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Quantum diffusion

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If you place a drop of ink into a glass of water, the ink will slowly dissipate into the surrounding water until it is perfectly mixed. If you record your experiment with a camera and play the film backwards, you will see something that is never observed in the real world. Such diffusive and irreversible behaviour is ubiquitous in nature. Nevertheless, the fundamental equations that describe the motion of individual particles – Newton's and Schrödinger's equations – are reversible in time: a film depicting the motion of just a few particles looks as realistic when played forwards as when played backwards.

In this snapshot, we discuss how one may try to understand the origin of diffusion starting from the fundamental laws of quantum mechanics.

1 Quantum mechanics on a lattice

Despite the spectacular success of Newtonian mechanics[1] for over two centuries, physicists realized at the beginning of the 20th century that it was woefully

[1] Newtonian mechanics was formulated in Newton's celebrated *Philosophiae Naturalis Principia Mathematica*, published in 1687 by the Royal Society of London. It constitutes the core of *classical mechanics*, a term coined in the beginning of the 20th century in contrast to the nascent theory of *quantum mechanics*.

inadequate in describing the structure of matter. This led to the development of quantum mechanics in the first quarter of the 20th century. According to Schrödinger's formulation of quantum mechanics (1925), the state of a quantum particle is given by a *wave function*, which replaces the three plus three coordinates of position and momentum from Newtonian mechanics.

Consider a particle moving on a lattice, as depicted in Figure 1. A physical interpretation is an electron moving on an atomic lattice. In this note, we focus on a lattice for simplicity of presentation, but all of the following ideas have counterparts in the continuum, where the particle is moving in Euclidean space. We call the lattice Λ, and suppose that it is equal to the d-dimensional lattice $\mathbb{Z}^d$, consisting of d-dimensional vectors whose coordinates are integers. Here, $d = 3$ is of course the most natural choice, but other values of d are also of interest, both mathematically and physically ($d = 2$ and $d = 1$ can in fact be realized in experiments).

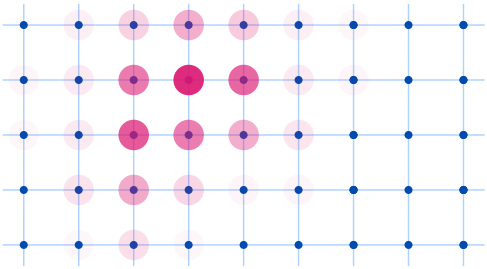

Figure 1: A portion of the two-dimensional lattice $\mathbb{Z}^2$. We draw a quantum particle schematically using red discs indicating the probability $|\psi(x)|^2$ of finding the particle at the lattice site x.

A *wave function* is a function, denoted by ψ, on the lattice Λ. It is of great importance in quantum mechanics that the value $\psi(x)$ of the wave function at the lattice point $x \in \Lambda$ be a *complex number*. This motivates a short digression on complex numbers[2]. Just as a real number may be regarded as a point on a line, a complex number may be regarded as a point in the plane consisting of two real numbers a and b. Conventionally, a complex number is written as $z = a + \mathrm{i}b$, where i is the *imaginary unit*, a formal object that satisfies the property $\mathrm{i}^2 = -1$. Complex numbers may be added and multiplied exactly like real numbers, with the simple convention that i^2 is always replaced by -1. A complex number $a + \mathrm{i}b$ is real whenever $b = 0$.

[2] If you would like to learn more about complex numbers, you might want to have a look at Bruce Reznick's snapshot *What does '>' really mean?* (No. 4/2014). This digression, however, is sufficient for our needs.

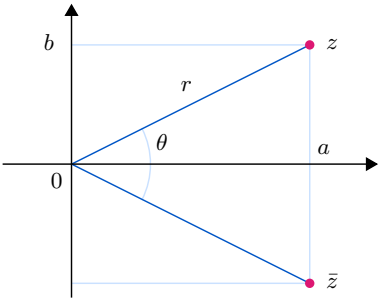

Figure 2: A complex number $z = a + \mathrm{i}b = r\mathrm{e}^{\mathrm{i}\theta}$ and its complex conjugate $\bar{z} = a - \mathrm{i}b = r\mathrm{e}^{-\mathrm{i}\theta}$, represented in Cartesian and polar coordinates.

