Remarks concerning

A Quantum Misdemeanor

and its circumvention

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Introduction. In a recent paper,[1] Carl Bender and co-authors have drawn attention to a point at which a line of formal argument frequently encountered in elementary expositions of quantum mechanics becomes so informal as to be fundamentally incorrect, and indicate how, by appeal to a device introduced by Euler, the defect can be circumvented. My objective here will be to provide an account BBP's interesting work—which relates not to the physics but only to the mathematics of quantum mechanics—to place it in a somewhat more general context, and to discuss some of its non-obvious ramifications.

Mathematical prelude. The BBP paper is an exercise in applied mathematics, the ideas that they take for a ride around the block are not physical but mathematical. By way of preparation I look here to a few of those.

The Fourier Integral Theorem asserts that for a broad class of "nice" functions $f(x)$

$$f(x) = \tfrac{1}{2\pi}\int_{-\infty}^{\infty}\Big\{\int_{-\infty}^{\infty} f(y)e^{-iky}dy\Big\}e^{ikx}dx$$

Written

$$f(x) = \int_{-\infty}^{\infty} f(y)\Big\{\tfrac{1}{2\pi}\int_{-\infty}^{\infty} e^{-ik(y-x)}dk\Big\}dy \tag{1}$$

[1] Carl M. Bender, Dorje C. Brody & Matthew F. Parry, "Making sense of the divergent series for reconstructing a Hamiltonian from its eigenstates and eigenvalues," AJP **88**, 148–152 (2020), henceforth denoted BBP.

this becomes the assertion that the functions

$$\varphi_k(x) = \tfrac{1}{\sqrt{2\pi}} e^{ikx}$$

are *complete*:

$$\int_{-\infty}^{\infty} \bar{\varphi}_k(y)\varphi_k(x)dk = \delta(y-x) \tag{2.1}$$

But

$$\text{if} \quad \tfrac{1}{2\pi}\int_{-\infty}^{\infty} e^{-ik(y-x)}dk = \delta(y-x) \quad \text{then} \quad \tfrac{1}{2\pi}\int_{-\infty}^{\infty} e^{-ix(k-j)}dx = \delta(k-j)$$

which written

$$\int_{-\infty}^{\infty} \bar{\varphi}_k(x)\varphi_j(x)dx = \delta(k-j) \tag{2.2}$$

asserts the *orthonormality* of the functions $\varphi_k(x)$. Equations (2) illustrate the sense in which "completeness" and "orthonormality" are sibling—though by no means equivalent—notions.

It the derivative $\partial_x f(x)$ of the nice function $f(x)$ is also nice, we expect—by (1) written

$$f(x) = \int_{-\infty}^{\infty} f(y)\delta(y-x)dy$$

—to have

$$\begin{aligned}
\partial_x f(x) &= \int_{-\infty}^{\infty} f(y)[-\partial_y \delta(y-x)]dy \quad \text{by } \partial_x g(y-x) = -\partial_y g(y-x) \\
&= \int_{-\infty}^{\infty} \partial_y f(y)\delta(y-x)dy \quad \text{after integrating by parts}
\end{aligned}$$

Which raises the question (a question for which the Gaussian representation of $\delta(y-x)$ provides a pretty answer): What kind of object is

$$\partial_y \delta(y-x) = \partial_y \Big\{ \tfrac{1}{2\pi} \int_{-\infty}^{\infty} e^{-ik(y-x)}dk \Big\}$$

Turning now from Fourier integrals to Fourier series, the functions

$$s_n(x) \equiv \sqrt{2/\pi}\,\sin(nx) : \; n = 1, 2, \ldots$$

are nice on the interval $x \in [0, \pi]$ and vanish on its boundaries. If so also is/does $f(x)$, then—with Fourier/Dirac—we expect by orthonormality

$$\int_0^{\pi} s_m(x)s_n(x)dx = \delta_{mn}$$

to have

$$f(x) = \sum_{n=1}^{\infty} f_n s_n(x)$$

$$f_n = \int_0^\pi f(y)s_n(y)\,dy$$

$$= \sum_{n=1}^{\infty} \int_0^\pi f(y)s_n(y)s_n(x)\,dy$$

$$= \int_0^\pi \sum_{n=1}^{\infty} f(y)s_n(y)s_n(x)\,dy = \int_0^\pi f(y)\delta(y-x)\,dy \tag{3}$$

which asserts the completeness of the functions $s_n(x)$:

$$\sum_{n=1}^{\infty} s_n(y)s_n(x) = \delta(y-x) \tag{4}$$

Plot $\sum_{n=1}^N s_n(y)s_n(x)$ as a function of y, with fixed $x \in [0,\pi]$ and ascending values of N to gain a sense of how completeness comes about.

Proceding formally from (3), we have

$$\begin{aligned}\partial_x f(x) &= \int_0^\pi f(y)\cdot\partial_x\delta(y-x)\,dy\\ &= -\int_0^\pi f(y)\cdot\partial_y\delta(y-x)\,dy\\ &= \underbrace{-f(y)\delta(y-x)\Big|_0^\pi}_{0} + \int_0^\pi \partial_y f(y)\cdot\delta(y-x)\,dy\end{aligned}$$

From (4) we are led formally to write

$$\begin{aligned}\partial_y\delta(y-x) &= \partial_y \sum_{n=1}^{\infty} s_n(y)s_n(x) && \star\\ &= \sum_{n=1}^{\infty} \partial_y s_n(y)\cdot s_n(x) && \star\star\\ &= \sum_{n=1}^{\infty} (2/\pi)n\cos(ny)\sin(nx)\end{aligned}$$

which actually makes a kind of sense when plotted. But[2] $\sum_n^N s_n(y)s_n(x)$ is not a uniformly convergent sequence of functions of y: it is manifestly *not* the case that for all $\epsilon > 0$ there exists a N_0 such that

$$\left|\delta(y-x) - \textstyle\sum_n^N s_n(y)s_n(x)\right| < \epsilon \quad : \quad \text{all } N > N_0$$

So the step $\star \longleftrightarrow \star\star$ is disallowed: uniform convergence is necessary (but not sufficient) for term-wise differentiation to be permitted. It is to a step taken

[2] Assign to x any fixed value in $[0,\pi]$.

violation of this fundamental fact that BBP draw attention, and for which they devise (borrow from Euler) a work-around.

The more general quantum context. An important role in expository classical/quantum mechanics is played by systems in which a mass m moves one-dimensionally in the presence of a time-independent potential $V(x)$. In classical Hamiltonian physics the dynamical motion of a phase point $\{p, x\}$ is regulated, *via* the canonical equations, by the Hamiltonian $H(p, x) = \frac{1}{2m}p^2 + V(x)$. In quantum physics the dynamical motion of the quantum state $|\psi)$ is regulated *via* the abstract Schrödinger equation

$$\mathbf{H}|\psi) = i\hbar\partial_t|\psi) \tag{5}$$

by the Hamiltonian operator $\mathbf{H} = \frac{1}{2m}\mathbf{p}^2 + V(\mathbf{x})$. In the x-representation (made natural by $V(x)$ and the way boundary conditions are usually phrased) (5) becomes

$$\begin{aligned} \int (x|\mathbf{H}|y)dy(y|\psi) &= i\hbar\partial_t(x|\psi) \\ (x|\psi) &= \psi(x,t) \end{aligned} \tag{6.1}$$

which is most commonly written[3]

$$\left\{\tfrac{1}{2m}\left(\tfrac{\hbar}{i}\partial_x\right)^2 + V(x)\right\}\psi(x,t) = i\hbar\partial_t\psi(x,t) \tag{6.2}$$

