APPLIED THETA FUNCTIONS

of one or several variables ‡

Nicholas Wheeler, Reed College Physics Department
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Introduction. My objective here will be to provide a concise account of the stark essentials of some of my recent work as it relates to that wonderful creation of the youthful Jacobi—the theory of theta functions. I will omit details except when they bear critically upon a point at issue.[1] And in the tradition of my field (which was a tradition also of Jacobi) I will make no pretense to mathematical rigor. Because my dinner guests are mathematicians, I will leave the phenomenological meat and interpretive spice in the kitchen, and serve only the boiled bare bones of the physics that motivates me.

My subject is remarkable for the variety of its parts: it lives at a point where analysis, geometry, number theory, group theory and the calculus of variations intersect—in service of issues that (in my opinion) lie close to the heart and soul of quantum mechanics. Both the mathematics and the physics suggest that the results I have to report are—though pretty in themselves—but the tip of the proverbial iceberg, symptoms of a much richer pattern of interrelationships that lies still hidden from (my) view. The actors in our play stand presently before scrim. My daunting assignment is to describe both actors and their skit in terms which, though brief, are likely to inspire speculation concerning the drama which will unfold when the scrim is lifted.

1. Physical & mathematical fundamentals in the one-dimensional case. Consider the heat equation (diffusion equation), which in the one-dimensional case (two-dimensional spacetime) reads

$$\alpha D^2\varphi(x,t) = \tfrac{\partial}{\partial t}\varphi(x,t) \quad : \quad \alpha \text{ (real)} > 0 \text{ and } D \equiv \tfrac{\partial}{\partial x} \tag{1}$$

Proceeding (because it leads efficiently to the heart of the matter) in language

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[1] Many of those can be found in *2-Dimensional Particle-in-a-Box Problems in Quantum Mechanics: Part I* (June/July 1997), to which I will make frequent reference.

of the operational calculus, we write[2]

$$\begin{gathered}\tfrac{\partial}{\partial t}\varphi = \alpha D^2\varphi\\ \downarrow\\ \varphi_t(x) = e^{\alpha t D^2}\varphi_0(x)\end{gathered}$$

From the familiar Gaussian integral formula

$$\int_{-\infty}^{+\infty} e^{-(ax^2+2bx+c)}\,dx = \sqrt{\frac{\pi}{a}}\exp\Big\{\frac{b^2-ac}{a}\Big\} \quad : \quad \Re(a)>0$$

we have this integral representation of the operator $e^{\alpha t D^2}$:

$$e^{\alpha t D^2} = \frac{1}{\sqrt{4\pi\alpha t}}\int_{-\infty}^{+\infty} e^{-\frac{1}{4\alpha t}\xi^2}e^{-\xi D}\,d\xi$$

so

$$\begin{aligned}\varphi_t(x) &= \frac{1}{\sqrt{4\pi\alpha t}}\int_{-\infty}^{+\infty} e^{-\frac{1}{4\alpha t}\xi^2}\varphi_0(x-\xi)\,d\xi \quad \text{by Taylor's theorem}\\ &= \int_{-\infty}^{+\infty} g(\xi,t)\varphi_0(x-\xi)\,d\xi \qquad (2)\\ g(x,t) &\equiv \frac{1}{\sqrt{4\pi\alpha t}}e^{-\frac{1}{4\alpha t}x^2} \qquad (3)\end{aligned}$$

One easily establishes that $g(x,t)$ is itself a solution of the heat equation, and has these special properties:

$$\begin{gathered}\int_{-\infty}^{+\infty} g(x,t)\,dx = 1\\ \lim_{t\downarrow 0} g(x,t) = \delta(x)\end{gathered}$$

It is called by Widder[3] the "source solution." Clearly $g(-\xi,t) = g(\xi,t)$. A change of variables $\xi \longrightarrow y = x-\xi$ therefore brings (2) to the form

$$\begin{aligned}\varphi_t(x) &= \int_{-\infty}^{+\infty} g(x-y,t)\varphi_0(y)\,dy \qquad (4)\\ &= \text{weighted superposition of } y\text{-centered source solutions}\end{aligned}$$

which shows $g(x-y,t)$ to be, in effect, the "Green function" of the heat equation. Widder (Chapter I, §6) describes nine modes of transformation that send

$$\text{solution} \longrightarrow \text{solution of the heat equation}$$

The last and most curious entry on his list is the *Appell transformation*:

$$\mathsf{A} \quad : \quad \varphi(x,t) \xrightarrow[\text{Appell}]{} g(x,t)\cdot\varphi(\tfrac{x}{t},-\tfrac{1}{t}) \qquad (5)$$

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[2] Here I borrow from §6 of *"Construction & Physical Application of the Fractional Calculus"* (1997).

[3] D. V. Widder, *The Heat Equation* (1975), p.10.

In some old notes[4] I have shown that the Appell transformations (1892) stand central to some wonderful mathematics, which in the light of what is to follow may acquire new interest.

The Schrödinger equation for a quantum mechanical free particle reads

$$-\tfrac{\hbar^2}{2m}D^2\psi = i\hbar\tfrac{\partial}{\partial t}\psi \tag{6}$$

which can be got from (1) by formal "complexification of the diffusion constant"

$$\alpha \longrightarrow \lim_{\epsilon\downarrow 0}\left\{i\tfrac{\hbar}{2m}+\epsilon\right\}$$

In place of (4) one obtains a result which is conventionally notated

$$\psi(x,t) = \int K(x,t;y,0)\,\psi(y,0)\,dy \tag{7}$$

Here $K(x,t;y,0)$—by nature a Green function—is called the free particle "propagator," and can be described

$$K(x,t;y,0) = \sqrt{\tfrac{m}{iht}}\exp\left\{\tfrac{i}{\hbar}\tfrac{m}{2t}(x-y)^2\right\} \tag{8}$$

It is (so far as its $\{x,t\}$-dependence is concerned) a solution of the Schrödinger equation, distinguished from other solutions by the circumstance that

$$\lim_{t\downarrow 0}K(x,t;y,0) = \delta(x-y) \tag{9}$$

At this point the story takes a curious turn, which I might symbolize this way:

$$\begin{aligned} \text{classical mechanics} &\longleftarrow \text{quantum mechanics}\\ \boxed{\text{EMPTY OF PHYSICS}} &\longleftarrow \text{theory of heat, diffusion theory} \end{aligned}$$

$\boxed{\text{EMPTY OF PHYSICS}}$ has, of course, nothing to say about anything, but classical mechanics and quantum mechanics have been engaged in intricate dialog since the since the day quantum mechanics was invented, and classical mechanics has in particular some fairly sharp things to say about the construction of the quantum propagator; we can, according to (8), write

$$K(x,t;y,0) = \sqrt{\tfrac{i}{\hbar}\tfrac{\partial^2 S}{\partial x\partial y}}\;e^{\frac{i}{\hbar}S(x,t;y,0)} \tag{10}$$

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[4] See APPELL, GALILEAN & CONFORMAL TRANSFORMATIONS IN CLASSICAL/QUANTUM FREE PARTICLE DYNAMICS: RESEARCH NOTES 1976. In that work my objective was to identify and study the *covariance group* of (in effect) the heat equation, which turns out to be a conformal group. Central to that group are the (inversive, nonlinear) "Möbius transformations," to which the Appell transformations are very closely related.

with

$$S(x,t;y,0) = \tfrac{m}{2t}(x-y)^2 \tag{11}$$

But $S(x,t;y,0)$ is, in the sense I will explain in a moment, precisely the *dynamical action function* associated with the classical motion $(x,t) \longleftarrow (y,0)$. It is pursuant to this elementary remark that we will soon find ourselves looking to classical motions in order to realize quantum objectives. The results to which we will be led will in many cases mimic results which were first obtained in connection with the theory of heat; it strikes me as a point of deep curiosity that the theory of heat is, however, informed by no analog of the concept of "classical particulate motion." It is my impression that "complexification of the diffusion coefficient" stands near the center of this little mystery; that it opened some unintended doors; that, in a manner of speaking, it was "complexification that called classical mechanics into being."

Orthodox quantum mechanics provides (at least when the Hamiltonian H is time-independent) a standard mechanism for moving from the time-dependent Schrödinger equation

$$\mathsf{H}\psi(x,t) = i\hbar\tfrac{\partial}{\partial t}\psi(x,t) \tag{12.1}$$

to the associated propagator $K(x,t;x_0,t_0)$. Writing $\psi(x,t) = \Psi(x)e^{-\frac{i}{\hbar}Et}$, one looks to the associated time-independent Schrödinger equation

$$\mathsf{H}\,\Psi(x) = E\Psi(x) \tag{12.2}$$

Having by calculation assembled the eigenfunctions $\Psi_n(x)$—which can be arranged/assumed to be orthonormal and complete

$$\int \Psi_m(x)\Psi_n^*(x) = \delta_{mn} \quad \text{and} \quad \sum_n \Psi_n(x)\Psi_n^*(y) = \delta(x-y)$$

—and the associated eigenvalues E_n, one constructs

$$K(x,t;y,0) = \sum_n e^{-\frac{i}{\hbar}E_n t}\Psi_n(x)\Psi_n^*(y) \tag{13}$$

The sum on the right describes what is in effect a $\Psi_n^*(y)$-weighted superposition of elementary solutions $\psi_n(x,t) \equiv e^{-\frac{i}{\hbar}E_n t}\Psi_n(x)$, and by completeness gives back $\delta(x-y)$ as $t\downarrow 0$.

In the case of an unconstrained free particle—the particular case of present interest—the time-dependent Schrödinger equation reads $-\frac{\hbar^2}{2m}\big(\frac{\partial}{\partial x}\big)^2\Psi = E\Psi$. The resulting eigenfunctions

$$\Psi_p(x) \equiv \tfrac{1}{\sqrt{h}}e^{\frac{i}{\hbar}px} \tag{14}$$

are orthonormal and complete in the sense standard to Fourier transform theory

$$\int_{-\infty}^{+\infty}\Psi_p(x)\Psi_q^*(x)\,dx = \delta(p-q) \quad \text{and} \quad \int_{-\infty}^{+\infty}\Psi_p(x)\Psi_p^*(y)\,dp = \delta(x-y)$$

The associated energy spectrum

$$E_p \equiv p^2/2m$$

is continuous and (except for the ground state) doubly degenerate; $\Psi_{+p}(x)$ and $\Psi_{-p}(x)$ share the same eigenvalue, but are, except at $p = 0$, distinct. Drawing upon (13) we have

$$K(x,t;y,0) = \tfrac{1}{h}\int_{-\infty}^{+\infty} e^{-\frac{i}{\hbar}[\frac{p^2}{2m}t - p(x-y)]}\,dp \tag{15}$$

which by formal Gaussian integration[5] gives back precisely (8). Equation (15) provides what might be called the "wave representation of the free propagator," since on the right we see a $\Psi_p^*(y)$-weighted superposition of elementary "running wave solutions"

$$\psi_p(x,t) = \tfrac{1}{\sqrt{h}}e^{-\frac{i}{\hbar}[\frac{p^2}{2m}t - px]} \tag{16}$$

of the time-dependent Schrödinger equation. We are in position now to understand why the propagator—which begins life as a δ spike—becomes progressively more diffuse: it is assembled from dispersive population $\{\psi_p(x,t)\}$ of waves, each member of which runs with its own characteristic

$$\text{phase velocity} = \tfrac{1}{2}(p/m)$$

Now let the (otherwise free) mass point m be constrained to move on a loop or *ring* of circumference a. Imposition of the periodic boundary condition

$$\psi_p(x,t) = \psi_p(x+a,t)$$

restricts the set of allowed p-values: $\frac{i}{\hbar}pa = i2\pi n$ entails

$$\begin{aligned} p \longrightarrow p_n &= \mathcal{P}n \quad : \quad n = 0, \pm1, \pm2, \ldots \\ \mathcal{P} &\equiv \tfrac{h}{a} \end{aligned}$$

and causes the energy spectrum to become discrete

$$\begin{aligned} E \longrightarrow E_n = \tfrac{1}{2m}p_n^2 &= \mathcal{E}n^2 \quad : \quad n = 0, 1, 2, \ldots \\ \mathcal{E} &\equiv \tfrac{1}{2m}\mathcal{P}^2 = \tfrac{h^2}{2ma^2} \end{aligned}$$

The eigenfunctions

$$\Psi_n(x) \equiv \tfrac{1}{\sqrt{a}}e^{\frac{i}{\hbar}p_n x}$$

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[5] Flagrant formalism can be avoided if one makes the replacement $\hbar \longrightarrow \hbar - i\epsilon$ and proceeds to the limit $\epsilon \downarrow 0$ at the end of the calculation, as was advocated by Feynman. Such a program creates a rather curious state of affairs; it places physical theory on the complex plane, and associates physical reality with the boundary values assumed by certain analytic functions.

are orthonormal and complete (within the space of periodic functions) in the sense that

$$\int_0^a \Psi_m(x)\Psi_n^*(x)\,dx = \delta_{mn} \quad \text{and} \quad \sum_{n=-\infty}^{\infty} \Psi_m(x)\Psi_m^*(y) = \delta(x-y)$$

The propagator becomes[6]

$$K(x,t;y,0) = \sum_{n=-\infty}^{\infty} \tfrac{1}{a} e^{-\frac{i}{\hbar}[\mathcal{E}n^2t - \mathcal{P}n(x-y)]} \tag{17.1}$$

$$= \tfrac{1}{a}\Big\{1 + 2\sum_{n=1}^{\infty} e^{-\frac{i}{\hbar}\mathcal{E}n^2t} cos[2n\pi\tfrac{x-y}{a}]\Big\} \tag{17.2}$$

$$= \tfrac{1}{a}\Big\{1 + 2\sum_{n=1}^{\infty} e^{-i\beta n^2} cos[2n(\xi-\zeta)]\Big\} \tag{17.3}$$

where the dimensionless variables ξ, ζ and β are defined

$$\xi \equiv \pi x/a \qquad \zeta \equiv \pi y/a \qquad \beta \equiv \mathcal{E}t/\hbar$$

Borrowing notation (which is by no means standard in this field) now from Abramowitz & Stegun **16.27** ∼ Whittaker & Watson Chapter XXI ∼ Bellman's *Brief Introduction to Theta Functions* §2, we write

$$\vartheta(z,\tau) \equiv \sum_{n=-\infty}^{\infty} e^{i[\pi\tau n^2 - 2zn]} = 1 + 2\sum_{n=1}^{\infty} q^{n^2}\cos 2nz \quad \text{with} \quad q = e^{i\pi\tau} \tag{18}$$

and find that (17) can be expressed

$$K(x,t;y,0) = \tfrac{1}{a}\vartheta\big(\xi-\zeta, -\tfrac{\beta}{\pi}\big) \tag{19}$$
$$\tfrac{\beta}{\pi} = \tfrac{ht}{2ma^2}$$
$$\xi - \zeta = \pi\tfrac{x-y}{a}$$

Quantum physics has at this point entered into conversation with (and has been put in position to ransack) the elaborately developed *theory of theta functions*[7] and all that radiates therefrom. As will soon emerge, each has things to teach the other.

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[6] Compare (15). The "Gaussian integral"—which was seen at (8) to describe an elementary function—is replaced here by a "Gaussian sum," which doesn't; it describes what will instantly declare itself to be a "theta function."

[7] When Jacobi (1829) pioneered in this area he had in mind not partial differential equations but the theory of elliptic functions. Reading from §134J of *The Encyclopedic Dictionary of Mathematics* (to which one must look for

The defining equation (18) can be notated

$$\begin{aligned}\vartheta(z,\tau) &= \sum_{n=-\infty}^{\infty} e^{(-i2n)z+\alpha(-i2n)^2\tau} \quad \text{provided we set } \alpha = -\tfrac{i\pi}{4} \qquad (20)\\ &= \text{superimposed solutions of the ``heat equation'' } \{\alpha\partial_z^2 - \partial_\tau\}\vartheta = 0\end{aligned}$$

The theta function $\vartheta(z,\tau)$ is therefore itself a solution of the heat equation, and so also therefore is its Appell transform

$$\mathsf{A}\,\vartheta(z,\tau) = \underbrace{\frac{1}{\sqrt{4\pi\alpha\tau}}e^{-\frac{1}{4\alpha\tau}z^2}}_{=\frac{1}{\pi}\sqrt{\frac{i}{\tau}}e^{\frac{1}{i\pi\tau}z^2} \quad \text{because } \alpha=-\frac{i\pi}{4}} \cdot\vartheta\big(\tfrac{z}{\tau},-\tfrac{1}{\tau}\big) \tag{21}$$

But fundamental to the theory of theta functions in the identity

$$\vartheta(z,\tau) = A\cdot\vartheta\big(\tfrac{z}{\tau},-\tfrac{1}{\tau}\big) \quad \text{where} \quad A\equiv\sqrt{i/\tau}\,e^{z^2/i\pi\tau} \tag{22}$$

which—idiosyncratically—I call "Jacobi's identity,"[8] and concerning which Bellman remarks that it

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

Returning with (22) to (21) we obtain this novel formulation of Jacobi's identity:

$$\vartheta(z,\tau) \text{ is an eigenfunction of the Appell operator: } \mathsf{A}\vartheta = \tfrac{1}{\pi}\vartheta \tag{23.1}$$

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the precise meaning of the notation) one has

$$\operatorname{sn} w = \frac{\theta_3(0)\theta_1(v)}{\theta_2(0)\theta_4(v)}, \quad \operatorname{cn} w = \frac{\theta_4(0)\theta_2(v)}{\theta_2(0)\theta_4(v)}, \quad \operatorname{dn} w = \frac{\theta_4(0)\theta_3(v)}{\theta_3(0)\theta_4(v)}, \quad \text{etc.}$$

which suggest the sense in which theta functions—of which there are actually four kinds; what I call $\vartheta(z,\tau)$ is actually $\vartheta_3(z,\tau)$—"cleave" the theory of elliptic functions, which they support as a kind of superstructure.

I note in passing that Fourier, in his *Analytic Theory of Heat* (1822), treats what has come to be called the "Fourier ring problem" and is led to a result essentially equivalent to (19). Widder (Chapter V, §8) speculates that this may have been the first use of ϑ_3.

[8] The standard appellation (!)—"Jacobi's imaginary transformation"—sounds to my ear too much (but maybe not inappropriately) like a magic act. I suspect that Jacobi himself obtained (22) by series manipulation. For an elementary proof, which hinges on the "Poisson summation formula," see Part I §4 or Courant & Hilbert, *Methods of Mathematical Physics I*, pp. 74–77.