Instead of using the Cartesian coordinates a and b, a complex number may also be represented using *polar coordinates*,

$$z \;=\; a + \mathrm{i}b \;=\; r\cos\theta + \mathrm{i}r\sin\theta \;=\; r\mathrm{e}^{\mathrm{i}\theta}\,, \tag{1}$$

where in the second equality we used *Euler's formula* $\cos\theta + \mathrm{i}\sin\theta = \mathrm{e}^{\mathrm{i}\theta}$; see Figure 2. We conclude our digression on complex numbers by defining the *complex conjugate* $\bar{z}$ of a complex number z, obtained from z by a reflection about the horizontal axis. Hence, for the complex number from (1) we have $\bar{z} = a - \mathrm{i}b = r\mathrm{e}^{-\mathrm{i}\theta}$. The simple rules $\overline{z+w} = \bar{z} + \bar{w}$ and $\overline{zw} = \bar{z}\bar{w}$ are easy to check from the definition of the complex conjugate. Finally, by Pythagoras' theorem, we find that the distance from 0 to z is equal to $|z| = \sqrt{a^2 + b^2} = \sqrt{z\bar{z}} = r$.

Let us now return to the wave function ψ, which, we recall, defines the state of our quantum particle. A fundamental principle of quantum mechanics states that, in general, the position of the particle in state ψ is not precisely known, and that ψ only gives us information about the *probability* of finding the particle at a given position. More precisely, the probability of the particle's being at position $x \in \Lambda$ is equal to $|\psi(x)|^2$. Since the sum of these probabilities over all lattice sites must be equal to one, we always impose the normalization

$$\sum_{x\in\Lambda} |\psi(x)|^2 \;=\; 1 \tag{2}$$

on our wave function ψ. See Figure 1 for an illustration of the probability distribution $|\psi(x)|^2$ for one choice of ψ.

Now that we know how to describe the state of a quantum particle, we have to determine how this state evolves in time. As formulated by Schrödinger in 1925, the dynamics of a quantum particle is governed by a *Hamiltonian* –

a linear map[3] H that assigns to each wave function ψ a new wave function $H\psi$. The choice of H defines the physical model (below we shall give several examples of Hamiltonians). Once the Hamiltonian H is given, the evolution of the time-dependent wave function ψ_t is given by *Schrödinger's equation*

$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}\psi_t(x) \;=\; (H\psi_t)(x)\,. \tag{3}$$

This is a *linear first-order differential equation*, which means that it is a linear equation in the wave function ψ_t and its time derivative $\frac{\mathrm{d}}{\mathrm{d}t}\psi_t$. The solution of such an equation is uniquely determined by the wave function ψ_0 at time $t = 0$. Despite being a linear first-order differential equation, the Schrödinger equation (3) can be extremely difficult to solve. This is because the evolving quantity ψ_t is a collection of *infinitely* many complex numbers $\psi_t(x)$, $x \in \Lambda$.

By definition, a Hamiltonian is always required to be *self-adjoint*. This means that $\sum_{x\in\Lambda} \overline{\psi(x)}(H\psi)(x)$ is a real number for all wave functions ψ. Using this fact, combined with the product rule of differentiation and Schrödinger's equation (3), we can compute the time derivative of the total probability:

