



Research Article

A Correspondence Principle

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Abstract. A single mathematical theme underpins disparate physical phenomena in classical, quantum and statistical mechanical contexts. This mathematical “correspondence principle”, a kind of wave–particle duality with glorious realizations in classical and modern mathematical analysis, embodies fundamental geometrical and physical order, and yet in some sense sits on the edge of chaos. Illustrative cases discussed are drawn from classical and anomalous diffusion, quantum mechanics of single particles and ideal gases, quasicrystals and Casimir forces.

Keywords. Classical analysis, quantum mechanics, statistical mechanics, random walks and Lévy flights, quasicrystals, Casimir forces.

Physics is not just Concerning the Natures of Things, but Concerning the Interconnectedness of all the Natures of Things [1]

1. INTRODUCTION

One of the more insightful critics of relatively recent mathematics—from inside the profession—is Morris Kline, who has made the following observation [2]. “It behooves us to learn why, despite its uncertain foundations and despite the conflicting theories of mathematicians, mathematics has proved so incredibly effective”. The views of Wigner [3] and Hamming [4] on the “unreasonable effectiveness of mathematics” are perhaps better known, are warmer towards the mathematical profession, and have likely been better received. Philosophers of mathematics have perhaps placed undue emphasis on the apparent rightness of mathematics for the formulation of physical theories.

The essential point of this article is that there is a single theme—though one which can be recast in many superficially distinct ways—that reappears in a bewildering array of mathematical and physical contexts. Its appearance is seldom in the direct formulation of models, but rather arises in the working out of the implications of those formulations. We venture to suggest, though with some diffidence, that this mathematics internal to theories may itself

contain some measure of physical insight, and perhaps even of physical reality.

Some of the ways in which the theme presents itself are collected in Table 1. It is particularly striking that the formulae in Table 1 vary from highly specific results about particular mathematical functions to results involving arbitrary functions, and include formulae that make sense in relatively elementary calculus, formulae that necessarily involve the theory of functions of a complex variable, and formulae that make no sense in classical real or complex analysis and need to be interpreted in the sense of generalized functions. The mathematical equivalence of the results in Table 1 has been addressed twenty years ago in a paper of Ninham, Hughes, Frankel and Glasser [5], and the reader may refer to that paper for a fuller account of the mathematical inter-relations and some relevant references that are not repeated here. What we offer here is a more compelling case for centrality of these relations to physics, rather than to mathematics.

In the context of physics, the “correspondence principle”, first enunciated by Bohr [6], requires quantum mechanics to be consistent with classical mechanics in an appropriate limit, initially in Bohr’s case in the limit of large quantum numbers, but now interpreted more broadly [7]. The “complementarity principle”, also due to Bohr [8], was enunciated in the context of the problem of measurement in quantum mechanics, and its consequence of most interest in the present paper (loosely expressed as “wave–particle duality”) is the requirement that quantum mechanical systems exhibit both wave and corpuscular characteristics, though never both at the same time. Echoes of these principles may be discerned in the discussion that follows.

In Section 2.1 we discuss various perspectives on the common theme underlying the entries in Table 1, which we regard, perhaps controversially, as the deepest “correspondence principle” in mathematical physics. There is an elegance and a tidiness in the formulae of Table 1, but these formulae are in some sense at the edge of chaos, as we discuss in Section 2.2. Moving towards specific physical contexts, we discuss time-evolving classical and quantum processes (Section 3), before turning our attention to questions of dilatational symmetry motivated by scattering data from quasicrystals (Section 4).

The examples in Sections 3 and 4 all involve intrinsically linear, non-cooperative phenomena and there is no explicit temperature dependence. In Section 5 we consider problems of quantum statistical mechanics, before concluding with perhaps the most elegant and intriguing appearance of our common theme in the context of Casimir forces (Section 6).

A collection of useful formulae for the theta functions is given in Appendix A. The variety of contexts from which our examples are drawn have their own popular notations and characteristic terminologies. For the most part we are able to avoid different uses of the same symbol, however force of habit and prevailing idiom oblige us to use τ in two different ways: as a complex number in the upper half-plane for the theory of theta functions and (in Section 4 and Appendix B) as the golden ratio $(1 + \sqrt{5})/2$. For brevity we use the usual notations \mathbb{Z} , \mathbb{N} , \mathbb{R} and \mathbb{C} for the integers, natural numbers (i.e., the strictly positive integers), real numbers and complex numbers, respectively. All computations were performed with MATHEMATICA.

2. THE MATHEMATICAL CONTEXT

2.1. Variations on a theme

An infinite sum of periodically spaced delta functions, $\sum_{n=-\infty}^{\infty} \delta(x - 2nL)$, corresponding to equally spaced “points” or “atoms” on a line, is one of the simplest conceptualizations of the atomic-scale granularity of real matter. Finite segments of such a function, stacked in two and three dimensions form visualizations of elementary crystals and at large scales, where the granularity cannot be resolved, produce apparently smooth structures.

By purely formal Fourier analysis—though a proper derivation within the theory of generalized functions is available [9]—we shall represent $\sum_{n=-\infty}^{\infty} \delta(x - 2nL)$ as a (classically divergent) series of classical functions. As $\sum_{n=-\infty}^{\infty} \delta(x - 2nL)$ is periodic, computing its Fourier expansion in the usual manner using

$$f(x) = \sum_{n=-\infty}^{\infty} \left[\frac{1}{2L} \int_{-L}^L e^{-in\pi y/L} f(y) dy \right] e^{in\pi x/L} \quad (1)$$

yields

$$\begin{aligned} \sum_{n=-\infty}^{\infty} \delta(x - 2nL) &= \frac{1}{2L} \sum_{n=-\infty}^{\infty} e^{in\pi x/L} \\ &= \frac{1}{2L} + \frac{1}{L} \sum_{n=1}^{\infty} \cos\left(\frac{n\pi x}{L}\right). \end{aligned} \quad (2)$$

Although Eq. (2) is valid only in the sense of generalized functions, it arises very cleanly as an extrapolation from a very classical result. Where

$$\theta_3(z|\tau) = \sum_{n=-\infty}^{\infty} \exp\{\pi i n^2 \tau + 2in z\} \quad (3)$$

Table 1. Five essentially equivalent results, identifiable as a single theme that is central to a broad range of problems in classical and quantum physics.

the correspondence principle or wave-particle duality	$\sum_{n=-\infty}^{\infty} \delta(x - 2nL) = \frac{1}{2L} \sum_{n=-\infty}^{\infty} e^{in\pi x/L} = \frac{1}{2L} + \frac{1}{L} \sum_{n=1}^{\infty} \cos\left(\frac{n\pi x}{L}\right)$
theta function transformations (many equivalent or related forms)	$\frac{1}{2L} \sum_{n=-\infty}^{\infty} \exp(-\epsilon\pi n^2 + in\pi x/L) = \sum_{n=-\infty}^{\infty} \frac{1}{\sqrt{4L^2\epsilon}} \exp\left[-\frac{\pi}{4L^2\epsilon}(x - 2nL)^2\right]$
(classical) Poisson summation formula	$\sum_{n=-\infty}^{\infty} f(n) = \sum_{n=-\infty}^{\infty} \int_{-\infty}^{\infty} e^{2\pi inx} f(x) dx$
Riemann relation for the analytic continuation of $\zeta(s) = \sum_{n=1}^{\infty} n^{-s}$	$\zeta(s) = 2^s \pi^{s-1} \sin\left(\frac{1}{2}\pi s\right) \Gamma(1-s) \zeta(1-s)$
transformation of Euler's product	$\prod_{k=1}^{\infty} (1 - e^{-kx}) = \left(\frac{2\pi}{x}\right)^{1/2} \exp\left(\frac{x}{24} - \frac{\pi^2}{6x}\right) \prod_{k=1}^{\infty} (1 - e^{-4\pi^2 k/x})$

denotes the third of the Jacobi theta functions [10] (see Appendix A) in what is now the traditional notation [11], the Jacobi theta function transformation

$$\theta_3(z|\tau) = \exp\left(\frac{i\pi}{4} - \frac{iz^2}{\pi\tau}\right) \tau^{-1/2} \theta_3\left(\frac{z}{\tau} \middle| -\frac{1}{\tau}\right) \quad (4)$$

is valid for all $z \in \mathbb{C}$ and for $\text{Im}\{\tau\} > 0$. If we divide Eq. (4) by $2L$ and set $\tau = i\epsilon$ ($\epsilon > 0$) and $z = \pi x/(2L)$, we find that

$$\begin{aligned} & \frac{1}{2L} \sum_{n=-\infty}^{\infty} \exp(-\epsilon\pi n^2 + in\pi x/L) \\ &= \frac{1}{2L} + \frac{1}{L} \sum_{n=1}^{\infty} \exp(-\epsilon\pi n^2) \cos\left(\frac{n\pi x}{L}\right) \\ &= \sum_{n=-\infty}^{\infty} \frac{1}{\sqrt{4L^2\epsilon}} \exp\left[-\frac{\pi}{4L^2\epsilon}(x - 2nL)^2\right]. \end{aligned} \quad (5)$$

For each fixed value of x , every term in the sum converges rapidly to zero as $\epsilon \rightarrow 0$, unless we have $x = nL$, in which case the n th term diverges, but we have

$$\begin{aligned} & \int_{-\infty}^{\infty} \frac{1}{\sqrt{4L^2\epsilon}} \exp\left[-\frac{\pi}{4L^2\epsilon}(x - 2nL)^2\right] dx \\ &= \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} e^{-X^2} dX = 1, \end{aligned}$$

showing that the right-hand side converges in an appropriate sense to $\sum_{n=-\infty}^{\infty} \delta(x - 2nL)$. We show the series (5)

for $\epsilon = 1/16, 1/4, 1$ and 4 in Fig. 1. The elegant identity (5) equates two conceptually distinct viewpoints: a sum of smooth waves and a sum of pulses that may be identified as individual particles [12]. The particle interpretation becomes increasingly more attractive as ϵ is reduced. The three other Jacobi theta functions have analogous transformations that connect classically divergent trigonometric series to periodically spaced delta functions [5]. Indeed a more general result can be obtained by writing

$$\vartheta_{a,b}(z|\tau) = \sum_{n=-\infty}^{\infty} \exp\{\pi i[(n+a)^2\tau + 2(n+a)(z+b)]\} \quad (6)$$

(so, for example, $\theta_3(z|\tau) = \vartheta_{0,0}(z/\pi|\tau)$) and noting that the generalization of Jacobi's transformation,

$$\vartheta_{a,b}(z|\tau) = \exp\left(\frac{i\pi}{4} - \frac{\pi iz^2}{\tau} + 2\pi iab\right) \tau^{-1/2} \vartheta_{-b,a}\left(\frac{z}{\tau} \middle| -\frac{1}{\tau}\right), \quad (7)$$

leads to

$$\begin{aligned} & \lim_{\epsilon \rightarrow 0} \frac{1}{2L} \sum_{n=-\infty}^{\infty} e^{-\pi(n+a)^2\epsilon} e^{\pi i(n+a)(x/L+2b)} \\ &= \sum_{n=-\infty}^{\infty} e^{2\pi ina} \delta(x - 2(n-b)L). \end{aligned} \quad (8)$$

The periodic delta function structures associated with the standard Jacobi theta functions $\theta_1, \theta_2, \theta_3$ and

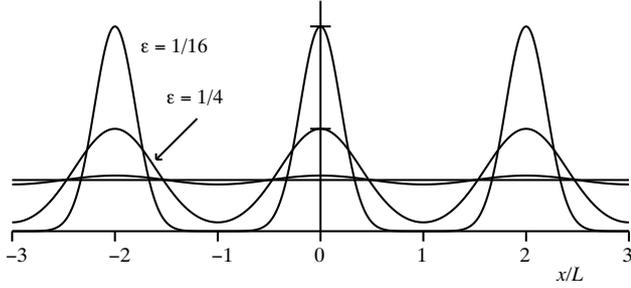


Figure 1. The series (5) interpolates between a uniformly flat profile ($\epsilon \rightarrow \infty$), a continuous wave (finite ϵ) and a train of particles ($\epsilon \rightarrow 0$). We illustrate this with the cases $\epsilon = 1/16$ (highest peaks), $1/4$ and 1 and 4 (nearly flat).