Among the solutions of (6.2) are solutions of the separated form

$$\psi_E(x)\cdot\exp\left(\tfrac{1}{i\hbar}Et\right)$$

where $\psi_E(x)$ is a boundary-condition-satisfying solution of the t-independent Schrödinger equation

$$\left\{\tfrac{1}{2m}\left(\tfrac{\hbar}{i}\partial_x\right)^2 + V(x)\right\}\psi_E(x) = E\psi_E(x) \tag{7}$$

where the allowed E-values comprise the "spectrum" of the differential operator $\left\{\frac{1}{2m}\left(\frac{\hbar}{i}\partial_x\right)^2 + V(x)\right\}$. Abstractly

$$\mathbf{H}|E) = E|E), \quad (x|E) = \psi_E(x) \tag{8}$$

Look to a case in which the eigenvalues are distinct. Write

$$\{E_0, E_1, E_2, \ldots\} \quad \text{and} \quad \{|0), |1), |2), \ldots\}$$

to denote the non-degenerate eigenvalues and associated eigenstates, whereupon

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[3] Discussion of how one gets from (6.1) to (6.2) can be found in my *Quantum Class Notes* (2000), New Chapter 0, pages 29–38.

has become

$$\mathsf{H}|n) = E_n|n), \quad (x|n) = \psi_n(x) \quad : \quad n = 0, 1, 2, \ldots$$

Using this apparatus—together with the spectral decomposition of the Hamiltonian

$$\mathsf{H} = \sum_n |n)E_n(n|$$

and the assumption that set $\{|n)\}$ of eigenstates is complete

$$\mathsf{I} = \sum_n |n)(n|$$

—to proceed formally from (6.1), we have

$$\begin{aligned}
\int (x|\,\mathsf{H}\,|y)dy(y|\psi) &= \int H(x,y)dy(y|\psi) \\
H(x,y) &= \sum_n (x|n)E_n(n|y) \\
&= \sum_n (x|n)\big\{\tfrac{1}{2m}\big(\tfrac{\hbar}{i}\partial_y\big)^2 + V(y)\big\}(n|y) \qquad \star \\
&= \big\{\tfrac{1}{2m}\big(\tfrac{\hbar}{i}\partial_y\big)^2 + V(y)\big\}\sum_n (x|n)(n|y) \qquad \star\star \\
&= \big\{\tfrac{1}{2m}\big(\tfrac{\hbar}{i}\partial_y\big)^2 + V(y)\big\}\delta(y-x) \\
\text{whence} \qquad &= \big\{\tfrac{1}{2m}\big(\tfrac{\hbar}{i}\partial_x\big)^2 + V(x)\big\}(x|\psi)
\end{aligned}$$

and so have recovered (6.2) from (6.1)? It is at $\star \longleftrightarrow \star\star$ that BBP blow their whistle, call foul, on the ground that the series on the right side of

$$\delta(y-x) = \lim_{N\uparrow\infty} \sum_n^N (x|n)(n|y)$$

is not uniformly convergent.

BBP resolution: case of a particle-in-a-box. Stripped to its bare bones,[4] the time-independent Schrödinger equation for a boxed particle reads

$$-\tfrac{1}{2}\partial_x^2\psi(x) = \mathcal{E}\psi(x)$$

which by the requirements $\psi(0) = \psi(\pi) = 0$ and $\int_0^\pi |\psi(x)|^2 dx = 1$ supply

[4] For the fully clothed theory, see (for example) David Griffiths & Darrell Schroeter, *Introduction to Quantum Mechanics* (3rd edition, 2018), §2.2. It is for mainly notational reasons that we set $\hbar = m = 1$ and place the box boundaries at $[0, \pi]$.

eigenvalues/functions

$$\mathcal{E}_n = \tfrac{1}{2}n^2, \qquad \psi_n(x) = \sqrt{2/\pi}\,\sin(nx) \quad : \quad n = 1, 2, \ldots$$

The BBP objective in this instance is to achieve

$$\int_0^\pi H(x,y)\psi(y)dy = -\tfrac{1}{2}\partial_x^2\psi(x)$$

Their problem: to get from

$$H(x,y) = \sum_{n=1} \sqrt{2/\pi}\,\sin(nx)\cdot\tfrac{1}{2}n^2\cdot\sqrt{2/\pi}\,\sin(ny)$$

to

$$= -\tfrac{1}{2}\partial_y^2\delta(y-x) \tag{9}$$

even though the non-convergence of

$$\begin{aligned} J(x,y) &\equiv \tfrac{2}{\pi}\sum_{n=1}^\infty \sin(nx)\cdot\sin(ny) \\ &= \tfrac{1}{\pi}\sum_{n=1}^\infty \big\{\cos[n(x-y)] - \cos[n(x+y)]\big\} \\ &= \tfrac{2}{\pi}\big\{1+0+1+0+1+0+\cdots\big\} \text{ at } x = y = \tfrac{1}{2}\pi \end{aligned}$$

causes the simple formal argument to fail.

To resolve this (seemingly fatal) difficulty, they look—with Euler, whose spirit seems to have inspired the following clever argument—to the tempered series

$$J(x,y;\lambda) \equiv \tfrac{1}{\pi}\sum_{n=1}^\infty \lambda^n\big\{\cos[n(x-y)] - \cos[n(x+y)]\big\}$$

Using $\cos(nu) = \frac{1}{2}(e^{inu} + e^{-inu})$ and

$$\begin{aligned} \sum_{n=1}^\infty (\lambda e^{iu})^n &= \sum_{n=0}^\infty (\lambda e^{iu})^n - 1 \\ &= \frac{1}{1-\lambda e^{iu}} - 1 \end{aligned}$$

we have

$$\sum_{n=1}^\infty \lambda^n\cos(nu) = \tfrac{1}{2}\Big[\frac{1}{1-\lambda e^{iu}} + \frac{1}{1-\lambda e^{-iu}}\Big] - 1$$

$$\begin{aligned} \sum_{n=1}^\infty \lambda^n\big\{\cos(nu) - \cos(nv)\big\} = \;& \tfrac{1}{2}\Big[\frac{1}{1-\lambda e^{iu}} + \frac{1}{1-\lambda e^{-iu}}\Big] \\ &- \tfrac{1}{2}\Big[\frac{1}{1-\lambda e^{iv}} + \frac{1}{1-\lambda e^{-iv}}\Big] \end{aligned}$$

Using `ComplexExpand` and `Simplify`, we find

$$\tfrac{1}{2}\Big[\frac{1}{1-\lambda e^{iu}}+\frac{1}{1-\lambda e^{-iu}}\Big]=\frac{1-\lambda\cos u}{1-2\lambda\cos u+\lambda^2}\equiv D(u,\lambda)$$

giving

$$J(x,y;\lambda)\equiv\tfrac{1}{\pi}\big\{D(x-y,\lambda)-D(x+y,\lambda)\big\} \tag{10}$$

BBF observe that

$$\begin{aligned} D(u,\lambda)&=\frac{1}{1-\lambda} &&:\quad \cos u=1;\, i.e.,\ u=n\pi : n=0,\pm2,\pm4,\ldots\\ \lim_{\lambda\to1}D(u,\lambda)&=1 &&:\quad \cos u\neq 1\end{aligned} \tag{11}$$

Let $\square$ denote the square inscribed on the xy-plane with opposite vertices at $\{0,0\}$ and $\{\pi,\pi\}$. On the diagonal we have $x-y=0$, while at other interior points and $x+y<2\pi$, so by (9, 10)

$$J(x,y;\lambda)=\begin{cases}[\pi(1-\lambda)]^{-1} &:\quad \text{on the diagonal: } x=y\\ 0 &:\quad \text{elsewhere within }\square\end{cases}$$

giving

$$\lim_{\lambda\to1}J(x,y;\lambda)=\begin{cases}\infty &:\quad x=y\\ 0 &:\quad \text{otherwise}\end{cases}$$

which suggests that

$$=\delta(y-x) \tag{12}$$

To properly *establish* (12) we show that in the limit $\lambda\uparrow 1$ we realize a condition of the $\delta(y-x)$-defining form

$$\int_a^b\delta(y-x)dy=\begin{cases}0 &:\quad a<b<x\\ 1 &:\quad a<x<b\\ 0 &:\quad x<a<b\end{cases} \tag{13}$$