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\sum_{x\in\Lambda}|\psi_t(x)|^2 \;&=\; \sum_{x\in\Lambda}\overline{\Big(\frac{\mathrm{d}}{\mathrm{d}t}\psi_t(x)\Big)}\psi_t(x) + \sum_{x\in\Lambda}\overline{\psi_t(x)}\Big(\frac{\mathrm{d}}{\mathrm{d}t}\psi_t(x)\Big)\\ &=\; \mathrm{i}\sum_{x\in\Lambda}\overline{\big((H\psi_t)(x)\big)}\psi_t(x) - \mathrm{i}\sum_{x\in\Lambda}\overline{\psi_t(x)}\big((H\psi_t)(x)\big) \;=\; 0\,,\end{aligned}$$

where in the last step we used the self-adjointness of H, combined with the fact that a complex number z is real if and only if $\bar{z} = z$. We conclude that the *normalization* (2) *is preserved under time evolution*: if ψ_0 is normalized in the sense of (2), then so is ψ_t for any time t. Hence, we may define for each time t a probability distribution

$$p_t(x) \;\coloneqq\; |\psi_t(x)|^2\,. \tag{4}$$

The quantity $p_t(x)$ has the interpretation of the probability of finding the quantum particle at position x at time t.

2 Diffusion

Let us shift our attention for a while to a classical particle, and consider, for simplicity, the one-dimensional lattice $\Lambda = \mathbb{Z}$. The simplest model exhibiting

[3] In general, a *linear map* between two vector spaces V and W is a function $H : V \to W$ satisfying $H(a\psi + b\varphi) = aH(\psi) + bH(\varphi)$ for any vectors $\psi, \varphi \in V$ and numbers a and b. In our case, $V = W$ is the vector space of wave functions. As is customary, we use the shorthand notation $H(\psi) \equiv H\psi$ for the value of a linear map.

diffusion is the *simple random walk*, where the particle successively jumps to a neighbouring site with uniform probability.

In order to make such ideas precise, it is helpful to recall some basic ideas of probability theory in another short digression[4]. For simplicity, we focus on the discrete case where all random variables take values in a countable set. (As you may know, similar ideas apply for general random variables, which may have a continuous distribution.) We have a *sample space* Ω, which is a set consisting of all possible *outcomes* or *realizations* of our random system. We have a collection of *events*, which are subsets of Ω. Moreover, we have a *probability* $\mathbb{P}$ that assigns to each event A a number $\mathbb{P}[A] \in [0,1]$, the probability of A. A *random variable* X is a function on Ω, so that $X(\omega)$ is the value that the random variable X takes in the realization ω. The probability that the random variable X is equal to some value x is written as $\mathbb{P}[X = x] \coloneqq \mathbb{P}[\{\omega : X(\omega) = x\}]$. We say that the random variables $X_1, \dots, X_n$ are *independent* if $\mathbb{P}[X_1 = x_1, \dots, X_n = x_n] = \mathbb{P}[X_1 = x_1] \cdots \mathbb{P}[X_n = x_n]$ for all $x_1, \dots, x_n$. Informally, this means that the distribution of X_i, $i = 1, \dots, n$, is not affected by the realization of the other random variables. Finally, we define the *expectation* of the random variable X as $\mathbb{E}[X] \coloneqq \sum_x x\, \mathbb{P}[X = x]$.

Let us now return to the simple random walk. It is obtained by constructing a sequence of independent random variables $Z_1, Z_2, Z_3, \dots$ taking values in $\{-1, 1\}$. The interpretation of Z_i is the i-th jump of the random walk, whereby $Z_i = -1$ means a jump to the left and $Z_i = +1$ a jump to the right. We require both directions to have the same probability, so that $\mathbb{P}[Z_i = -1] = \mathbb{P}[Z_i = +1] = 1/2$ for all $i \in \mathbb{N}$.