And if, with Magnus & Oberhettinger (Chapter VII, §1) and others, we adopt this modified definition

$$\theta(z,\tau) \equiv \vartheta(\pi z,\tau) = \sum_{n=-\infty}^{\infty} e^{(-i2\pi n)z+\hat{\alpha}(-i2\pi n)^2\tau} \quad \text{with } \hat{\alpha} \equiv \tfrac{1}{\pi^2}\alpha$$

we are led to the following more vivid variant of (23.1):

$$\theta(z,\tau) \text{ is Appell-invariant: } \mathbf{A}\theta = \theta \tag{23.2}$$

Equations (23) derive interest from the fact that they serve to establish a direct link between the theory developed in these pages—a theory dominated by the theta function—and theory pertaining to the group of transformations that map $\mathcal{S} \longrightarrow \mathcal{S}$, where $\mathcal{S}$ is the *solution set* that arises when to the heat equation (Schrödinger equation) are conjoined certain side conditions

We take now a quantum mechanical step which Fourier, working the thermal side of the street, was neither analytically positioned nor physically motivated to take. Bringing Jacobi's identity (22) to (19), we obtain

$$\begin{aligned} K(x,t;y,0) &= \tfrac{1}{a}\sqrt{-\tfrac{i\pi}{\beta}}\; \underbrace{e^{-\frac{1}{i\beta}(\xi-\zeta)^2}\vartheta(-\pi\tfrac{\xi-\zeta}{\beta},+\tfrac{\pi}{\beta})} \\ &\qquad\qquad\qquad = \sum_{n=-\infty}^{\infty} e^{\frac{i}{\beta}(\xi+n\pi-\zeta)^2} \text{ after simplifications} \\ &= \sqrt{\tfrac{m}{iht}}\sum_{n=-\infty}^{\infty} e^{\frac{i}{\hbar}\frac{m}{2t}[(x+na)-y]^2} \end{aligned} \tag{24}$$

and it is to provide an interpretation of this result that I turn now to review of some ideas essential to classical mechanics.

Let $q^1, q^2, \ldots, q^n$ coordinatize the configuration space of a mechanical system, and let $L(\dot{q},q)$ be the Lagrangian (the "system characterizer"). In Lagrangian mechanics the dynamical problem presents itself as the problem of constructing solutions (subject to side conditions) of the equations of motion

$$\Big\{\frac{d}{dt}\frac{\partial}{\partial \dot{q}^k} - \frac{\partial}{\partial q^k}\Big\}L(\dot{q},q) = 0 \quad (k = 1,2,\ldots,n)$$

Hamilton's principle[9] as us to think of those as the Euler-Lagrange equations that result from stipulating that the *action functional*

$$S[q(t)] \equiv \int_{t_0}^{t_1} L(\dot{q}(t),q(t))\,dt$$

be (in the fixed-endpoint sense of Figure 1) extremal:

$$\delta S[q(t)] = 0$$

[9] Which is only one (though certainly the most important) of the numerous "variational principles of mechanics." Note particularly that the "Principle of Leasst Action" is—surprisingly—something quite else.

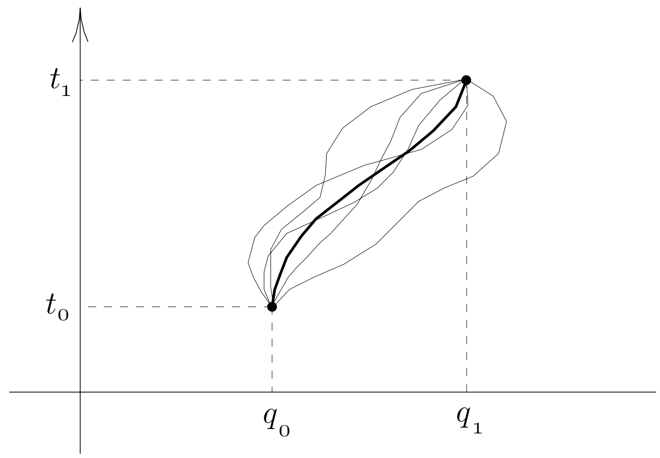

FIGURE 1: *The construction basic to the "fundamental problem of the calculus of variations" generally, and to Hamilton's principle in particular. A "dynamical path" linking the specified endpoints—which is to say: an extremizer of the action functional* S[path]—*is indicated by a heavy curve.*

I will write

$$q_{\text{dynamical}}(t) \sim \text{ dynamical path } (q_1, t_1) \longleftarrow (q_0, t_0)$$

when I want to emphasize that I have in mind a *solution* of the equations of motion, an "extremizer of the action functional." Clearly

$$\begin{aligned} S[q_{\text{dynamical}}(t)] &= \text{ function only of endpoint data that determines the path} \\ &= S(q_1, t_1; q_0, t_0), \text{ the } \textit{dynamical action function} \end{aligned}$$

in which connection it is important to note that whereas

- the dynamical path consistent with given initial data $(q_0, \dot{q}_0)$ is unique,
- one, several or infinitely many dynamical paths can conform to given endpoint data $(q_1, t_1; q_0, t_0)$.

Turning now from generalities to particulars: to describe (relative to an inertial frame) the one-dimensional dynamics of a free mass point m one writes

$$L = \tfrac{1}{2}m\dot{x}^2$$

Then $\ddot{x} = 0$ gives

$$x(t) = \begin{cases} x_0 + v(t - t_0) & \text{solution identified by initial data} \\[2ex] x_0 + \frac{x_1 - x_0}{t_1 - t_0}(t - t_0) & \text{solution identified by endpoint data} \end{cases}$$

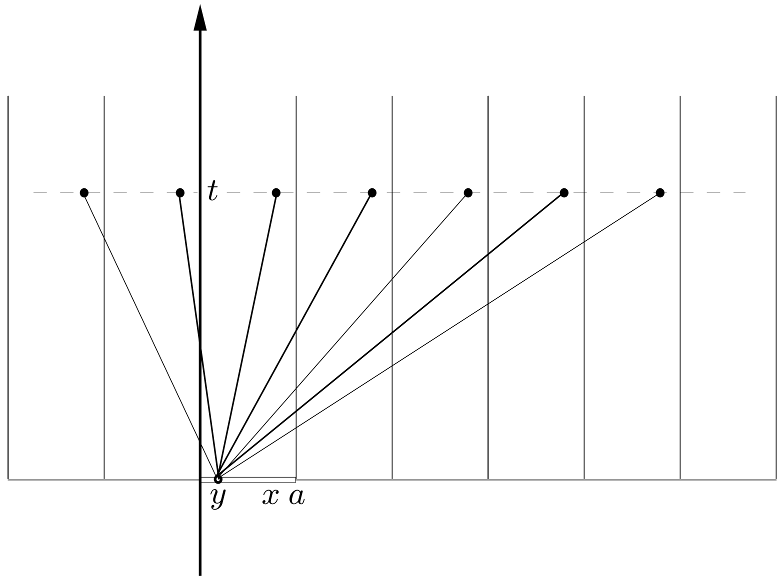

FIGURE 2: *On a ring (of circumference a, with x taken to mean arc length) the points x and $x+na$ $(n=0,\pm1,\pm2,\ldots)$ are physically identical. There are therefore an infinitude of distinct dynamical paths linking a specified pair of physical endpoints. In our treatment of the ring problem we have, by the way, set aside all considerations having to do with the fact that x coordinatizes a* curved *manifold.*

and we compute

$$\begin{aligned} S_{\text{free}}(x_1,t_1;x_0,t_0) &= \frac{m}{2}\frac{(x_1-x_0)^2}{(\,t_1-\,t_0)} \\ &= \frac{m}{2}\frac{(\text{distance traveled})^2}{\text{duration of flight}} \end{aligned} \tag{25}$$

This result—this explicit description[10] of the extreme value (actually the least value) assumed by the action functional $S_{\text{free}}[\text{path}]$—exposes the meaning of (11), and supplies at the same time an interpretation of (24), for we are in position now to recognize that

$$\tfrac{m}{2t}[(x+na)-y]^2 = \begin{array}{l}\text{dynamical action of a free particle that circuits the}\\ \text{ring } n \text{ times while } \textit{en route} \text{ from } (y,0) \text{ to } (x,t)\end{array}$$

and therefore to write (see Figure 2)

$$\begin{aligned} K(x,t;y,0) &= \sqrt{\tfrac{m}{iht}}\sum_{n=-\infty}^{\infty} e^{\frac{i}{\hbar}S[n\text{-loop dynamical path: }(x,t)\leftarrow(y,0)]} \\ &= \sqrt{\tfrac{m}{iht}}\sum_{\text{all such paths}} e^{\frac{i}{\hbar}S[\text{dynamical path: }(x,t)\leftarrow(y,0)]} \end{aligned}$$

[10] It is a curious fact that the literature supplies only a few such examples.

Study of the ring problem has brought us to the realization that the propagator can (at least within the context of that particular problem) be described in either of two distinct ways:

$$K(x,t;y,0) = \begin{cases} \displaystyle\sum_n e^{-\frac{i}{\hbar}E_n t}\Psi_n(x)\Psi_n^*(y) \\ \displaystyle\sqrt{\tfrac{m}{iht}} \sum_{\text{all such paths}} e^{\frac{i}{\hbar}S[\text{dynamical path }(x,t)\leftarrow(y,0)]} \end{cases} \tag{26}$$

We were led from the top statement (WAVE REPRESENTATION) to the bottom statement (PARTICLE REPRESENTATION) by appeal to Jacobi's identity, and know on those grounds that the two representations are "Appell equivalent" in the sense that the Appell transformation sends either into the other. I draw attention in Part I §2 to the fact that, while Jacobi's formula does enjoy the status of an "identity," its left and right sides are *compationally quite distinct*. A similar remark pertains to (26); the "particle representation" is computationally most useful—in this context and others—when t is small:

> *Quantum mechanics becomes "classical" (in a sense often symbolized $\hbar \downarrow 0$) in the short-time approximation $t \downarrow 0$*

Note particularly in this connection that the time variable t is "upstairs" in the wave representation, but "downstairs" in the particle representation.

Now let the mass point be confined not to a ring but to the interior of a "one-dimensional box:" $0 \le x \le a$. From the clamped boundary conditions[11]

$$\psi(0,t) = \psi(a,t) = 0 \qquad (\text{all } t)$$

we are led to the orthonormal eigenfunctions

$$\Psi_n(x) = \sqrt{\tfrac{2}{a}}\sin(n\pi\tfrac{x}{a}) \quad : \quad n = 1,2,3,\ldots$$

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[11] "Probability conservation" is expressed $\partial_t P + \partial_x J = 0$, where

$$\begin{aligned} P &\equiv \psi^*\psi &&: \quad \text{probability density} \\ J &\equiv i\tfrac{\hbar}{2m}(\psi\psi_x^* - \psi_x\psi^*) &&: \quad \text{probability current} \end{aligned}$$

The clamped boundary condition is consistent with, but not enforced by, the more general requirement

$$J(0,t) = J(a,t) = 0 \qquad (\text{all } t)$$

The alternatives are, however, physically more natural to thermal physics than to quantum mechanics. Our methods extend straightforwardly to *all* cases.

The associated eigenvalues can still be described $E_n = \mathcal{E}n^2$, but $\mathcal{E}$ has now a quarter of its former value:[12]

$$\mathcal{E}_{\text{box}} = \tfrac{h^2}{8ma^2} = \tfrac{1}{4}\mathcal{E}_{\text{ring}}$$

And the spectrum has now lost its former degeneracy.

Working in the wave representation, it is now immediate that

$$\begin{aligned} K(x,t;y,0) &= \tfrac{1}{a}\sum_{n=1}^{\infty} e^{-i\beta n^2}\underbrace{2\sin n\xi\cdot\sin n\zeta}_{=\cos n(\xi-\zeta)-\cos n(\xi+\zeta)} \\ &= \tfrac{1}{2a}\Big[\vartheta\big(\tfrac{\xi-\zeta}{2},-\tfrac{\beta}{\pi}\big)-\vartheta\big(\tfrac{\xi+\zeta}{2},-\tfrac{\beta}{\pi}\big)\Big] \end{aligned} \tag{27.1}$$

Drawing upon Jacobi's identity, we pass to the particle representation:

$$\begin{aligned} &= \tfrac{1}{2a}\sqrt{\tfrac{\pi}{i\beta}}\Big[e^{\frac{i}{\beta}(\frac{\xi-\zeta}{2})^2}\vartheta\big(-\tfrac{\pi(\xi-\zeta)}{2\beta},\tfrac{\pi}{\beta}\big)-e^{\frac{i}{\beta}(\frac{\xi+\zeta}{2})^2}\vartheta\big(-\tfrac{\pi(\xi+\zeta)}{2\beta},\tfrac{\pi}{\beta}\big)\Big] \\ &= \sqrt{\tfrac{\pi}{4a^2 i\beta}}\sum_{-\infty}^{\infty}\Big[e^{\frac{i\pi^2}{\beta}\left(\frac{\xi-\zeta}{2\pi}+n\right)^2}-e^{\frac{i\pi^2}{\beta}\left(\frac{\xi+\zeta}{2\pi}+n\right)^2}\Big] \\ &= \sqrt{\tfrac{m}{iht}}\sum_{-\infty}^{\infty}\Big[e^{\frac{i}{\hbar}\{\frac{m}{2}\frac{(x-y+2an)^2}{t}\}}-e^{\frac{i}{\hbar}\{\frac{m}{2}\frac{(x+y+2an)^2}{t}\}}\Big] \end{aligned} \tag{27.2}$$

It was this result—interpreted as suggested by Figures 3 & 4—that gave rise to the terminology "quantum mechanical method of images," and inspired the present research effort.[13] Since

- paths represented $(x+2na,t) \longleftarrow (y,0)$ entail an even number of reflections, while
- paths represented $(-x+2na,t) \longleftarrow (y,0)$ entail an odd number

we can consider the minus sign in (27.2) to arise from a factor of the form

$$(-)^{\text{number of reflections}}$$

And we would obtain such a factor if the action function acquired a jump discontinuity

$$\Delta S = (\text{integer} + \tfrac{1}{2})h$$

at each reflection point. Physical grounds on which one might account for such jump discontinuity terms ΔS are presented near the end of Part I §1. In connection with the allusion to "Stokes' phenomenon" presented there in a footnote, see also §253.C in *Encyclopedic Dictionary of Mathematics*. Note

[12] Retaining the abbreviation $\beta = \mathcal{E}t/\hbar$, this entails $\beta_{\text{box}} = \frac{1}{4}\beta_{\text{ring}}$. The physics here is analogous to that of closing the ends of an organ pipe previously open at both ends, and the analogy could be made perfect if only organ builders had thought to make *toroidal* pipes.

[13] For historical remarks, see Part I §2.

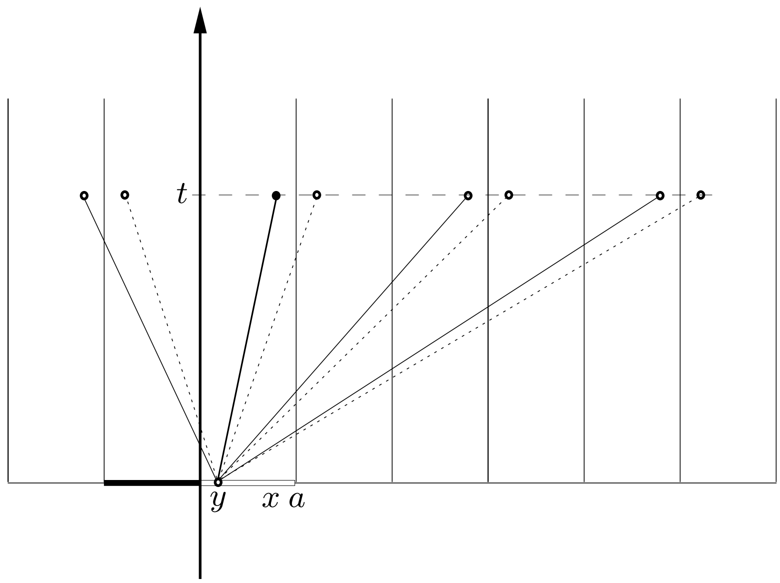


FIGURE 3: *Direct and image paths associated with the box problem (compare Figure 2). The "fundamental unit" contains two cells—the physical box and an image box. "Tessellation of the line" results from translated replication of the fundamental unit:* $x \to x + nT$ *with* $T \equiv 2a$. *Translates of* $x_0 \equiv x$ *are even, translates of* $x_1 \equiv -x$ *are odd.*

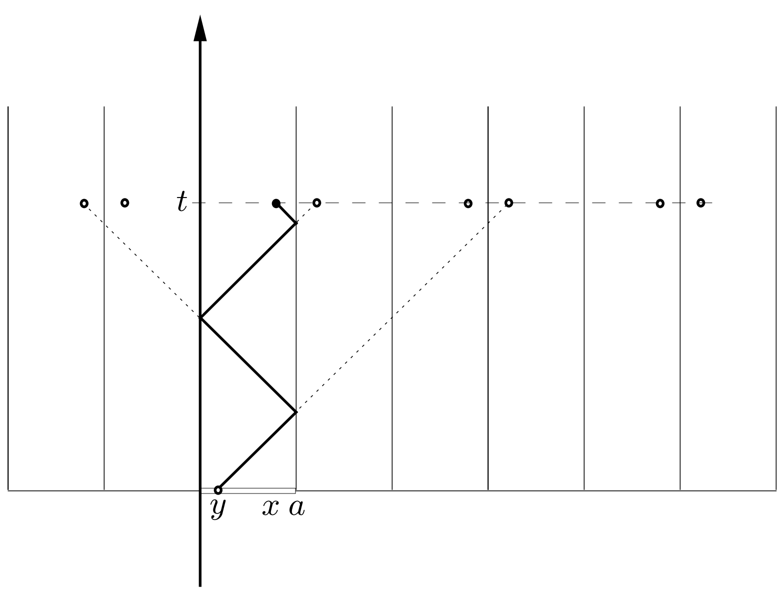


FIGURE 4: *Construction by which fictitious image paths give rise in physical spacetime to multiply reflected paths.*

how utterly elementary was the mechanism by which—at (27.1)—the even/odd distinction was forced upon us. Note also that by this interpretation (26) pertains not only to the ring problem but also to the box problem; we have made spontaneous contact with a simplified instance of the "Feynman formalism," according to which one can expect to write

$$K_{\text{particle representation}}(x,t;x_0,t_0) \sim \int e^{\frac{i}{\hbar}S[\text{path}]}d[\text{paths}]$$

where the "path integral" embraces not just the dynamical paths but (in the sense of Figure 1) *all* the Hamiltonian comparison paths $(x,t) \longleftarrow (x_o,t_0)$.[14]

RESEARCH PROBLEM: The intrusion of the theta function (theory of elliptic functions) stands as an invitation to *establish explicit contact with the theory of automorphic functions*.

RESEARCH PROBLEM: To the extent that a Feynman formalism remains in force when

$$L = \tfrac{1}{2}m\dot{x}^2 \quad \text{is generalized to} \quad L = \tfrac{1}{2}m\dot{x}^2 - U(x)$$

there should exist a "generalized Appell transformation" such that

$$K_{\text{wave}} \xleftrightarrow[\text{generalized Appell}]{} K_{\text{particle}}$$

Find it. One might, as a first step, be well-advised to look closely to the cases $U(x) = mgx$ and $U(x) = \frac{1}{2}m\omega^2x^2$ in which both representations of the propagator are known in explicit detail. Such a theory, if it could be developed, would give back Jacobi's identity —and all that flows from it—as a special case!