θ_4 are recovered by replacing (a, b) with $(1/2, 1/2)$, $(1/2, 0)$, $(0, 0)$ and $(0, 1/2)$, respectively. Some of these choices yield coefficients with alternating plus or minus signs in the string of delta functions, and so can represent microscopically charged but macroscopically neutral matter. The generalized function $\sum_{n=-\infty}^{\infty} \delta(x - 2nL)$ is sometimes called a (or the) “Dirac comb” and its implications on the interpretation of diffraction data from solid crystals have received some attention [13, 14], especially in the context of its invariance (up to dilation and multiplication) under Fourier transformation:

$$\begin{aligned} \int_{-\infty}^{\infty} e^{2\pi i f x} \sum_{n=-\infty}^{\infty} \delta(x - 2nL) dx &= \sum_{n=-\infty}^{\infty} e^{4\pi i n L f} \\ &= \frac{1}{2L} \sum_{n=-\infty}^{\infty} \delta\left(f - \frac{n}{2L}\right). \end{aligned} \quad (9)$$

The generalized function identity (2) is sometimes called the Poisson summation formula, a forgivable appropriation of terminology [15] that we shall not adopt. For us the Poisson summation formula is [16]

$$\sum_{n=-\infty}^{\infty} f(n) = \sum_{n=-\infty}^{\infty} \int_{-\infty}^{\infty} e^{2\pi i n x} f(x) dx. \quad (10)$$

This follows immediately from the observation that

$$\begin{aligned} \sum_{n=-\infty}^{\infty} f(n) &= \int_{-\infty}^{\infty} f(x) \sum_{n=-\infty}^{\infty} \delta(x - n) dx \\ &= \int_{-\infty}^{\infty} f(x) \sum_{n=-\infty}^{\infty} e^{2\pi i n x} dx \\ &= \sum_{n=-\infty}^{\infty} \int_{-\infty}^{\infty} f(x) e^{2\pi i n x} dx. \end{aligned}$$

Jacobi’s transformations, which we have seen produce such things as generalized function identity (2), can also be regarded as consequences of Eq. (10). For example, by taking $f(x) = \exp(-\pi x^2 \epsilon)$ in Eq. (10), we obtain $\theta_3(0|i\epsilon) = \epsilon^{-1/2} \theta_3(0|i\epsilon^{-1})$. Riemann [17, 18] used this relationship to establish his famous functional relationship

$$\zeta(s) = 2^s \pi^{s-1} \sin\left(\frac{1}{2}\pi s\right) \Gamma(1-s) \zeta(1-s), \quad (11)$$

where the Riemann zeta function $\zeta(s)$ and the gamma function $\Gamma(s)$ are defined initially by

$$\zeta(s) = \sum_{n=1}^{\infty} n^{-s} \quad \text{for } \text{Re}\{s\} > 1, \quad (12)$$

and

$$\Gamma(s) = \int_0^{\infty} e^{-t} t^{s-1} dt \quad \text{for } \text{Re}\{s\} > 0, \quad (13)$$

and extend by analytic continuation to functions holomorphic except for simple poles at $s = 1$ and at $s = 0, 1, 2, \dots$, respectively [11, 17, 19].

The Riemann zeta function is profoundly important in number theory, but surprisingly frequently encountered also in physics [20]. Although a rigorous account of those of its properties that are rigorously established requires serious work [11, 19], some results fall out very simply [21]. Since

$$\zeta(s) = 1 + \frac{1}{2^s} + \sum_{m=2}^{\infty} \frac{1}{(m+1)^s},$$

inserting the binomial expansion

$$(m+1)^{-s} = \sum_{j=0}^{\infty} \frac{(-1)^j s(s+1) \cdots (s+j-1)}{j! m^{j+s}}$$

and interchanging orders of summation (the double series is absolutely convergent for $\text{Re}\{s\} > 1$) we find after a little algebra that

$$\sum_{j=1}^{\infty} \frac{(-1)^{j-1} s(s+1) \cdots (s+j-1)}{j!} [\zeta(s+j) - 1] = \frac{1}{2^s}. \quad (14)$$

Analytic continuation of this result, which we obtained initially on the assumption that $\text{Re}\{s\} > 1$, shows immediately that

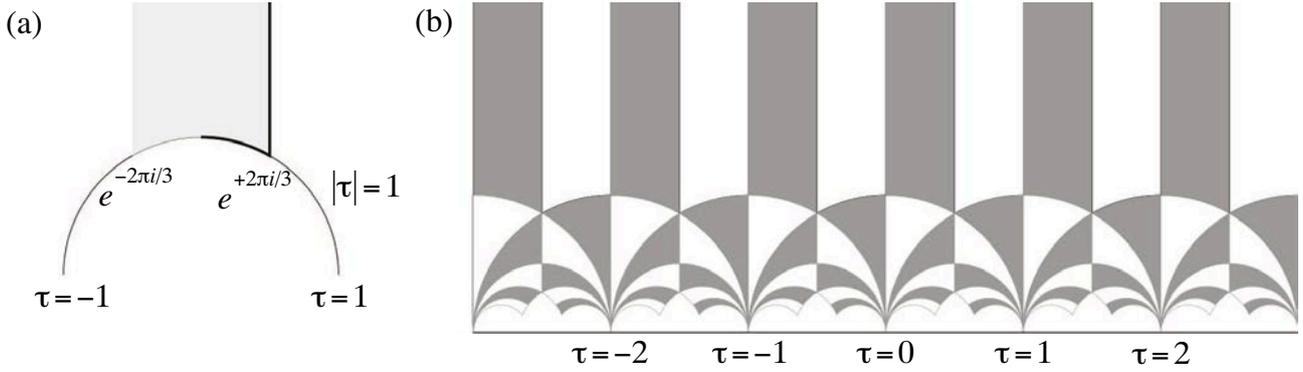


Figure 2. (a) The shaded region shows the fundamental set \mathbb{M} for the modular group. We include only the right half of the boundary, that is, boundary points with $0 \leq \text{Re} \leq \{\tau\} \leq \frac{1}{2}$, shown as a dark curve. There are no modular transformations connecting any pair of distinct points in \mathbb{M} . (b) The images of the fundamental set \mathbb{M} under the modular group tessellate the plane. We have shaded the right half of \mathbb{M} and all its images, while the left half of \mathbb{M} and all its images are left white, though their boundaries are drawn in gray. The images of \mathbb{M} shown here were obtained from those modular transformations with $a = 0, b = -1, c = 1$ and $-2 \leq d \leq 2$ (corresponding to $\tau' = \tau + d$, followed by $\tau'' = -1/\tau'$), or these transformations followed by a translation. The region close to the real axis is progressively filled as further transformations of \mathbb{M} are considered, but it become increasingly hard to portray the images without increasing the magnification of the figure.

$$\lim_{s \rightarrow 0} s\zeta(1 + s) = 1, \quad \zeta(0) = -\frac{1}{2}, \quad \zeta(-1) = -\frac{1}{12}, \quad \zeta(-2) = 0,$$

and so on, and the Riemann relation (11) then yields $\zeta(2) = \pi^2/6, \zeta(4) = \pi^4/90, \dots$, although closed-form elementary evaluations of $\zeta(3), \zeta(5), \dots$ have never been found. Some of the known simple exact values of the zeta function will be needed in Section 6, as will the equation

$$\Gamma(s)\zeta(s) = \int_0^\infty \frac{x^{s-1} dx}{e^x - 1} \quad (15)$$

that results from writing $t = nx$ in Eq. (13) and summing over n .

As noted in the Introduction, but worth emphasizing again, the five results collected in Table 1—four of which we have already discussed, with the fifth (an infinite product transformation)—are essentially a single result [5]. It is possible to obtain all of the results from any one of them, and they establish a link between many substantial fields of mathematics, including complex analysis, number theory, harmonic analysis and numerical analysis [5, 22, 23]. It is the centrality of this common theme to physics that we begin to address in Section 3.

2.2. Analytical irregularity

There is surprising irregularity and complexity lurking behind the five equivalent identities in Table 1. We illustrate this first by considering the special case of the

theta function $\theta_3(z|\tau)$ with $z = 0$. If we write for brevity $\theta(\tau) = \theta_3(0|\tau)$, then $\theta(\tau)$ is well-defined as a holomorphic (that is, complex-differentiable) function of the complex variable τ in the upper half plane $\text{Im}\{\tau\} > 0$. From Eqs (3) and (4) we find that

$$\theta(\tau + 1) = \theta(\tau) \quad \text{and} \quad \theta(\tau) = \left(\frac{i}{\tau}\right)^{1/2} \theta(-\tau^{-1}). \quad (16)$$

Both of the transformations $\tau \rightarrow \tau + 1$ and $\tau \rightarrow -\tau^{-1}$ are bijections of the upper half plane (that is, one-to-one correspondences between two copies of the upper half plane). These two fundamental transformations are the generators of a group of transformations of the upper half-plane known as the modular group [24]. Modular transformations have the form $\tau \mapsto (a\tau + b)/(c\tau + d)$, where $a, b, c, d \in \mathbb{Z}$ and $ad - bc = 1$.

Figure 2(a) shows a subset \mathbb{M} of the upper half-plane known as the fundamental region for the modular group. Every point in the upper half-plane is the image of a point in \mathbb{M} under a modular transformation, but there is no modular transformation connecting any two points of \mathbb{M} . Figure 2(b) shows the remarkable way in which successive applications of simple modular transformations carry \mathbb{M} into regions of progressively smaller total area, located closer and closer to the real τ axis. It follows that along the line segment defined by $\tau = \sigma + i\varepsilon$, with $-1 \leq \sigma \leq 1$ and $0 < \varepsilon \ll 1$, there is enormous variation in $\theta(\sigma + i\varepsilon)$, as shown in Fig. 3.

If we write $q = e^{i\pi\tau}$, the upper half-plane $\text{Re}\{\tau\} > 0$ corresponds to the disk $|q| < 1$ and we have

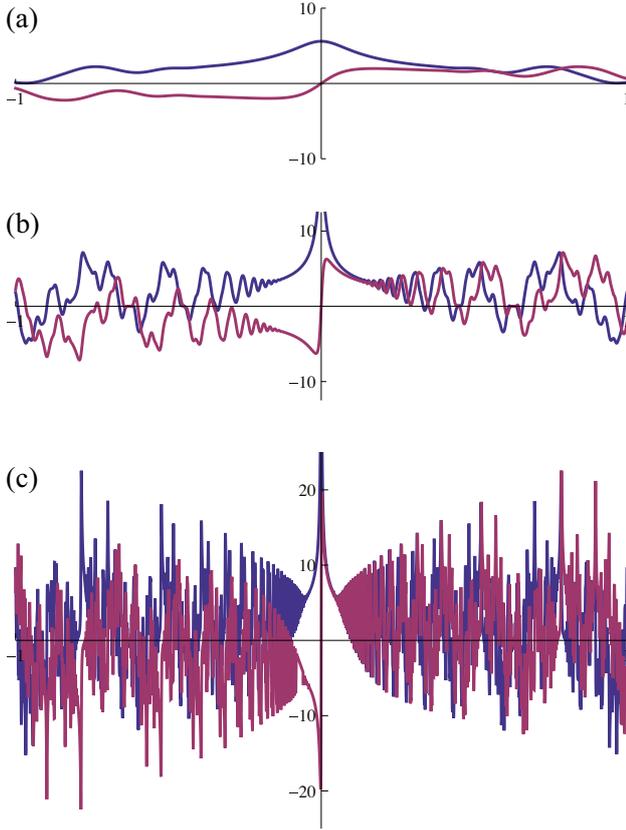


Figure 3. We show the real part (blue curves) and the imaginary part (red curves) of $\theta_3(\sigma + i\varepsilon)$ for $-1 \leq \sigma \leq 1$: (a) $\varepsilon = 0.1$; (b) $\varepsilon = 0.01$; (c) $\varepsilon = 0.001$.

$$\theta_3(\tau) = 1 + 2 \sum_{n=1}^{\infty} q^{n^2} = 1 + 2q + 2q^4 + 2q^9 + \dots \quad (17)$$

This is a power series in q , with the unit circle as its circle of convergence, and gaps of rapidly increasing length between powers of q with nonzero coefficients. Indeed, for fixed z , all of the theta functions $\theta_k(z|\tau)$, $k \in \{1, 2, 3, 4\}$, have the form

$$\theta_k(z|\tau) = q^\kappa \sum_{n=0}^{\infty} a_{k,n}(z) q^{\lambda_n} \quad (18)$$

where $\kappa \in \{0, 1/2\}$ and either $\lambda_n = n^2$ or $\lambda_n = n(n+1)$, with the series always convergent for $|q| < 1$ and always divergent for $|q| > 1$.