Termwise integration gives

$$\int_a^b J(x,y;\lambda)dy=-\tfrac{2}{\pi}\sum_{n=1}^\infty\tfrac{1}{n}\lambda^n\sin(nx)\big\{\cos(nb)-\cos(na)\big\}$$

and *Mathematica* supplies

$$\begin{aligned}-\tfrac{2}{\pi}\sum_{n=1}^\infty\tfrac{1}{n}\lambda^n\sin(nx)\cos(nb)&\\ =-i\tfrac{1}{2\pi}\Big\{&\log\big(1-\lambda e^{i(x+b)}\big)\\ &+\log\big(1-\lambda e^{i(x-b)}\big)\\ &-\log\big(1-\lambda e^{-i(x+b)}\big)\\ &-\log\big(1-\lambda e^{-i(x-b)}\big)\Big\}\\ =-i\tfrac{1}{2\pi}\log\frac{f(x+b)f(x-b)}{\bar f(x+b)\bar f(x-b)}&\quad\text{where}\quad f(u)\equiv1-\lambda e^{iu}\\ &\qquad\qquad\quad \bar f(u)=f(-u)\end{aligned}$$

Similarly

$$\begin{aligned}+\tfrac{2}{\pi}\sum_{n=1}^{\infty}\tfrac{1}{n}\lambda^n\sin(nx)\cos(na) &= +i\tfrac{1}{2\pi}\log\frac{f(x+a)f(x-a)}{\bar{f}(x+a)\bar{f}(x-a)}\\ &= -i\tfrac{1}{2\pi}\log\frac{\bar{f}(x+a)\bar{f}(x-a)}{f(x+a)f(x-a)}\\ &= -i\tfrac{1}{2\pi}\log\frac{f(-x-a)f(-x+a)}{\bar{f}(-x-a)\bar{f}(-x+a)}\end{aligned}$$

so

$$\int_a^b J(x,y;\lambda)\,dy = -i\tfrac{1}{2\pi}\log\frac{f(x+b)f(x-b)f(-x-a)f(-x+a)}{\bar{f}(x+b)\bar{f}(x-b)\bar{f}(-x-a)\bar{f}(-x+a)}$$

From

$$f(u) = 1-\lambda e^{iu} = \sqrt{1-2\lambda\cos u+\lambda^2}\,\exp\Big\{i\arctan\Big[\frac{\lambda\sin u}{\lambda\cos u-1}\Big]\Big\}$$

we obtain

$$\begin{aligned}-i\tfrac{1}{2\pi}\log\frac{f(u)}{\bar{f}(u)} = -i\tfrac{1}{2\pi}\cdot 2i\arctan\Big[\frac{\lambda\sin u}{\lambda\cos u-1}\Big] &= \tfrac{1}{\pi}\arctan\Big[\frac{\lambda\sin u}{\lambda\cos u-1}\Big]\\ &= \tfrac{1}{\pi}\arctan\big[-\cot\tfrac{1}{2}u\big]\ \text{ at } \lambda=1\\ &\equiv g(u)\end{aligned}$$

From the graph of $g(u)$ we learn that (contrary to what BBP report at $u=0$)

$$g(u) = \begin{cases}\tfrac{1}{2\pi}(u-\pi) & : \quad u>0\\ \text{indeterminate} & : \quad u=0\\ \tfrac{1}{2\pi}(u+\pi) & : \quad u<0\end{cases} \tag{14}$$

Therefore

$$\mathcal{J}(x;a,b) \equiv \int_a^b J(x,y;\lambda\uparrow 1)dy = g(x+b)+g(x-b)+g(-x-a)+g(-x+a)$$

so working from the following table

	$x+b$	$x-b$	$-x-a$	$-x+a$
$0\leqslant x<a<b\leqslant\pi$	$+$	$-$	$-$	$+$
$0\leqslant a<x<b\leqslant\pi$	$+$	$-$	$-$	$-$
$0\leqslant a<b<x\leqslant\pi$	$+$	$+$	$-$	$-$

we by (14) have—in those respective cases—

$$\mathcal{J} = \begin{cases}\tfrac{1}{2\pi}\big[(x+b-\pi)+(x-b+\pi)+(-x-a+\pi)+(-x+a-\pi)\big]=0\\ \tfrac{1}{2\pi}\big[(x+b-\pi)+(x-b+\pi)+(-x-a+\pi)+(-x+a+\pi)\big]=1\\ \tfrac{1}{2\pi}\big[(x+b-\pi)+(x-b-\pi)+(-x-a+\pi)+(-x+a+\pi)\big]=0\end{cases}$$

So we have achieved a realization of (13), which asserts the completeness of the orthonormal eigenfunctions. From the established convergence of

$$J(x,y;\lambda)=\tfrac{2}{\pi}\sum_{n=1}^{\infty}\lambda^n\sin(nx)\cdot\sin(ny)$$

we are permitted to write

$$\begin{aligned}\sum_{n=1}^{\infty}\lambda^n\sin(nx)\cdot\tfrac{1}{2}n^2\cdot\sin(ny)&=-\tfrac{1}{2}\partial_y^2\sum_{n=1}^{\infty}\lambda^n\sin(nx)\cdot\sin(ny)\\&=-\tfrac{1}{2}\partial_y^2J(x,y;\lambda)\end{aligned}$$

which in the limit $\lambda\uparrow 1$ becomes $\qquad =-\tfrac{1}{2}\partial_y^2\delta(y-x)$

which is the result that at (9) we sought. It was Euler's trick that allowed the argument to get off the ground; the argument thereafter was simple in concept, but at several points hinged on information of a sort that only a resource like *Mathematica* can provide, and upon an inventive genius that reveals the hand of Carl Bender.

Alternative approach to the particle-in-a-box problem. Supposing the Hamiltonian H to be t-independent, we have this

$$|\psi)_t=\exp\big\{\tfrac{1}{i\hbar}\mathsf{H}t\big\}|\psi)_0$$

formal solution of the time-dependent Schrödinger equation $\mathsf{H}|\psi)=i\hbar\partial_t|\psi)$. In the x-representation

$$(x|\psi)_t=\int(x|\exp\big\{\tfrac{1}{i\hbar}\mathsf{H}t\big\}|y)dy(y|\psi)_0$$

If the spectrum is discrete/non-degenerate we can use $\mathsf{H}=\sum_n|n)E_n(n|$ to obtain

$$\begin{aligned}\psi(x,t)&=\int K(x,y;t)\psi(y,0)dy\\K(x,y;t)&=\sum_n(x|n)e^{E_nt/i\hbar}(n|y)\end{aligned}$$

where the "propagator" (or "Green function") is a solution of the Schrödinger equation, distinguished from others by the property

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

Returning in this light to our boxed particle, we have

$$\begin{aligned}K_{\text{box}}(x,y;t)&=\tfrac{2}{\pi}\sum_{n=1}^{\infty}e^{-\frac{1}{2}in^2t}\sin(nx)\sin(ny)\\&=\tfrac{1}{\pi}\sum_{n=1}^{\infty}e^{-\frac{1}{2}in^2t}\big\{\cos[n(x-y)]-\cos[n(x+y)]\big\}\end{aligned}$$

Recalling the definition of the Jacobi theta function[5]

$$\vartheta_3(z,\tau) = \sum_{-\infty}^{\infty} e^{i[\pi\tau n^2 - 2zn]} = 1 + 2\sum_{n=1}^{\infty} e^{i\pi\tau n^2}\cos 2nz$$

we have

$$K_{\text{box}}(x,y;t) = \tfrac{1}{2\pi}\Big\{\vartheta\Big(\frac{x-y}{2},-\frac{t}{2}\Big) - \vartheta\Big(\frac{x+y}{2},-\frac{t}{2}\Big)\Big\} \tag{15}$$

Fundamental to the theory of theta functions is **Jacobi's Identity**

$$\vartheta(z,\tau) = \sqrt{i/\tau}\, e^{z^2/i\pi\tau}\cdot\vartheta\big(\tfrac{z}{\tau},-\tfrac{1}{\tau}\big) \tag{16}$$

in which—remarkably—τ appears upstairs on the left, but downstairs on the right.[6] Drawing upon (16) we obtain[7] this "Jacobi transform" of (15):[8]

$$K_{\text{box}}(x,y;t) = \sqrt{1/2\pi it}\sum_{n=-\infty}^{\infty}\Big[e^{i\frac{(x-y+2\pi n)^2}{2t}} - e^{i\frac{(x+y+2\pi n)^2}{2t}}\Big] \tag{17}$$

Setting $it=\sigma$, we have

$$= \sum_{n=-\infty}^{\infty}\Big[\tfrac{1}{\sqrt{2\pi\sigma}}\,e^{-\frac{(x-y+2\pi n)^2}{2\sigma}} - \tfrac{1}{\sqrt{2\pi\sigma}}\,e^{-\frac{(x+y+2\pi n)^2}{2\sigma}}\Big]$$

and in the limit $t\!\downarrow\!0$ obtain a pair of "Dirac combs"

$$\lim_{t\downarrow 0} K_{\text{box}}(x,y;t) = \sum_{n=-\infty}^{\infty}\Big[\delta(x-y+2\pi n) - \delta(x+y+2\pi n)\Big]$$
$$\downarrow$$
$$= \delta(x-y) \text{ if } x,y \text{ are both interior to the box}$$

[5] This is one of four functions (from which I will henceforth omit the identifying subscript) introduced by Carl Jacobi (1804–1851) to provide a platform for his theory of elliptic functions (1829). In the following I will draw frequently upon material in my "Applied theta functions of one or several variables," (October, 1997).