Our particle starts at $X_0 = 0$ and undergoes a simple random walk, making a jump Z_i at time i. Its position X_t at an integer time $t \in \mathbb{N}$ is therefore given by the sum of all jumps up to time t:

$$X_t \;\coloneqq\; Z_1 + Z_2 + \cdots + Z_t\,. \tag{5}$$

Since $\mathbb{E}[Z_i] = 1 \cdot \mathbb{P}[Z_i = +1] - 1 \cdot \mathbb{P}[Z_i = -1] = 1/2 - 1/2 = 0$ for all $i \in \mathbb{N}$, we find that $\mathbb{E}[X_t] = 0$ for all $t \in \mathbb{N}$: the expected position is always the origin. A more interesting quantity is the *expected squared distance* from X_0 to X_t,

$$\mathbb{E}\big[X_t^2\big] \;=\; \mathbb{E}\big[(Z_1 + Z_2 + \cdots + Z_t)^2\big] \;=\; \mathbb{E}\big[Z_1^2 + Z_2^2 + \cdots + Z_t^2\big] \;=\; t\,, \tag{6}$$

where in the second step we used that if $i \neq j$ then Z_i and Z_j are independent and hence $\mathbb{E}[Z_i Z_j] = \mathbb{E}[Z_i]\mathbb{E}[Z_j] = 0$, and in the third step we used that $\mathbb{E}[Z_i^2] = 1^2 \cdot \mathbb{P}[Z_i = +1] + (-1)^2 \cdot \mathbb{P}[Z_i = -1] = 1$.

[4] If you would like to learn more about probability theory, the book *Probability essentials* by Jean Jacod and Philip Protter [8] is an excellent place to start.

This calculation shows that the typical displacement from the origin at time t, given by $\sqrt{\mathbb{E}[X_t^2]}$, is proportional to $\sqrt{t}$. Such a relation is the hallmark of *diffusion*.

In contrast, suppose that instead of making jumps in a random direction, the particle always moves to the right. (In the above probabilistic language, this means that $\mathbb{P}(Z_i = +1) = 1$ and $\mathbb{P}(Z_i = -1) = 0$.) Then, clearly, $X_t = t$ and we have $\mathbb{E}[X_t^2] = t^2$. This type behaviour is called *ballistic*, and corresponds to a particle moving linearly at a constant speed. Finally, if the particle never leaves a neighbourhood of 0 (for instance if the particle does not move or if it jumps alternately left and right), the quantity $\mathbb{E}[X_t^2]$ remains bounded as t grows. This corresponds to a *trapped particle*. Summarizing, we have seen three different types of behaviour as t goes to infinity:

$$\sqrt{\mathbb{E}\big[X_t^2\big]} \;\sim\; \begin{cases} t & \text{for ballistic motion} \\ \sqrt{t} & \text{for diffusive motion} \\ \text{constant} & \text{for trapped motion}\,. \end{cases}$$

They are illustrated in Figure 3.

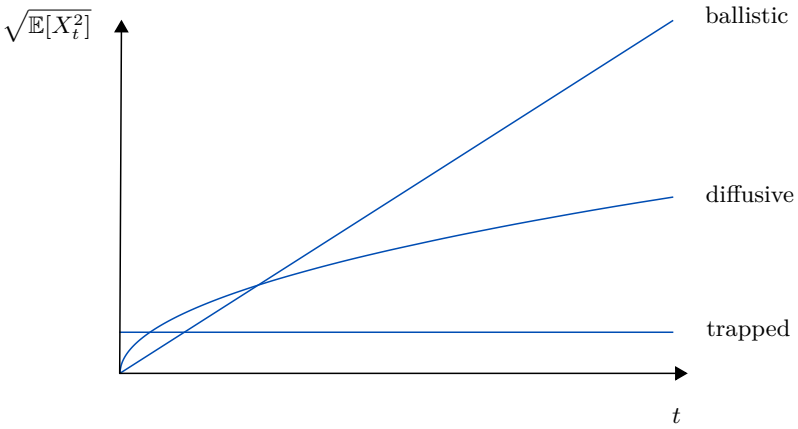

Figure 3: The behaviour of the typical displacement from the origin for the three types of dynamics.