More generally, if λ_n is a strictly increasing sequence of non-negative integers, then $\sum_n a_n q^{\lambda_n}$ is a power series in the complex variable q . If $\lambda_n/n \rightarrow \infty$ as $n \rightarrow \infty$ the power series is called a “lacunary series”, the name referring to the gaps between powers of q that have nonzero coef-

ficients. A beautiful theorem of Fabry [25, 26] states that if $\sum_n a_n q^{\lambda_n}$ is a lacunary power series with radius of convergence 1, then the function defined by $f(q) = \sum_n a_n q^{\lambda_n}$ for $|q| < 1$ cannot be continued analytically beyond $|q| = 1$. As functions of q , the theta functions meet the conditions of Fabry’s Theorem. Analytic continuation across the unit circle $|q| = 1$ is prevented by the presence of a dense fence of singular points on this circle. Figure 3 manifests the existence of this fence.

It is interesting that the five equivalent identities in Table 1, which involve either smooth functions or periodic functions, are the gateway to revealing dense, non-smooth behavior.

3. TIME-EVOLVING CLASSICAL AND QUANTUM PROCESSES

Our point of departure in Section 2.1 was already associated with physical concepts, namely periodically spaced point masses or point charges, but no physical models or processes have really been addressed.

3.1. Classical Diffusion

For $-\infty < z < \infty$ and $\text{Im}\{\tau\} > 0$, all four Jacobi theta functions satisfy the partial differential equation

$$\frac{\pi i}{4} \frac{\partial^2 u}{\partial z^2} + \frac{\partial u}{\partial \tau} = 0, \quad (19)$$

as indeed does the more general function $\theta_{a,b}(z|\pi|\tau)$.

If we take $\tau = (4D/\pi)it$ with t real, replace z by x , and write $u(x, \tau) = v(x, t)$, Eq. (19) reduces to the one-dimensional diffusion equation

$$\frac{\partial v}{\partial t} = D \frac{\partial^2 v}{\partial x^2}. \quad (20)$$

The theta function transformations connect optimally structured short-time and long-time solutions of one-dimensional diffusion problems in finite domains, with one theta function expression corresponding to an expansion of the solution in spatial trigonometric functions with exponentially decaying time-dependent coefficients (a good solution from at long times) and the other corresponding to a “method of images” solution constructed from Gaussian propagators (a good solution at short times) [22]. For example, if we write $\varepsilon = \pi Dt/L^2$, then Eq. (5) equates these two solutions in the case of impenetrable reflecting boundaries (zero flux: $-D\partial v/\partial x = 0$) at $x = \pm L$, and initial condition $v(x, 0) = \delta(x)$:

$$\begin{aligned} & \frac{1}{2L} + \frac{1}{L} \sum_{n=1}^{\infty} \exp\left(-\frac{n^2\pi^2Dt}{L^2}\right) \cos\left(\frac{n\pi x}{L}\right) \\ &= \sum_{n=-\infty}^{\infty} \frac{1}{\sqrt{4\pi Dt}} \exp\left[-\frac{1}{4Dt}(x - 2nL)^2\right]. \end{aligned} \quad (21)$$

3.2. Anomalous diffusion

In one dimension and in the absence of boundaries, the mean-square displacement for the diffusion process (20) grows linearly with time [27]:

$$\int_{-\infty}^{\infty} x^2 v(x, t) dx = \int_{-\infty}^{\infty} x^2 v(x, 0) dx + 2Dt. \quad (22)$$

The study of diffusion processes based on Eq. (20) was initiated by Fick [28] in 1855. Much more recently there has been intense interest in transport processes that are not diffusive in character [29, 30, 31, 32]. In one-dimensional unbiased non-diffusive processes the mean-square displacement may grow more slowly than linearly with time (sub-diffusive processes), or faster than linearly (super-diffusive processes). An extreme case of one-dimensional super-diffusion has an infinite mean-square displacement and this can lead to a statistically self-similar or fractal [33] footprint structure (the set of points visited has a fractal dimension less than 1).

Hughes, Shlesinger and Montroll [34] considered a random walk model in which the random displacement made at any step has the probability density function

$$p(x) = \frac{a-1}{2a} \sum_{n=0}^{\infty} a^{-n} [\delta(x - \Delta b^n) + \delta(x + \Delta b^n)], \quad (23)$$

with $a > 1$ and $b > 1$. Since motions on the length scale Δb^n are a times more abundant than motions on the next shortest length scale Δb^{n+1} , the stepping law has fractal character built in (with fractal dimension $\mu = \ln(a)/\ln(b)$), and the only question is whether fractal footprints are left visible at long times, or the legacy of the walk is smeared. If $\mu < 2$ the mean-square displacement per step is infinite, the central limit theorem fails, and the continuum limit of the process does not have the standard Gaussian propagator familiar from classical diffusion [30, 35]. The walk is transient if $\mu < 1$ (any interval is visited only finitely many times with probability 1) and fractal footprints are left.

To analyze features of this model, it is necessary to understand the behavior near the origin of the Fourier transform of the probability density function (23), and this is equivalent to requiring the small- k behavior of

$$\lambda(k) = \frac{a-1}{a} \sum_{n=0}^{\infty} a^{-n} \cos(b^n k). \quad (24)$$

It is easy to see that $\lambda(k)$ satisfies the rather simple-looking functional equation

$$\lambda(k) = \frac{a-1}{a} \cos(k) + a^{-1} \lambda(bk), \quad (25)$$

which is reminiscent of equations obtained in real-space renormalization treatments of lattice spin systems [36, 37]. The apparent simplicity of the functional equation is illusory. Hughes et al. [34] were able to show using the Poisson summation formula (10) that for $k > 0$ and $\ln(a)/\ln(b) \notin \{2, 4, 6, \dots\}$,

$$\lambda(k) = \frac{a-1}{a} \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n)!} \frac{k^{2n}}{1 - b^{2n}/a} + k^\mu Q(k), \quad (26)$$

where [38]

$$Q(k) = \frac{a-1}{a \ln b} \sum_{n=-\infty}^{\infty} \Gamma(s_n) \cos\left(\frac{\pi s_n}{2}\right) \exp\left(-\frac{2n\pi i \ln k}{\ln b}\right) \quad (27)$$

and we have written for brevity $s_n = -\mu + 2n\pi i / \ln b$. The appearance in $Q(k)$ of “log-periodic oscillations” (periodic in $\ln k$ with period $\ln b$) is striking (see Fig. 4). Similar oscillations occur in real-space renormalisation group transformations for lattice spin systems [39], in a model for the distribution of family names in a society [40] and in a variety of other systems that exhibit a form of discrete scale invariance [41].

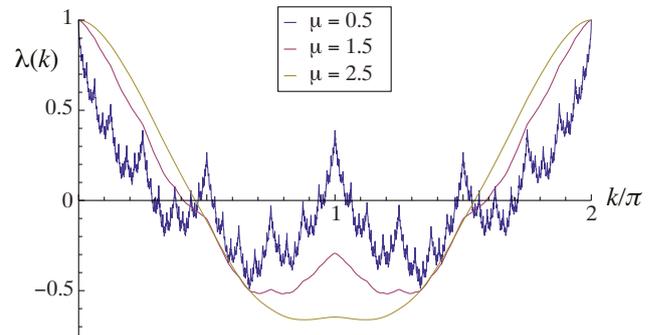


Figure 4. The structure function (24) of the Weierstrass random walk step probability density function (23). In each case, $b = 2$, and we choose a values so that so that $\mu = \ln(a)/\ln(b)$ takes the values 0.5 [blue (most irregular) curve], 1.5 (red curve) and 2.5 (gold curve).

If b is a positive integer and $b \geq 2$ then we can recognize $\lambda(k)$ as a constant multiple of the real part of the lacunary power series $\sum_{n=0}^{\infty} a^{-n} z^{bn}$ evaluated on its circle of convergence ($|z| = 1$), so a dense set of singular points must be present and indeed for appropriate values of a and b the series for $\lambda(k)$ is the celebrated nowhere-differentiable function of Weierstrass [42].

There is a second perspective on Eq. (23) that is also worth considering [30, 34]. By considering the contour integral of $e^{-z} z^{s-1}$ around a simple closed contour in the z -plane consisting of the arc of the circle $|z| = R$ within the first quadrant, and straight lines along the real and imaginary axis linking the ends of the arc to the origin, it is easy to prove that for $0 < \text{Re}\{s\} < 1$,

$$\int_0^{\infty} e^{ix} x^{s-1} dx = \Gamma(s) \exp(\frac{1}{2}i\pi s). \quad (28)$$

Adding this equation and its complex conjugate we find that for $0 < \text{Re}\{s\} < 1$,

$$\int_0^{\infty} \cos(x) x^{s-1} dx = \Gamma(s) \cos(\frac{1}{2}\pi s). \quad (29)$$

The definition of the Mellin transform and the associated inversion formula [16],

$$\bar{f}(s) = \int_0^{\infty} x^{s-1} f(x) dx, \quad (30)$$

$$f(x) = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} x^{-s} \bar{f}(s) ds, \quad (31)$$

with the Bromwich contour $\text{Re}\{s\} = c$ placed inside a strip in which the Mellin transform integral converges, are another manifestation of the relations collected in Table 1, since they can be used to obtain both the Riemann relation and the theta function transformation in relatively straightforward ways.

Using Eqs (29) and (31) we can write

$$\cos(b^n k) = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} b^{-ns} k^{-s} \Gamma(s) \cos(\frac{1}{2}\pi s) ds, \quad (32)$$

for $k > 0$ and $0 < c < 1$. Inserting this representation into Eq. (24), interchanging the order of integration and summation and recognizing a geometric series, we find [30, 34] that

$$\lambda(k) = \frac{a-1}{a} \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} \frac{k^{-s} \Gamma(s) \cos(\frac{1}{2}\pi s) ds}{1 - a^{-1} b^{-s}}. \quad (33)$$

Translating the contour of integration to the left and taking account of the residues at the poles crossed, we recover Eqs (26) and (27). The power series arises from the simple poles along the real axis at $s = 0, -2, -4, \dots$, while $k^\mu Q(k)$ comes from the line of poles at $s_n = -\mu + 2n\pi i / \ln b$. The small- k behavior, which governs the limiting behavior of the random walk, is dominated by which pole or poles the contour next encounters after we have translated it past the origin. For $\mu > 2$ the next pole encountered is a simple pole at $s = -2$, so that $1 - \lambda(k) \propto k^2$ as $k \rightarrow 0$ (ensuring a diffusive limit). However for $0 < \mu < 2$ we meet the line of poles at $s = s_n$, and this is how the term $k^\mu Q(k)$ arises, precluding diffusion.

These kinds of calculations using Mellin transforms are closely connected to the powerful role of Mellin transforms in asymptotic analysis [43] and also give one link between several identities in Table 1. Whichever approach is used to reveal the small- k behavior of $\lambda(k)$, the simplest limiting behavior is obtained as $\Delta \rightarrow 0$ and $t_0 \rightarrow 0$ (where t_0 is the time between successive steps) if we also make $a \rightarrow 1$ and $b \rightarrow 1$, while holding both $\mu = \ln a / \ln b$ and Δ^μ / t_0 constant. Then if $\mu < 2$, the evolution of the random position X_t of the moving agent satisfies

$$\frac{\partial}{\partial t} \mathbf{E}\{\exp(iqX_t)\} = -c|q|^\mu \mathbf{E}\{\exp(iqX_t)\}, \quad (34)$$

where c is a positive real constant, $q \in \mathbb{R}$, and \mathbf{E} denotes mathematical expectation or averaging. The ‘‘characteristic function’’ $\mathbf{E}\{\exp(iqX_t)\}$ is just a spatial Fourier transform of the probability density function for the agent’s location at time t . Solving the evolution equation (34) with the initial condition $X_0 = 0$ gives $\mathbf{E}\{\exp(iqX_t)\} = \exp(-c|q|^\mu t)$ and inverting the Fourier transform gives the celebrated symmetric stable densities [29, 30] of Lévy [44],

$$S_\mu(x, t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \exp(-iqx - c|q|^\mu t) dq. \quad (35)$$

The borderline case $\mu = 2$ corresponds to the Gaussian density, while for $\mu < 2$, the density decays algebraically rather than exponentially, with $\text{Pr}\{X_t > x\} \propto x^{-\mu}$ as $x \rightarrow \infty$. The only other case where the symmetric stable density has a simple closed form expression [45] is $\mu = 1$, which is the Cauchy density $(c/\pi)(x^2 + c^2)^{-1}$.