2. General remarks concerning classical motion within a polygonal box. The objective of our effort thus far has been to extract insight into the "principles of classical assembly" of K_{particle} from knowledge of how eigenvalues E_n and eigenfunctions $\Psi_n(x)$ (independently computed) enter into the assembly of K_{wave}. At this point the flow of the argument reverses its drift: we will use classical physics (and the principles now at our command) to construct K_{particle}, which we will process in such a way as to premit extraction of information concerning the spectrum and eigenfunctions—information which we would (in at least some cases) be unable to obtain by independent means. That program

[14] The Feynman integral—the "Feynman quantization procedure"—has, for all of its technical imperfections, become an indispensible tool of contemporary quantum physics. Both the Feynman integral and (in diffusion/heat theory) its cousin, the Wiener integral, are very "Gaussian" in spirit and detail. That circumstance can be traced to the circumstance that $L = T - U$ and the kinetic energy T is *quadratic* in velocity. And beyond that, to the circumstance that physics in a relativistic world is necessarily (nearest-neighbor) *local*, whence the intrusion of ∇^2 operators.

can, however, be carried to completion only in certain favorable cases. The following remarks are intended to highlight what is so "special" about those favorable cases.

Two-dimensional boxes have diverse shapes (all one-dimensional boxes have, on the other hand, the same shape), and the reflective adventures of a free particle confined to the interior of such a box are correspondingly diverse.

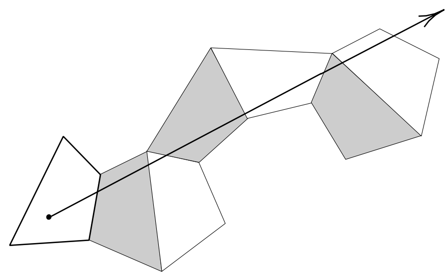


FIGURE 5: *A particle is launched from a prescribed point in a prescribed direction. Its subsequent reflective adventures can be constructed by reflective covering of the prolonged ray. See also Figure 44 in Part I. Adjustment of the initial data would result in quite a different figure, and superposition of all such figures would yield unintelligible hash.*

The adventures implicit in given *initial* data are easy to construct (see the figure), but the (diverse) adventures consistent with given *endpoint* data appear to yield to ennumeration only in those exceptional cases in which all such figures are in fact the same figure. This happens in a subset of the cases in which the box "reflectively tessellates the plane." Tom Wieting (1980) has established that there exist precisely eight such tessellations. Of those, four (Figure 6) are, for our purposes, "tractable," while another four (Figure 7) remain (in the present state of the art) intractable. The tractable cases are distinguished from intractable cases in several (interrelated) respects:

- only in the "tractable" cases is is possible to assign unambiguous orientation and parity to reflective images of the physical box, and therefore to set up constructions of the type illustrated in Figure 8;
- wedges are known from the theory of waves[15] to be "diffractive" unless

$$\text{wedge angle} = \frac{\pi}{\text{integer}}$$

  All of the intractable cases—and none of the tractable ones—contain angles in violation of this condition.

See, in this connection, also the captions of Figures 6 & 7.

[15] Oberhettinger (1958); see footnote 54 in Part I for the detailed citation. See also R. E. Crandall, "Exact propagator for motion confined to a sector," J. Phys. A Math. Gen. **16**, 513 (1983).

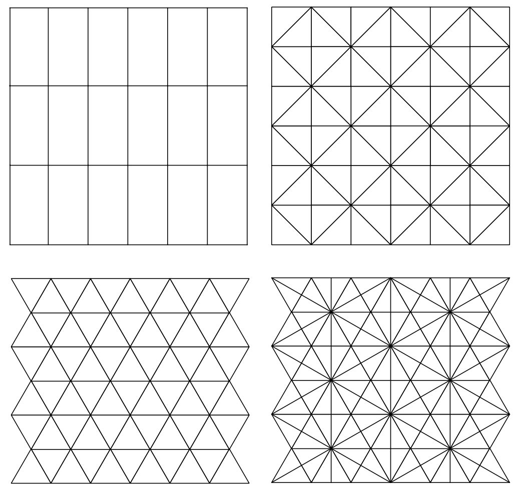


FIGURE 6: *The four "tractable" tessellations of the plane. All vertices are, in each case, of even order, and each tessellation serves to rule the plane.*

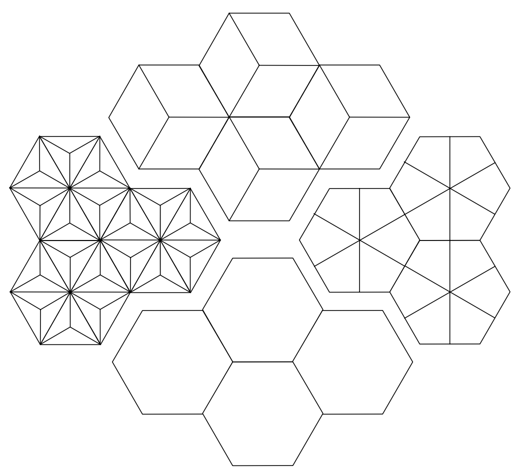


FIGURE 7: *The four "intractable" tessellations. Each contains vertices of odd order, and (since each contains interrupted line segments) none serves to rule the plane.*

Details relating to each of the tractable cases are presented in Part I. Here I present a synoptic account of the method of images as it pertains only to the equilateral box problem. This is, in several respects, the most characteristic —also the most interesting—of the simple box problems; it leads to a spectrum of number-theoretic interest, and to eigenfunctions that cannot be obtained the method of separation.

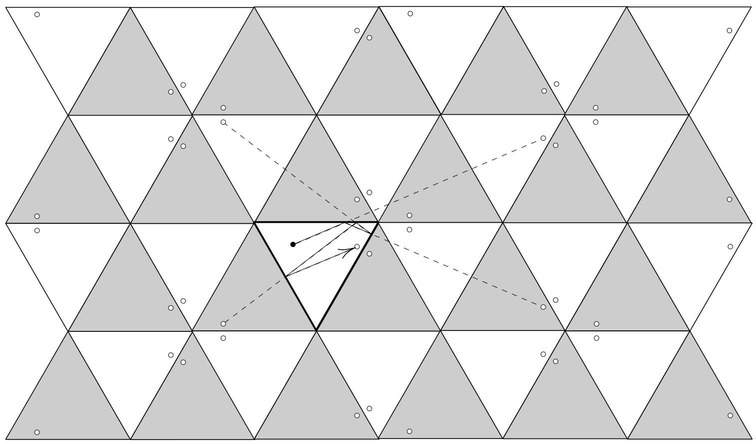
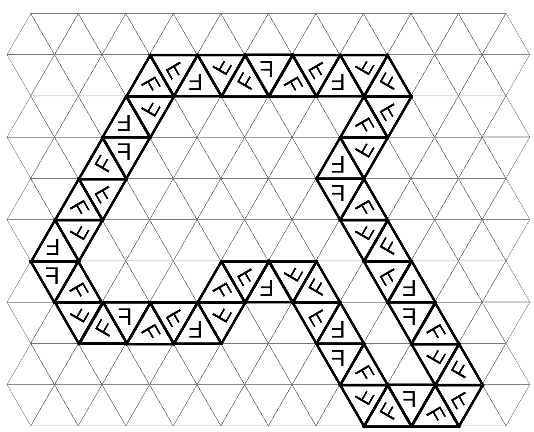


FIGURE 8: *Construction of a* 4^{th}*-order cushion shot on a triangular billiard table. The motion becomes periodic when the source point occupies a position from which the targeted image point is seen to eclipse the image point in a similarly-oriented image of the physical box. Similar constructions are possible in all the tractable cases; the rectangular analog appears as Figure 10 in Part I.*

RESEARCH PROBLEM: The following figure demonstrates that *"reflective transport" around a closed curve brings about no change in orientation*…just as, in flat space, parallel transport around a



loop has no effect. The tractable tessellations are, in this sense, "flat," and the intractable ones "curved." Develop theory adequate to account for the path-dependence of orientation and parity. Such a theory would presumably provide a kind of "reflective imitation" of some standard differential geometry.

3. Setting up the equilateral box problem. Our objective is quantum mechanical, but—characteristically of the method of images—we look first to the classical problem. Figure 10 establishes the dimension of the physical box, and its position/orientation with respect to a Cartesian coordinate system. A total

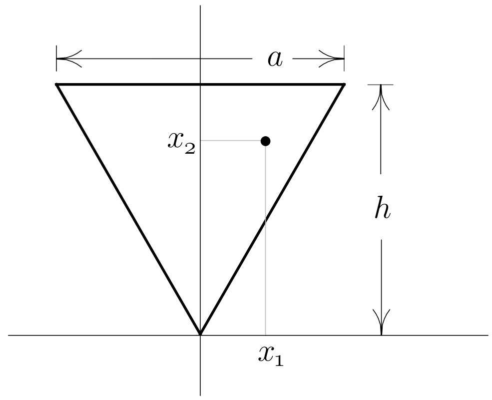


FIGURE 10: *Coordinate system used in analysis of the equilateral box problem.*

of six orientational variants of the physical box occur on the tessellated plane. A sample of each is present in the conventionally-defined "fundamental unit" (Figure 11). Working out the coordinates of the "fundamental images" of $\boldsymbol{x}$, we obtain

$$\begin{aligned}
\boldsymbol{x}_0 &= \begin{pmatrix} +1 & 0 \\ 0 & +1 \end{pmatrix}\boldsymbol{x} \quad \text{with} \quad \boldsymbol{x} \equiv \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \\
\boldsymbol{x}_1 &= \tfrac{1}{2}\begin{pmatrix} -1 & -\sqrt{3} \\ -\sqrt{3} & +1 \end{pmatrix}\boldsymbol{x}_0 \\
\boldsymbol{x}_2 &= \tfrac{1}{2}\begin{pmatrix} -1 & -\sqrt{3} \\ +\sqrt{3} & -1 \end{pmatrix}\boldsymbol{x}_0 \\
\boldsymbol{x}_3 &= \begin{pmatrix} +1 & 0 \\ 0 & -1 \end{pmatrix}\boldsymbol{x}_0 \\
\boldsymbol{x}_4 &= \tfrac{1}{2}\begin{pmatrix} -1 & +\sqrt{3} \\ -\sqrt{3} & -1 \end{pmatrix}\boldsymbol{x}_0 \\
\boldsymbol{x}_5 &= \tfrac{1}{2}\begin{pmatrix} -1 & +\sqrt{3} \\ +\sqrt{3} & +1 \end{pmatrix}\boldsymbol{x}_0
\end{aligned}$$

"Siblings" of $\boldsymbol{x}_\alpha$ reside at the points $\boldsymbol{x}_\alpha + n_1\boldsymbol{T}_1 + n_2\boldsymbol{T}_2$, where

$$\boldsymbol{T}_1 = \tfrac{a}{2}\begin{pmatrix} 3 \\ +\sqrt{3} \end{pmatrix} \quad \text{and} \quad \boldsymbol{T}_2 = \tfrac{a}{2}\begin{pmatrix} 3 \\ -\sqrt{3} \end{pmatrix}$$

In Part I §3 I develop the "semi-miraculous proof" that the squared length of

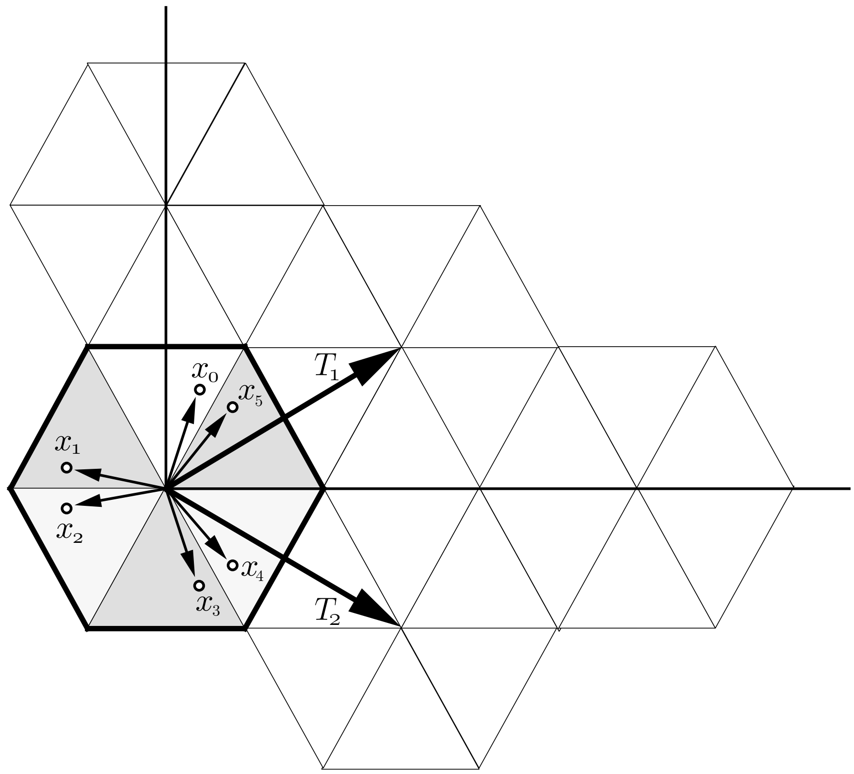


FIGURE 11: *Identification of the six elements that will be taken to comprise the "fundamental unit," names assigned to the associated "fundamental images" of the physical target point* $\boldsymbol{x} \equiv \boldsymbol{x}_0$*, and the (non-orthogonal) translation vectors* $\boldsymbol{T}_1$ *and* $\boldsymbol{T}_2$ *that serve to replicate the fundamental unit. White elements are even (in the sense theat they give rise to paths with an even number of reflection points), shaded elements are odd; by notational contrivance*

$$\text{parity of } \boldsymbol{x}_\alpha = (-)^\alpha$$

the displacement vector $\boldsymbol{x}_{\text{image point}} \equiv \boldsymbol{x}_\alpha + n_1\boldsymbol{T}_1 + n_2\boldsymbol{T}_2 - \boldsymbol{y}$ (source point to target image) can be described

$$|\boldsymbol{x}_{\text{image point}} - \boldsymbol{y}|^2 = (\boldsymbol{v}_\alpha + \boldsymbol{n})\cdot\mathbb{T}(\boldsymbol{v}_\alpha + \boldsymbol{n})$$

where

$$\boldsymbol{v}_\alpha \equiv \mathbb{T}^{-1}\begin{pmatrix} \boldsymbol{S}_\alpha\cdot\boldsymbol{T}_1 \\ \boldsymbol{S}_\alpha\cdot\boldsymbol{T}_2 \end{pmatrix} \quad \text{with} \quad \mathbb{T} \equiv \begin{pmatrix} \boldsymbol{T}_1\cdot\boldsymbol{T}_1 & \boldsymbol{T}_1\cdot\boldsymbol{T}_2 \\ \boldsymbol{T}_2\cdot\boldsymbol{T}_1 & \boldsymbol{T}_2\cdot\boldsymbol{T}_2 \end{pmatrix} \text{ and } \boldsymbol{S}_\alpha \equiv \boldsymbol{x}_\alpha - \boldsymbol{y}$$

In service of clarity I will not introduce the explicit descriptions of $\boldsymbol{v}_\alpha$ and $\mathbb{T}$ until we have actual need of them.

We expect now to have (in the particle representation)[16]

$$\begin{aligned} K(\boldsymbol{x},t;\boldsymbol{y},0) &= \sqrt{\left(\tfrac{m}{iht}\right)^{\text{dimension}}} \sum_{\text{all images}} \exp\left\{\tfrac{i}{\hbar}S\big((\boldsymbol{x}_{\text{image}},t)\longleftarrow(\boldsymbol{y},0)\big)\right\} \\ &= \tfrac{m}{iht}\sum_{\alpha=0}^{5}(-)^\alpha\sum_{\boldsymbol{n}}\exp\left\{\tfrac{i}{\hbar}S_\alpha\right\} \qquad (28) \\ &\qquad\qquad \tfrac{i}{\hbar}S_\alpha \equiv \beta(\boldsymbol{v}_\alpha+\boldsymbol{n})\cdot\mathbb{T}(\boldsymbol{v}_\alpha+\boldsymbol{n}) \end{aligned}$$

where—beware!—β has acquired (compare p. 6) a new definition:

$$\beta \equiv im/2\hbar t$$

At (28) we encounter an expression of the form

$$\sum_{\boldsymbol{n}} e^{i[\text{term quadratic in } \boldsymbol{n} \,+\, \text{term linear in } \boldsymbol{n}]}$$

and it is that circumstance (compare (18)) which motivates the following digression:

4. Theta functions of several variables. Let $g(x_1,x_2,\ldots,x_p)$ be some nice function of several variables, and form

$$G(x_1,x_2,\ldots,x_p) \equiv \sum_{\boldsymbol{n}} g(x_1+n_1,x_2+n_2,\ldots,x_p+n_p)$$

which exhibits the periodicity of the unit lattice in p-space. We have this "p-dimensional generalization of the Poisson summation formula"[17]

$$\sum_{\boldsymbol{n}} g(\boldsymbol{x}+\boldsymbol{n}) = \sum_{\boldsymbol{n}} e^{2\pi i\boldsymbol{n}\cdot\boldsymbol{x}}\int_{-\infty}^{+\infty} g(\boldsymbol{y})e^{-2\pi i\boldsymbol{n}\cdot\boldsymbol{y}}\,dy_1dy_2\cdots dy_p \qquad (29)$$

In the particular case $g(\boldsymbol{x}) = e^{-\boldsymbol{x}\cdot\mathbb{A}\boldsymbol{x}}$ (the matrix can without loss of generality be assumed to be symmetric, and by explicit assumption its eigenvalues all lie on the right half-plane) we have

$$\sum_{\boldsymbol{n}} e^{-(\boldsymbol{x}+\boldsymbol{n})\cdot\mathbb{A}(\boldsymbol{x}+\boldsymbol{n})} = \sum_{\boldsymbol{n}} e^{2\pi i\boldsymbol{n}\cdot\boldsymbol{x}}\int_{-\infty}^{+\infty} e^{-(\boldsymbol{y}\cdot\mathbb{A}\boldsymbol{y}+2\boldsymbol{b}\cdot\boldsymbol{y})}\,dy_1dy_2\cdots dy_p$$

with $\boldsymbol{b} \equiv i\pi\boldsymbol{n}$. Drawing now upon the famous "multidimensional Gaussian integral formula"

$$\int_{-\infty}^{+\infty} e^{-(\boldsymbol{y}\cdot\mathbb{A}\boldsymbol{y}+2\boldsymbol{b}\cdot\boldsymbol{y})}\,dy_1dy_2\cdots dy_p = \sqrt{\frac{\pi^p}{\det\mathbb{A}}}\,e^{\boldsymbol{b}\cdot\mathbb{A}^{-1}\boldsymbol{b}}$$

[16] Compare PartI §5.
[17] See Part I §4 for supporting details and references.

we obtain—as a particular implication of (29)—

$$\sum_{\boldsymbol{n}} e^{-(\boldsymbol{x}+\boldsymbol{n})\cdot\mathbb{A}\,(\boldsymbol{x}+\boldsymbol{n})} = \sqrt{\frac{\pi^p}{\det\mathbb{A}}}\sum_{\boldsymbol{n}} e^{2\pi i\,\boldsymbol{n}\cdot\boldsymbol{x}-\pi^2\boldsymbol{n}\cdot\mathbb{A}^{-1}\boldsymbol{n}} \tag{30}$$