Returning to the probability distribution (4) defined in terms of the quantum-mechanical wave function that solves Schrödinger's equation, we may ask whether the behaviour of p_t is ballistic, diffusive, or trapped. To answer this question, we choose the initial state of the wave function to correspond to a

particle located at the origin with probability one,

$$\psi_0(x) \coloneqq \begin{cases} 1 & \text{if } x = 0 \\ 0 & \text{if } x \neq 0\,, \end{cases} \tag{7}$$

and we define p_t as in (4) in terms of the solution ψ_t of the Schrödinger equation (3). Then we investigate the large-time behaviour of the expected squared distance from the origin

$$\sum_{x\in\Lambda} |x|^2\, p_t(x)\,, \tag{8}$$

where $|x|$ is the distance from the lattice point $x \in \Lambda$ to the origin 0.

The answer to the above question clearly depends on the choice of the Hamiltonian. In general, and in many physically interesting cases, it is extremely difficult to answer. However, it is easy to concoct examples of Hamiltonians that result in ballistic or trapped motion.

Suppose first that $(H\psi)(x) = v(x)\psi(x)$ for some real-valued function v on Λ. As required by the definition of a Hamiltonian, H is a self-adjoint linear map (you can verify this as a simple exercise). Moreover, the solution of Schrödinger's equation (3) is easy to write down: $\psi_t(x) = \mathrm{e}^{-\mathrm{i}tv(x)}\psi_0(x)$. You can easily check that this ψ_t solves (3). Hence, $p_t(x) = p_0(x)$ for all times t, and we conclude that (8) does not depend on t. The motion is therefore *trapped*.

A slightly more interesting Hamiltonian is the *discrete Laplacian* Δ, defined through

$$(\Delta\psi)(x) \coloneqq \sum_{y:|y-x|=1} (\psi(x) - \psi(y))\,, \tag{9}$$

where the summation ranges over points y of the lattice that are nearest neighbours of x. (There are $2d$ of them.) Again, a short calculation shows that Δ is self-adjoint. Using *Fourier analysis*[5], one can prove that for $H = \Delta$ the behaviour of (8) is *ballistic*: it grows like t^2 for large t. The physical interpretation of the Hamiltonian Δ is a *free particle* moving on the lattice. This model is the quantum analogue of the naive classical ballistic particle introduced above.

Of course, both of these models are very simple and not particularly realistic. Moreover, neither leads to diffusive motion. In order to remedy these deficiencies, we introduce *disorder* into our Hamiltonian.

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[5] Fourier analysis is a powerful way of writing arbitrary functions as superpositions of simple waves. In Chapter 3 of his snapshot *The ternary Goldbach problem* (No. 3/2014), Harald Helfgott gives an introduction to Fourier analysis.

3 Random Hamiltonians and quantum diffusion

Think of our quantum particle as an itinerant electron moving on an atomic lattice. A perfect lattice can be modelled by a Hamiltonian similar to Δ, and, as explained above, results in ballistic motion[6]. However, a more realistic, and interesting, model should include imperfections caused for instance by impurities and thermal fluctuations of the lattice. It is neither possible nor desirable to define these imperfections precisely one by one; rather, we seek a statistical description that reproduces an appropriate distribution of imperfections. In other words, we choose a large collection, or *ensemble*, of Hamiltonians, and pick one *realization* from this ensemble at random. From a physical point of view, the different realizations of H could correspond to different states of thermal fluctuation of the atomic lattice, or to different distributions of defects or impurities in the atomic lattice. Mathematically, considering an ensemble of Hamiltonians means that the Hamiltonian $H \equiv H(\omega)$ depends on the realization ω in some sample space Ω equipped with a probability $\mathbb{P}$.

If we choose the ensemble of Hamiltonians appropriately, we expect that a randomly chosen realization will give rise to a diffusive behaviour with high probability. The randomness is therefore used to rule out exceptional "regular" realizations of H that occur only with small probability. Hence, taking a random ensemble of Hamiltonians allows one to make precise the statement that a "typical" Hamiltonian leads to diffusive behaviour. Such mathematical modelling of complex disordered systems using randomness has proved extremely fruitful in many sciences.