Super-diffusive processes, such as the stable density, are naturally formulated in unbounded space, but it may be of interest to seek solutions in finite intervals. Appropriate boundary conditions for reflecting boundaries are debatable (for $\mu < 1$ the path is discontinuous), but we can use method of images arguments [cf. Eq. (21)]

to obtain a solution which conserves probability in the interval $(-L, L)$. The following analysis is very much in the sense of generalised functions, as we work with classically divergent series and use the identity (2):

$$\begin{aligned}
& \sum_{n=-\infty}^{\infty} S_{\mu}(x - 2nL) \\
&= \sum_{n=-\infty}^{\infty} \frac{1}{2\pi} \int_{-\infty}^{\infty} \exp(-iq(x - 2nL) - c|q|^{\mu}t) dq \\
&= \frac{1}{2\pi} \int_{-\infty}^{\infty} \sum_{n=-\infty}^{\infty} \exp(2inLq) \exp(-iqx - c|q|^{\mu}t) dq \\
&= \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{\pi}{L} \sum_{n=-\infty}^{\infty} \delta\left(q - \frac{n\pi}{L}\right) \exp(-iqx - c|q|^{\mu}t) dq \\
&= \frac{1}{2L} + \frac{1}{L} \sum_{n=1}^{\infty} \cos\left(\frac{n\pi x}{L}\right) \exp\left[-\left(\frac{n\pi}{L}\right)^{\mu} ct\right]. \tag{36}
\end{aligned}$$

It is perhaps curious that for this system, the relaxation to the uniform density $1/(2L)$ on the interval is a simple exponential, rather than some form of stretched exponential, despite the transport process being highly super-diffusive.

Clearly there are many subtleties that can arise when stochastic ideas intersect with self-similarity. For another manifestation of this, see Appendix B.

3.3. One quantum particle

Let h denote Planck's constant and $\hbar = h/(2\pi)$. If we write $\tau = -2\hbar t/(\pi m)$ with t complex (with a negative imaginary part) and $u(z, \tau) = \psi(z, t)$, we obtain from Eq. (19) the one-dimensional Schrödinger equation in free space,

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial z^2}. \tag{37}$$

Thus linear combinations of theta functions with the complex time extrapolated to the real axis should be able to be used to construct non-trivial time-dependent solutions of Schrödinger equation. Although we are aware of no systematic study of this, for an investigation of some cognate issues the reader may consult the beautiful paper of Fulling and Güntürk [46] on the one-dimensional Schrödinger equation with periodic boundary conditions. Less direct applications of theta functions to solving Schrödinger's equation have been considered by Gaveau and Schulman [47].

The formal connection between theta functions and Schrödinger's equation (obtained by letting the artificial negative imaginary part of the time approach 0) corresponds to moving radially outwards towards the circle of convergence of a lacunary series, as discussed in Section 2.2. The highly irregular form of the propagator discussed by Fulling and Güntürk should therefore come as no surprise.

If we don't observe the connection to theta functions, and instead use an energy eigenfunction approach to solve the d -dimensional Schrödinger equation $i\hbar \partial \psi / \partial t = -[\hbar^2/(2m)] \nabla^2 \psi$ in the box $(0, L)^d$ (with the wave function vanishing on the boundary) we obtain the general solution

$$\psi(\mathbf{x}, t) = \sum_{\mathbf{n} \in \mathbb{N}^d} c(\mathbf{n}) \exp\left[-\frac{iE(\mathbf{n})t}{\hbar}\right] \prod_{j=1}^d \sin\left(\frac{n_j \pi x_j}{L}\right), \tag{38}$$

where $\mathbf{n} = (n_1, n_2, \dots, n_d)$ and

$$E(\mathbf{n}) = \frac{\hbar^2 \pi^2 |\mathbf{n}|^2}{2mL^2} = \frac{\hbar^2 |\mathbf{n}|^2}{8mL^2}. \tag{39}$$

If we take the initial condition $\psi(\mathbf{x}, t') = \delta(\mathbf{x} - \mathbf{x}')$ with $\mathbf{x}' \in (0, L)^d$, we obtain the (never classically convergent) generalized function propagator

$$\begin{aligned}
\psi(\mathbf{x}, t | \mathbf{x}', t') &= \left(\frac{2}{L}\right)^d \sum_{\mathbf{n} \in \mathbb{N}^d} \exp\left[-\frac{iE(\mathbf{n})(t - t')}{\hbar}\right] \\
&\quad \times \prod_{j=1}^d \sin\left(\frac{n_j \pi x_j}{L}\right) \sin\left(\frac{n_j \pi x'_j}{L}\right). \tag{40}
\end{aligned}$$

Perhaps the connection to theta functions makes the strangeness of this result easier to comprehend.

Despite the irregular propagator for finite intervals, the free-space Schrödinger equation does have some comparatively simple, well-behaved normalizable solutions on the real line, such as the spreading Gaussian wave packet found by Darwin [48] and Kennard [49] and the Airy function solution of Lekner [50].

4. QUASICRYSTALS

Diffraction experiments probe the structure of condensed matter using electrons, neutrons or X rays. In systems with long-range order, this order is revealed by observed intensity distributions exhibiting sharp peaks [51, 52]. Experimental realities and the finiteness

of the atoms scattering the incident radiation broaden the peaks, but basically in an idealized but substantially correct way, the observed density in many cases is a set of delta functions, whose locations encode information about the atomic locations, which are also delta functions. This picture is clearest and most apt for crystals, where the diffraction data corresponds to the Fourier transform of the crystal [53]. For the one-dimensional case with equal spacing between atoms, Eq. (9) shows that the Fourier transform is simply the original lattice structure with a changed lattice spacing (the Fourier transform of the Dirac comb is a Dirac comb). Similar results hold in two and three dimensions [54].

The discovery in 1984 by Shechtman et al. [55] of a metallic phase with long-range orientational order but no translational symmetry challenged established paradigms in crystallography, which assume that crystals consist of unit cells of atoms of various species arranged periodically. Within six weeks, Levine and Steinhardt [56] had dubbed these structures “quasicrystals”—a name the structures have retained [57]—and suggested analogies to nonperiodic tilings of space with local pentagonal symmetry previously studied by Penrose [58]. Shechtman received the 2011 Nobel Prize in Chemistry for the discovery of quasicrystals.

The appearance in a physical context of long-range order without translational symmetry naturally motivated a number of fundamental studies of a purely mathematical character, including a careful definition of diffraction on aperiodic structures [59]. Many important observations concerning cognate mathematical issues can be found in Senechal [60, 61], Senechal and Taylor [62, 63] and Baake and Grimm [64].

When translational invariance breaks down in the observed crystallographic data, the unambiguous connection to the original lattice is lost. How is the structure of a quasicrystal to be inferred? To begin, the attempt to fit the diffraction data $\tilde{\rho}(\mathbf{k})$ to delta functions with a non-zero minimal spacing and recover well-spaced delta functions for $\rho(\mathbf{r})$ is doomed to failure [65].

Ninham and Lidin [66] suggested the possible relevance to quasicrystals of dilatational rather than translational symmetry, using the following example, which has interesting historical antecedents. The gnomon ($\gamma\nu\acute{\omega}\mu\omega\nu$) is the shadow-casting blade on a sundial, but also refers to triangles or rectangles produced by internal subdivision of triangles or rectangles in a special way. In particular, if an isosceles triangle with two sides of length $\tau > 1$ and third side of length 1 is subdivided by drawing a straight line from one of the equal angles to the opposite face to create an isosceles triangle with two sides of length 1, the other triangle created in this

subdivision is the gnomon. A simple argument based on similar triangles establishes that the gnomon is itself an isosceles triangle if and only if

$$\tau^2 - \tau - 1 = 0, \quad (41)$$

from which it follows that

$$\tau = (1 + \sqrt{5})/2 \approx 1.618 \quad (42)$$

(see Fig. 5(a), in which the gnomon is shaded in gray). For this special choice of τ , the internal angles of the triangles produced in the subdivision are all integer multiples of $\pi/5$, as shown. In Fig. 5(b) we take the scaled replica of the original triangle produced by the subdivision, subdivide it in a similar manner, and repeat this process several times, always producing isosceles triangles with the same angles, but with the lengths of sides diminishing by a factor of τ at each stage. The number τ is the famous golden mean, golden ratio or golden number, which figures prominently in aesthetics [67] and in nature [68]. The logarithmic spirals

$$\frac{\ln r}{\ln \tau} = \frac{\theta + a\pi/5}{\pi/5}, \quad a \in \{0, \pm 2, \pm 4, \pm 6, \pm 8\}, \quad (43)$$

are shown as grey curves in Fig. 5(c). Their intersections generate a distribution of points with five-fold rotational symmetry about the origin. The logarithmic spiral $\ln r / \ln \tau = \theta/(3\pi/5)$ passes through these points of intersection, with the distance from the origin increasing by a factor of τ between any two consecutive intersections. With suitable scaling and rotation, the inscribed triangles shown in Fig. 5(b) can be placed with their vertices located at the intersection points [66, 69].

We consider the Fourier-space signature of the mass distribution

$$\begin{aligned} \rho(\mathbf{r}) = & \sum_{j=1}^{10} \sum_{m=-\infty}^{\infty} a^{-|m|} \delta(x - \tau^m \cos(\pi j/5)) \\ & \times \delta(y - \tau^m \sin(\pi j/5)), \end{aligned} \quad (44)$$

which places all mass on rays through the origin, with angular separation $\pi/5$ between rays, and on each ray, we have dilatational invariance in the locations of the masses, with a scaling factor τ . The convergence factor $a^{-|m|}$ (with $a > 1$) is present to keep finite total mass in the system. We find that where $\mathbf{k} = (k_1, k_2)$,

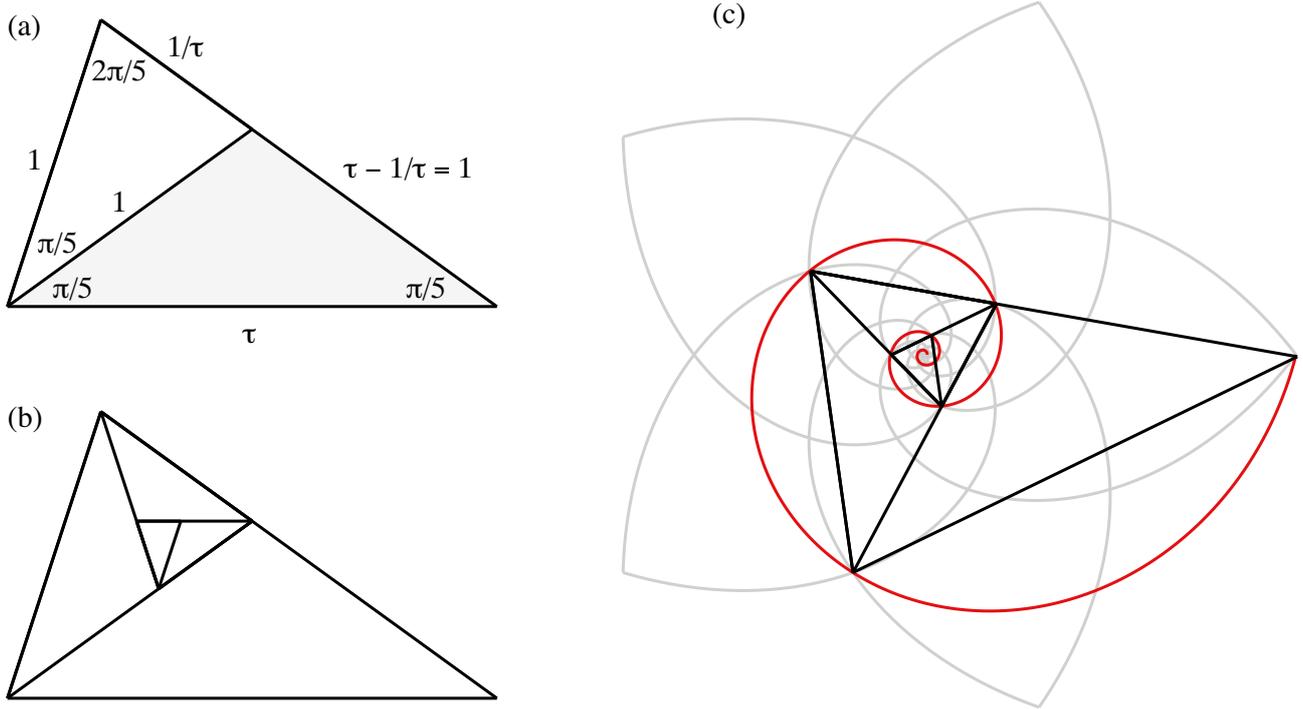


Figure 5. (a) With τ given by Eq. (42), an isosceles triangle with side lengths ratios $\tau : \tau : 1$, can be subdivided into two isosceles triangles, one of which (white interior) has side length ratios $\tau : \tau : 1$ but side lengths a factor τ smaller than those in the original triangle. (b) We can continue the process of subdivision to generate a nested set of isosceles triangles with side length ratios $\tau : \tau : 1$, but at each step of the process, the side length of the triangle just produced is reduced from that of its parent by a factor of τ . (c) The intersections of the logarithmic spirals (43) generate a distribution of points with five-fold rotational symmetry about the origin. The logarithmic spiral $\ln r / \ln \tau = \theta / (3\pi/5)$, shown in red, passes through these points of intersection, with the distance from the origin increasing by a factor of τ between any two consecutive intersections. With suitable scaling and rotation, the inscribed triangles shown in diagram (b) can be placed with their vertices located at the intersection points (figure adapted from Ninham and Lidin [66]).

