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LETTER TO THE EDITOR

The Schrödinger and diffusion propagators coexisting on a lattice

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Abstract. The Schrödinger and diffusion equations are normally related only through a formal analytic continuation. There are apparently no intermediary partial differential equations with physical interpretations that can form a conceptual bridge between the two. However, if one starts off with a symmetric binary random walk on a lattice then it is possible to show that both equations occur as approximate descriptions of *different aspects* of the same classical probabilistic system. This suggests that lattice calculations may prove to be a useful intermediary between classical and quantum physics.

The partial differential equation

$$\frac{\partial u}{\partial t} = D\frac{\partial^2 u}{\partial x^2} \tag{1}$$

has two distinct contexts. Where D is real and positive the diffusion or heat equation is a familiar starting point for classical systems. As originally shown by Einstein, the equation itself has an underlying microscopic model, namely Brownian motion. When D is imaginary, the equation is the free-particle Schrödinger equation and forms the starting point for much of non-relativistic quantum mechanics. In this context the equation has no known underlying stochastic model that is as direct as the Brownian motion model of diffusion. If one tries to consider intermediary equations with complex D the behaviour of the solutions is dominated by the real part of D unless the real part is identically 0. This means that such intermediary equations are of little help in interpreting the Schrödinger equation since, in a sense, the Schrödinger equation is embedded in a sea of equations whose solutions are qualitatively different.

In this letter we point out that if we go back to a particular lattice random walk model of Brownian motion and ask for not only a position probability density, but also for correlations in the particle paths, we end up with the diffusion equation as an approximate description of the probability density, and the Schrödinger equation as an approximate description of the correlations. This unites the two equations as being the result of different projections in the same system, and suggests that it may be advantageous to pay closer attention to discrete systems.

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The difference equation

Difference equations have been used effectively to connect quantum and classical equations in the relativistic domain [1, 2] and some interesting features of the lattice–continuum transition may be found in [3]. There is also a growing interest in the relationship between diffusion, fractals and quantum mechanics [4–7], and here we hope to further that interest by showing that Schrödinger's free-particle equation is directly applicable to ensembles of lattice random walks. To this end we write down the difference equation for a random walk on a lattice, taking into account the direction of motion and the geometry of the path.

Let $p_\mu(m\delta, s\epsilon)$ be the probability that a walker on a lattice, with (x, t) spacings δ and ϵ, respectively, arrives in state $\mu(\mu = 1, 2, 3, 4)$ at $x = m\delta$ with $t = s\epsilon$. Here $m = 0, \pm 1, \ldots$ and $s = 0, 1, 2, \ldots$. States 1 and 3 correspond to right-moving particles and states 2 and 4 correspond to left-moving particles. At each time step a particle can move one step either to the left or right. A particle starting in state 1 changes to state 2 at the first direction change, 3 at the second, 4 at the third and back to state 1 at the fourth direction change. States 1 and 3 differ only by the *parity* of their trajectories. For example, a trajectory which starts in state 1 and ends in state 3 will have an odd number of plus to minus direction changes in it. By contrast a trajectory which starts in state 1 and ends in state 1 will have an even number of such direction changes. The difference equation for $p_\mu(m\delta, s\epsilon)$ is simply the difference equation for a random walk on a lattice where we keep track of both the direction and parity of the trajectory. The difference equations are

$$\begin{aligned}
p_1(m\delta, (s+1)\epsilon) &= \frac{\alpha}{2} p_1((m-1)\delta, s\epsilon) + \frac{\alpha}{2} p_4((m+1)\delta, s\epsilon) \\
p_2(m\delta, (s+1)\epsilon) &= \frac{\alpha}{2} p_2((m+1)\delta, s\epsilon) + \frac{\alpha}{2} p_1((m-1)\delta, s\epsilon) \\
p_3(m\delta, (s+1)\epsilon) &= \frac{\alpha}{2} p_3((m-1)\delta, s\epsilon) + \frac{\alpha}{2} p_2((m+1)\delta, s\epsilon) \\
p_4(m\delta, (s+1)\epsilon) &= \frac{\alpha}{2} p_4((m+1)\delta, s\epsilon) + \frac{\alpha}{2} p_3((m-1)\delta, s\epsilon)\,.
\end{aligned} \tag{2}$$

Notice that the *physical process* represented by these equations is that of the simple binary random walk. In equations (2), if we merge states 1 and 3 as well as 2 and 4 thus ignoring parity, we see that the resulting system is just that of the symmetric binary random walk (see equation (7)). The 'extra' two states add nothing to the dynamics of the process, their presence allows us to partition the trajectories into classes of even and odd parity. Having said this, although we call the parity states 'extra' there is nothing arbitrary about them. They are extra only in the sense that we can choose not to retain information on them, just as we need not distinguish the two directions if all we want to end up with is the diffusion equation in the continuum limit.