[6] Jacobi's Identity—often called "Jacobi's imaginary transformation"—plays a central role in so many such diverse applications that Richard Bellman (in his *A Brief Introduction to Theta Functions* (1961)) has remarked that "it is not easy to find another identity of comparable significance."

[7] See "Applied theta functions,"[5] page 12.

[8] If points x and y lie within the box ($0 < x, y < \pi$) there is a direct path $y \to x$ and infinitely many reflected paths, some of which are first reflected at the right wall, others at the left wall (see figures 2, 3, 4 in "Applied theta functions"[5]). Feynman summation over that population of paths (effectively, a "method of images") leads directly to (17).

We have established completeness of the functions $\{\sin nx\}$ by an alternative to the elegantly belabored method described on pages 6–8.

Note finally that if the Schrödinger equation is written

$$\mathcal{D}\psi(x,t)=0 \quad \text{with} \quad \mathcal{D}\equiv \tfrac{1}{2}\partial_x^2+i\partial_t$$

then

$$\begin{aligned}\mathcal{D}K_{\rm box}(x,y;t)&=\mathcal{D}\Big\{\tfrac{2}{\pi}\sum_{n=1}^{\infty}e^{-\frac{1}{2}in^2t}\sin(nx)\sin(ny)\Big\}\\&=\tfrac{2}{\pi}\sum_{n=1}^{\infty}\underbrace{\mathcal{D}\Big\{e^{-\frac{1}{2}in^2t}\sin(nx)\sin(ny)\Big\}}_{0}=0\end{aligned}$$

This is usually phrased as the statement that

$$\theta(x,t)\equiv\vartheta(\pi z,it)=1+2\sum_{n=1}^{\infty}e^{-\pi n^2t}\cos(2\pi nz) \quad : \quad t>0$$

satisfies the heat equation: $\frac{1}{4\pi}\partial_z^2\theta(z,t)=\partial_t\theta(z,t)$.

BBP resolution: case of a harmonic oscillator. The standard theory,[9] stripped to its bare bones (set $\hbar=m=\omega=1$), reads

$$\begin{aligned}\mathbf{H}&=-\tfrac{1}{2}\partial_x^2+\tfrac{1}{2}x^2 \qquad (18)\\ \mathbf{H}\phi_n(x)&=(n+\tfrac{1}{2})\phi_n(x)\\ \phi_n(x)&=\frac{1}{\sqrt{2^n n!\sqrt{\pi}}}H_n(x)e^{-x^2/2} \quad : \quad n=0,1,2,\ldots\end{aligned}$$

Our objective is, as before, to recover the operator (18) from the spectral decomposition of $\mathbf{H}$. Proceeding as we did on page 5, we write

$$\int(x\,\mathbf{H}|y)dy(y|\psi)=\int\sum_{n=0}(x|n)(n+\tfrac{1}{2})(n|y)dy(y|\psi)$$

whence

$$\begin{aligned}H(x,y)\equiv(x|\,\mathbf{H}\,|y)&=\sum_{n=0}\phi_n(x)(n+\tfrac{1}{2})\phi_n(y)\\&=\sum_{n=0}\big[-\tfrac{1}{2}\partial_y^2+\tfrac{1}{2}y^2\big]\phi_n(x)\phi_n(y) \qquad \star\\&=\big[-\tfrac{1}{2}\partial_y^2+\tfrac{1}{2}y^2\big]\sum_{n=0}\phi_n(x)\phi_n(y) \qquad \star\star\\&=\big[-\tfrac{1}{2}\partial_y^2+\tfrac{1}{2}y^2\big]\delta(y-x) \quad \text{by completeness}\end{aligned}$$

giving

$$\begin{aligned}\int(x\,\mathbf{H}|y)dy(y|\psi)&=\int\big[-\tfrac{1}{2}\partial_y^2+\tfrac{1}{2}y^2\big]\delta(y-x)\psi(y)dy\\&=\big[-\tfrac{1}{2}\partial_x^2+\tfrac{1}{2}x^2\big]\psi(x)\end{aligned}$$

[9] See Griffiths & Schroeter,[4] §2.3.

The argument fails at $\star \longrightarrow \star\star$ for the same reason as before: $\sum_n \phi(x)\phi_n(y)$ does not converge uniformly.

BBP resort to the same work-around as before: they look to the tempered series $\sum_n \lambda^n \phi(x)\phi_n(y)$ with the intention of finally letting the Euler parameter $\lambda \uparrow 1$. In this instance, *Mathematica* has nothing useful to say, but the problem was studied by Gustav Ferdinand Mehler (1835–1895), who in 1866 produced **Mehler's formula**,[10] of which one formulation reads

$$\sum_{n-0}^{\infty} \tfrac{\lambda^n}{2^n n!} H_n(x)H_n(y) = \frac{1}{\sqrt{1-\lambda^2}} \exp\Big\{\frac{2xy\lambda - (x^2+y^2)\lambda^2}{1-\lambda^2}\Big\} \tag{19}$$

which by $H_n(x) = \sqrt{2^n n!\sqrt{\pi}}\, e^{\frac{1}{2}x^2}\phi_n(x)$ becomes

$$\begin{aligned} J(x,y;\lambda) &\equiv \sum_{n=0}^{\infty} \lambda^n \phi_n(x)\phi_n(y) \\ &= \tfrac{1}{\sqrt{\pi}} e^{-\frac{1}{2}(x^2+y^2)} \frac{1}{\sqrt{1-\lambda^2}} \exp\Big\{\frac{2xy\lambda - (x^2+y^2)\lambda^2}{1-\lambda^2}\Big\} && (20.1) \\ &= \frac{1}{\sqrt{\pi(1-\lambda^2)}} \exp\Big\{\frac{4xy\lambda - (x^2+y^2)(1+\lambda^2)}{2(1-\lambda^2)}\Big\} && (20.2) \\ &= \frac{1}{\sqrt{\pi(1-\lambda^2)}} \exp\Big\{\frac{\lambda-1}{\lambda+1}\frac{(x+y)^2}{4} + \frac{\lambda+1}{\lambda-1}\frac{(x-y)^2}{4}\Big\} && (20.3) \end{aligned}$$

These are alternative statements of what E. T. Whittaker has called the "quantum Mehler formula." BBP reproduce what they consider to be "perhaps the simplest derivation of the Mehler formula" (of which there are—as will emerge—a great many, notable for their diversity), namely one presented by G. H. Hardy in some orthogonal polynomial lectures (1933) as later recorded in a publication of G. N. Watson; Hardy's result, as it happens, lacks the xy-summetry that is manifest on both sides of the equations (19) and (20). The right sides of (20) provide alternative descriptions of what is in effect the generating function of the bivariate functions $\phi_n(x)\phi_n(y)$, and announce the uniform convergence of $\sum_n \lambda^n \phi_n(x)\phi_n(y) : |\lambda| < 1$. The special utility of (20.3) lies in the observation that as $\lambda \uparrow 1$ we obtain (use $1-\lambda^2 = (1+\lambda)(1-\lambda)$ and write $1-\lambda = \sigma$)

$$\begin{aligned} \lim_{\lambda\uparrow 1} J(x,y;\lambda) &= \lim_{\sigma\downarrow 0} \frac{1}{\sqrt{2\pi\sigma}} \exp\Big\{-\frac{(x-y)^2}{2\sigma}\Big\} \\ &= \text{Gaussian representation of } \delta(y-x) \end{aligned} \tag{21}$$

We have, in this instance, established completeness directly, without appeal to the $\delta(y-x)$-defining condition (13).