$$\tilde{\rho}(\mathbf{k}) = \sum_{j=1}^{10} \sum_{m=-\infty}^{\infty} a^{-|m|} \exp\left\{i\tau^m \left[k_1 \cos\left(\frac{\pi j}{5}\right) + k_2 \sin\left(\frac{\pi j}{5}\right) \right]\right\}. \quad (45)$$

We show $|\rho(\mathbf{k})|$ for $a = 1.1$ in Fig. 6. It is not surprising that the rotational symmetry in the mass distribution is reflected in the Fourier transform domain: this is clear from Eq. (45). What is more interesting, and more beautiful, is that in the Fourier transform domain, where the signal is continuous (rather than localized on lines, as in the original space domain), we see a rich structure with local intensity maxima occurring at many points in the sectors between the ten lines on which the brightest peaks are located. Also, it is by no means obvious from the formula (45) where the intensity maxima on the bright lines will occur. In Fig. 7, we show $|\rho(\mathbf{k})|$ on the vertical axis in the \mathbf{k} -plane. There are many local maxima, but a sequence of locally outstanding maxima can be identified at the k_2 values 4.775, 7.732, 12.51, 20.25, 32.77. The successive ratios of these k_2 values are all close to (but not exactly) 1.618, and we see the golden

ratio from physical space recurring (to a decent approximation) in intensity maxima in Fourier space.

The convergence factor $a^{|m|}$ in Eq. (45) stops $|\tilde{\rho}(\mathbf{k})|$ from having exact dilatational symmetry. If we were able to set $a = 1$, then we would recover $|\tilde{\rho}(\mathbf{k})| = |\tilde{\rho}(\tau\mathbf{k})|$. Berry and Lewis [70] have considered what they call the Weierstrass–Mandelbrot fractal function

$$W(t) = \sum_{n=-\infty}^{\infty} \frac{[(1 - e^{i\gamma^n t})e^{i\phi_n}]}{\gamma^{(2-D)n}}, \quad 1 < D < 2, \gamma > 1, \quad (46)$$

where ϕ_n represents a constant phase added onto each term. The series is convergent and, if ϕ_n is constant, has perfect self-similarity: $W(\gamma t) = \gamma^{2-D}W(t)$. Ninham and Lidin [66] have considered another way of overcoming the problem of infinite mass accumulating in the neighborhood of the origin by using the formal series

$$\sum_{m=-\infty}^{\infty} [\cos(2\pi r \tau^{-m}) - \cos(2\pi \tau^{-m})]$$

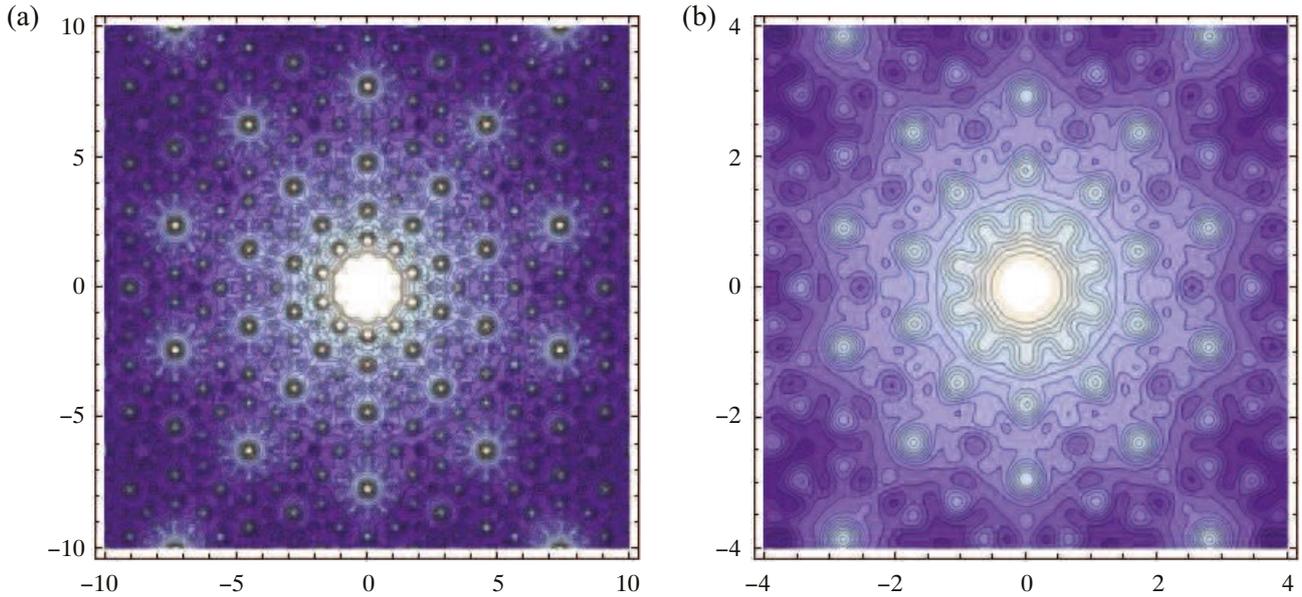


Figure 6. The \mathbf{k} -plane is colored (with 20 levels) to show $|\tilde{\rho}(\mathbf{k})|$, where the Fourier transform $\tilde{\rho}(\mathbf{k})$, given by Eq. (45), arises from the mass distribution (44). Lighter shades represent larger values of $|\tilde{\rho}(\mathbf{k})|$. (a) $-10 \leq k_1, k_2 \leq 10$; (b) $-4 \leq k_1, k_2 \leq 4$. For the convergence factor $a^{|m|}$ we have taken $a = 1.1$.

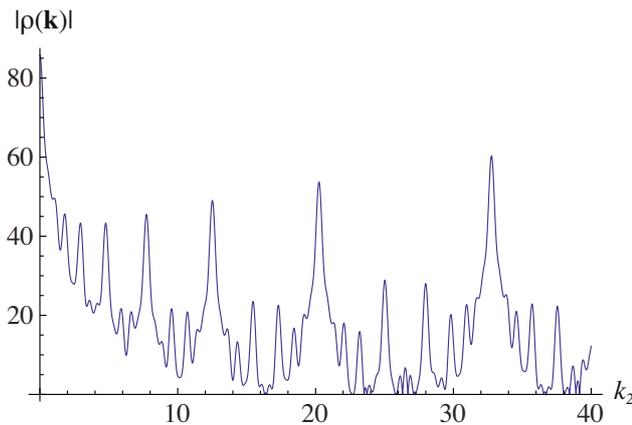


Figure 7. We show $|\tilde{\rho}(\mathbf{k})|$ on the line $\mathbf{k} = (0, k_2)$, where the Fourier transform $\tilde{\rho}(\mathbf{k})$, given by Eq. (45) arises from the mass distribution (44). For the convergence factor $a^{|m|}$ we have taken $a = 1.1$.

for the mass distribution along a ray through the origin, where r is the distance from the origin.

Quasicrystals are not the only context in which wild oscillations and apparent self-similar structure arise in the amplitude of diffracted light. Berry [71] gives a beautiful example, in which theta functions play a key role.

5. QUANTUM STATISTICAL MECHANICS

We consider several models from quantum statistical mechanics, for which we use standard notation and terminology [72, 73], so that k is Boltzmann's constant and T is the absolute temperature.

5.1. The harmonic oscillator

The free energy $g(\omega)$ associated with a harmonic oscillator of frequency ω and energy levels $(n + 1/2)\hbar\omega$ ($n = 0, 1, 2, \dots$) is given in terms of the canonical partition function $\mathcal{Z}(\omega)$ by

$$\exp\left[-\frac{g(\omega)}{kT}\right] = \mathcal{Z}(\omega) = \sum_{n=0}^{\infty} \exp\left[-\frac{(n + 1/2)\hbar\omega}{kT}\right]. \quad (47)$$

$$g(\omega) = kT \ln\left[2 \sinh\left(\frac{\hbar\omega}{2kT}\right)\right] = \frac{\hbar\omega}{2} - \sum_{n=1}^{\infty} \frac{kT}{n} \exp\left(-\frac{n\hbar\omega}{kT}\right). \quad (48)$$

For brevity, we have suppressed in the notation the dependence of the free energy on the temperature. Hence

$$g'(\omega) = \frac{\hbar}{2} + \hbar \sum_{n=1}^{\infty} \exp\left(-\frac{n\hbar\omega}{kT}\right), \quad (49)$$

leading to the formal identification [74]

$$\begin{aligned} \operatorname{Re}\{g'(i\omega)\} &= \frac{\hbar}{2} + \hbar \sum_{n=1}^{\infty} \cos\left(\frac{n\hbar\omega}{kT}\right) \\ &= \pi kT \sum_{n=-\infty}^{\infty} \delta\left(\omega - \frac{2\pi kTn}{\hbar}\right). \end{aligned} \quad (50)$$

This superficially bizarre result connecting the oscillator free energy to a string of delta functions, arising from the mathematical correspondence principle, proves surprisingly useful. If the modes of oscillation of a system are given by a secular equation of the form $D(\omega) = 0$, then the free energy can be computed as a sum over the contributions from the various modes by the contour integral

$$F = \frac{1}{2\pi i} \oint g(\omega) \frac{d}{d\omega} \ln[D(\omega)] d\omega, \quad (51)$$

the contour integral being taken over a simple closed contour that surrounds all zeros of $D(\omega)$ on the positive real axis. If there are infinitely many such zeros with the spacing bounded below as $\omega \rightarrow \infty$, an appropriate limiting construction is made. Integrating by parts, deforming the contour and making formal use of Eq. (50) enables the free energy to be computed conveniently [74, 75]. This is especially convenient in the calculation of dispersion (van der Waals) forces between dielectric media [74, 75].

5.2. Particle in a box

Using the energy eigenvalues (39), the free energy \mathcal{G} associated with a single (non-elementary [76]) particle of mass m in the d -dimensional box $[0, L]^d$ is given by

$$\begin{aligned} \exp\left[-\frac{\mathcal{G}}{kT}\right] &= \sum_{n_1=1}^{\infty} \sum_{n_2=1}^{\infty} \cdots \sum_{n_d=1}^{\infty} \exp\left[-\frac{\hbar^2 \sum_{j=1}^d n_j^2}{8mL^2kT}\right] \\ &= \left\{ \sum_{n=1}^{\infty} \exp\left[-\frac{\hbar^2 n^2}{8mL^2kT}\right] \right\}^d \\ &= \left\{ \frac{1}{2} \theta_3\left(0, \exp\left[-\frac{\hbar^2}{8mL^2kT}\right]\right) - \frac{1}{2} \right\}^d. \end{aligned} \quad (52)$$

Here we adopt the usual notational convenience of writing $\theta_k(z|\tau) = \theta_k(z, q)$, where $q = e^{i\pi\tau}$. If we consider N identical non-interacting particles in the same box, Eq. (52) becomes the equation for the free energy \mathcal{G} per

particle. Fixing T , the right-hand side can be evaluated asymptotically in the limit $L \rightarrow \infty$, using the Jacobi theta function transformation (4), which in the special case $z = 0$ and $\tau = it$ ($t \in \mathbb{R}$, with $t > 0$) becomes $\theta_3(0, it) = t^{-1/2} \theta_3(0|it^{-1})$. We find that

$$\exp\left[-\frac{\mathcal{G}}{kT}\right] = \left\{ \frac{L}{\lambda_T} \theta_3\left(0, \exp\left[-\frac{4\pi L^2}{\lambda_T^2}\right]\right) - \frac{1}{2} \right\}^d \quad (53)$$

$$\sim \left(\frac{L}{\lambda_T}\right)^d \quad \text{as } L \rightarrow \infty, \quad (54)$$

where for brevity in notation we have introduced the thermal wavelength $\lambda_T = h(2\pi mkT)^{-1/2}$. The single-term approximation (54) is well known [73], but the theta function representations (52) and (53) enable us to compute \mathcal{G} and the associated thermodynamic observables to high precision for any value of L/λ_T .