Equivalently[18]

$$\begin{aligned}\sum_{\boldsymbol{n}} e^{-\pi^2\boldsymbol{n}\cdot\mathbb{B}\boldsymbol{n}-2\pi i\,\boldsymbol{n}\cdot\boldsymbol{x}} &= \frac{1}{\sqrt{\pi^p\det\mathbb{B}}}\sum_{\boldsymbol{n}} e^{-(\boldsymbol{x}+\boldsymbol{n})\cdot\mathbb{B}^{-1}(\boldsymbol{x}+\boldsymbol{n})}\\ &= \frac{1}{\sqrt{\pi^p\det\mathbb{B}}}\,e^{-\boldsymbol{x}\cdot\mathbb{B}^{-1}\boldsymbol{x}}\sum_{\boldsymbol{n}} e^{-\boldsymbol{n}\cdot\mathbb{B}^{-1}\boldsymbol{n}-2\boldsymbol{x}\cdot\mathbb{B}^{-1}\boldsymbol{n}}\end{aligned}$$

which by notational adjustment[19]

$$\mathbb{B} = \frac{1}{i\pi}\mathbb{W} \quad\text{and}\quad \boldsymbol{x} = \frac{\boldsymbol{z}}{\pi}$$

reads

$$\underbrace{\sum_{\boldsymbol{n}} e^{i(\pi\boldsymbol{n}\cdot\mathbb{W}\boldsymbol{n}-2\boldsymbol{n}\cdot\boldsymbol{z})}}_{\equiv\,\vartheta(\boldsymbol{z},\mathbb{W})\quad\text{by proposed definition}} = \sqrt{\frac{i^p}{\det\mathbb{W}}}\,e^{-i\frac{1}{\pi}\boldsymbol{z}\cdot\mathbb{M}\boldsymbol{z}}\sum_{\boldsymbol{n}} e^{-i(\pi\boldsymbol{n}\cdot\mathbb{M}\boldsymbol{n}+2\boldsymbol{n}\cdot\mathbb{M}\boldsymbol{z})} \tag{31}$$

In this notation (31) becomes

$$\vartheta(\boldsymbol{z},\mathbb{W}) = \sqrt{\frac{i^p}{\det\mathbb{W}}}\,e^{-i\frac{1}{\pi}\boldsymbol{z}\cdot\mathbb{M}\boldsymbol{z}}\cdot\vartheta(\mathbb{M}\boldsymbol{z},-\mathbb{M}) \tag{32}$$

which is the multivariable generalization of Jacobi's identity (22). Writing

$$\vartheta(\boldsymbol{z},\mathbb{W}) = \sum_{\boldsymbol{n}} e^{i\pi\boldsymbol{n}\cdot\mathbb{W}\boldsymbol{n}}\{\cos 2\boldsymbol{n}\cdot\boldsymbol{z} - i\sin 2\boldsymbol{n}\cdot\boldsymbol{z}\}$$

we observe that only the cosine term survives the summation process, so we have

$$\vartheta(\boldsymbol{z},\mathbb{W}) = \sum_{\boldsymbol{n}} e^{i\pi\boldsymbol{n}\cdot\mathbb{W}\boldsymbol{n}}\,\cos 2\boldsymbol{n}\cdot\boldsymbol{z} \tag{33}$$

which gives back (18) in the one-dimensional case, and proves especially useful in our intended applications.

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[18] I find it convenient at this point to introduce the notation $\mathbb{B}\equiv\mathbb{A}^{-1}$.

[19] I encounter here a small problem: I need a matrix analog of τ, but $\mathbb{T}$ has been preempted. I give the assignment to $\mathbb{W}$ because it lends itself to the easily remembered clutter-reducing usage $\mathbb{M}\equiv\mathbb{W}^{-1}$. In (31) below I will on one occasion draw upon the symmetry of $\mathbb{M}$ to write $\boldsymbol{n}\cdot\mathbb{M}\boldsymbol{z}$ in place of $\boldsymbol{z}\cdot\mathbb{M}\boldsymbol{n}$.

We are in position now to contemplating writing a multidimensional book about the *properties* of $\vartheta(\boldsymbol{z},\mathbb{W})$ and its relationships to multi-variable generalizations of other functions central to higher analysis. But this is not the place, nor am I the man to undertake such an assignment. I return to the main line of my story, content to develop specific properties in response to specific needs, as they arise.[20]

5. Passage to the wave representation of the propagator. In notation supplied by (31) we have

$$\sum_{\boldsymbol{n}} e^{\beta(\boldsymbol{v}+\boldsymbol{n})\cdot\mathbb{T}(\boldsymbol{v}+\boldsymbol{n})} = e^{\beta\boldsymbol{v}\cdot\mathbb{T}\boldsymbol{v}}\cdot\vartheta\big(i\beta\mathbb{T}\boldsymbol{v}, -\tfrac{i\beta}{\pi}\mathbb{T}\big) \tag{34.1}$$

which, by appeal to Jacobi's identity (32) and after a good deal of tedious simplification (during the course of which the exponential prefactor disappears), becomes

$$= \sqrt{\big(-\tfrac{\pi}{\beta}\big)^p\tfrac{1}{\det\mathbb{T}}}\,\vartheta\big(\pi\boldsymbol{v}, \tfrac{\pi}{i\beta}\mathbb{T}^{-1}\big) \tag{34.2}$$

Returning with this information to (28) we have

$$\begin{aligned}
K(\boldsymbol{x},t;\boldsymbol{y},0) &= \underbrace{\tfrac{m}{iht}\big(-\tfrac{\pi}{\beta}\big)\sqrt{\tfrac{1}{\det\mathbb{T}}}}_{=\sqrt{\frac{1}{\det\mathbb{T}}}=\frac{1}{6\cdot\text{area}}}\sum_{\alpha=0}^{5}(-)^\alpha\vartheta\big(\pi\boldsymbol{v}_\alpha, \tfrac{\pi}{i\beta}\mathbb{T}^{-1}\big)\\
&\qquad\qquad\qquad \text{area of physical box} = \tfrac{1}{4}\sqrt{3}a^2\\
&= \tfrac{1}{6\cdot\text{area}}\sum_{\alpha=0}^{5}(-)^\alpha\sum_{\boldsymbol{n}} e^{i\pi\boldsymbol{n}\cdot\frac{\pi}{i\beta}\mathbb{T}^{-1}\boldsymbol{n}}\cos 2\pi\boldsymbol{n}\cdot\boldsymbol{v}_\alpha\\
&= \tfrac{1}{6\cdot\text{area}}\sum_{\boldsymbol{n}} e^{-\frac{i}{\hbar}\mathcal{E}(n_1^2-n_1n_2+n_2^2)t}\sum_{\alpha=0}^{5}(-)^\alpha\cos 2\pi\boldsymbol{n}\cdot\boldsymbol{v}_\alpha
\end{aligned}\tag{35}$$

$$\mathcal{E}\equiv\tfrac{2}{9}\frac{h^2}{ma^2}$$

The fact that t resides now *upstairs* in the exponent is clear indication that we have achieved a formulation of K_{wave}. Our assignment now is to bring (35) into precise and explicit structural agreement with (13), so that we can simply *read off* the eigenvalues and associated eigenfunctions.

---

[20] It is interesting to note that

$$\Theta(\mathbb{W},\boldsymbol{z})\equiv\sum_{\boldsymbol{n}} e^{i(\pi\boldsymbol{n}\cdot\mathbb{W}\boldsymbol{n}+2\pi\boldsymbol{n}\cdot\boldsymbol{z})}$$

—which differs from my $\vartheta(\boldsymbol{z},\mathbb{W})$ only by in inconsequential sign and an almost inconsequential factor of π—is known to *Mathematica* as `SiegelTheta[W,z]`, and is called up by the command `<<NumberTheory‘SiegelTheta‘`. Concerning this function, the author of p. 320 in *Standard Add-on Packages 3.0* remarks that it "was initially investigated by Riemann and Weierstrass and further studies were done by Frobenius and Poincaré. These investigations represent some of the most significant accomplishments of 19th Century mathematics."

6. Number-theoretic properties of the spectrum. In the exponent of (35) we encounter

$$n_1^2 - n_1 n_2 + n_2^2 = \tfrac{1}{2}\boldsymbol{n}^{\mathsf{T}}\begin{pmatrix} 2 & -1 \\ -1 & 2 \end{pmatrix}\boldsymbol{n}$$

The following equations

$$\begin{pmatrix} 2 & -1 \\ -1 & 2 \end{pmatrix}\begin{pmatrix} 1 \\ 1 \end{pmatrix} = 1\cdot\begin{pmatrix} 1 \\ 1 \end{pmatrix} \quad\text{and}\quad \begin{pmatrix} 2 & -1 \\ -1 & 2 \end{pmatrix}\begin{pmatrix} 1 \\ -1 \end{pmatrix} = 3\cdot\begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

summarize the spectral properties of the symmetric matrix, and put us in position to write

$$\begin{pmatrix} 2 & -1 \\ -1 & 2 \end{pmatrix} = \tfrac{1}{2}\cdot\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}^{\mathsf{T}}\begin{pmatrix} 1 & 0 \\ 0 & 3 \end{pmatrix}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

The immediate implication is that

$$\begin{aligned} n_1^2 - n_1 n_2 + n_2^2 &= \tfrac{1}{4}\hat{\boldsymbol{n}}^{\mathsf{T}}\begin{pmatrix} 1 & 0 \\ 0 & 3 \end{pmatrix}\hat{\boldsymbol{n}} \quad\text{with}\quad \hat{\boldsymbol{n}} \equiv \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}\boldsymbol{n} \equiv \mathbb{R}\boldsymbol{n} \\ &= \tfrac{1}{4}\big[(n_1+n_2)^2 + 3(n_1-n_2)^2\big] \\ &= \tfrac{1}{4}\underbrace{\big[\hat{n}_1^2 + 3\hat{n}_2^2\big]}_{\equiv N(\hat{\boldsymbol{n}})} = \tfrac{1}{4}(\hat{n}_1 + i\sqrt{3}\hat{n}_2)(\hat{n}_1 - i\sqrt{3}\hat{n}_2) \end{aligned} \tag{36}$$

By these elementary remarks we are plunged into the world of algebraic number theory, and more specifically into what L. W. Reid calls[21] "the realm $k(\sqrt{-3})$."

It is at this point that we pick our first indication that the numbers $\hat{\boldsymbol{n}}$ serve more naturally to index the objects of interest to us—eigenvalues and eigenfunctions—than do the numbers $\boldsymbol{n}$. But

$$\begin{aligned} n_1 &= \tfrac{1}{2}(\hat{n}_1 + \hat{n}_2) \\ n_2 &= \tfrac{1}{2}(\hat{n}_1 - \hat{n}_2) \end{aligned}$$

will be integers if an only $\hat{n}_1$ and $\hat{n}_2$ are either both ever or both odd; it will be, therefore, our understanding[22] that

$$\hat{\mathbf{n}} \in \text{same-parity sublattice}$$

By this adjustment, and with this understanding, (35) has become

$$K(\boldsymbol{x},t;\boldsymbol{y},0) = \tfrac{1}{6\cdot\text{area}}\sum_{\hat{\boldsymbol{n}}}{}' e^{-\frac{i}{\hbar}\hat{\mathcal{E}}(\hat{n}_1^2+3\hat{n}_2^2)t}\sum_{\alpha=0}^{5}(-)^\alpha\cos\pi\hat{\boldsymbol{n}}\cdot\hat{\boldsymbol{v}}_\alpha \tag{37}$$

---

[21] I quote the title of Chapter VI in his *Elements of the Theory of Algebraic Numbers* (1910). Reid taught at Haverford College, and his text (introduction by David Hilbert) is so old-fashioned as to be intelligible even to this physicist. I myself have only incidental interest in the theory of algebraic numbers, but from bibliographic remarks appended by Bellman to the final sections of his little monograph I gain the impression that algebraic numbers were a *primary* interest of the people—giants with names like Landau, Hecke, Siegel, Mordell—who, during years 1919–1940, were mainly responsible for cultivation of the theory of what Bellman calls "multidimensional theta functions."

[22] See Figure 24 in Part I §8.

where the prime on the $\sum'$ signifies constraint to the sublattice; also

$$\hat{\mathcal{E}} \equiv \tfrac{1}{4}\mathcal{E} = \tfrac{1}{18}\tfrac{h^2}{ma^2}$$

and[23]

$$\hat{\boldsymbol{v}}_\alpha \equiv \mathbb{R}\boldsymbol{v}_\alpha = \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}\boldsymbol{v}_\alpha$$

Critical use will be made of ramifications of the observation that

$$\hat{n}_1^2 + 3\hat{n}_2^2 = \Big(\frac{-\hat{n}_1 + 3\hat{n}_2}{2}\Big)^2 + 3\Big(\frac{-\hat{n}_1 - \hat{n}_2}{2}\Big)^2$$

which can be phrased

$$N(\hat{\boldsymbol{n}}) = N(\mathbb{A}\hat{\boldsymbol{n}}) \quad \text{with} \quad \mathbb{A} \equiv \tfrac{1}{2}\begin{pmatrix} -1 & +3 \\ -1 & -1 \end{pmatrix}$$

and traced to the circumstance that

$$\mathbb{A} \quad : \quad \text{same-parity lattice points} \longmapsto \text{same-parity lattice points}$$

and has the property that

$$\mathbb{A}^\mathsf{T}\mathbb{G}\mathbb{A} = \mathbb{G} \quad \text{with} \quad \mathbb{G} \equiv \begin{pmatrix} 1 & 0 \\ 0 & 3 \end{pmatrix}$$

From $\det(\mathbb{A} - \lambda\mathbb{I}) = \lambda^2 + \lambda + 1$ we learn that the eigenvalues of $\mathbb{A}$ are the complex cube roots of unity, while the Hamilton-Jacobi theorem supplies

$$\mathbb{A}^2 + \mathbb{A} + \mathbb{I} = \mathbb{O} \quad \text{whence} \quad \mathbb{A}^3 = \mathbb{I}$$

The practical upshot of preceding remarks is this: the norm $N(\hat{\boldsymbol{n}})$ is invariant under action of $\mathbb{A}$

$$\hat{\boldsymbol{n}} \longrightarrow \mathbb{A}\hat{\boldsymbol{n}} \longrightarrow \mathbb{A}^2\hat{\boldsymbol{n}} \longrightarrow \hat{\boldsymbol{n}} \text{ again}$$

and also under all reflective transformations.[24] So each non-axial lattice point $\hat{\boldsymbol{n}}$ has a set of eleven companions (and each axial point a set of five companions)

[23] The argument runs this way: $\hat{\boldsymbol{n}} = \mathbb{R}\boldsymbol{n}$ entails $\boldsymbol{n}^\mathsf{T} = \hat{\boldsymbol{n}}^\mathsf{T}\mathbb{Q}$ with $\mathbb{Q} \equiv (\mathbb{R}^{-1})^\mathsf{T}$, so we have $\boldsymbol{n}\cdot\boldsymbol{v} = \boldsymbol{n}^\mathsf{T}\boldsymbol{v} = \hat{\boldsymbol{n}}^\mathsf{T}\mathbb{Q}\,\boldsymbol{v}$. As it happens, $\mathbb{Q} = \frac{1}{2}\mathbb{R}$. So we define $\hat{\boldsymbol{v}} \equiv \mathbb{R}\,\boldsymbol{v}$ and obtain $\boldsymbol{n}\cdot\boldsymbol{v} = \frac{1}{2}\,\hat{\boldsymbol{n}}\cdot\hat{\boldsymbol{v}}$. We see now, by the way, why in (37) the 2 has disappeared from the argument of the cosine.

[24] By which phrase I understand these

$$\hat{\boldsymbol{n}} \longrightarrow \begin{pmatrix} - & 0 \\ 0 & + \end{pmatrix}\hat{\boldsymbol{n}}, \text{ else } \begin{pmatrix} + & 0 \\ 0 & - \end{pmatrix}\hat{\boldsymbol{n}}, \text{ else } \begin{pmatrix} - & 0 \\ 0 & - \end{pmatrix}\hat{\boldsymbol{n}}$$

which will be distinct except when $\hat{\boldsymbol{n}}$ lies on one axis or the other.

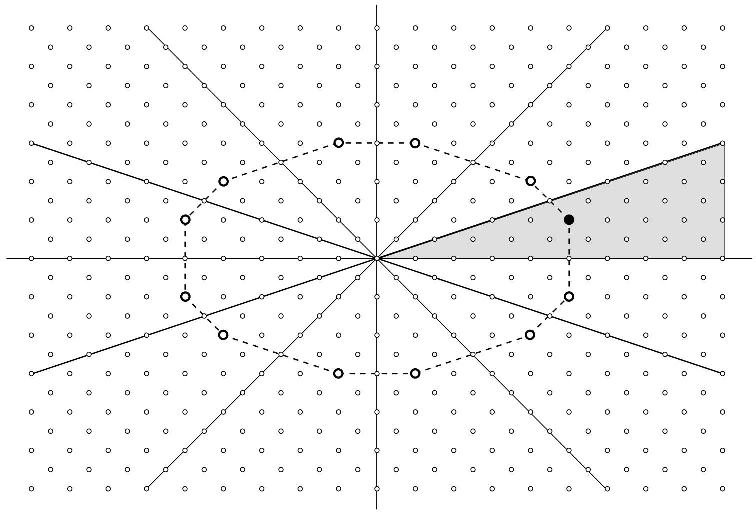

FIGURE 12: *The same-parity sublattice of the $\hat{\boldsymbol{n}}$-lattice is resolved by action of $\mathbb{A}$ into twelve sectors. An arbitrarily selected sector (shaded) will be called the "fundamental sector" or* "wedge." *Each point interior to the wedge has eleven companions with which it shares the value of its norm; collectively, those points comprise the elements of a 12-element* "orbit." *Points on the upper/lower edge of the wedge are elements of 6-element orbits; for representations of those, see Figure 26 in Part I.*

with which it shares the value of its norm. The situation is illustrated in the preceding figure.

What we have gained by this excursion into the theory of algebraic numbers in an ability to resolve one of the summation processes that enter into (37), writing

$$\sum_{\hat{\boldsymbol{n}}}{}' e^{-\frac{i}{\hbar}\hat{\mathcal{E}}(\hat{n}_1^2+3\hat{n}_2^2)t}\cdot(\text{etc})$$
$$= \sum\nolimits'_{\text{wedge points}} e^{-\frac{i}{\hbar}\hat{\mathcal{E}}(\hat{n}_1^2+3\hat{n}_2^2)t}\cdot\underbrace{\Big\{\sum\nolimits_{\text{orbit identified by a wedge point}}\Big\}}_{\text{“sum over spectral symmetries”}}(\text{etc})$$

This step will be shown in the next section to play a key role in the...