[10] "Hermite polynomials"—of which anticipations (1810) can be found already in the work of Laplace—were studied in detail by Chebyshev (1859) in work that did not attract much attention. Hermite's independent contributions to the subject date from 1864, so the subject was still quite new when Mehler entered the picture.

With the uniform convergence of the series $J(x, y; \lambda)$ now established, we can write

$$\begin{aligned} H_{\rm osc}(x, y; \lambda) &= \sum_{n=0}^{\infty} \lambda^n \phi_n(x)\big[n + \tfrac{1}{2}\big]\phi_n(y) \\ &= \sum_{n=0}^{\infty} \lambda^n \phi_n(x)\big[-\tfrac{1}{2}\partial_y^2 + \tfrac{1}{2}y^2\big]\phi_n(y) \\ &= \big[-\tfrac{1}{2}\partial_y^2 + \tfrac{1}{2}y^2\big]\sum_{n=1}^{\infty} \lambda^n \phi_n(x)\phi_n(y) \end{aligned}$$

which in the limit $\lambda\uparrow 1$ becomes $H_{\rm osc}(x, y) = [-\frac{1}{2}\partial_y^2 + \frac{1}{2}y^2]\delta(y - x)$, giving

$$\int H_{\rm osc}(x, y)\psi(y)dy = \big[-\tfrac{1}{2}\partial_x^2 + \tfrac{1}{2}x^2\big]\psi(x)$$

Alternative approach to the oscillator problem. The oscillator propagator

$$K_{\rm osc}(x, t; y, 0) = \sum_{n=0}^{\infty} e^{-i(n+\frac{1}{2})\,t}\phi_n(x)\phi_n(y)$$

can be written

$$= e^{-i\frac{1}{2}t}\cdot \sum_{n=0}^{\infty}(e^{-it})^n\phi_n(x)\phi_n(y)$$

If, on the right side of (20), we make the replacement $\lambda \to e^{-it}$ (where the Euler parameter λ has now acquired direct physical significance) and command `ExpToTrig//Simplify` we obtain

$$K_{\rm osc}(x, t; y, 0) = \text{prefactor}\cdot \exp\big\{iS(x, t; y, 0)\big\}$$

$$S(x, t; y, 0) = \frac{(x^2 + y^2)\cos t - 2xy}{2\sin t} \tag{22.1}$$

where the prefactor, which derives partly from the zero-point shift of the oscillator spectrum, is given by

$$\text{prefactor} = \frac{\sqrt{\lambda}}{\sqrt{\pi\lambda(\lambda^{-1} - \lambda^{+1})}}\Bigg|_{\lambda\,\to\, e^{-it}} = \frac{1}{\sqrt{2\pi i \sin t}} \tag{22.2}$$

The function $S(x, t; y, 0)$ is a familiar object. For a classical oscillator with $m = \omega = 1$ the Lagrangian reads $L(\dot\xi, \xi) = \frac{1}{2}(\dot\xi^2 - \xi^2)$. Let $\xi(\tau)$ be any path with these specified endpoints: $\xi(0) = y$; $\xi(t) = x$. The "action functional" is defined

$$S[\xi(\tau)] \equiv \int_0^t L(\dot\xi(\tau), \xi(\tau))\,d\tau$$

By Hamilton's Principle

$$\delta S[\xi(t)] = 0 \quad\Longrightarrow\quad \frac{d}{d\tau}\frac{\partial L}{\partial\dot\xi} - \frac{\partial L}{\partial\xi} = 0$$

the solutions of which are "*dynamical* paths." In the present instance

$$\begin{aligned} \ddot\xi(\tau) + \xi(\tau) = 0 \quad\Longrightarrow\quad \xi_{\rm dynamical}(\tau) &= A\cos\tau + B\sin\tau \\ &= y\cos\tau + \frac{x - y\cos t}{\sin t}\sin\tau \end{aligned}$$

The "dynamical action function" (extremizer of the action functional) is the 2-point function defined

$$S(x,t;y,0) = S[\xi_{\text{dynamical}}(t)] = \int_0^t L(\dot{\xi}(\tau),\xi(\tau))\,d\tau\Big|_{\xi=\xi_{\text{dynamical}}}$$

which in the present instance becomes

$$= \frac{(x^2+y^2)\cos t - 2xy}{2\sin t}$$

From $L(\dot{\xi},\xi) = \frac{1}{2}(\dot{\xi}^2 - \xi^2)$ we obtain the Hamiltonian $H(\wp,\xi) = \frac{1}{2}(\wp^2+\xi^2)$ and *Mathematica* confirms that $S(x,t;y,0)$ satisfies the Hamilton-Jacobi equation

$$H\big(\tfrac{\partial S}{\partial x}, x\big) + \tfrac{\partial S}{\partial t} = 0$$

Reverting now to the quantum side of the story,[11] in 1941 23-year-old Richard Feynman asked Herbert Jehle (formerly a student of Schrödinger, then a visitor at Princeton) whether he had ever encountered a quantum allusion to the classical Principle of Least Action. Jehle directed him to a paper[12] in which Dirac draws attention —as he did again later in §32 of his *Principles of Quantum Mechanics*—to the structural resemblance of certain action-based classical constructions and their purported quantum analogs. Feynman asked whether Dirac's "analogies" might read as actual *equations*, and promptly demonstrated a sense in which they could be: thus was the sum-over-paths formalism born (Feynman dissertation: "The principle of least action in quantum mechanics," 1942). Fundamental to that formalism are (1) the construction

$$\begin{aligned}&K(x,t;y,0)\\ &= \sum_{\text{paths}} \iint K(x,t;x_n,n\tau)\cdots K(x_2,2\tau;x_1,\tau)K(x_1,\tau;y,0)dx_1dx_2\cdots dx_n\end{aligned}$$

$$\text{path} \quad : \quad \{x,t\} \leftarrow \{x_n,n\tau\} \leftarrow \cdots \leftarrow \{x_2,2\tau\} \leftarrow \{x_1,\tau\} \leftarrow \{y,0\}$$
$$\tau = t/(n+1)$$

and (2) the proposition that *quantum mechanics is briefly classical*:

$$K(x,t;y,0) \approx A(t)\exp\big\{\tfrac{i}{\hbar}S(x,t;y,0)\big\} \quad : \quad t \text{ small}$$

Feynman fixed $A(t)$ by the requirement that $\lim_{t\downarrow 0} K(x,t;y,0) = \delta(y-x)$.

[11] I borrow from my Quantum Lecture Notes (2000), Chapter 3, "Feynman Quantization."

[12] P.A.M.Dirac, "The Lagrangian in quantum mechanics," Physicalische Zeitschrift der Sowjetunion **3**, 61 (1933), reproduced in J. Schwinger, *Selected Papers on QED* (1958).

