figure truncation was at $k = 30$.*

From

$$\int_0^1 1\cdot\psi_n(x)\,dx = \frac{2\sqrt{2}}{\pi}\{1, 0, \tfrac{1}{3}, 0, \tfrac{1}{5}, 0, \tfrac{1}{7}, 0, \ldots\}$$

we see that the coefficients in (32) are precisely those that appear in the Fourier sine-series development of the unit function; *i.e.*, when the unit function is construed to be an element of $\mathcal{H}$.

While all derivatives of the unit function $U(x)$ vanish, the same cannot be said of $\tilde{U}(x)$. Looking to

$$\tilde{U}_p(x) \equiv (-\partial_{xx})^p\,\tilde{U}(x) = 2\sqrt{2}\,\pi^{2p-1}\sum_{k=0}^{\infty}(2k+1)^{2p-1}\psi_{2k+1}(x) \tag{33}$$

(which follows from (32), and gives back (32) at $p = 0$), we observe that all such functions vanish at the boundaries of the unit interval (as is required of the elements of $\mathcal{H}$), but that the coefficients

$$u_{2k+1,p} = 2\sqrt{2}\,\pi^{2p-1}(2k+1)^{2p-1}$$

diverge if $p \geqslant 1$ and their sum diverges even at $p = 0$. More to the point, we find

$$\sum_{k=0}^{\infty} |u_{2k+1,p}|^2 = \begin{cases} 1 & : \quad p = 0 \\ \infty & : \quad p = 1, 2, 3, \ldots \end{cases}$$

The functions $\tilde{U}_p(x)$ are, for $p \geqslant 1$, *not square integrable* so—compliance with the boundary conditions $\tilde{U}_p(0) = \tilde{U}_p(1) = 0$ notwithstanding—cannot be elements of $\mathcal{H}$. When truncated versions of $\tilde{U}_{p=1}(x)$ are plotted they are found to exhibit very pronounced Gibbs phenomena, and to oscillate about zero with frequencies *and amplitudes* that grow as the truncation point is pushed farther out, and those effects are amplified when p is made larger. The form of such figures suggests that the *averaged* value of $\tilde{U}_p(x)$ might be zero, but from

$$\int_0^1 \sin[\pi(2k+1)x]\,dx = \frac{2}{\pi(2k+1)}$$

we obtain

$$\int_0^1 \tilde{U}_p(x)\,dx = 8\pi^{2p-2}\sum_{k=0}^{\infty}(2k+1)^{2p-2} = \begin{cases} 1 & : \quad p = 0 \\ \infty & : \quad p = 1, 2, 3, \ldots \end{cases}$$

We will have occasion to revisit these disturbing facts.

So much for the results that follow when the parabolic wavepacket $\Psi(x)$ is developed in the $\psi_n(x)$-basis, and construed to be an element of $\mathcal{H}$. I turn now discussion of the results that follow when—alternatively—$\Psi(x)$ is developed in the $\phi_n(x)$-basis, and construed to be an element of $\mathcal{H}^\star$. We proceed from

$$\Psi(x) \longmapsto \tilde{\Psi}^\star(x) = \sum_{n=1}^{\infty} c_n^\star \phi_n(x)$$

where *Mathematica* supplies

$$c_n^\star = \int_0^1 \Psi(x)\phi_n(x)\,dx = \begin{cases} \sqrt{\tfrac{5}{6}} & : \quad n = 0 \\ 0 & : \quad n \text{ odd} \\ -\tfrac{4\sqrt{15}}{\pi^2 n^2} & : \quad n \text{ even} \end{cases}$$

and confirms that

$$\sum_{n=1}^{\infty} |c_n^\star|^2 = \tfrac{5}{6} + \Big(-\tfrac{4\sqrt{15}}{\pi^2}\Big)^2 \sum_{k=1}^{\infty} \frac{1}{(2k)^2} = 1$$

Since the coordinates $c_n^\star$ fall off only as n^{-2} (compare (30), where the c_n were seen to fall off as n^{-3}), one must truncate at relatively high order to obtain good approximations, but when that is done one finds that graphs of $\Psi(x)$ and $\Psi^\star(x)$ are nicely coincident save for one detail: the slope of $\Psi^\star(x)$ flattens in the immediate neighborhood of the boundary points, the size of the neighborhood shrinking as the truncation point is pushed farther out.