7. Assembly of the eigenfunctions. By computation—in service of clarity I omit the details,[25] even though it was from those patterned details that I first apprehended the importance of $\mathbb{A}$—one obtains

[25] Those are spelled out on pp. 40–46 of Part I, and with the assistance of *Mathematica* are not really too burdensome.

$$\sum_{\alpha=0}^{5}(-)^\alpha \cos\pi\,\hat{\boldsymbol{n}}\cdot\hat{\boldsymbol{v}}_\alpha = 2\Big\{\;F_{\hat{\boldsymbol{n}}}(\xi_1,\xi_2)\cdot\sin[2\hat{n}_1\zeta_1]\sin[2\hat{n}_2\zeta_2] + G_{\hat{\boldsymbol{n}}}(\xi_1,\xi_2)\cdot\cos[2\hat{n}_1\zeta_1]\sin[2\hat{n}_2\zeta_2]\Big\} \tag{38}$$

where the dimensionless variables $\boldsymbol{\xi}$ and $\boldsymbol{\zeta}$ have been defined

$$\begin{aligned}\xi_1 &\equiv \tfrac{\pi}{3a}x_1 & \zeta_1 &\equiv \tfrac{\pi}{3a}y_1\\ \xi_2 &\equiv \tfrac{\pi}{3a}\sqrt{3}\,x_2 & \zeta_2 &\equiv \tfrac{\pi}{3a}\sqrt{3}\,y_2\end{aligned}$$

and where

$$\begin{aligned}F_{\hat{\boldsymbol{n}}}(\xi_1,\xi_2) \equiv \sin[2\hat{n}_1\xi_1]\sin[2\hat{n}_2\xi_2] &- \sin[\hat{n}_1(\xi_1+\xi_2)]\sin[\hat{n}_2(3\xi_1-\xi_2)]\\ &+ \sin[\hat{n}_1(\xi_1-\xi_2)]\sin[\hat{n}_2(3\xi_1+\xi_2)]\end{aligned} \tag{39.1}$$

$$\begin{aligned}G_{\hat{\boldsymbol{n}}}(\xi_1,\xi_2) \equiv \cos[2\hat{n}_1\xi_1]\sin[2\hat{n}_2\xi_2] &+ \cos[\hat{n}_1(\xi_1+\xi_2)]\sin[\hat{n}_2(3\xi_1-\xi_2)]\\ &- \cos[\hat{n}_1(\xi_1-\xi_2)]\sin[\hat{n}_2(3\xi_1+\xi_2)]\end{aligned} \tag{39.2}$$

Observe that $\boldsymbol{\xi}$ and $\boldsymbol{\zeta}$ enter *asymmetrically* into the expression on the right side of (38). Our effort now will be focused on the removal of that surprising defect. We begin by noticing that the following equations

$$\left.\begin{aligned}&\sin(a_1z_1+a_2z_2)\sin(b_1z_1+b_2z_2)-\sin(a_1z_1-a_2z_2)\sin(b_1z_1-b_2z_2)\\ &\qquad=\sin(a_1+b_1)z_1\sin(a_2+b_2)z_2-\sin(a_1-b_1)z_1\sin(a_2-b_2)z_2\\ &\cos(a_1z_1+a_2z_2)\sin(b_1z_1+b_2z_2)-\cos(a_1z_1-a_2z_2)\sin(b_1z_1-b_2z_2)\\ &\qquad=\cos(a_1+b_1)z_1\sin(a_2+b_2)z_2-\cos(a_1-b_1)z_1\sin(a_2-b_2)z_2\end{aligned}\right. \tag{40}$$

have the status of *identities*.

> RESEARCH PROBLEM: The identities (40)—which play a magical role in the present application, and give indication of being representative of a broader *class* of little-known identities—almost "prove themselves" once they have been stated, but do not "beg to be stated." Develop a theoretical framework which provides a natural context for such identities, and makes transparent their validity.

Using the first of those identites to manipulate the last two terms on the right side of (39.1), and the second to do the same to (39.2), we obtain

$$\left.\begin{aligned}F_{\hat{\boldsymbol{n}}}(\xi_1,\xi_2) = \sin[2\hat{n}_1\xi_1]\sin[2\hat{n}_2\xi_2] &+ \sin[2\tfrac{-\hat{n}_1+3\hat{n}_2}{2}\xi_1]\sin[2\tfrac{-\hat{n}_1-\hat{n}_2}{2}\xi_2]\\ &+ \sin[2\tfrac{-\hat{n}_1-3\hat{n}_2}{2}\xi_1]\sin[2\tfrac{+\hat{n}_1-\hat{n}_2}{2}\xi_2]\\ G_{\hat{\boldsymbol{n}}}(\xi_1,\xi_2) = \cos[2\hat{n}_1\xi_1]\sin[2\hat{n}_2\xi_2] &+ \cos[2\tfrac{-\hat{n}_1+3\hat{n}_2}{2}\xi_1]\sin[2\tfrac{-\hat{n}_1-\hat{n}_2}{2}\xi_2]\\ &+ \cos[2\tfrac{-\hat{n}_1-3\hat{n}_2}{2}\xi_1]\sin[2\tfrac{+\hat{n}_1-\hat{n}_2}{2}\xi_2]\end{aligned}\right\} \tag{41}$$

The significance of this wonderful result is brought vividly to light if we define

$$\begin{aligned} f_{\hat{\boldsymbol{n}}}(\xi_1,\xi_2) &\equiv \sin[2\hat{n}_1\xi_1]\sin[2\hat{n}_2\xi_2] \\ g_{\hat{\boldsymbol{n}}}(\xi_1,\xi_2) &\equiv \cos[2\hat{n}_1\xi_1]\sin[2\hat{n}_2\xi_2] \end{aligned}$$

and recall the action of $\mathbb{A}$, for then we have

$$\begin{aligned} F_{\hat{\boldsymbol{n}}}(\xi_1,\xi_2) &= f_{\hat{\boldsymbol{n}}}(\xi_1,\xi_2) + f_{\mathbb{A}\hat{\boldsymbol{n}}}(\xi_1,\xi_2) + f_{\mathbb{A}^2\hat{\boldsymbol{n}}}(\xi_1,\xi_2) \\ G_{\hat{\boldsymbol{n}}}(\xi_1,\xi_2) &= g_{\hat{\boldsymbol{n}}}(\xi_1,\xi_2) + g_{\mathbb{A}\hat{\boldsymbol{n}}}(\xi_1,\xi_2) + g_{\mathbb{A}^2\hat{\boldsymbol{n}}}(\xi_1,\xi_2) \end{aligned}$$

Manifestly

$$\begin{aligned} F_{\hat{\boldsymbol{n}}}(\xi_1,\xi_2) &= F_{\mathbb{A}\hat{\boldsymbol{n}}}(\xi_1,\xi_2) = F_{\mathbb{A}^2\hat{\boldsymbol{n}}}(\xi_1,\xi_2) \\ G_{\hat{\boldsymbol{n}}}(\xi_1,\xi_2) &= G_{\mathbb{A}\hat{\boldsymbol{n}}}(\xi_1,\xi_2) = G_{\mathbb{A}^2\hat{\boldsymbol{n}}}(\xi_1,\xi_2) \end{aligned}$$

while it follows by inspection from (41) that

$$\begin{aligned} \hat{\boldsymbol{n}} \longmapsto \begin{pmatrix} -\hat{n}_1 \\ \hat{n}_2 \end{pmatrix} \quad &\text{induces} \quad \begin{cases} F_{\hat{\boldsymbol{n}}}(\boldsymbol{\xi}) \longmapsto -F_{\hat{\boldsymbol{n}}}(\boldsymbol{\xi}) \\ G_{\hat{\boldsymbol{n}}}(\boldsymbol{\xi}) \longmapsto +G_{\hat{\boldsymbol{n}}}(\boldsymbol{\xi}) \end{cases} \\ \hat{\boldsymbol{n}} \longmapsto \begin{pmatrix} \hat{n}_1 \\ -n_2 \end{pmatrix} \quad &\text{induces} \quad \begin{cases} F_{\hat{\boldsymbol{n}}}(\boldsymbol{\xi}) \longmapsto -F_{\hat{\boldsymbol{n}}}(\boldsymbol{\xi}) \\ G_{\hat{\boldsymbol{n}}}(\boldsymbol{\xi}) \longmapsto -G_{\boldsymbol{n}}(\boldsymbol{\xi}) \end{cases} \\ \hat{\boldsymbol{n}} \longmapsto \begin{pmatrix} -\hat{n}_1 \\ -\hat{n}_2 \end{pmatrix} \quad &\text{induces} \quad \begin{cases} F_{\hat{\boldsymbol{n}}}(\boldsymbol{\xi}) \longmapsto +F_{\hat{\boldsymbol{n}}}(\boldsymbol{\xi}) \\ \hat{G}_{\hat{\boldsymbol{n}}}(\boldsymbol{\xi}) \longmapsto -G_{\boldsymbol{n}}(\boldsymbol{\xi}) \end{cases} \end{aligned}$$

Finally we notice that (again by implication of (41))

$$\begin{aligned} &F_{\hat{\boldsymbol{n}}}(\boldsymbol{\xi}) = G_{\hat{\boldsymbol{n}}}(\boldsymbol{\xi}) = 0 && \text{if } \hat{\boldsymbol{n}} \in \text{ lower edge of wedge: } \hat{\boldsymbol{n}} = \big(\begin{smallmatrix} 0 \\ 2k \end{smallmatrix}\big) \\ &\left.\begin{aligned} &F_{\hat{\boldsymbol{n}}}(\boldsymbol{\xi}) = 0 \\ &G_{\hat{\boldsymbol{n}}}(\boldsymbol{\xi}) = 2\cos 6k\xi_1 \sin 2k\xi_2 - \sin 4k\xi_2 \end{aligned}\right\} && \text{if } \hat{\boldsymbol{n}} \in \text{upper edge of wedge: } \hat{\boldsymbol{n}} = \big(\begin{smallmatrix} k \\ 3k \end{smallmatrix}\big) \end{aligned}$$

Drawing upon these facts, we have

$$\sum_{\text{orbit}} \sum_{\alpha=0}^{5} (-)^\alpha \cos \pi \hat{\boldsymbol{n}}\hat{\boldsymbol{v}}_\alpha = 2 \begin{cases} 4\big\{F_{\hat{\boldsymbol{n}}}(\boldsymbol{\xi})F_{\hat{\boldsymbol{n}}}(\boldsymbol{\zeta}) + G_{\hat{\boldsymbol{n}}}(\boldsymbol{\xi})G_{\hat{\boldsymbol{n}}}(\boldsymbol{\zeta})\big\} & \text{if } \hat{\boldsymbol{n}} \in \text{interior} \\ 2\big\{\quad 0 \quad + G_{\hat{\boldsymbol{n}}}(\boldsymbol{\xi})G_{\hat{\boldsymbol{n}}}(\boldsymbol{\zeta})\big\} & \text{if } \hat{\boldsymbol{n}} \in \text{upper edge} \\ 2\big\{\quad 0 \quad + \quad 0 \quad \big\} & \text{if } \hat{\boldsymbol{n}} \in \text{lower edge} \end{cases}$$

Our goal has now been achieved. For upon returning to (37) with the information just gained, we have

$$K(\boldsymbol{x},t;\boldsymbol{y},0) = {\sum_{\text{Wedge}}}' e^{-\frac{i}{\hbar}\hat{\mathcal{E}}(\hat{n}_1^2+3\hat{n}_2^2)t}\,\Psi_{\hat{\boldsymbol{n}}}(\boldsymbol{x})\Psi^*_{\hat{\boldsymbol{n}}}(\boldsymbol{y}) \tag{42}$$

where "Wedge" means "interior and upper edge of the wedge," and where

$$\Psi_{\hat{\boldsymbol{n}}}(\boldsymbol{x}) \equiv \begin{cases} \sqrt{\frac{8}{6\cdot\text{area}}}\big[G_{\hat{\boldsymbol{n}}}(\boldsymbol{\xi}) + iF_{\hat{\boldsymbol{n}}}(\boldsymbol{\xi})\big] & \text{if } \hat{\boldsymbol{n}} \in \text{interior of wedge} \\ \sqrt{\frac{4}{6\cdot\text{area}}}\; G_{\hat{\boldsymbol{n}}}(\boldsymbol{\xi}) & \text{if } \hat{\boldsymbol{n}} \in \text{upper edge of wedge} \end{cases} \tag{43}$$

The orthonormality of the eigenfunctions $\Psi_{\hat{\boldsymbol{n}}}(\boldsymbol{x})$ is manifest, since it provided the basis of the argument that gave us (13). To establish completeness one returns to the particle representation (28) and observes that

$$\lim_{t\downarrow 0} K(\boldsymbol{x},t;\boldsymbol{y},0) = \delta(\boldsymbol{x}-\boldsymbol{y}) + \text{image spikes}$$

For graphical representations of some low-order eigenfunctions (which reproduce the physical box and its images as a pattern of nodal lines) see Figure 30 in Part I.

It is striking that the functions $\Psi_{\hat{\boldsymbol{n}}}(\boldsymbol{x})$ do not possess product structure, and therefore could not have been obtained by the separation of variables method. They can, however, be written in a variety of alternative ways; drawing upon *Mathematica*'s `TrigReduce[`*expr*`]` resource, we obtain for example

$$\begin{aligned} G_{\hat{\boldsymbol{n}}}(\boldsymbol{\xi}) \equiv \cos[2\hat{n}_1\xi_1]\sin[2\hat{n}_2\xi_2] &+ \cos[\hat{n}_1(\xi_1+\xi_2)]\sin[\hat{n}_2(3\xi_1-\xi_2)] \\ &- \cos[\hat{n}_1(\xi_1-\xi_2)]\sin[\hat{n}_2(3\xi_1+\xi_2)] \end{aligned}$$

$$\begin{aligned} = \tfrac{1}{2}\big\{ -\sin[2\hat{n}_1\xi_1 - 2\hat{n}_2\xi_2] &+ \sin[2\hat{n}_1\xi_1 + 2\hat{n}_2\xi_2] \\ &- \sin[(\hat{n}_1-3\hat{n}_2)\xi_1 + (\hat{n}_1+\hat{n}_2)\xi_2] \\ &+ \sin[(\hat{n}_1+3\hat{n}_2)\xi_1 + (\hat{n}_1-\hat{n}_2)\xi_2] \\ &+ \sin[(\hat{n}_1-3\hat{n}_2)\xi_1 - (\hat{n}_1+\hat{n}_2)\xi_2] \\ &- \sin[(\hat{n}_1+3\hat{n}_2)\xi_1 - (\hat{n}_1-\hat{n}_2)\xi_2]\big\} \end{aligned}$$

$$F_{\hat{\boldsymbol{n}}}(\boldsymbol{\xi}) = \text{similar expression}$$

which prove useful in connection with the work of Part II.

8. Spectral degeneracy. The quantum mechanical equilateral box problem has been seen to yield energy eigenvalues of the form

$$E_{\hat{\boldsymbol{n}}} = \tfrac{h^2}{18ma^2}N(\hat{\boldsymbol{n}})$$

where

$$N(\hat{\boldsymbol{n}}) \equiv \hat{n}_1^2 + 3\hat{n}_2^2$$

is called by me the "norm" of $\hat{\boldsymbol{n}}$, though literally it is the norm of $n_1 + \sqrt{-3}n_2$. From (43) we learn that

$$E_{\hat{\boldsymbol{n}}} \text{ is } \begin{cases} \text{doubly degenerate if } \hat{\boldsymbol{n}} \in \text{interior of wedge} \\ \text{non-degenerate if } \hat{\boldsymbol{n}} \in \text{upper edge of wedge} \end{cases}$$

Examination of the tabulated values of $N(\hat{\boldsymbol{n}})$ reveals that some entries appear multiply; those give rise to "accidental" spectral degeneracy. In such cases, distinct lattice points $\hat{\boldsymbol{n}}', \hat{\boldsymbol{n}}'', \ldots$ support orbits that *happen* to fall on the *same* ellipse $\hat{n}_1^2 + 3\hat{n}_2^2 =$ constant. In Part I §9 I belabor (as first-time visitors to a

$* * *$		912		948		1008		1092		1200
	844		$\boxed{868}$		916		988		1084	
$* * *$		796		832		892		976		
	732		756		804		876		972	
$* * *$		688		724		784		$\boxed{868}$		
	628		652		700		772			
$* * *$		$\boxed{588}$		624		684		768		
	$\boxed{532}$		556		604		676			
$* * *$		496		$\boxed{532}$		592				
	444		468		516		$\boxed{588}$			
$* * *$		412		448		508				
	$\boxed{364}$		388		436					
$* * *$		336		372		432				
	292		316		$\boxed{364}$					
$* * *$		268		304						
	228		252		300					
$* * *$		208		244						
	172		196							
$* * *$		156		192						
	124		148							
$* * *$		112								
	84		108							
$* * *$		76								
	52									
$* * *$		48								
	28									
$* * *$										
	12									
$* * *$										
$* * *$										

TABLE 1: *Values assumed by* $N(\hat{n}_1, \hat{n}_2) = \hat{n}_1^2 + 3\hat{n}_2^2$ *on the interior and upper edge of the wedge.* $\hat{n}_1$ *ranges* $\uparrow$ *and* $\hat{n}_2$ *ranges* $\rightarrow$ *on* $\{0, 1, 2, \ldots\}$. *Repeated entries are* $\boxed{\textit{boxed}}$, *and are the entries of special interest.*

strange land are inclined to do), but am content here simply to summarize, the number-theoretic mechanism that underlies spectral degeneracy. One begins by establishing that[26]

$$N(\hat{n}_1, \hat{n}_2) \equiv \begin{cases} 0 \pmod 4 & \text{if } \hat{n}_1 \text{ and } \hat{n}_2 \text{ have the same parity} \\ \pm 1 \pmod 4 & \text{otherwise} \end{cases}$$

Only the former case is of interest to us; we have

$$N(\hat{\mathbf{n}}) = 4^\alpha \cdot \text{product of odd primes, with } \alpha \geq 1$$

Now we resolve the odd primes into two classes: an odd prime

$$P > 3 \text{ will be called} \begin{cases} \text{a } p\text{-prime if } P \equiv +1 \,(\text{mod}\, 6) \\ \text{a } q\text{-prime otherwise; i.e., if } P \equiv -1 \,(\text{mod}\, 6) \end{cases}$$

Establish that every q-prime enters *squared* into the factorization of $N(\hat{\mathbf{n}})$

$$\begin{aligned} N(\hat{\mathbf{n}}) &= 4^\alpha 3^\beta p_1^{\mu_1} \cdots p_k^{\mu_k} Q^2 \\ &\qquad\qquad Q \equiv q_1^{\nu_1} \cdots q_\ell^{\nu_\ell} \end{aligned} \tag{44}$$

Establish that 3, 4 and every p-prime (but no q-prime) can be written

$$p = m^2 + 3n^2$$

and is therefore "composite" in the sense

$$\begin{aligned} p &= (m + jn)(m - jn) \\ &\qquad j \equiv \sqrt{-3} \text{ by extension of the notation } i \equiv \sqrt{-1} \\ &= \text{"norm" } \pi\bar{\pi} \text{ of the algebraic number } \pi \equiv m + jn \end{aligned}$$

made evident by the following data (see also Table 2 in Part I):

$$\begin{aligned} 3 &= 0^2 + 3 \cdot 1^2 \\ 4 &= 2^2 + 3 \cdot 0^2 = 1^2 + 3 \cdot 1^2 \\ \\ 7 &= 2^2 + 3 \cdot 1^2 \\ 13 &= 1^2 + 3 \cdot 2^2 \\ 19 &= 4^2 + 3 \cdot 1^2 \\ 31 &= 2^2 + 3 \cdot 3^2 \\ &\vdots \end{aligned}$$

We observe that m and n are necessarily of *opposite* parity, and that necessarily $mn \neq 0$. We find ourselves now in position to write

[26] We touch here on some number theory I have come to realize is entirely standard, the principles of which were first explained to me by Ray Mayer.