5.3. Ideal gas of elementary particles

Consider now ideal gases of elementary particles, which may be bosons (such as photons or mesons, for which an arbitrary number of particles can occupy any state) or fermions (such as electrons or neutrinos, for which any state may be occupied by at most one particle). It is more convenient to work with the grand partition function $Q = \prod_n \mathcal{Z}_n$, where \mathcal{Z}_n is the canonical partition function for occupancy of the n th state, in which each particle present has energy ε_n and chemical potential μ . Thus we have

$$\mathcal{Z}_n = \sum_{j=0}^{\infty} e^{-j(\varepsilon_n - \mu)/(kT)} = \frac{1}{1 - e^{-(\varepsilon_n - \mu)/(kT)}} \quad (\text{bosons});$$

$$\mathcal{Z}_n = \sum_{j=0}^1 e^{-j(\varepsilon_n - \mu)/(kT)} = 1 + e^{-(\varepsilon_n - \mu)/(kT)} \quad (\text{fermions}).$$

If we define the fugacity as usual by $z = \exp[\mu/(kT)]$ we obtain [77]

$$Q_B(T) = \prod_n \left[1 - z \exp\left(-\frac{\varepsilon_n}{kT}\right) \right]^{-1} \quad (\text{bosons});$$

$$Q_F(T) = \prod_n \left[1 + z \exp\left(-\frac{\varepsilon_n}{kT}\right) \right] \quad (\text{fermions}).$$

Consider the case of fugacity $z = 1$. If zero point energy is neglected and we write $\varepsilon_n = n\hbar\omega$ as in black-body radiation, then on writing $x = \exp[-\hbar\omega/(kT)]$ we find [5] that

$$\begin{aligned}
Q_B(T) &= \prod_{n=1}^{\infty} (1 - x^n)^{-1} = \frac{1}{\varphi(x)} : \\
Q_F(T) &= \prod_{n=1}^{\infty} (1 + x^n) = \frac{\prod_{n=1}^{\infty} (1 - x^{2n})}{\prod_{n=1}^{\infty} (1 - x^n)} = \frac{\varphi(x^2)}{\varphi(x)},
\end{aligned} \tag{55}$$

where Euler's product $\varphi(x) = \prod_{n=1}^{\infty} (1 - x^n)$, intimately related to the Jacobi theta functions, is discussed in Appendix A and has the transformation formula

$$\varphi(e^{-x}) = \left(\frac{2\pi}{x}\right)^{1/2} \exp\left(\frac{x}{24} - \frac{\pi^2}{6x}\right) \varphi(e^{-4\pi^2/x}), \tag{56}$$

which is one of the mathematical correspondence principle relations from Table 1. The original expressions for the grand partition function are able to be used for computation for high temperatures, but are useless at low temperatures. However, Eq. (56) gives immediate access to low temperature expansions, since we can eliminate $\varphi(\exp[-\hbar\omega/(kT)])$ in favor of $\varphi(\exp[-4\pi^2 kT/(\hbar\omega)])$. Planat [78] has pursued the implications of the relation between Euler's product and the theory of partitions [79] in the context of the massless Bose gas.

If we retain the zero point energy and consider a general value of the fugacity, we can represent the grand partition functions in terms of the q -Pochhammer function [80]

$$(a; q)_{\infty} = \prod_{n=0}^{\infty} (1 - aq^n) = \sum_{n=0}^{\infty} \frac{(-1)^n q^{n(n-1)/2} a^n}{\prod_{m=1}^n (1 - q^m)}. \tag{57}$$

Building on the work of Rogers and Ramanujan [81], there is now an impressive corpus of transformations and identities related to theta functions and q -Pochhammer functions, and they arise frequently in mathematical physics [82].

6. CASIMIR FORCES

The famous prediction of Casimir [83, 84] that the zero temperature energy of interaction of two perfectly conducting plates a distance ℓ apart in vacuum provides an attractive force per unit area $\pi^2 \hbar c / (240 \ell^4)$ between the plates was a landmark result. Direct experimental verification was challenging, with Sparnaay [85] in 1958 finding that “the attractive interactions do not contradict Casimir's theoretical prediction” (the experiments had

problematically large uncertainty). Finally, in 1997, Lamoreaux [86] effectively settled the basic issue [87]: “we have given an unambiguous demonstration of the Casimir force with accuracy of order 5%. Our data is not of sufficient accuracy to demonstrate the finite temperature correction ...”. (Casimir's original discussion did not address either finite temperature nor limitations on conductivity.) Crudely described, the Casimir effect demonstrates the consequences of geometrically constraining free oscillations of a system (here, the electromagnetic field) compared to the unconstrained state. Entirely classical analogues of the Casimir effect in macroscopic physics have been identified in a maritime context [88], and in an acoustic system suitable for lecture demonstrations [89].

The literature related to the Casimir effect is already voluminous and connections of papers with apparently cognate keywords to physics can be highly tenuous. At one extreme end of the literature [90, 91], since the evaluations of $\zeta(-1)$ and $\zeta(-3)$ are needed in the discussion of the physical Casimir effect (depending on the geometry), the evaluation for $s = -1$ of the analytic continuation of a series of the form $Z(s) = \sum_{\lambda} \lambda^{-s}$, where λ runs through a set of values with an interpretation related to energy levels, has been called the “Casimir energy”. The sign of $Z(-1)$ “reflects certain dynamical and arithmetical properties” [91] and formulae related to the so-called Casimir energy can be obtained for compact Riemann surfaces of genus $g \geq 2$.

Of greater physical interest is the embedding of the original Casimir effect in a broader context that admits predictions of interactions between more general classes of matter than perfect conductors at zero temperature [75, 92]. Profoundly important papers by Lifshitz [93, 94, 95] and his subsequent work with Dzyaloshinskii and Pitaevskii [96, 97], also appearing in a later textbook [98], replaced perfect conductors in vacuum by dielectric materials separated by an intervening dielectric material. By permitting the dielectrics to have a frequency-dependent dielectric susceptibility, a wide variety of physical (and even biological) systems could be discussed, and subsequent work of Ninham and Parsegian [99, 100] showed how the required dielectric properties could be determined from spectroscopic data, leading to the ability to make quantitative predictions in experimentally accessible systems. The original Casimir problem arises as an extreme limit of the Lifshitz theory approach, and Lifshitz theory permits the computation of temperature-dependent effects [74, 75, 101]. Experimental validation of the predictions of Lifshitz theory has been obtained in many cases [102].

We focus on the original Casimir problem—plates separated by vacuum—because it exhibits most simply

the importance of the mathematical correspondence principle. Let $F(\ell, T)$ denote the free energy of interaction per unit area between two infinite parallel conducting plates separated by a distance ℓ , in vacuum, at finite temperature T . It is instructive to see how extensive use of results of classical analysis such as the Riemann relation for the zeta function and various properties of the gamma function enable the free energy to be expressed in a highly informative way that enables dangerous issues concerning non-uniformity of asymptotic expansions to be dealt with [103]. Where we have already set the dielectric constant of the region between the plates to be unity, then from Lifshitz theory [75] we have

$$F(\ell, T) = \frac{kT}{8\pi\ell^2} \lim_{\Delta \rightarrow 1^-} \lim_{\bar{\Delta} \rightarrow 1^-} \sum'_{n=0} I(\xi_n, \ell), \quad (58)$$

where the prime on the sum indicates that the $n = 0$ term is to be weighted with a factor of 1/2, the parameter ξ_n is defined by

$$\xi_n = \frac{2\pi n k T}{h} \quad (59)$$

and

$$I(\xi_n, \ell) = \left(\frac{2\xi_n \ell}{c}\right)^2 \int_1^\infty p \left\{ \ln \left[1 - \Delta^2 \exp\left(-\frac{2p\xi_n \ell}{c}\right) \right] + \ln \left[1 - \bar{\Delta}^2 \exp\left(-\frac{2p\xi_n \ell}{c}\right) \right] \right\} dp. \quad (60)$$

To avoid an indeterminacy [104] in the case $n = 0$, we evaluate $I(\xi_n, \ell)$ for small positive real n by use of the change of variables $y = 2p\xi_n \ell/c$ and then take the limit $n \rightarrow 0$. The Riemann zeta function first arises from the $n = 0$ contribution from the $s = 3$ case of the integral (15).

For convenience in the asymptotic analysis we write

$$x = \frac{2kT\ell}{hc}. \quad (61)$$

The coupling between the temperature T and the plate spacing ℓ is very important. The limit $x \rightarrow 0$ corresponds to the low-temperature limit, provided that the plate separation is constrained, or to the small-spacing limit, provided that the temperature is not too high. The analysis of Ninham and Daicic [103] to this point has

$$F(\ell, T) = \frac{kT}{8\pi\ell^2} \left\{ -\zeta(3) + \sum_{n=1}^{\infty} (2\pi n x)^2 \int_1^\infty 2p \ln(1 - e^{-2\pi n x p}) dp \right\}. \quad (62)$$

To evaluate the sum over n we may begin by expanding the logarithm using the series

$$\ln(1 - Z) = - \sum_{m=1}^{\infty} \frac{Z^m}{m} \quad (-1 \leq Z < 1).$$

Since Eq. (13) shows that the gamma function is the Mellin transform [43] of the decaying exponential, using the Mellin inversion theorem [Eqs (30) and (31)] we have the contour integral representation

$$e^{-z} = \frac{1}{2\pi i} \int_{\kappa - i\infty}^{\kappa + i\infty} z^{-s} \Gamma(s) ds,$$

with the positive constant κ that places the vertical Bromwich contour $\text{Re}(s) = \kappa$ selected to secure convergence in the subsequent analysis based on this integral ($\kappa > 3$ suffices). We now have

$$\ln(1 - e^{-2\pi n x p}) = - \sum_{m=1}^{\infty} \int_{\kappa - i\infty}^{\kappa + i\infty} \frac{(2\pi m n x p)^{-s} \Gamma(s) ds}{2\pi i m},$$

so we can eliminate the logarithm factor from the integrand in Eq. (62), evaluate the resulting elementary integral over p and recognize the sums over m and n as series for the Riemann zeta function [Eq. (12)]. In this way one arrives at the scaled free energy

$$\mathcal{F} = \frac{hc\ell}{(kT)^2} F(\ell, T) \quad (63)$$

$$= -\frac{\zeta(3)}{4\pi x} - \frac{1}{2\pi i} \int_{\kappa - i\infty}^{\kappa + i\infty} \frac{\zeta(s-2)\zeta(s+1)\Gamma(s) ds}{(2\pi x)^{s-1}(s-2)}. \quad (64)$$

The integrand has only four singularities, namely the simple poles at $s = -1, 0, 2$ and 3 . To see this, we note that the gamma function has simple poles of residue $(-1)^j/j!$ at $s = -j$ ($j = 0, 1, 2, 3, \dots$), while $\zeta(s-2)\zeta(s+1)$ has a simple pole at $s = 3$ and simple zeros at $s = -2, -3, -4, \dots$ (noting that $\zeta(z)$ has a simple pole at $z = 1$ and simple zeros at $z = -2, -4, -6, \dots$).