The WKB approximation was invented simultaneously/independently (in 1926) by Gregor Wentzel, H. A. Kramers & Léon Brillouin, all of whom worked in one dimension. John Van Vleck (1899–1980) sought in 1928 to show that the deeper significance of a certain detail becomes evident only when one works in higher dimension.[13] He established that for small t

$$K(\boldsymbol{x},t;\boldsymbol{y},0)\approx(i2\pi\hbar)^{-n/2}\sqrt{D}\,\exp\left\{\tfrac{i}{\hbar}S(\boldsymbol{x},t;\boldsymbol{y},0)\right\} \tag{23}$$
$$D(\boldsymbol{x},t;\boldsymbol{y},0)=(-)^n\det\left\|\frac{\partial^2 S(\boldsymbol{x},t;\boldsymbol{y},0)}{\partial x^r\partial y^s}\right\|$$

and that this result is exact for systems (free particles, particles in free fall, oscillators) in which the Hamiltonian H depemds at most quadratically on p and x. Van Vleck's accomplishment attracted little notice at the time (which is why, when he spoke at Brandeis in the late 1950s, he still possessed nearly all of his reprints. . . and how I acquired mine). When—after an interval of nearly thirty years—the relevance of (23) to the Feynman formalism was appreciated D came to be called "the Van Vleck determinant." In the one-dimensional case (23) reads

$$K(x,t;y,0)\approx\sqrt{\frac{i}{2\pi\hbar}\frac{\partial^2 S(x,t;y,0)}{\partial x\,\partial y}}\,\exp\left\{\tfrac{i}{\hbar}S(x,t;y,0)\right\}$$

which(set $\hbar=1$) becomes—in precise agreement with (22)—

$$K_{\rm osc}(x,t;y,0)=\sqrt{\frac{1}{2\pi i\sin t}}\,\exp\left\{i\,\frac{(x^2+y^2)\cos t-2xy}{2\sin t}\right\} \tag{24}$$

Mathematica confirms that $K_{\rm osc}(x,t;y,0)$ satisfies the Schrödinger equation

$$\tfrac{1}{2}\big[-\partial_x^2+x^2\big]\psi=i\,\partial_t\psi$$

It is a solution distinguished from others by the circumstance that (compare (21))

$$\lim_{it\downarrow 0}K_{\rm osc}(x,t;y,0)=\lim_{it\downarrow 0}\frac{1}{\sqrt{2\pi it}}\exp\left\{-\frac{(x-y)^2}{2it}\right\}=\delta(y-x)$$

which again establishes the completeness of the oscillator eigenfunctions.[14]

All of which is well and good, and supports the assertion that working from the propagator—rather than from the spectral representation of H—obviates any need to resort to Euler's trick, pretty though ramifications of the latter strategy can be.

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[13] "The correspondence principle in the statistical interpretation of quantum mechanics," PNAS **14**, 178 (1928).

[14] Equation (19) can be obtained by a variety of other means. See, for example, Quantum Lecture Notes, Chapter 3, pages 43–46, and New Chapter 0, page 40. Each of those arguments can be considered to provide a derivation of Mehler's formula.

Laguerre polynomials & the Lebedeff / Hardy-Hille formula. I am not aware of antique occurances of Hermite/Laguerre polynomials in the work of physicists, but since 1926, when Schrödinger announced the invention of the equation that bears his name, every mention of "Hermite polynomials" has caused every physicist to think of harmonic oscillators, and at every mention of "associated Laguerre polynomials" $L_n^{(\alpha)}(x) =$`LaguerreL[`n,α,x`]` to think of the hydrogen atom. Spherical separation of the time-independent wave equation implicit in the Hamiltonian

$$\mathsf{H} = \tfrac{1}{2m}(\mathsf{p}_1^2 + \mathsf{p}_2^2 + \mathsf{p}_3^2) - k\frac{1}{\sqrt{\mathsf{x}_1^2 + \mathsf{x}_2^2 + \mathsf{x}_3^2}}$$

leads[15] to $\Psi_{n\ell m}(r,\theta,\phi) = R_{n\ell}(r)\cdot Y_\ell^m(\theta,\phi)$ where

$$R_{n\ell}(r) \sim e^{-\frac{1}{2}x}x^\ell L_{n-l-1}^{(2\ell+1)}(x) \quad : \quad \begin{cases} n = 1,2,3,\dots \\ \ell = 0,1,2,\dots,n-1 \end{cases}$$
$$x \equiv \frac{2r}{na}$$

while polar separation of the in case of the Hamiltonian

$$\mathsf{H} = \tfrac{1}{2m}(\mathsf{p}_1^2 + \mathsf{p}_2^2) - k\frac{1}{\sqrt{\mathsf{x}_1^2 + \mathsf{x}_2^2}}$$

that defines "2-dimensional hydrogen"[16] leads[17] to

$$R_{n\ell}(r) \sim e^{-\frac{1}{2}x}x^\ell L_{n-\ell-1}^{(2\ell)}(x)$$
$$x \equiv \frac{2x}{(n-\frac{1}{2})a}$$

Laguerre polynomials come into play also when, in the phase space formulation of quantum mechanics, one looks to the Wigner distributions[18]

$$P_n(x,p) = \tfrac{1}{\pi\hbar}\int_{-\infty}^{\infty}\bar{\phi}_n(x+\xi)\phi_n(x-\xi)\exp[2(i/\hbar)p\xi]\,d\xi$$

associated with the oscillator eigenstates $\phi_n(n) = \frac{1}{\sqrt{2^n n!\sqrt{\pi}}}H_n(x)e^{-x^2/2}$ we

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[15] See Griffiths & Schroeter,[4] equation (4.89).

[16] Interest in this formal system springs from the fact that the classical Kepler problem gives rise to orbits that are confined to a plane. In a 2-dimensional world one would expect—if central forces fall off geometrically—to have, on the other hand,

$$\mathsf{H} = \tfrac{1}{2m}(\mathsf{p}_1^2 + \mathsf{p}_2^2) - k\log\sqrt{\mathsf{x}_1^2 + \mathsf{x}_2^2}$$

[17] See "Classical/quantum theory of 2-dimensional hydrogen" (1999), page 12.

[18] See Quantum Lecture Notes, Chapter 2, pages 10, 11.

obtain (after again setting $\hbar = m = \omega = 1$)

$$
\begin{aligned}
P_0(x,p) &= +\tfrac{1}{\pi}e^{-\frac{1}{2}\mathcal{E}}L_0(\mathcal{E}) \quad \text{where} \quad \mathcal{E} \equiv 2(p^2+x^2)\\
P_1(x,p) &= -\tfrac{1}{\pi}e^{-\frac{1}{2}\mathcal{E}}L_1(\mathcal{E}) = -\tfrac{1}{\pi}e^{-\frac{1}{2}\mathcal{E}}(1-\mathcal{E})\\
P_2(x,p) &= +\tfrac{1}{\pi}e^{-\frac{1}{2}\mathcal{E}}L_2(\mathcal{E}) = +\tfrac{1}{\pi}e^{-\frac{1}{2}\mathcal{E}}(1-2\,\mathcal{E}+\tfrac{1}{2}\mathcal{E}^2)\\
&\vdots\\
P_n(x,p) &= (-)^n\tfrac{1}{\pi}e^{-\frac{1}{2}\mathcal{E}}L_n(\mathcal{E})
\end{aligned}
$$

where the addition formula $L_n^{(\alpha+\beta+1)}(x+y) = \sum_{i=0}^n L_i^{(\alpha)}(x)L_{n-i}^{(\beta)}(y)$ supplies

$$
L_n(\mathcal{E}) = \sum_{i=0}^n L_i^{(-\frac{1}{2})}(2p^2)L_{n-i}^{(-\frac{1}{2})}(2x^2)
$$

One fine day—while still a grad student, now more than sixty years ago—I went to the Brandeis University library to consult a paper to which I had encountered a reference.[19] I took advantage of the opportunity to browse a bit, and—quite by accident—came upon a paper by E. T. Whittaker,[20] which I recognized to have much in common with a (belatedly influential) paper by Dirac[12] and to have anticipated in some respects the work of Schwinger and Feynman. Perhaps it is because we usually think of Whittaker (1873–1956, rough contemporary therefore of Arnold Sommerfeld and Einstein) as a distinguished *classical* mathematician/physicist, or perhaps World War II was a fatal distraction that caused 1941 publications to attract few readers. I have, in any event, never encountered a reference to Whittaker's paper (except for his own, in his *The History of the Theories of Aether & Electricity* [1910, revised 1951], to which in 1953 he added a Volume II in which he traced the history of quantum mechanics 1900–1926 and alludes to his own work on page 279). Whittaker's quantum paper is listed as the 55$^{\text{th}}$ of 56 RESEARCH PAPERS IN

[19] Neil H. McCoy, "Certain expansions in the algebra of quantum mechanics," Proc. Edinburgh Math Soc. (2$^{\text{nd}}$ Series) **3**, 118 (1932). I gave an account of McCoys paper—which addresses the operator ordering/reordering problem, and provides a valuable adjunct to Campbell-Baker-Hausdorff theory—at a Reed College physics seminar "An operator ordering technique with quantum mechanical applications" (12 October 1966 [see Collected Seminars, 1963–1970]) where I used McCoy's technique (as it pertains to $e^{\mathsf{p}^2+\mathsf{x}^2}$) to obtain

$$
K_{\text{osc}}(x,t;y,0) = \sqrt{\frac{m\omega}{2\pi i\hbar}}\exp\left\{\frac{i}{\hbar}m\omega\frac{(x^2+y^2)\cos\omega t - 2xy}{2\sin\omega t}\right\}
$$

which at $m = \omega = \hbar = 1$ gives back (24).