Prime factors of $N(\hat{\boldsymbol{n}})$	Continuation
$12 = 4 \cdot 3$	$444 = 4 \cdot 3 \cdot 37$
$28 = 4 \cdot 7$	$448 = 4^3 \cdot 7$
$48 = 4^2 \cdot 3$	$468 = 4 \cdot 3^2 \cdot 13$
$52 = 4 \cdot 13$	$496 = 4^2 \cdot 31$
$76 = 4 \cdot 19$	$508 = 4 \cdot 127$
$84 = 4 \cdot 3 \cdot 7$	$516 = 4 \cdot 3 \cdot 43$
$108 = 4^2 \cdot 3^3$	$\boxed{532} = 4 \cdot 7 \cdot 19$
$112 = 4^2 \cdot 7$	$556 = 4 \cdot 139$
$124 = 4 \cdot 31$	$\boxed{588} = 4 \cdot 3 \cdot 7^2$
$148 = 4 \cdot 37$	$592 = 4^2 \cdot 37$
$156 = 4 \cdot 3 \cdot 13$	$604 = 4 \cdot 151$
$172 = 4 \cdot 43$	$624 = 4^2 \cdot 3 \cdot 13$
$192 = 4^3 \cdot 3$	$628 = 4 \cdot 157$
$196 = 4 \cdot 7^2$	$652 = 4 \cdot 163$
$208 = 4^2 \cdot 13$	$676 = 4 \cdot 13^2$
$228 = 4 \cdot 3 \cdot 19$	$684 = 4 \cdot 3^2 \cdot 19$
$244 = 4 \cdot 61$	$688 = 4^2 \cdot 43$
$252 = 4 \cdot 3^2 \cdot 7$	$700 = 4 \cdot 7 \cdot \langle 5 \rangle^2$
$268 = 4 \cdot 67$	$724 = 4 \cdot 181$
$292 = 4 \cdot 73$	$732 = 4 \cdot 3 \cdot 61$
$300 = 4 \cdot 3 \cdot \langle 5 \rangle^2$	$756 = 4 \cdot 3^3 \cdot 7$
$304 = 4^2 \cdot 19$	$768 = 4^4 \cdot 3$
$316 = 4 \cdot 79$	$772 = 4 \cdot 193$
$336 = 4^2 \cdot 3 \cdot 7$	$784 = 4^2 \cdot 7^2$
$\boxed{364} = 4 \cdot 7 \cdot 13$	$796 = 4 \cdot 199$
$372 = 4 \cdot 3 \cdot 31$	$804 = 4 \cdot 3 \cdot 67$
$388 = 4 \cdot 97$	$832 = 4^3 \cdot 13$
$412 = 4 \cdot 103$	$844 = 4 \cdot 211$
$432 = 4^2 \cdot 3^3$	$\boxed{868} = 4 \cdot 7 \cdot 31$
$436 = 4 \cdot 109$	$876 = 4 \cdot 3 \cdot 73$

TABLE 2: *The entries have been taken (in ascending order) from Table 1, and their factors displayed in conformity with (44). Only two entries possess q-factors; those are the* $\langle 5 \rangle$*'s at 300 and 700, and each enters squared, as (44) stipulates.*

$$N = 4^\alpha(\pi_0\bar{\pi}_0)^\beta(\pi_1\bar{\pi}_1)^{\mu_1}\cdots(\pi_k\bar{\pi}_k)^{\mu_k}Q^2 \tag{45}$$

which can be rendered

$$N = \nu\bar{\nu} \quad \text{with} \quad \nu \equiv \hat{n}_1 + j\hat{n}_2$$

in multiple ways. Each way supports an orbit. The spectral degeneracy function $g(N)$ answers this essentially combinatorial question: How many of those orbits are distinct, and of those how many contain elements either interior to or on the upper edge of the wedge? By an easy argument, one can (since an orbital *tour* is in prospect) assume without loss of generality that

$$\nu = 2^\alpha j^\beta Q \underbrace{\left(\begin{smallmatrix}\pi_1\\ \bar{\pi}_1\end{smallmatrix}\right)\cdots\left(\begin{smallmatrix}\pi_1\\ \bar{\pi}_1\end{smallmatrix}\right)}_{\mu_1\ \text{factors}}\underbrace{\left(\begin{smallmatrix}\pi_2\\ \bar{\pi}_2\end{smallmatrix}\right)\cdots\left(\begin{smallmatrix}\pi_2\\ \bar{\pi}_2\end{smallmatrix}\right)}_{\mu_2\ \text{factors}}\cdots\underbrace{\left(\begin{smallmatrix}\pi_k\\ \bar{\pi}_k\end{smallmatrix}\right)\cdots\left(\begin{smallmatrix}\pi_k\\ \bar{\pi}_k\end{smallmatrix}\right)}_{\mu_k\ \text{factors}}$$

where one is, at each bracket, asked to "choose upper else lower." Pretty clearly, spectral multiplicity can occur only when has choices to make. Table 2 provides therefore only these candidates:

Interesting Cases
$196 = 4\cdot 7^2$
$\boxed{364} = 4\cdot 7\cdot 13$
$\boxed{532} = 4\cdot 7\cdot 19$
$\boxed{588} = 4\cdot 3\cdot 7^2$
$676 = 4\cdot 13^2$
$784 = 4^2\cdot 7^2$
$\boxed{868} = 4\cdot 7\cdot 31$

TABLE 3: *Here, extracted from Table 2, are the only cases in which two or more p-primes (the same or different) enter into the prime factorization of $N(\hat{\boldsymbol{n}})$.*

To see how the argument now runs, look to the case 196; we confront (apart from signs) two choices:

$$\nu = 2(2+j)(2+j) = 2 + j8 \quad \text{else} \quad \nu = 2(2+j)(2-j) = 14 + j0$$

It becomes computationally useful at this point to notice that the action

$$\hat{\boldsymbol{n}} \longrightarrow \mathbb{A}\hat{\boldsymbol{n}} \longrightarrow \mathbb{A}^2\hat{\boldsymbol{n}} \longrightarrow \hat{\boldsymbol{n}} \text{ again}$$

of $\mathbb{A}$ is reproduced by the action

$$(\hat{n}_1 + j\hat{n}_2) \longrightarrow A(\hat{n}_1 + j\hat{n}_2) \longrightarrow A^2(\hat{n}_1 + j\hat{n}_2) \longrightarrow (\hat{n}_1 + j\hat{n}_2) \text{ again}$$

of

$$A \equiv \tfrac{1}{2}(-1-j) = \text{a cube root of unity}$$

Proceeding thus, we have $(2+j8) \rightarrow (11-j5) \rightarrow (-13-j3)$ which (by inclusion of all reflective companions) defines an orbit, one member of which—namely $(13+j3)$—lies interior to the wedge; this I symbolize

$$(2+j8) \looparrowright (13+j3) \quad : \quad \text{compare Table I}$$

where $\looparrowright$ means "tour the orbit and land in the wedge." On the other hand, $(14+j0) \looparrowright (14+j0)$ lies on the excluded *lower edge* of the wedge. So 196 is in fact *non*-degenerate.[27] A similar remark pertains to 676 and 784. Looking next to 364, we have

$$\nu = 2(2+j)(1+j2) = (-8+j10) \quad \text{else} \quad \nu = 2(2+j)(1-j2) = (16-j6)$$

By computation

$$(-8+j10) \looparrowright (19+j) \quad \text{and} \quad (16-j6) \looparrowright (17+j5)$$

so—consistently with data presented in Table I—364 is, because it supports two distinct orbits, doubly degenerate.[28] Analysis of the cases 532 and 868 proceeds similarly. In the sole remaining case 588 we have

$$\nu = 2(j)(2+j)(2+j) = (-24+j2) \quad \text{else} \quad \nu = 2(j)(2+j)(2-j) = (0+j14)$$

giving

$$(-24+j12) \looparrowright (24+j2) \quad \text{and} \quad (0+j14) \looparrowright (21+j7)$$

and since $(21+j7)$ lies on the *upper* edge of the wedge we again have double degeneracy.[29]

We are, on the basis of the preceding remarks, not surprised to discover that $4 \cdot 7 \cdot 13 \cdot 19 = 6916$ is four-fold degenerate:

$$\begin{aligned} 6916 &= 73^2 + 3 \cdot 23^2 \\ &= 79^2 + 3 \cdot 15^2 \\ &= 82^2 + 3 \cdot 8^2 \\ &= 83^2 + 3 \cdot 3^2 \end{aligned}$$

Joe Roberts once directed my attention to number-theoretic literature wherein we are informed that

$$\text{degeneracy of } N(\boldsymbol{n}) = \sum_{\text{divisors } d \text{ of } M} (-3|d)$$

---

[27] But two states attach to each interior lattice point, so a quantum physicist would say of the associated eigenvalue that it is "doubly degenerate."

[28] Meaning four states, whence quadruple degeneracy in the language of physics.

[29] But edge-of-the-wedge states are singlets, so we have triple degeneracy in quantum terminology.

where $M \equiv N/4^\alpha$ and $(-3|d)$ is known to *Mathematica* as `JacobiSymbol[-3,d]` By numerical experimentation I have satisfied myself that the preceding formula does indeed work, but that it contributes no actual power that it not already ours; it does, in particular, not *identify* the states (lattice points) in question. However one proceeds, one has first to *factor* $N(\boldsymbol{n})$, which when $\hat{n}_1$ and/or $\hat{n}_2$ are large becomes problematic. Curiously, the circumstance that makes factorization difficult is the very circumstance that calls into play the approximation method to which I now turn.

9. Semi-classical approximation of spectral density. We are in the habit of saying that "quantum mechanics goes over into classical mechanics in the limit $\hbar \downarrow 0$." But consider: we live in a quantum world, yet look about and see classical mechanics operative all around us... even though no one has "turned off $\hbar$." To speak of "quantum mechanics in the limit $\hbar \downarrow 0$)" is, in this light, to speak of an analytically informative physical fiction (and to risk sweeping some deep physical questions under the carpet); it would be fairer to the physics of the matter to say that (compare p. 11)

Quantum mechanics becomes "classical"
as the "quantum numbers" become large

This is, in fact (and as use of the antique terminology suggests), an ancient insight—familiar already to Planck. And it is in the spirit of Planck that we now proceed.

The equation[30] $x^2 + 3y^2 = N$ describes an ellipse on the (x, y)-plane. Drawing inspiration from Figure 12, we ask: "How many lattice points can, in plausible approximation, be expected to lie within the shaded sector in the

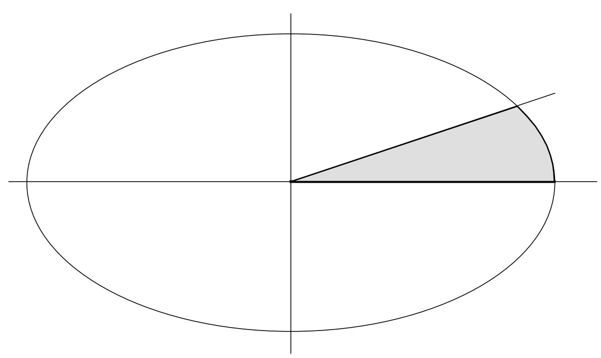

FIGURE 13: *How many same-parity lattice points are interior to the shaded sector?*

[30] For purposes of the present discussion I find it convenient to adopt this simplified notation: $\hat{n}_1 \mapsto x$, $\hat{n}_2 \mapsto y$.

preceding figure?"[31] Introducing polar coordinates in the usual way, we have

$$\begin{aligned}\text{sector area} &= \int_0^{\theta_{\max}} \tfrac{1}{2}r^2\,d\theta\\ &= \tfrac{N}{2}\int_0^{\arctan\frac{1}{3}} \frac{1}{\cos^2\theta + 3\sin^2\theta}\,d\theta\\ &= \tfrac{\pi}{12\sqrt{3}}N \quad \text{according to } \textit{Mathematica}\end{aligned}$$

Since each lattice point preempts unit area, and only half the lattice points are same-parity points, we expect in leading approximation to have

$$\{\text{number of wedge points with } N(\hat{\boldsymbol{n}}) \le N\} \approx \tfrac{\pi}{24\sqrt{3}}N = 0.075575N$$

Since *two* quantum states associate with each interior wedge point (and one state with each edge-of-the-wedge point) we expect in that same approximation (which entails general neglect of edge effects) to have

$$\{\text{number } \mathcal{N}(E) \text{ of states with energy} \le E \equiv \tfrac{h^2}{18ma^2}N\} \approx \tfrac{\pi}{12\sqrt{3}}N$$

which, since the equilateral box has area $\frac{1}{4}\sqrt{3}a^2$, can be written

$$\mathcal{N}(E) \approx \tfrac{\pi}{12\sqrt{3}}\tfrac{18ma^2}{h^2}E = \tfrac{(\text{box area})\cdot(2\pi mE)}{h^2} \tag{45}$$

Digressing now to pick up the other thread in this story: the conditions

$$\boldsymbol{x} \in \text{box} \qquad \& \qquad p^2 = 2mE$$

mark the boundaries of a "bubble" in 4-dimensional phase space, which has

$$\text{phase volume} = (\text{box area})\cdot(2\pi mE)$$

Quantum mechanics came into being as a ramification of Planck's stipulation that

$$= (\text{integer})\cdot h^2$$

which Planck interprets to mean that only certain energies are "allowed" (i.e., that the energy spectrum has become discrete):

$$\begin{aligned}E_n &= \tfrac{h^2}{2\pi m(\text{box area})}\,n \quad : \quad (n = 1, 2, 3, \ldots) \\ &\downarrow \\ &= \tfrac{h^2}{(\frac{1}{2}\pi\sqrt{3})\,ma^2}\,n \quad \text{when the box is equilateral}\end{aligned} \tag{46}$$

---

[31] The question brings to mind *Gauss' circle problem* and places us in contact with "geometic number theory;" see, for example, Chapter 15 of G. E. Andrews' *Number Theory* (1971).

Since Planck has, in this instance, been led to an *incorrect energy spectrum*, it is becomes a point of curiosity that he is led from (46) to a description of $\mathcal{N}(E)$—namely

$$\begin{aligned}\mathcal{N}(E) &\equiv \text{number of states with energy } E \le E_n\\ &= n\\ &= \tfrac{(\text{box area})\cdot(2\pi mE)}{h^2}\end{aligned}$$

—that agrees precisely with (45). In this respect, Planck computed more accurately than he knew (or than is commonly acknowledged), but he computed the wrong thing!

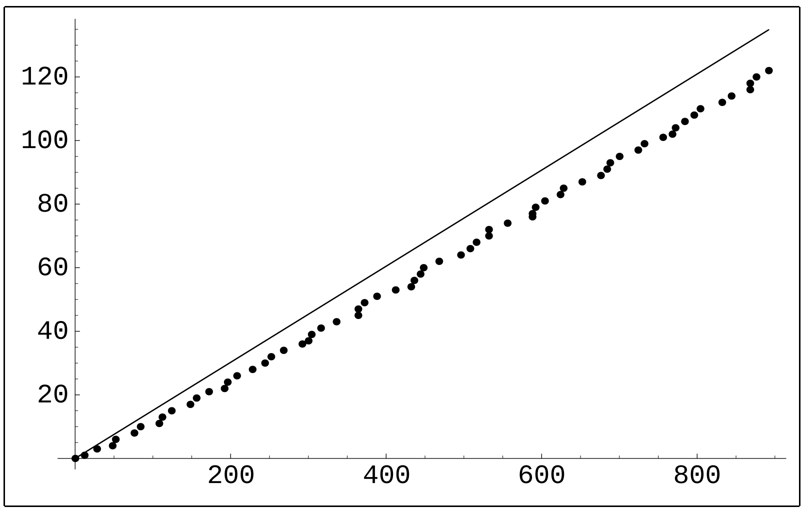

FIGURE 14: *The dots (the data comes from Table 1, and takes into account the fact that interior wedge points are doublets, upper edge points are singlets) describe the* actual *E-dependence of $\mathcal{N}(E)$, while the curve derives from the approximation formula (45). Ticks on the abcissa refer to the dimensionless energy parameter $N \equiv E/\mathcal{E}$, where $\mathcal{E} \equiv \frac{h^2}{18ma^2}$. The approximation is systematically too large.*

In deriving (45)—which it becomes conveneient at this point to write

$$\mathcal{N}(E) \approx \tfrac{1}{4\pi}\big[\tfrac{2mE}{\hbar^2}\big]\cdot(\text{box area})$$

—we systematically neglected edge effects, and achieved the accuracy illustrated in the preceding figure. In 1957, F. H. Brownell—working in a tradition which had been established already in 1911 by the young Hermann Weyl[32] —obtained

[32] For an account of how Weyl came to be concerned with problems of this sort, see Part I §9 Footnote 43. For Brownell's own account of his work, see J. Math. Mech. **6**, 119 (1957).

this improvement

$$\mathcal{N}(E) \approx \tfrac{1}{4\pi}\left[\tfrac{2mE}{\hbar^2}\right]\cdot(\text{box area}) - \tfrac{1}{4\pi}\left[\tfrac{2mE}{\hbar^2}\right]^{\frac{1}{2}}\cdot(\text{box perimeter})$$

which was found in 1971 to admit of still further refinement:[33]

$$\begin{aligned}\mathcal{N}(E) \approx \tfrac{1}{4\pi}\left[\tfrac{2mE}{\hbar^2}\right]\cdot(\text{box area}) - \tfrac{1}{4\pi}\left[\tfrac{2mE}{\hbar^2}\right]^{\frac{1}{2}}\cdot(\text{box perimeter})\\ + \tfrac{1}{12\pi}\left\{\oint(\text{curvature})\,ds + \sum_{\text{vertices}}\frac{\pi^2-(\text{angle})^2}{2(\text{angle})}\right\}\end{aligned} \tag{47}$$

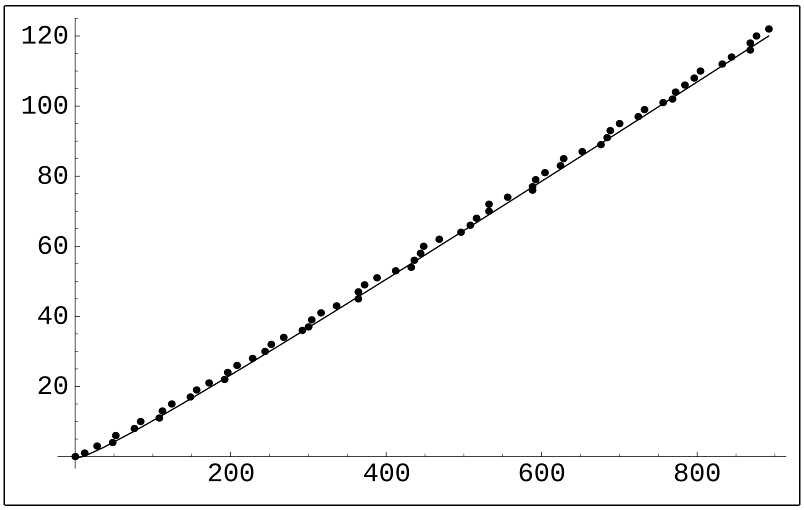

FIGURE 15: *Effect (compare Figure 14) of refinements incorporated into the spectral approximation formula (47).*

Such formulæ—which serve to relate spectral structure to geometrical properties of the enclosure—are, as a class, known as "Weyl expansions." Much of the recent monograph by Brack & Bhaduri[34] is given over to review of diverse methods for obtaining and improving upon such formulæ. In the case of special interest to us, one has

$$\begin{aligned} \text{box area} &= \tfrac{1}{4}\sqrt{3}\,a^2\\ \text{box perimeter} &= 3a\\ \oint(\text{curvature})\,ds &= 0 \qquad \text{(because the sides are straight)}\\ \text{angle} &= \tfrac{2}{3}\pi \qquad \text{(of which there are 3)}\\ E &= \tfrac{h^2}{18ma^2}N \end{aligned}$$

[33] K. Stewartson & R. T. Waechter, Proc. Camb. Phil. Soc. **69**, 353 (1971).