So what should we choose as our ensemble of random Hamiltonians? One important example is the *Anderson model*

$$(H\psi)(x) \;\coloneqq\; (\Delta\psi)(x) + v(x)\psi(x)\,, \tag{10}$$

where $(v(x) : x \in \Lambda)$ is a collection of independent identically distributed[7] real-valued random variables[8]. Another important example is the *random band matrix*

$$(H\psi)(x) \;\coloneqq\; \sum_{y:|x-y|\leqslant W} \big(A_{xy} + A_{yx}\big)\psi(y)\,, \tag{11}$$

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[6] This seemingly simple fact is in fact a remarkable feature of quantum mechanics, called *Bloch's theorem*. In contrast, in classical mechanics, a particle moving on a regular lattice (the so-called periodic Lorentz gas) undergoes highly erratic motion. (The precise mathematical notion is *ergodicity* of the particle's motion.)

[7] "Identically distributed" means that each $v(x)$ has the same probability distribution.

[8] A common and convenient choice for the distribution of $v(x)$ is the famous *standard normal distribution*, which you may have encountered in probability theory. Its density is given by f_1 in (12) below.

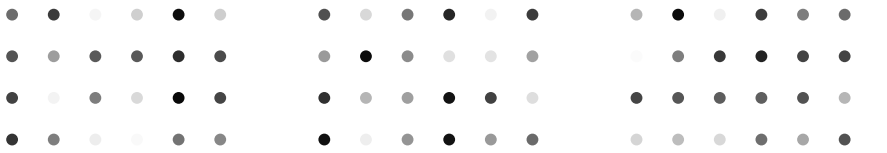

Figure 4: Three realizations of the Anderson model (10) for $\Lambda = \mathbb{Z}^2$. Each lattice site $x \in \Lambda$ is represented by a dot whose brightness depends on $v(x)$.

where $W > 0$ is a parameter called the *band width*, and $(A_{xy} : x, y \in \Lambda)$ is a collection of independent identically distributed real-valued random variables. You may check that both of these random Hamiltonians are self-adjoint. Moreover, they are *invariant under time reversal*. This means that if ψ_t is the solution of the Schrödinger equation (3), then the *time-reversed* wave function $\varphi_t(x) := \overline{\psi_{-t}(x)}$ is also a solution of (3). Informally, the quantum time evolution generated by (10) or (11) runs equally well forwards and backwards in time.

Both models (10) and (11) have been extensively studied in the physics literature, ever since the seminal paper of Anderson [1]. There is compelling evidence to suggest that, on the three-dimensional lattice $\Lambda = \mathbb{Z}^3$ and under appropriate assumptions on the distribution of the random variables, a randomly chosen realization of H gives rise to *quantum diffusion* with very high probability: (8) grows like t for large t. (In contrast, on the one-dimensional lattice $\Lambda = \mathbb{Z}$ it is known [7] that a randomly chosen realization of H leads to trapped motion with very high probability.)

A rigorous mathematical understanding of quantum diffusion for the models (10) and (11) is a formidable task. So far, quantum diffusion has only been established for relatively short time scales, in a so-called *scaling limit* where the time t cannot go to infinity arbitrarily fast but is coupled to some internal parameters of the model, such as the band width W from (11). This analysis was achieved for the model (10) in [4–6] and for the model (11) in [2, 3].

In fact, in these works it is not only proved that (8) is of order t for large t, but the actual profile of the probability distribution p_t is computed. Roughly, in [2–6] it is proved that for large t the profile p_t is well approximated by a *normal distribution* with *variance* σ^2 of order t. Here, a (mean-zero) normal distribution with variance σ^2 is by definition the Gaussian probability density

$$f_{\sigma^2}(x) \;:=\; \frac{1}{\sqrt{2\pi\sigma^2}}\, \mathrm{e}^{-\frac{x^2}{2\sigma^2}}\,. \tag{12}$$

(As you may have learned in probability theory, f_{σ^2} is indeed a probability density on $\mathbb{R}$ in the sense that $\int \mathrm{d}x\, f_{\sigma^2}(x) = 1$ for all $\sigma > 0$.)