[20] "On Hamilton's principal function in quantum mechanics," Proc. Roy. Soc. (Edinburgh), Section A, **61**, 1–19 (1941).

MATHEMATICS & MATHEMATICAL PHYSICS in G. Temple's biography (available on the web), but seems otherwise to have vanished without trace ... with one sole exception: Google responds to the keyword "Whittaker quantum" with my own "E. T. Whittaker's quantum formalism: forgotten precursor to Schwinger's variational principle" (2001), which provides a 43-page account of the subject and some of its ramifications, and will be my source for what now follows.[21]

To illustrate his methods, Whittaker looks first (inevitably) to the harmonic oscillator,[22] and then to systems of the seemingly preposterous design

$$\mathsf{H} = \tfrac{1}{2m}\Big\{\tfrac{1}{\ell}\,\mathsf{p}\,\mathsf{x}\,\mathsf{p} + \frac{A}{\mathsf{x}} + B\,\mathsf{x}\Big\} \tag{25}$$

(here $[\ell]$ = length, while A and B have obvious physical dimension), which he plucks out of the air with mathematical malace aforethought. Whittaker, broadly informed classical analyst that he was, was aware that Mehler's formula —fundamental to the theory of Hermite polynomials—is representative of a *class* of such formulae. And that within that class falls "Lebedeff's formula," fundamental to the theory of generalized Laguerre polynomials.[23] Whittaker's primary objective—but by no means his only valuable accomplishment in this paper—was to construct a "quantum mechanical deduction of the Lebedeff formula."

So much for setting the stage. Turning now to the particulars of Whittaker's argument:

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[21] A much briefer synopsis of Whittaker's theory can be found in my handwritten *Lectures on Quantum Mechanics* (1967–68), Chapter III, pages 68–75.

[22] Whittaker's argument leads him to what he calls a "quantum mechanical deduction of Mehler's formula." A similar result was obtained by Feynman in 1947 (and used by him to illustrate the power of the path-integral method), and by Schwinger (who in unpublished class notes used an elegant operator-ordering terchnique) a bit later, but neither seems to have been aware of the Mehler connection... or that Whittaker had been there already. Whittaker, for his own part, appears to have been more interested in the mathematics than the physics, and neglected to mention (did not notice? seems odd) that the $S(x,t;y,0)$ in (24) is precisely the *classical action* for an oscillator—a point of which Feynman, at least, was very well aware.

[23] W. Lebedeff worked with Hilbert and took his PhD from Göttingen in 1906. Lebedeff's formula appears for the first time in Mathematische Annalen **64**, 388 (1907). Whittaker remarks that the formula was rediscovered by Einar Hille (1926), G. H. Hardy (1932) and by many others. It is today most commonly known as the "Hille-Hardy formula," else "Hardy-Hille formula," with never a mention of Lebedeff.

The polynomials $L_n^{(\alpha)}(z)$ are generated[24]

$$\sum_{n=0}^{\infty} \lambda^n L_n^{(\alpha)}(z) = \frac{1}{(1-\lambda)^{\alpha+1}} e^{-\lambda z/(1-\lambda)} \quad : \quad \alpha > -1$$

Explicitly

$$\begin{aligned} L_n^{(\alpha)}(z) &= \tfrac{1}{n!} z^{-\alpha} e^z \partial_z^n \big\{ e^{-z} z^{n+\alpha} \big\} \\ &= \sum_{k=0}^{n} C_{n,k}(\alpha)\, z^k \end{aligned}$$

$$C_{n,k}(\alpha) = (-)^k \frac{(n+\alpha)!}{k!(n-k)!(k+\alpha)!}$$

where the "shifted factorial" $(n+\alpha)! \equiv (1+\alpha)(2+\alpha)\cdots(n+\alpha) = \Gamma(n+\alpha+1)$ would, if it included the factor $(0+\alpha)$, be a "Pochhammer polynomial." From

$$\begin{aligned} C_{3,0} &= +\frac{(3+\alpha)!}{0!3!1} = \frac{(1+\alpha)(2+\alpha)(3+\alpha)}{6} \\ C_{3,1} &= -\frac{(3+\alpha)!}{1!2!(1+\alpha)!} = -\frac{(2+\alpha)(3+\alpha)}{2} \\ C_{3,2} &= +\frac{(3+\alpha)!}{2!1!(2+\alpha)!} = +\frac{(3+\alpha)}{2} \\ C_{3,3} &= -\frac{(3+\alpha)!}{3!0!(3+\alpha)!} = -\frac{1}{6} \end{aligned}$$

we obtain, for example,

$$L_3^{(\alpha)}(z) = -\tfrac{1}{6}z^3 + \tfrac{1}{2}(3+\alpha)z^2 - \tfrac{1}{2}(2+\alpha)(3+\alpha)z^1 + \tfrac{1}{6}(1+\alpha)(2+\alpha)(3+\alpha)z^0$$

which at $\alpha = 0$ gives $L_3(z) = L_3^{(0)}(z) = -\tfrac{1}{6}z^3 + \tfrac{3}{2}z^2 - 3z + 1$. Semi–inversely,

$$L_n^{(k)}(z) = (-\partial_z)^k L_{n+k}(z) \quad : \quad k \text{ an integer}$$

The polynomials $L_n^{(\alpha)}(z)$ are orthogonal in this sense

$$\int_0^\infty z^\alpha e^{-z} L_m^{(\alpha)}(z) L_n^{(\alpha)}(z)\, dz = \frac{(n+\alpha)!}{n!}\delta_{mn}$$

and are regular solutions of (it is here that the dimensionlessness of z becomes critical)

$$\big\{ z\,\partial_z^2 + (1+\alpha-z)\,\partial_z + n \big\} f(z) = 0$$

[24] Here and below z is a generic dimensionless real variable; x, when it reappears, will be a physical variable with the dimensionality $[x] = \text{length}$.

The functions

$$\varPhi_n^{(\alpha)}(z) \equiv N z^{\frac{1}{2}\alpha} e^{-\frac{1}{2}z} L_n^{(\alpha)}(z) \quad : \quad N \equiv \Big[\frac{n!}{(n+\alpha)!}\Big]^{\frac{1}{2}}, \quad \alpha > -1$$

are therefore orthonormal

$$\int_0^\infty \varPhi_m^{(\alpha)}(z)\varPhi_n^{(\alpha)}(z)\,dz = \delta_{mn} \tag{26}$$

and (see Abramowitz & Stegun, §22.6) are solutions of

$$\Big\{z\,\partial_z^2 + \partial_z + \Big[-\frac{\alpha^2}{4z} - \frac{1}{4}z + n + \frac{\alpha+1}{2}\Big]\Big\}f(z) = 0$$

as can be verified by computation in illustrative cases. But $z\,\partial_z = \partial_z z - 1$, so we have

$$\Big\{\partial_z z\,\partial_z - \frac{\frac{1}{4}\alpha^2}{z} - \tfrac{1}{4}z\Big\}f(z) = -\big\{n + \tfrac{1}{2}(\alpha+1)\big\}f(z) \tag{27}$$

Bringing the physical variable x now into play, we write $z = x/\ell$ and by $dz = (1/\ell)\,dx$ from (26) obtain the orthonomality statement

$$\int_0^\infty \varphi_m^{(\alpha)}(x)\varphi_n^{(\alpha)}(x)\,dx = \delta_{mn} \quad \text{with} \quad \varphi_n^{(\alpha)}(x) \equiv (1/\sqrt{\ell}\,)\,\varPhi_n^{(\alpha)}(x/\ell)$$

while by $\partial_z = \ell\,\partial_x$ we from (27) obtain

$$\Big\{\ell\,\partial_x x\,\partial_x - \frac{\frac{1}{4}\ell\alpha^2}{x} - \frac{x}{4\ell}\Big\}\varphi_n^{(\alpha)}(x) = -\big[n + \tfrac{1}{2}(\alpha+1)\big]\varphi_n^{(\alpha)}(x)$$