[34] M. Brack & R. K. Bhaduri, *Semiclassical Physics* (1997). See especially §4.5.2 and the discussion of the triangular box problem that appears in §3.2.7.

The approximation formula (47) becomes

$$\mathcal{N}(E) \approx \tfrac{\pi}{12\sqrt{3}}N - \tfrac{1}{2}\sqrt{N} + \tfrac{5}{48}$$

and achieves the success shown in Figure 15.

In many physical/theoretical connections, the object of most immediate interest is not the spectral number function $\mathcal{N}(E)$ but the "spectral density function" $\rho(E)$. When the spectrum is continuous the relationship between $\mathcal{N}(E)$ and $\rho(E)$ is very easy to describe:

$$\mathcal{N}(E) = \int_0^E \rho(E')\,dE' \quad \text{and} \quad \rho(E) = \tfrac{d}{dE}\mathcal{N}(E)$$

When the spectrum ($\{0 < E_1 < E_2 < \cdots\}$, with degeneracies $g(E_n)$) is discrete the situation is a bit more awkward in its details

$$\mathcal{N}(E) = \sum_n g(E_n)\,\underbrace{\theta(E-E_n)}_{} = \text{irregular staircase} \tag{48.1}$$

$$\equiv \int_0^E \delta(E'-E_n)\,dE' \;:\; \text{Heaviside step function}$$

$$= \int_0^E \underbrace{\Big\{\sum_n g(E_n)\delta(E'-E_n)\Big\}}_{}\,dE'$$

$$= \rho(E') = \text{row of weighted spikes} \tag{48.2}$$

but remains unchanged in its essentials; in view of my interest in boxed systems (and since confinement implies spectral discreteness) it is in language specific to the discrete case that I proceed.

Generally, one expects to have

$$\mathcal{N}(E) = \mathcal{N}_0(E) + \tilde{\mathcal{N}}(E) \tag{49}$$

where

$\mathcal{N}_0(E)$ describes the mean trend of $\mathcal{N}(E)$

$\tilde{\mathcal{N}}(E)$ describes detailed fluctuations about the mean

Suppose, for example, that E_n can be described $E_n = \mathcal{E}n$.[35] The staircase is

[35] We recover Planck's box spectrum (46) by setting $\mathcal{E} = \frac{h^2}{2\pi m(\text{box area})}$. The exact harmonic oscillator spectrum $E_n = \hbar\omega(n - \frac{1}{2})$ is also regular in a slight variant of this same sense.

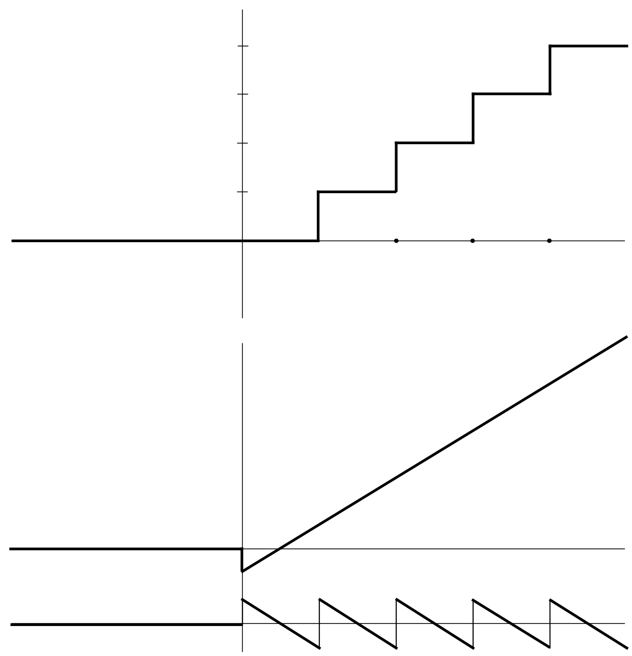

FIGURE 16: *At top is the regular staircase described in the text. At bottom are the functions $\mathcal{N}_0(E)$ and $\tilde{\mathcal{N}}(E)$ described by (50).*

then regular; it becomes natural (see the figure) to set

$$\mathcal{N}_0(E) = \theta(E)\cdot\left\{\tfrac{1}{\mathcal{E}}\cdot E - \tfrac{1}{2}\right\} \tag{50.1}$$

and[36]

$$\begin{aligned}\tilde{\mathcal{N}}(E) &= \begin{cases}\text{descending sawtooth} & : \quad E \geq 0\\ 0 & : \quad E < 0\end{cases}\\ &= \theta(E)\cdot\tfrac{1}{\pi}\Big\{\sin 2\pi\tfrac{E}{\mathcal{E}} + \sin 4\pi\tfrac{E}{\mathcal{E}} + \sin 6\pi\tfrac{E}{\mathcal{E}} + \cdots\Big\}\end{aligned} \tag{50.2}$$

From these equations it follows by differentiation that

$$\begin{aligned}\rho_0(E) &= -\tfrac{1}{2}\delta(E) + \tfrac{1}{\mathcal{E}}\theta(E)\\ \tilde{\rho}(E) &= \theta(E)\cdot\Big\{2\cos 2\pi\tfrac{E}{\mathcal{E}} + 4\cos 4\pi\tfrac{E}{\mathcal{E}} + 6\cos 6\pi\tfrac{E}{\mathcal{E}} + \cdots\Big\}\end{aligned}$$

Direct recovery of such information from

$$\rho(E) = \rho_0(E) + \tilde{\rho}(E) = \sum_{n=1}^{\infty}\delta(E - \mathcal{E}n)$$

poses an analytical challenge which I must on this occasion be content to pass by.

[36] I have borrowed my description of the descending sawtooth from p. 447 of Bartsch's *Handbook of Mathematical Formulas* (9th edition, 1974).

Returning in the light of these remarks to the equilateral box problem, we have

$$\rho(E) = \sum_{\text{Wedge}} \delta(E - \mathcal{E}N(\hat{\boldsymbol{n}})) \tag{51}$$
$$\mathcal{E} = \tfrac{h^2}{18ma^2}$$

from which we expect to recover

$$\mathcal{N}(E) = \int_0^E \rho(E')\,dE' = \underbrace{\mathcal{N}_0(E)}_{\text{known already from (47)}} + \tilde{\mathcal{N}}(E)$$

But *how* does one proceed from (51) to (47)? And, more particularly, what of an exact/approximate nature can one say concerning the structure of $\tilde{\mathcal{N}}(E)$?

10.Trace formulæ. In statistical mechanics, the central object is the so-called "partition function" (also called the "sum-over-states," and in German the "zustandsumme"), which is defined

$$\begin{aligned} Z(T) &\equiv \sum_{\text{states}} e^{-\frac{1}{kT}E(\text{state})} \\ &= \int_0^\infty e^{-\frac{E}{kT}}\rho(E)\,dE \\ &= \text{essentially the LAPLACE TRANSFORM of } \rho(E) \end{aligned} \tag{52}$$

This I mention partly to illustrate the "immediate physical interest" that (as claimed above) attaches in some contexts to the density of states function $\rho(E)$, but mainly to cast a certain light upon the remarks that now follow:

Look again to the wave representation (13) of the quantum dynamical propagator; setting $y = x$ and integrating over all x-values, we (by normality: $\int \Psi(x)\Psi^*(x)\,dx = 1$) obtain

$$\begin{aligned} K(t) &\equiv \int K(x,t;x,0)\,dx \\ &\equiv \text{"trace" of the propagator} \\ &= \int_{-\infty}^{+\infty} e^{-\frac{i}{\hbar}Et}\rho(E)\,dE \quad \text{with } \rho(E) = 0 \text{ when } E < 0 \\ &= \text{essentially the FOURIER TRANSFORM of } \rho(E) \end{aligned} \tag{53}$$

Generally, formation of the trace

$$\mathbb{K} \longmapsto K \equiv \text{trace}(\mathbb{K})$$

entails loss of all the off-diagonal information written into a matrix $\mathbb{K}$, and provides only a lumped summary of the information written onto the diagonal.

So it is at (53): all information relating to properties (beyond normality) of the eigenfunctions $\Psi_n(x)$ has been washed out; only spectral information survives. But we have in $K(t)$ a t-parameterized *family* of traces. By looking to the t-dependence of the trace function $K(t)$ one can expect to recover properties of the energy spectrum (even, in favorable cases, a description of the spectrum $\{E_n\}$ itself).

Formulæ of such a nature are, in general, called "trace formulæ." It is, for example, an immediate consequence of (53) that

$$\rho(E) = \tfrac{1}{h}\int_{-\infty}^{+\infty} e^{+\frac{i}{\hbar}Et}K(t)\,dt \tag{54}$$

and—if we work in the wave representation, where all spectral information is presumed to be known beforehand—we have

$$K(t) = \sum_n g(E_n)e^{-\frac{i}{\hbar}E_n t}$$

from which we recover (48):

$$\rho(E) = \sum_n g(E_n)\cdot \underbrace{\tfrac{1}{h}\int_{-\infty}^{+\infty} e^{\frac{i}{\hbar}(E-E_n)t}\,dt}_{=\,\delta(E-E_n)}$$

But suppose we elect to work in the particle representation (as we might be inclined to do if we did *not* possess advance knowledge of the spectrum). Then[37]

$$K(x,t;x,0) = \sqrt{\tfrac{m}{iht}}\sum_{\text{all such "excursions"}} e^{\frac{i}{\hbar}S[\text{dynamical path }(x,t)\leftarrow(x,0)]}$$

and we expect to have

$$\rho(E) = \tfrac{1}{h}\int_{-\infty}^{+\infty} e^{\frac{i}{\hbar}Et}\sqrt{\tfrac{m}{iht}}\bigg\{\int\sum_{\text{excursions}} e^{\frac{i}{\hbar}S[(x,t)\leftarrow(x,0)]}\,dx\bigg\}dt \tag{55}$$

To see how the idea works out in practice, we look again to the quantum mechanical version of Fourier's ring problem. We found in §1 that the eigenvalues can be described

$$E_n = \tfrac{h^2}{2ma^2}n^2 \quad \text{with} \quad g(E_n) = \begin{cases} 1 & \text{if } n = 0 \\ 2 & \text{if } n = 1, 2, 3, \ldots \end{cases}$$

[37] See again (26). I formulate the following remarks in one-dimensional language, but the extension to two or more dimensions is straightforward. I use the term "excursion" to suggest a *path that ends where it began*.

and that in the particle representation

$$K(x,t;y,0) = \sqrt{\tfrac{m}{iht}}\sum_{n=-\infty}^{\infty} e^{\frac{i}{\hbar}\frac{m}{2t}[(x+na)-y]^2}$$

$$\downarrow$$

$$K(t) = \sqrt{\tfrac{m}{iht}}\sum_{n=-\infty}^{\infty} e^{\frac{i}{\hbar}\frac{m}{2t}[na]^2}\int_0^a dx \;:\; \text{“trace” of the ring propagator}$$

Returning with this information to (55) we have

$$\rho(E) = \tfrac{1}{h}\int_{-\infty}^{+\infty} e^{\frac{i}{\hbar}Et}\Big\{\sqrt{\tfrac{ma^2}{iht}}\sum_{n=-\infty}^{\infty} e^{\frac{i}{\hbar}\frac{m}{2t}[na]^2}\Big\}\,dt$$

But

$$\begin{aligned}
\big\{\text{etc.}\big\} = K(t) &= \sqrt{\tfrac{i}{\tau}}\sum_{n=-\infty}^{\infty} e^{-\frac{i\pi n^2}{\tau}} && \text{provided we define } \tau \equiv -\tfrac{h}{ma^2}t\\
&= \sqrt{i/\tau}\cdot\vartheta(0,-\tfrac{1}{\tau}) && \text{by the definition (18) of } \vartheta(z,\tau)\\
&= \vartheta(0,\tau) && \text{by Jacobi's identity (22)}\\
&= \sum_{n=-\infty}^{\infty} e^{i\pi\tau n^2}
\end{aligned}$$

so we have

$$\rho(E) = \tfrac{1}{h}\int_{-\infty}^{+\infty} e^{\frac{i}{\hbar}Et}\sum_{n=-\infty}^{\infty} e^{i\pi\tau n^2}\,dt$$

which (recall the meaning of τ and the definition of E_n) becomes

$$\begin{aligned}
&= \tfrac{1}{h}\int_{-\infty}^{+\infty}\sum_{n=-\infty}^{\infty} e^{\frac{i}{\hbar}[E-E_n]t}\,dt\\
&= \delta(E-E_0) + 2\sum_{n=1}^{\infty}\delta(E-E_n)
\end{aligned}$$

That we have in this example managed to recover an already known exact result is not really very surprising, for when we drew upon Jacobi's identity we in effect crossed the street—from the particle representation to the wave representation.

Consider now again the case of a particle confined to the interior of a one-dimensional box; quoting from (27.2), we have

$$K(x,t;y,0) = \sqrt{\tfrac{m}{iht}}\sum_{-\infty}^{\infty}\Big[e^{\frac{i}{\hbar}\{\frac{m}{2}\frac{(x-y+2an)^2}{t}\}} - e^{\frac{i}{\hbar}\{\frac{m}{2}\frac{(x+y+2an)^2}{t}\}}\Big]$$

$$\downarrow$$

$$K(t) = \underbrace{\sqrt{\tfrac{m}{iht}}\sum_{-\infty}^{\infty}\int_0^a e^{\frac{i}{\hbar}\{\frac{m}{2}\frac{(2an)^2}{t}\}}\,dx}_{A} - \underbrace{\sqrt{\tfrac{m}{iht}}\sum_{-\infty}^{\infty}\int_0^a e^{\frac{i}{\hbar}\{\frac{m}{2}\frac{(2x+2an)^2}{t}\}}\,dx}_{B}$$

The A-term is easy; we have

$$\begin{aligned}
A &= \tfrac{1}{2}\sqrt{\tfrac{4ma^2}{iht}}\sum_{-\infty}^{\infty} e^{i\pi[\frac{4ma^2}{ht}]n^2}\\
&= \tfrac{1}{2}\sqrt{\tfrac{i}{\tau}}\sum_{-\infty}^{\infty} e^{-i\pi\tau n^2} \quad \text{provided we define } \tau \equiv -\tfrac{h}{4ma^2}t\\
&= \tfrac{1}{2}\vartheta(0,\tau) \qquad\qquad \text{by the same argument as before}
\end{aligned}$$

Evaluation of the B-term is even easier, and foreshadows things to come. We have (as becomes clear upon a moment's thought)

$$B = \sqrt{\tfrac{m}{iht}}\cdot\tfrac{1}{2}\int_{-\infty}^{+\infty} e^{i\pi[\frac{m}{ht}]x^2}\,dx = \tfrac{1}{2}$$

Therefore

$$K(t) = \tfrac{1}{2}\vartheta(0,\tau) - \tfrac{1}{2} = \sum_{n=1}^{\infty} e^{i\pi\tau n^2}$$

giving

$$\begin{aligned}
\rho(E) &= \tfrac{1}{h}\int_{-\infty}^{+\infty} e^{\frac{i}{\hbar}Et}\sum_{n=1}^{\infty} e^{-\frac{i}{\hbar}E_n t}\,dt\\
&= \sum_{n=1}^{\infty}\delta(E-E_n)
\end{aligned}$$

where (compare p. 12) $E_n \equiv \frac{h^2}{8ma^2}n^2$. Here again, we have recovered an already known exact result; the spectrum (relative to that encountered in connection with the ring problem) has shifted by a factor of $\frac{1}{4}$, and has lost its former degeneracy.

Returning now to the equilateral box problem ... we learned at (28) that (in the particle representation)

$$\begin{aligned}
K(\boldsymbol{x},t;\boldsymbol{x},0) &= \tfrac{m}{iht}\sum_{\text{all images}}\exp\Big\{\tfrac{i}{\hbar}S\big((\boldsymbol{x}_{\text{image}},t)\longleftarrow(\boldsymbol{x},0)\big)\Big\}\\
&= \tfrac{m}{iht}\sum_{\alpha=0}^{5}(-)^{\alpha}\sum_{\boldsymbol{n}}\exp\big\{\tfrac{i}{\hbar}S_\alpha\big\} \qquad (56)\\
&\qquad\qquad \tfrac{i}{\hbar}S_\alpha \equiv \beta(\boldsymbol{v}_\alpha+\boldsymbol{n})\cdot\mathbb{T}\,(\boldsymbol{v}_\alpha+\boldsymbol{n})
\end{aligned}$$

where

$$\mathbb{T} = \tfrac{3}{2}a^2\begin{pmatrix}2 & 1\\ 1 & 2\end{pmatrix}$$

$$\beta = \tfrac{im}{2\hbar t} = \tfrac{m}{iht}(-\pi)$$

and where the vectors $\boldsymbol{v}_\alpha$ can, when $\boldsymbol{y}=\boldsymbol{x}$, be described[38]

[38] Here I borrow from p. 41 of Part I.