The Bromwich contour may be translated an arbitrary finite distance, provided that we account correctly for the residues at poles across which the contour is dragged. If we move the contour to $\text{Re}(s) = 1$, then the term that must be added to account for the pole at $s = 2$ is easily shown to cancel with the first term on the right in Eq. (64). The pole at $s = 3$ leads to a term proportional to $1/x^2$, whose coefficient can be evaluated by recalling that $\zeta(0) = -1/2$ and $\zeta(4) = \pi^4/90$. We find that

$$\mathcal{F} = -\frac{\pi^2}{180x^2} - \frac{1}{2\pi i} \int_{1-i\infty}^{1+i\infty} \frac{\zeta(s-2)\zeta(s+1)\Gamma(s)ds}{(2\pi x)^{s-1}(s-2)}. \quad (65)$$

Since $\zeta(s-2) = -2^{s-2}\pi^{s-3}\sin(\pi s/2)\Gamma(3-s)\zeta(3-s)$ from the Riemann relation (11) and

$$\Gamma(3-s)\Gamma(s) = (2-s)(1-s)\Gamma(1-s)\Gamma(s) = \frac{(2-s)(1-s)\pi}{\sin(\pi s)} \quad (66)$$

we deduce that

$$\mathcal{F} = -\frac{\pi^2}{180x^2} + J(x), \quad (67)$$

where the first term on the right corresponds to the Casimir formula, while

$$J(x) = -\frac{1}{2\pi i} \int_{1-i\infty}^{1+i\infty} \frac{(1-s)\zeta(3-s)\zeta(s+1)ds}{4\pi \cos(\pi s/2)x^{s-1}}. \quad (68)$$

the change of variables $s = 1 + it$ produces

$$\begin{aligned} J(x) &= -\frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{t\zeta(2-it)\zeta(2+it)dt}{4\pi \sinh(\pi t/2)x^{it}} \\ &= -\int_0^{\infty} \frac{t\zeta(2-it)\zeta(2+it) \cos[t \ln(x)]dt}{4\pi^2 \sinh(\pi t/2)}. \end{aligned} \quad (69)$$

Since $\ln(x) = -\ln(1/x)$, Eq. (69) reveals the remarkable inversion symmetry

$$J(x) = J(x^{-1}). \quad (70)$$

The Casimir term is temperature-independent when one returns to the original variables, but the function $J(x)$ encapsulates genuine temperature dependence. The Riemann relation, one avatar of our central theme summarized in Table 1, has been used to expose the inversion symmetry (a previously observed result [107, 108]), but is also crucial for an efficient extraction of the x dependence. It may be noted in passing that a computer algebra software (such as Mathematica) is very helpful in checking that the intricate manipulations involved are correct, but is presently (and in the foreseeable future may well continue to be) unable to offer much help in guiding the analysis.

We digress for a moment. The function

$$\zeta(2+it)\zeta(2-it)$$

in the integrand in Eq. (69) is easily shown to be real-valued, but is by no means simple in structure: see Fig. 8. In qualitative terms, it appears roughly periodic, but

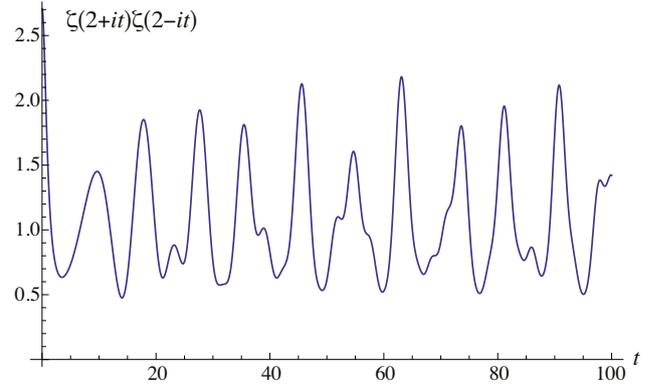


Figure 8. The function $\zeta(2+it)\zeta(2-it)$ in the integrand in Eq. (69): $0 < \zeta(2+it)\zeta(2-it) \leq \zeta(2)^2 = \pi^4/36 \approx 2.7$ for all $t \in \mathbb{R}$.

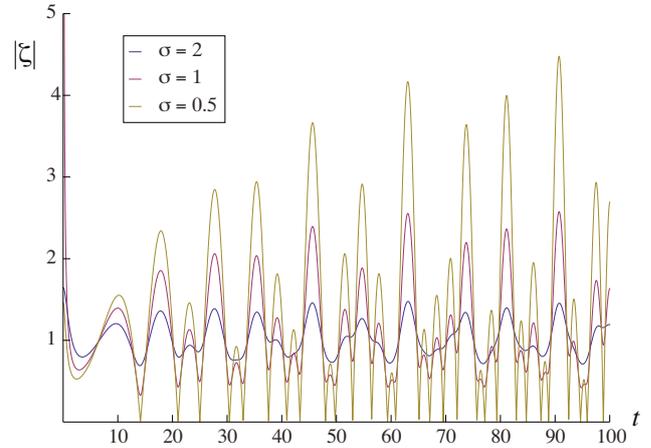


Figure 9. $|\zeta(\sigma+it)| = \sqrt{\zeta(\sigma+it)\zeta(\sigma-it)}$ for $\sigma \in \{1/2, 1, 2\}$, $0 < t < 100$.

the amplitudes of successive peaks and troughs and their spacing vary in an apparently random manner. More generally, for real σ and t , we have

$$\zeta(\sigma+it)\zeta(\sigma-it) = |\zeta(\sigma+it)|^2. \quad (71)$$

and the strange behavior of $|\zeta(2+it)|^2$ revealed in Fig. 8 arises also for other values of σ . When studying the response to changes in σ it is helpful to consider $|\zeta(\sigma+it)|$ rather than $|\zeta(\sigma+it)|^2$ to reduce the height of the maxima. We plot $|\zeta(\sigma+it)|$ in Fig. 9 for $\sigma = 2$, $\sigma = 1$ and $\sigma = 0.5$. It may be observed that the spacing of the peaks and troughs hardly changes, but the peak heights grow and the trough heights fall as σ decreases. It is relatively easy to prove that $\zeta(\sigma+it)$ is nonzero whenever $\sigma > 1$. That $\zeta(\sigma+it)$ is also never 0 for $\sigma = 1$ is much more difficult to prove. Establishing this was an essential ingredient of the proofs in 1896 by Hadamard [105] and de la Vallée

Poussin [106] that the number of prime numbers less than or equal to n has the asymptotic form $n/\ln n$ as $n \rightarrow \infty$. In the context of our discussion, the still-unresolved Riemann hypothesis [17, 19], asserts that $\zeta(\sigma + it) \neq 0$ for $\sigma > 1/2$. It is strangely beautiful that the mathematics of the Casimir effect comes so close to such subtle matters.

Returning to matters more overtly connected to physics, if F_{Casimir} denotes the original single-term Casimir energy prediction for the energy per unit area, we have

$$\frac{F(\ell, T)}{F_{\text{Casimir}}} = 1 + \eta(x), \quad \eta(x) = \frac{180x^2}{\pi^2} J(x). \quad (72)$$

In assessing the accuracy of the Casimir term, the role of the composite parameter x is crucial. We note that with ℓ measured in metres and T in Kelvin, we have

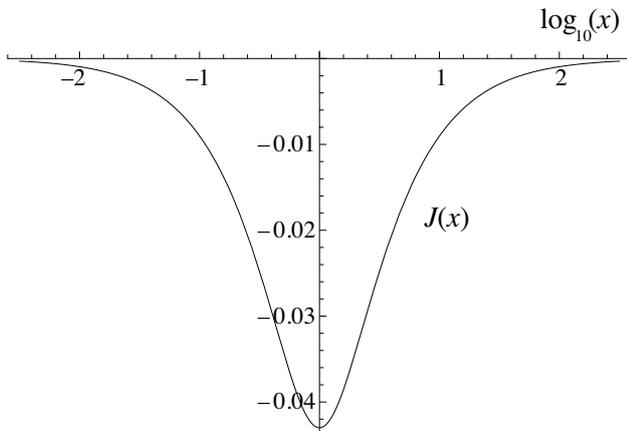


Figure 10. The function $J(x)$ computed from the integral (69) by numerical integration.

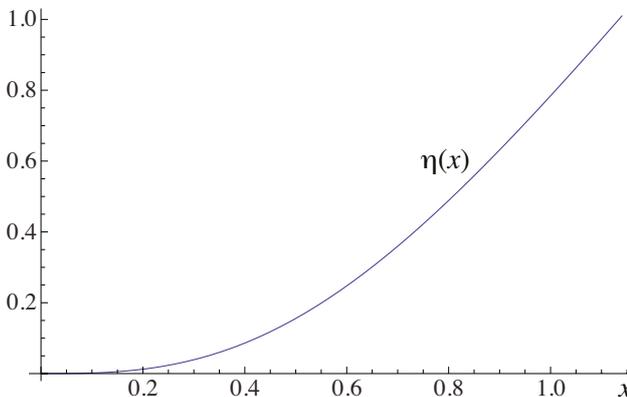


Figure 11. The fractional error $\eta(x)$ in the single-term Casimir formula, defined by Eq. (72), inferred from the numerically evaluated integral (69).

$$x = \frac{2kT\ell}{\hbar c} \approx 873T\ell. \quad (73)$$

In principle the numerical evaluation of the integral (69) requires some care because of the rapid oscillation of the cosine factor when $x \gg 1$ or $0 < x \ll 1$ and the erratic behavior of the real-valued function $\zeta(2 + it)\zeta(2 - it)$ (see Fig. 8). However, the Riemann–Lebesgue Lemma ensures that $J(x) \rightarrow 0$ as $x \rightarrow 0$ or as $x \rightarrow \infty$ and for the region where $J(x)$ differs perceptibly from zero, MATHEMATICA is up to the task. We show $J(x)$ for $10^{-2} \leq x \leq 10^2$ in Fig. 10. The fractional error η in the one-term Casimir formula, defined in Eq. (72), exceeds 1 for $x > 1.14$ but is less than 5×10^{-5} for $x \leq 0.03$.

In applications of the Casimir formula to experimental situations, relative errors associated with finite conductivity, departure of the real geometry from infinite parallel plates and other practical realities may dominate over the errors arising from the finiteness of the temperature that we have quantified through $\eta(x)$. Having acknowledged that caveat, we note that the case $x \approx 0.5$ arises for atomic dimensions ($\ell \approx 10^{-10}\text{m}$) when $T \approx 6 \times 10^6 \text{ K}$, within the range of estimated temperatures for the sun ($\approx 4 \times 10^3\text{K}$ at the surface, $1.6 \times 10^7\text{K}$ at the center [109]).

The analytic structures that have been revealed with the techniques illustrated above have a number of interesting consequences for the Casimir problem in vacuum and for analogous problems involving dielectric or conducting films. Some of these, including connections with nuclear and particle physics, have been explored elsewhere [110, 111]. The point to be made is that viewing physical problems from a mathematical perspective in the spirit of Table 1 leads both to efficient practical analysis and to new insights, though deep and subtle mathematical exotica are seldom far away.

7. CONCLUSIONS

We opened this paper with a reference to the conundrum of the surprising effectiveness of mathematics in physics. Berry has proposed one possible explanation [112].

We are beings of finite intelligence in an infinite inscrutable universe. In science, our individual intelligences cooperate, and we can understand more. But still, we are able to comprehend only those structures in the natural world that mirror our mental constructs. And at any stage of humanity's development, the most sophisticated constructs are those of our mathematics. Therefore our deepest penetration into the natural world is limited by our latest mathematics. As mathematics develops, more subtle features of

the universe become accessible to our understanding... So, 'The unreasonable effectiveness of mathematics in the natural sciences' is not unreasonable at all; on the contrary, it is inevitable.

This is not the only possible explanation, and in some areas, there are credible alternatives. We have shown that what is essentially one grand mathematical idea, which comes expressed in various ways, such as those collected in Table 1, underlies a wide range of apparently disparate physical phenomena. If one is a mathematical platonist—that is, a believer in the existence of abstract mathematical objects that are independent of intelligent agents and their language, thought and practices [113]—it is perhaps not such a leap of faith to conceive of a profound connection between some of these mathematical objects and physical reality.

Amongst a charming collection of pithy quotes and witticisms relevant to science collected by Berry [114] one finds what he calls “three laws of discovery”.

1. Discoveries are rarely attributed to the correct person [115].
2. Nothing is ever discovered for the first time [116].
3. Everything of importance has been said before by someone who did not discover it [117].

The existence of a common underlying mathematical theme in many contexts may be an explanation for the applicability of Berry’s laws in the sociology of physics.