Multiplication by $(1/2m\ell^2)(\frac{\hbar}{i})^2$ gives

$$\begin{aligned}\tfrac{1}{2m}\Big\{\tfrac{1}{\ell}(\tfrac{\hbar}{i}\partial_x)x(\tfrac{\hbar}{i}\partial_x) + \frac{\frac{1}{4}\hbar^2\alpha^2/\ell}{x} + \frac{\hbar^2}{4\ell^3}x\Big\}\varphi_n^{(\alpha)}(x)&\\ = \frac{\hbar^2}{2m\ell^2}\big[n + \tfrac{1}{2}(\alpha+1)\big]\,\varphi_n^{(\alpha)}(x)&\end{aligned} \tag{28}$$

where {etc.} is the x-representation of a Hamiltonian of the Whittaker's form (25), where A and B have acquired the special form

$$A(\alpha) = \hbar^2\alpha^2/4\ell, \quad B = \hbar^2/4\ell^3$$

It is by now clear that it was mathematical opportunism, not physics, that ignited Whittaker's interest in Hamiltonians of type (25), which refers actually to an α-paramterized population of systems.

Let (28) be abbreviated

$$\begin{aligned}\mathsf{H}^{(\alpha)}\varphi_n^{(\alpha)} &= E_n^{(\alpha)}\varphi_n^{(\alpha)}\\ E_n^{(\alpha)} &= \hbar\,\omega_n^{(\alpha)} \quad \text{with} \quad \omega_n^{(\alpha)} \equiv \omega\big[n + \tfrac{1}{2}(\alpha+1)\big]\\ &\qquad\qquad\qquad\qquad\;\; \equiv \omega n + \omega_\alpha\\ &\qquad\qquad\qquad\qquad\;\;\; \omega \equiv \hbar/2m\ell^2\end{aligned} \tag{29}$$

where $n = 0, 1, 2, \ldots$ and $\alpha > -1$. It is interesting that the spectra of such systems are "displaced oscillator spectra," which I take to be yet another symptom of the ever on-going conversation between Laguerre polynomials and Hermite polynomials.

The **Hardy-Hille formula** can be rendered[25]

$$\sum_{n=0}^{\infty}\frac{n!}{(n+\alpha)!}L_n^{(\alpha)}(x)L_n^{(\alpha)}(y)\,\lambda^n = HH(x,y,\lambda;\alpha)$$

with $\quad HH(x,y,\lambda;\alpha)=\dfrac{1}{(xy\lambda)^{\alpha/2}(1-\lambda)}e^{-(x+y)\lambda/(1-\lambda)}I_\alpha\Big(\dfrac{2\sqrt{xy\lambda}}{1-\lambda}\Big)$

where $I_\alpha(\bullet)=$ `BesselI[`$\alpha,\bullet$`]` is a modified Bessel functxion of the first kind. BBP might be expected to have interest in a variant of the form

$$\sum_{n=0}^{\infty}\lambda^n\varphi_n^{(\alpha)}(x)\varphi_n^{(\alpha)}(y)=BBP(x,y,\lambda;\alpha) \tag{30}$$

and to consider λ to be an Euler parameter. The function $BBP(x,y,\lambda;\alpha)$ is simply a generating function of the bivariate functions $\varphi_n^{(\alpha)}(x)\varphi_n^{(\alpha)}(y)$, but BBP's objective would be to establish completeness

$$\sum_{n=0}^{\infty}\varphi_n^{(\alpha)}(x)\varphi_n^{(\alpha)}(y)=\delta(y-x)\quad : \quad \text{any given/fixed } \alpha$$

in the limit $\lambda\uparrow 1$.[26]

Whittaker interprets his "quantum mechanical deduction of the Lebedeff formula" assignment to mean "construct a closed-form description of the propagator"

$$\begin{aligned}K_\alpha(x,y;t)&=(x|e^{-(i/\hbar)\mathsf{H}_\alpha t}|y)\quad : \quad \mathsf{H}_\alpha=\tfrac{1}{2m}\big\{\tfrac{1}{\ell}\,\mathsf{p}\,\mathsf{x}\,\mathsf{p}+A(\alpha)\mathsf{x}^{-1}+B(\alpha)\mathsf{x}\big\}\\&=\sum_{n=0}^{\infty}\varphi_n^{(\alpha)}(x)e^{-(i/\hbar)E_n^{(\alpha)}t}\varphi_n^{(\alpha)}(x)\end{aligned}$$

which by $E_n^{(\alpha)}=(\hbar^2/2m\ell^2)\big[n+\tfrac{1}{2}(\alpha+1)\big]\equiv\hbar(\omega n+\omega_\alpha)$ reads

$$=e^{-i\omega_\alpha t}\sum_{n=0}^{\infty}\big(e^{-i\omega t}\big)^n\varphi_n^{(\alpha)}(x)\,\varphi_n^{(\alpha)}(y) \tag{31}$$

[25] See the Wikipedia article "Laguerre polynomials."

[26] Convincing numerical evidence of completeness can be based upon (12). Use numerical integration to examine

$$\int_a^b\sum_{n=0}^{N}\varphi_n^{(\alpha)}(x)\varphi_n^{(\alpha)}(y)\,dy$$

for ascending values of N and three relative positionings of $\{a,x,b\}$.

A lengthy argument[27] takes Whittaker from (31) to his formulation of the **Lebedeff formula**

$$K_\alpha(x,y;t) = \frac{e^{-\frac{1}{2}i\pi\alpha}}{2i\ell\sin(\frac{1}{2}\theta)}\exp\Big\{i\,\frac{x+y}{2\ell}\cot(\tfrac{1}{2}\theta)\Big\}J_\alpha\Big(\frac{\sqrt{xy}}{\ell\sin(\frac{1}{2}\theta)}\Big) \tag{32}$$

where $\theta \equiv \omega t$ denotes "dimensionless time" and $J_\alpha(\bullet) = \texttt{BesselJ}[\alpha,\bullet]$ is a Bessel function of the first kind. The mere existence of such a formula is sufficient (except when $\sin\big(\frac{1}{2}\theta\big)$ vanishes) to permit BBP to execute their $\sum \mathcal{D} = \mathcal{D}\sum$ step. But to complete their argument we must establish that

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

This is accomplished on page 19 of WQF.[31]

Though Lebedeff's formula (32) was obtained here from a Hamiltonian that may seem contrived, it illustrates a point of fundamental physical significance —a point noted already in connection with the boxed particle problem (and attributed there to the structure of Jacobi's identity (16)) and encountered again at (24) in connection with the oscillator problem (a consequence there of the structure of Mehler's fomula):

t lives upstairs on the left, but downstairs on the right.

In Max Born's terminology, we encounter
- the "wave representation" of quantum mechanics on the left,
- the "particle representation" on the right.

And as has been emphasized successively by Dirac, Whittaker and Feynman, it is the latter that speaks most directly to the classical-quantum connection.[28] I have encountered the claim that every quantum problem that has been solved by ordinary means (producing eigenfunctions that are higher functions of one sort or another) has by now been solved also by Feynmanesque means. Which leads one to speculate that the Mehler and Lebedeff/Hardy-Hille formulae are citizens in a vast population of such formulae, that are as varied and richly interconnected as the higher functions are known to be. On pages 30–32 of WQF I show how Mehler's formula can be recovered from (the α-parameterized population of) Lebedeff/Hardy-Hille formulae.

On pages 20–27 of WQF I explore the classical physics of Whittaker's system, and its relationship to the construction of the quantum propagator; *i.e.*, to the Lebedeff/Hardy-Hill formula.

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[27] For my account of the details, see "E. T. Whittaker's quantum formalism" (2001), pages 13–18. This essay will be denoted WQF in what follows.

[28] Modern students of that connection might take strenuous exception to such an assertion.