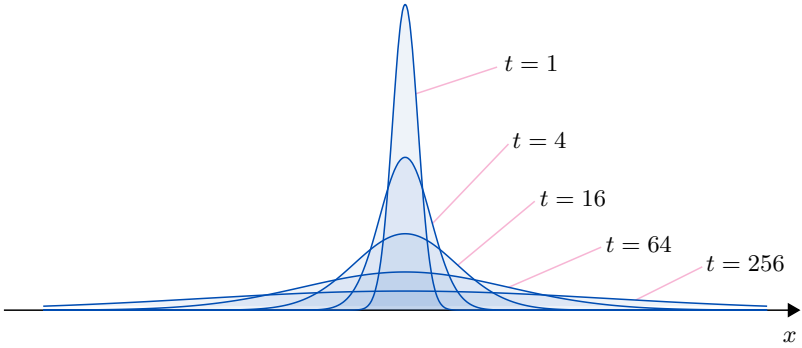

Figure 5: The evolution of the probability distribution p_t under quantum diffusion on $\mathbb{Z}^3$. For increased clarity, we only plot the first coordinate of x and draw x as a continuous variable. At each time t, the distribution p_t is approximately a normal distribution f_t from (12) with variance t.

The simple random walk from the previous section exhibits exactly the same behaviour: by the *central limit theorem*[9] of probability theory, the distribution of the random variable X_t defined in (5) is well approximated by a mean-zero normal distribution (12) with variance $\sigma^2 = t$. See Figure 5 for an illustration of the evolution of the distribution p_t in the diffusive case.

Having discussed diffusion and its emergence from reversible quantum dynamics, we now return to the question of irreversibility raised in the abstract. Indeed, diffusion is a hallmark of irreversible motion. To understand why, consider a particle at a fixed location x_0 at time 0, and suppose that we want to predict its position x_t at a later time $t > 0$. If its motion is ballistic with velocity v, then x_t is *uniquely determined* to be $x_t = x_0 + vt$. On the other hand, if its motion is diffusive, our best prediction for x_t is a *random variable* whose density is f_t from (12). Hence, diffusive motion introduces uncertainty, which grows with time, into the motion of the particle, while ballistic motion entails no uncertainty.

[9] The central limit theorem applies in fact to more general random variables than the Z_i defined above. It states that if $Z_1, Z_2, \ldots$ are independent identically distributed random variables with expectation $\mathbb{E}[Z_i] = 0$ and variance $\mathbb{E}[Z_i^2] = 1$, then the distributions of the rescaled sums $\frac{1}{\sqrt{t}}(Z_1 + Z_2 + \cdots + Z_t)$ converge as $t \to \infty$ to a mean-zero normal distribution with variance 1. This is a remarkable result, since the details of the distribution of the individual variables Z_i are completely washed out. This is the simplest instance of a "universality result" in probability. See the book [8] of Jacod and Protter for full details, including a proof.

How to reconcile irreversible diffusion with reversible microscopic dynamics? The solution is that diffusion only emerges from reversible microscopic dynamics in a certain *limit*, whereby information about the original dynamics is discarded. This may also be regarded as a *separation of scales* into microscopic and macroscopic scales. The *microscopic scale* is the scale of the individual lattice sites; on this scale the dynamics is reversible. The *macroscopic scale* is arrived at by "zooming out" so that we cannot distinguish individual lattice sites any more, and they blend together to form a continuum. We observe diffusion on the macroscopic scale, having discarded large amounts of microscopic information. It is precisely this loss of microscopic information that accounts for the loss of reversibility. From a physical point of view, the microscopic scale is the atomic scale of individual electrons and atomic nuclei, while the macroscopic scale is the scale that we see with the naked eye or even through an optical microscope.

Establishing quantum diffusion for the models (10) and (11) for arbitrarily large times t remains a major open problem. Its solution will most likely yield deep insights into the emergence of diffusion from deterministic, reversible quantum dynamics.

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