Most physicists will wisely choose to limit their pondering of metaphysical questions to the bar or coffee shop, but the contemplation of what may be the most natural mathematical framework for physical theory and the pursuit of the implications of the mathematics is a more defensible use of one’s office hours. While physical intuition and accumulated conventional wisdom are always worthy of respect, careful analyses with appropriate mathematical insight can yield surprising results. Recently, Lekner [118] has shown that at small separations, charged conducting spheres always attract each other, even when the charges on the spheres are of the same sign, except when the spheres have charges in the ratio that would make them an equipotential surface on contact. This refutation of the rule that “like charges repel” in classical physics is indeed striking. In quantum mechanics, where physical intuition is a more contentious matter (and in the view of many, not even appropriate), accumulated conventional wisdom has still developed, but as noted recently by Ball [119] it is by no means a settled matter that we have either the optimal perspective on the subject or the optimal formulation.

What is the appropriate mathematical training for the modern physicist may be hotly debated, but what

we have styled a correspondence principle (embodied in Table 1) and the associated treasures of classical real and complex analysis have legitimate claim for inclusion.

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APPENDIX A. JACOBI THETA FUNCTIONS

Where $\text{Im}\{\tau\} > 0$ to secure convergence in the sense of classical analysis and $q = e^{i\pi\tau}$ (so that $|q| < 1$), the four Jacobi theta functions $\theta_k(z|\tau) = \theta_k(z, q)$ are

$$\begin{aligned} \theta_1(z|\tau) &= 2 \sum_{n=0}^{\infty} (-1)^n \exp\{\pi i(n + \frac{1}{2})^2 \tau\} \sin[(2n + 1)z] \\ &= 2 \sum_{n=0}^{\infty} (-1)^n q^{(n+1/2)^2} \sin[(2n + 1)z] \\ &= 2G(q)q^{1/4} \sin z \prod_{n=1}^{\infty} [1 - 2q^{2n} \cos(2z) + q^{4n}]; \\ \theta_2(z|\tau) &= 2 \sum_{n=0}^{\infty} \exp\{\pi i(n + \frac{1}{2})^2 \tau\} \cos[(2n + 1)z] \\ &= 2 \sum_{n=0}^{\infty} q^{(n+1/2)^2} \cos[(2n + 1)z] \\ &= 2G(q)q^{1/4} \cos z \prod_{n=1}^{\infty} [1 + 2q^{2n} \cos(2z) + q^{4n}]; \\ \theta_3(z|\tau) &= \sum_{n=-\infty}^{\infty} \exp\{\pi i n^2 \tau + 2inz\} = 1 + 2 \sum_{n=1}^{\infty} q^{n^2} \cos(2nz) \\ &= G(q) \prod_{n=1}^{\infty} [1 + 2q^{2n-1} \cos(2z) + q^{4n-2}]; \\ \theta_4(z|\tau) &= \sum_{n=-\infty}^{\infty} (-1)^n \exp\{\pi i n^2 \tau + 2inz\} \\ &= 1 + 2 \sum_{n=1}^{\infty} (-1)^n q^{n^2} \cos(2nz) \\ &= G(q) \prod_{n=1}^{\infty} [1 - 2q^{2n-1} \cos(2z) + q^{4n-2}]. \end{aligned}$$

Here

$$G(q) = \prod_{n=1}^{\infty} (1 - q^{2n}) = \varphi(q^2)$$

and Euler's product $\varphi(x) = \prod_{n=1}^{\infty} (1 - x^n)$ has the remarkable property [5] that

$$\varphi(e^{-x}) = \left(\frac{2\pi}{x}\right)^{1/2} \exp[x/24 - \pi^2/(6x)] \varphi(e^{-4\pi^2/x}).$$

Where $0 < \arg(\tau) < \pi$, the Jacobi transformation formulae are

$$\theta_1(z|\tau) = -i \exp\left(\frac{i\pi}{4} - \frac{iz^2}{\pi\tau}\right) \tau^{-1/2} \theta_1\left(\frac{z}{\tau} \middle| -\frac{1}{\tau}\right),$$

$$\theta_2(z|\tau) = \exp\left(\frac{i\pi}{4} - \frac{iz^2}{\pi\tau}\right) \tau^{-1/2} \theta_4\left(\frac{z}{\tau} \middle| -\frac{1}{\tau}\right),$$

$$\theta_3(z|\tau) = \exp\left(\frac{i\pi}{4} - \frac{iz^2}{\pi\tau}\right) \tau^{-1/2} \theta_3\left(\frac{z}{\tau} \middle| -\frac{1}{\tau}\right),$$

$$\theta_4(z|\tau) = \exp\left(\frac{i\pi}{4} - \frac{iz^2}{\pi\tau}\right) \tau^{-1/2} \theta_2\left(\frac{z}{\tau} \middle| -\frac{1}{\tau}\right).$$

We observe that in a formal sense, if not within classical analysis (with the limits taken under the restrictions that $|q| < 1$ or $\text{Re}\{\tau\} > 0$, respectively) that

$$\lim_{q \rightarrow 1} \theta_3\left(\frac{\pi x}{2L}, q\right) = \lim_{\tau \rightarrow 0} \theta_3\left(\frac{\pi x}{2L} \middle| \tau\right) = L \sum_{n=-\infty}^{\infty} \delta(x - 2nL).$$

APPENDIX B. DIFFUSION WITH INCREASING LETHARGY

There is another interesting model for a kind of anomalous diffusion that raises mathematical questions that are at least as subtle as those discussed in Section 3.2 and partly related to them [120]. Consider a random walk in one dimension, for which steps to the left and right are equally likely at each stage, but the length of the n th step is c_n , where $c_n > 0$ and $\sum_{n=1}^{\infty} c_n < \infty$. The walker exhibits increasing lethargy, and asymptotically comes to rest at a random position X relative to the starting location, where $X = \sum_{n=1}^{\infty} \epsilon_n c_n$, the random variables $\{\epsilon_n\}$ are independent, and $\Pr\{\epsilon_n = 1\} = \Pr\{\epsilon_n = -1\} = 1/2$. In the probability literature, the random variable X is described as an ‘‘infinite Bernoulli convolution’’ and it

can be proved [121] that provided that $\sum_{n=1}^{\infty} c_n^2 < \infty$, the characteristic function (Fourier transform) associated with the distribution of this random variable exists, and is given by $E\{\exp(iqX)\} = \prod_{n=1}^{\infty} \cos(c_n q)$.

The case $c_n = \alpha^{n-1}$, where $0 < \alpha < 1$, for which $E\{\exp(iqX)\} = \prod_{n=0}^{\infty} \cos(\alpha^n q)$, is especially fascinating [122, 123, 124, 125]. This model builds in self-similarity in a way reminiscent of, but different to, Section 3.2. We have $X = \epsilon_1 + \alpha X_1$, where X and X_1 are identically distributed random variables, while ϵ_1 and X_1 are independent. Since $\sum_{n=0}^{\infty} \alpha^n = (1 - \alpha)^{-1}$, we know that $-(1 - \alpha)^{-1} \leq X \leq (1 - \alpha)^{-1}$. For the case $\alpha = 1/2$, it can be proved [127] that X is uniformly distributed on $[-2, 2]$, but for many other values of $\alpha \in (0, 1)$ the distribution of X does not apportion the probability so smoothly.

In general [126], the cumulative distribution function $F(x) = \Pr\{X \leq x\}$ of a real random variable X consists of either a single one, or a linear combination of both, of the following components: (i) an ‘‘absolutely continuous’’ component, corresponding to classical probability density function; (ii) a ‘‘singular’’ component, in which the probability all resides on a set of measure zero. For the increasingly lethargic walk with $0 < \alpha < 1/2$, X has a singular distribution: the nonzero probability all resides on a Cantor set of measure zero [123]. The rapid attenuation of the step lengths prevents the walker from exploring the apparent support decently. For $1/2 < \alpha < 1$, it has been proved [122] that the distribution of X for any given value of α is either entirely absolutely continuous or entirely singular. The simplicity of the case $\alpha = 1/2$ might suggest that absolute continuity always prevails for $1/2 < \alpha < 1$, and it has been proven that the set of values of $\alpha \in (1/2, 1)$ for which the distribution is singular has measure zero [128], but a countable number of values of $\alpha \in (1/2, 1)$ for which the distribution is singular were found by Erdős [124] and the search for other anomalous α values continues.

Diffusion with accumulating lethargy also has interesting connections to the discussion of Section 4, where the golden ratio $\tau = (1 + \sqrt{5})/2$ plays a significant role. Hu [129] has shown that for $\alpha = 1/\tau = (\sqrt{5} - 1)/2$ and for $-(1 - \alpha)^{-1} < x < (1 - \alpha)^{-1}$, the local fractal dimension

$$d(x) = \lim_{r \rightarrow 0^+} \log[\Pr\{x - r \leq X \leq x + r\}] / \log(r)$$

of the distribution of the random variable has maximum value $\log(2)/\log(\tau) \approx 1.4404$ and minimum value $\log(2)/\log(\tau) - 1/2 \approx 0.9404$. For additional related results see Lau and Ngai [130].

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- [17] B. Riemann, “Ueber die Anzahl der Primzahlen unter einer gegebenen Grösse,” *Monatsberichte der Königl. Preussische Akademie der Wissenschaften zu Berlin aus der Jahre 1859*, 671–680 (1860).
- [18] Riemann shows that where $\psi(x) = \sum_{n=1}^{\infty} e^{-n^2\pi x}$ and $\text{Re}\{s\} > 1$, we have $\zeta(s)\pi^{-s/2}\Gamma(s/2) = \int_0^{\infty} x^{s/2-1}\psi(x)dx$. He uses the transformation formula for $\theta_3(0|ix)$ to construct an analytic continuation for $\zeta(s)\pi^{-s/2}\Gamma(s/2)$ that is symmetric under replacement of s by $1-s$, and the Riemann relation follows.
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- $$1 - s\zeta(s+1) + \frac{s(s+1)}{2!}\zeta(s+2) - \frac{s(s+1)(s+2)}{3!}\zeta(s+3) + \dots = 0.$$
- from which the same conclusions about simple known values of $\zeta(-m)$ for m a non-negative integer be drawn. The method given in the present paper is classically rigorous. For an alternative rigorous approach, leading to the identity
- $$\sum_{q=0}^{\infty} \frac{(s-1)(s)_q}{(q+1)!} [\zeta(s+q) - 1] = 1,$$
- see §68 of E. Landau, *Handbuch der Lehre von der Verteilung der Primzahlen* (1st edition, Leipzig and Berlin, Teubner, 1909; 3rd edition, Providence, Rhode Island, AMS Chelsea, 1974).
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rier transform of the mass distribution $\rho(\mathbf{r}) = \sum_{\ell \in \mathcal{L}} \delta(\mathbf{r} - \ell)$ defined by placing unit mass at each point of \mathcal{L} is given by $\tilde{\rho}(\mathbf{k}) = \sum_{\ell^* \in \mathcal{L}^*} \delta(\mathbf{k} - \ell^*)$. More general results which essentially account for all simple cases have been established by Córdoba [13], who has shown that if μ and ν are two discrete subsets of \mathbb{R}^d (this requires the existence of a nonzero lower bound for the spacing between pairs of points) and $c(\mathbf{s}) > 0$ for all $\mathbf{s} \in \mu$ then the relations

$$\rho(\mathbf{r}) = \sum_{\mathbf{s} \in \mu} \delta(\mathbf{r} - \mathbf{s}), \quad \tilde{\rho}(\mathbf{k}) = \sum_{\mathbf{s} \in \nu} c(\mathbf{s}) \delta(\mathbf{k} - \mathbf{s}),$$

between a mass distribution $\rho(\mathbf{r})$ and its Fourier transform

$$\tilde{\rho}(\mathbf{k}) = \int_{\mathbb{R}^d} \exp(2\pi i \mathbf{k} \cdot \mathbf{r}) f(\mathbf{r}) d^d \mathbf{r}$$

can hold simultaneously if and only if the following conditions hold: $c(\mathbf{s}) = 1$ and there exists a linear transformation A of \mathbb{R}^d with determinant 1 such that $\mu = A\mathbb{Z}^d$ and $\nu = (A^{-1})^T \mathbb{Z}^d$, where T denotes the transpose. It may be noted that because the definitions of the Fourier transform and its inverse are simply complex conjugates, the factor of $c(\mathbf{s})$ can be placed in either one of the sums over μ and ν without altering the result. We have used this in rephrasing Córdoba's result to suit our notation and our application of interest, where it is more natural to assert that all masses are the same in physical space and allow position-dependent coefficients in the sum obtained on taking the Fourier transform.

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