$$\left.\begin{aligned}
-\pi\boldsymbol{v}_0 &= \begin{pmatrix} X_2 - X_2 \\ X_1 - X_1 \end{pmatrix} = \mathbf{0}\\
-\pi\boldsymbol{v}_1 &= \begin{pmatrix} X_0 - X_2 \\ X_1 - X_1 \end{pmatrix}\\
-\pi\boldsymbol{v}_2 &= \begin{pmatrix} X_1 - X_2 \\ X_0 - X_1 \end{pmatrix}\\
-\pi\boldsymbol{v}_3 &= \begin{pmatrix} X_1 - X_2 \\ X_2 - X_1 \end{pmatrix}\\
-\pi\boldsymbol{v}_4 &= \begin{pmatrix} X_0 - X_2 \\ X_2 - X_1 \end{pmatrix}\\
-\pi\boldsymbol{v}_5 &= \begin{pmatrix} X_2 - X_2 \\ X_0 - X_1 \end{pmatrix}
\end{aligned}\right\} \tag{57}$$

where X_1, X_2 and X_3 are dimensionless variables defined

$$\left.\begin{aligned}
X_0 &\equiv \tfrac{\pi}{3a}(\,2x_1)\\
X_1 &\equiv \tfrac{\pi}{3a}(-x_1 + \sqrt{3}x_2)\\
X_2 &\equiv \tfrac{\pi}{3a}(-x_1 - \sqrt{3}x_2)
\end{aligned}\right\} \tag{58}$$

and subject therefore to the redundancy condition $X_0 + X_1 + X_2 = 0$. We will acquire interest in the geometric meaning of the variables $\boldsymbol{v}_1 \dots \boldsymbol{v}_5$, but for the moment I concentrate on implications of the condition $\boldsymbol{v}_0 = \mathbf{0}$. We have

$$\begin{aligned}
K(t) &= \tfrac{m}{iht}\sum_{\boldsymbol{n}} e^{\beta\boldsymbol{n}\cdot\mathbb{T}\boldsymbol{n}}\,(\text{box area}) + \int_{\text{box}}(\text{remaining five terms})\,dx_1dx_2\\
&= \tfrac{m}{iht}(\tfrac{1}{4}\sqrt{3}a^2)\sum_{\boldsymbol{n}} e^{i\pi\boldsymbol{n}\cdot\mathbb{W}\boldsymbol{n}} \ + \ \text{etc.}\\
&\qquad\qquad \mathbb{W} \equiv \tfrac{3ma^2}{2ht}\left(\begin{smallmatrix} 2 & 1\\ 1 & 2\end{smallmatrix}\right)\\
&= \tfrac{m}{iht}(\tfrac{1}{4}\sqrt{3}a^2)\cdot\vartheta(\mathbf{0},\mathbb{W}) \ + \ \text{etc.}\\
&= \underbrace{\tfrac{m}{iht}(\tfrac{1}{4}\sqrt{3}a^2)\cdot\frac{i}{\sqrt{\det\mathbb{W}}}}_{\frac{1}{6}}\,\vartheta(\mathbf{0},-\mathbb{M}) \ + \ \text{etc.}\quad\text{by Jacobi's identity (32)}\\
&\qquad\qquad \mathbb{M} \equiv \mathbb{W}^{-1} = \tfrac{2ht}{9ma^2}\left(\begin{smallmatrix} 2 & -1\\ -1 & 2\end{smallmatrix}\right)\\
&= \tfrac{1}{6}\sum_{\boldsymbol{n}} e^{-\frac{i}{\hbar}\mathcal{E}4(n_1^2 - n_1n_2 + n_2^2)t} \ + \ \text{etc.}\\
&\qquad\qquad \mathcal{E} = \tfrac{h^2}{18ma^2}\\
&= \tfrac{1}{6}\sum_{\hat{\boldsymbol{n}}} e^{-\frac{i}{\hbar}\mathcal{E}(\hat{n}_1^2 + 3\hat{n}_2^2)t} \ + \ \text{etc.}
\end{aligned} \tag{59}$$

where (see again p. 23) $\hat{n}_1 \equiv n_1 + n_2$ and $\hat{n}_2 \equiv n_1 - n_2$ range on the familiar same-parity lattice. It follows from this result that

$$\rho(E) = \tfrac{1}{6}\sum_{\hat{\boldsymbol{n}}}\delta(E - E_{\hat{\boldsymbol{n}}}) + \underbrace{\tfrac{1}{h}\int_{-\infty}^{+\infty} e^{\frac{i}{\hbar}E\,t}(\text{etc.})\,dt}_{B}$$

$$E_{\hat{\boldsymbol{n}}} \equiv \tfrac{h^2}{18ma^2}(\hat{n}_1^2 + 3\hat{n}_2^2)$$

From prior study of the symmetry structure of $N(\hat{\boldsymbol{n}}) \equiv \hat{n}_1^2 + 3\hat{n}_2^2$—which can be done (and in §5 was done) independently of any appeal to properties of the wave functions—we know (see again Figure 12) that

$$\sum_{\hat{\boldsymbol{n}}} \text{any convergent function of } N(\hat{\boldsymbol{n}})$$
$$= \Big\{12\sum_{\text{interior}} + \quad 6\sum_{\text{upper edge}} + \quad 6\sum_{\text{lower edge}}\Big\} f\big(N(\hat{\boldsymbol{n}})\big)$$

where (to avoid a double count, and to avoid ambiguity in following statements) I consider the origin to lie on the "lower edge of the wedge." So we have

$$\rho(E) = \Big\{2\sum_{\text{interior}} + \sum_{\text{upper edge}}\Big\}\delta(E - E_{\hat{\boldsymbol{n}}}) + \underbrace{\Big\{B + \sum_{\text{lower edge}}\delta(E - E_{\hat{\boldsymbol{n}}})\Big\}}_{\text{extra term}}$$

But if we had been working from the *wave* representation of the propagator[39] we would know already that

$$\rho(E) = \Big\{2\sum_{\text{interior}} + \sum_{\text{upper edge}}\Big\}\delta(E - E_{\hat{\boldsymbol{n}}}) \qquad \text{is exact as it stands}$$

Our assignment, therefore, is to show that the "extra term" actually vanishes.

The vectors $\boldsymbol{v}_\alpha$ arise, by the mechanism described on p. 19, from the separation vectors $\boldsymbol{S}_\alpha \equiv \boldsymbol{x}_\alpha - \boldsymbol{x}$, and are found, by calculation based upon (57) and (58), to have these explicit meanings: $\boldsymbol{v}_\alpha = \mathbb{V}_\alpha \boldsymbol{x}$ where

$$\mathbb{V}_1 = \tfrac{1}{\sqrt{3}a}\begin{pmatrix} -\sqrt{3} & -1 \\ 0 & 0\end{pmatrix}, \quad \mathbb{V}_2 = \tfrac{1}{\sqrt{3}a}\begin{pmatrix} 0 & -2 \\ -\sqrt{3} & +1\end{pmatrix}, \quad \mathbb{V}_3 = \tfrac{1}{\sqrt{3}a}\begin{pmatrix} 0 & -2 \\ 0 & +2\end{pmatrix}$$
$$\mathbb{V}_4 = \tfrac{1}{\sqrt{3}a}\begin{pmatrix} -\sqrt{3} & -1 \\ 0 & +2\end{pmatrix}, \quad \mathbb{V}_5 = \tfrac{1}{\sqrt{3}a}\begin{pmatrix} 0 & 0 \\ -\sqrt{3} & +1\end{pmatrix}$$

Our interest in the vectors $\boldsymbol{v}_\alpha$ derives from their entry—*via* the constructions $(\boldsymbol{v}_\alpha + \boldsymbol{n})\cdot\mathbb{T}(\boldsymbol{v}_\alpha + \boldsymbol{n})$—into (56). On pp. 23 & 24 we had occasion to write

$$\hat{\boldsymbol{n}} = \mathbb{R}\boldsymbol{n} \quad \text{and} \quad \hat{\boldsymbol{v}}_\alpha = \mathbb{R}\boldsymbol{v}_\alpha \quad : \quad \mathbb{R} \equiv \begin{pmatrix} 1 & 1 \\ 1 & -1\end{pmatrix}$$

[39] Such procedure would be entirely alien to the spirit of the present calculation, since we are making a determined effort to avoid all the distracting tedium that goes into construction of the wave functions—labor that is wasted as soon as one passes from the propagator to its trace.

which entail

$$\boldsymbol{n} = \mathbb{S}\hat{\boldsymbol{n}} \quad \text{and} \quad \boldsymbol{v}_\alpha = \mathbb{S}\hat{\boldsymbol{v}}_\alpha \quad : \quad \mathbb{S} \equiv \mathbb{R}^{-1} = \tfrac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

and yield

$$(\boldsymbol{v}_\alpha + \boldsymbol{n})\cdot\mathbb{T}\,(\boldsymbol{v}_\alpha + \boldsymbol{n}) = (\hat{\boldsymbol{v}}_\alpha + \hat{\boldsymbol{n}})\cdot\hat{\mathbb{T}}\,(\hat{\boldsymbol{v}}_\alpha + \hat{\boldsymbol{n}})$$

where

$$\hat{\mathbb{T}} \equiv \mathbb{S}^{\mathsf{T}}\mathbb{T}\,\mathbb{S} = \tfrac{3}{4}a^2\begin{pmatrix} 3 & 0 \\ 0 & 1 \end{pmatrix}$$

is diagonal (which is the immediate point of these remarks). Additionally we have $\hat{\boldsymbol{v}}_\alpha = \hat{\mathbb{V}}_\alpha \boldsymbol{x}$ with $\hat{\mathbb{V}}_\alpha \equiv \mathbb{R}\,\mathbb{V}_\alpha$:

$$\hat{\mathbb{V}}_1 = \tfrac{1}{\sqrt{3}a}\begin{pmatrix} -\sqrt{3} & -1 \\ -\sqrt{3} & -1 \end{pmatrix}, \quad \hat{\mathbb{V}}_2 = \tfrac{1}{\sqrt{3}a}\begin{pmatrix} -\sqrt{3} & -1 \\ +\sqrt{3} & -3 \end{pmatrix}, \quad \hat{\mathbb{V}}_3 = \tfrac{1}{\sqrt{3}a}\begin{pmatrix} 0 & 0 \\ 0 & -4 \end{pmatrix}$$

$$\hat{\mathbb{V}}_4 = \tfrac{1}{\sqrt{3}a}\begin{pmatrix} -\sqrt{3} & +1 \\ -\sqrt{3} & -3 \end{pmatrix}, \quad \hat{\mathbb{V}}_5 = \tfrac{1}{\sqrt{3}a}\begin{pmatrix} -\sqrt{3} & +1 \\ +\sqrt{3} & -1 \end{pmatrix}$$

These results put us in position to look serially to the terms that enter into this refinement[40]

$$\text{etc.} = -(\text{etc.})_3 + \big\{(\text{etc.})_2 - (\text{etc.})_5\big\} + \big\{(\text{etc.})_4 - (\text{etc.})_1\big\}$$

of a notation introduced at (59). Looking first to $(\text{etc.})_3$—and taking into explicit account the facts that

$$\hat{\boldsymbol{v}}_3 = \tfrac{1}{\sqrt{3}a}\begin{pmatrix} 0 \\ -4x_2 \end{pmatrix} \text{ and } \hat{\mathbb{T}} \text{ is diagonal}$$

—we have

$$\begin{aligned}(\text{etc.})_3 &= \tfrac{m}{iht}\int_{\text{box}} \underbrace{\sum_{\hat{\boldsymbol{n}}} e^{\beta(\hat{\boldsymbol{v}}_3+\hat{\boldsymbol{n}})\cdot\hat{\mathbb{T}}\,(\hat{\boldsymbol{v}}_3+\hat{\boldsymbol{n}})}}\,dx_1dx_2\\ &= \underbrace{\sum_{\hat{n}_1} e^{-i\pi[-\frac{9ma^2}{4ht}]\hat{n}_1^2}}_{A_3}\cdot\underbrace{\sum_{\hat{n}_2} e^{\beta\frac{3}{4}a^2(-\frac{4}{\sqrt{3}a}x_2+\hat{n}_2)^2}}_{B_3}\end{aligned}$$

and, arguing as we did in connection with the ring problem (p. 42), obtain

$$\begin{aligned}A_3 &= \sum_{n=-\infty}^{\infty} e^{-i\pi[-\frac{9ma^2}{ht}]n^2} && \text{by adjustment: } \hat{n}_1 = 2n\\ &= \sqrt{\frac{iht}{m}\cdot\frac{1}{9a^2}}\sum_{n=-\infty}^{\infty} e^{-\frac{i}{\hbar}\left[\frac{h^2}{18ma^2}n^2\right]t} && \text{by Jacobi's identity (22)}\end{aligned}$$

[40] My organizing principle derives from Figure 12, which establishes the sense in which $\boldsymbol{x}_3$ stands "opposite" to $\boldsymbol{x}_0 \equiv \boldsymbol{x}$, $\boldsymbol{x}_5$ stands opposite to $\boldsymbol{x}_2$, and $\boldsymbol{x}_1$ stands opposite to $\boldsymbol{x}_4$.

Looking next to the factor

$$\int_{\text{box}} B_3\,dx_1dx_2 = \int_{\text{box}} \sum_{\hat{n}_2} e^{\beta\frac{3}{4}a^2(-\frac{4}{\sqrt{3}a}x_2+\hat{n}_2)^2}\,dx_1dx_2$$

The box (see again Figure 10) has height $h = \frac{\sqrt{3}}{2}a$ and its width can be described

$$\text{width } w(x_2) = \tfrac{2}{\sqrt{3}}x_2$$

so we have

$$\text{area} = \int_0^{\frac{1}{2}\sqrt{3}a} \tfrac{2}{\sqrt{3}}\,x_2\,dx_2 = \tfrac{1}{4}\sqrt{3}a^2$$

and, proceeding in the spirit of this elementary remark, obtain

$$\begin{aligned}
\int_{\text{box}} B_3\,dx_1dx_2 &= \int_0^{\frac{1}{2}\sqrt{3}a} \sum_{\hat{n}_2} e^{\beta\frac{3}{4}a^2(-\frac{4}{\sqrt{3}a}x_2+\hat{n}_2)^2} w(x_2)\,dx_2\\
&= \tfrac{1}{2}\sqrt{3}a\cdot\int_0^1 \sum_{\hat{n}_2} e^{\beta\frac{3}{4}a^2(2y+\hat{n}_2)^2} ay\,dy \quad \text{with } x_2 = \tfrac{1}{2}\sqrt{3}a\cdot y\\
&= \tfrac{1}{2}\sqrt{3}a^2\cdot\int_0^1 \sum_{n=-\infty}^{\infty} e^{\beta\,3a^2(y+n)^2} y\,dy \quad \text{with } \hat{n}_2 = 2n\\
&= \tfrac{1}{2}\sqrt{3}a^2\cdot\int_{-\infty}^{+\infty} e^{\beta\,3a^2y^2}\cdot\text{sawtooth}(y)\,dy
\end{aligned}$$

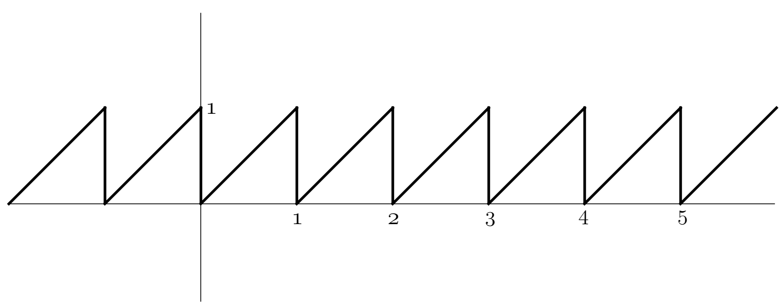

FIGURE 17: *Graph of the function* sawtooth(y) *that is central to the integration trick encountered just above. In the text I again look to Bartsch's* Handbook of Mathematical Formulas *for the associated Fourier series.*

where (see the figure)

$$\text{sawtooth}(y) = \tfrac{1}{2} - \tfrac{1}{\pi}\big\{\sin\tfrac{y}{2\pi} + \tfrac{1}{2}\sin 2\tfrac{y}{2\pi} + \tfrac{1}{3}\sin 3\tfrac{y}{2\pi} + \cdots\big\}$$

The sine terms, since odd functions of y, make no contribution to the Gaussian integral; we obtain therefore this simple result:

$$\int_{\text{box}} B_3 \, dx_1 dx_2 = \tfrac{1}{2}\sqrt{3}a^2 \cdot \tfrac{1}{2}\sqrt{-\tfrac{\pi}{\beta 3a^2}} = \tfrac{1}{4}a\sqrt{\tfrac{iht}{m}}$$

Assembling the results now in hand, we have

$$\begin{aligned}(\text{etc.})_3 &= \tfrac{m}{iht} \cdot \sqrt{\tfrac{iht}{m} \cdot \tfrac{1}{9a^2}} \sum_{n=-\infty}^{\infty} e^{-\frac{i}{\hbar}\left[\frac{h^2}{18ma^2}n^2\right]t} \cdot \tfrac{1}{4}a\sqrt{\tfrac{iht}{m}} \\ &= \tfrac{1}{12} \sum_{n=-\infty}^{\infty} e^{-\frac{i}{\hbar}\left[\frac{h^2}{18ma^2}n^2\right]t}\end{aligned}$$

Looking next to $\{(\text{etc.})_2 - (\text{etc.})_5\}$, we note by way of preparation that

$$\hat{\boldsymbol{v}}_2 = \begin{pmatrix} \hat{v}_{21} \\ \hat{v}_{22} \end{pmatrix} = \tfrac{1}{\sqrt{3}a} \begin{pmatrix} -\sqrt{3}x_1 - x_2 \\ +\sqrt{3}x_1 - 3x_2 \end{pmatrix}$$

and

$$\hat{\boldsymbol{v}}_5 = \begin{pmatrix} \hat{v}_{51} \\ \hat{v}_{52} \end{pmatrix} = \tfrac{1}{\sqrt{3}a} \begin{pmatrix} -\sqrt{3}x_1 + x_2 \\ +\sqrt{3}x_1 - x_2 \end{pmatrix}$$

We have

$$(\text{etc.})_2 = \tfrac{m}{iht} \int_{\text{box}} \sum_{\hat{n}_1} e^{\beta \frac{9a^2}{4}(\hat{v}_{21}+\hat{n}_1)^2} \cdot \sum_{\hat{n}_2} e^{\beta \frac{3a^2}{4}(\hat{v}_{22}+\hat{n}_2)^2} \, dx_1 dx_2$$

which in the variables

$$\begin{aligned}\hat{v}_{21} &= \phantom{-\sqrt{3}x} y - 1 \\ \hat{v}_{22} &= -\sqrt{3}x - 1\end{aligned}$$

suggested by Figure 18 becomes

$$(\text{etc.})_2 = \tfrac{m}{iht} \int_{\text{box}} \sum_{\hat{n}_1} e^{\beta \frac{9a^2}{4}(y+\hat{n}_1)^2} \cdot \sum_{\hat{n}_2} e^{\beta \frac{3a^2}{4}(\sqrt{3}x+\hat{n}_2)^2} \cdot \tfrac{3a^2}{4} dx \, dy$$

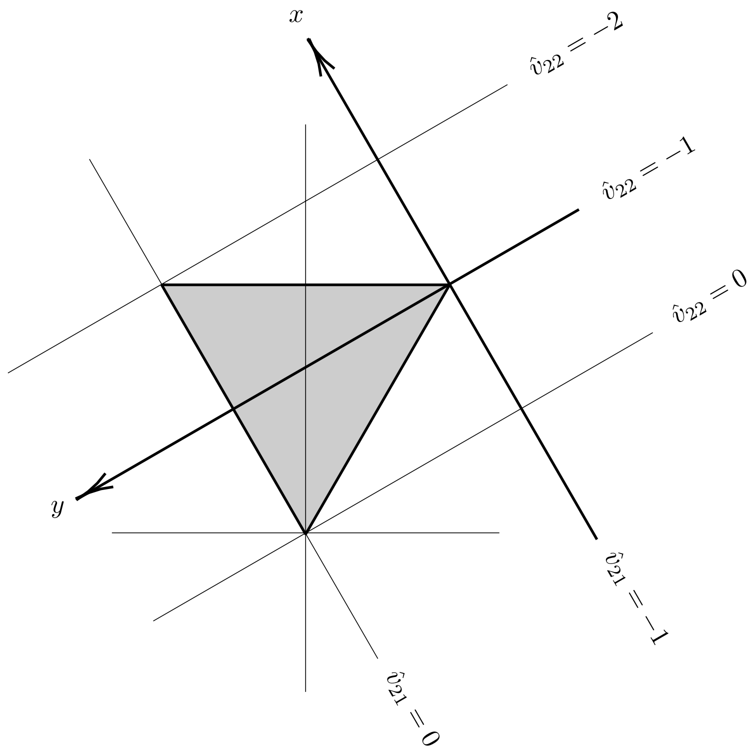

FIGURE 18: *The figure shows lines of constant $\hat{v}_{21}$ and $\hat{v}_{22}$ in relation to the physical box, and motivates the introduction of new variables of integration x and y.*