For normalization corresponding to interpretations of the p's as probabilities, α would be 1. However, we leave α as an unspecified positive constant for reasons which will soon become clear. equations (2) may be written as

$$\boldsymbol{p}(m\delta, (s+1)\epsilon) = \mathcal{E}\boldsymbol{p}(m\delta, s\epsilon) \tag{3}$$

with $\boldsymbol{p} = (p_1, p_2, p_3, p_4)^T$ and

$$\mathcal{E} = \frac{\alpha}{2} \begin{pmatrix} E^{-1} & 0 & 0 & E \\ E^{-1} & E & 0 & 0 \\ 0 & E & E^{-1} & 0 \\ 0 & 0 & E^{-1} & E \end{pmatrix} \tag{4}$$

where E is a shift operator such that $Ep(m\delta, s\epsilon) = p((m+1)\delta, s\epsilon)$.

Now let

$$\phi_1 = \frac{p_1 - p_3}{2} \qquad \phi_2 = \frac{p_2 - p_4}{2} \qquad z_1 = \frac{p_1 + p_3}{2} \qquad \text{and} \qquad z_2 = \frac{p_2 + p_4}{2}\,.$$

Here $\phi_{1(2)}$ is the expected difference in the number of particles of opposite parity arriving moving to the right (left). Similarly $z_{1(2)}$ is the expected total number of particles arriving moving to the right (left). In terms of these new variables (2) becomes

$$\begin{pmatrix} \phi_1(m\delta, (s+1)\epsilon) \\ \phi_2(m\delta, (s+1)\epsilon) \\ z_1(m\delta, (s+1)\epsilon) \\ z_2(m\delta, (s+1)\epsilon) \end{pmatrix} = \frac{\alpha}{2} \begin{pmatrix} E^{-1} & -E & 0 & 0 \\ E^{-1} & E & 0 & 0 \\ 0 & 0 & E^{-1} & E \\ 0 & 0 & E^{-1} & E \end{pmatrix} \begin{pmatrix} \phi_1(m\delta, s\epsilon) \\ \phi_2(m\delta, s\epsilon) \\ z_1(m\delta, s\epsilon) \\ z_2(m\delta, s\epsilon) \end{pmatrix}. \tag{5}$$

Note that the change of variables has rendered the system block diagonal and we can consider the two systems:

$$\begin{pmatrix} \phi_1(m\delta, (s+1)\epsilon) \\ \phi_2(m\delta, (s+1)\epsilon) \end{pmatrix} = \frac{\alpha}{2} \begin{pmatrix} E^{-1} & -E \\ E^{-1} & E \end{pmatrix} \begin{pmatrix} \phi_1(m\delta, s\epsilon) \\ \phi_2(m\delta, s\epsilon) \end{pmatrix} \tag{6}$$

and

$$\begin{pmatrix} z_1(m\delta, (s+1)\epsilon) \\ z_2(m\delta, (s+1)\epsilon) \end{pmatrix} = \frac{\alpha}{2} \begin{pmatrix} E^{-1} & E \\ E^{-1} & E \end{pmatrix} \begin{pmatrix} z_1(m\delta, s\epsilon) \\ z_2(m\delta, s\epsilon) \end{pmatrix}. \tag{7}$$

The block diagonalization effected by our change of variables is both mathematically and physically very significant. Mathematically it means that the ϕ_i and z_i may be analysed independently. Physically, this factoring into two separate systems is the result of a projection caused by recording excess parity. All we have to do to observe the ϕ_i of equation (6) is to measure excess parity in the symmetric binary random walk. We shall shortly see that the ϕ_i have very unexpected behaviour especially in view of the fact that the model we are examining is no more than a simplified version of Einstein's 1905 model. Although equations (6) are the ones of interest, equations (7) correspond to retaining only the directional information, and we consider them first. We are interested in the usual diffusive limit:

$$\left\{\delta \to 0,\ \epsilon \to 0,\ \frac{\delta^2}{\epsilon} \to 2D,\ m\delta \to x,\ s\epsilon \to t\right\}. \tag{8}$$

Consider the generating function (discrete fourier transform)

$$z_k(p, s\epsilon) = \sum_{m=-\infty}^{+\infty} z_k(m\delta, s\epsilon)\mathrm{e}^{-\mathrm{i}pm\delta}\delta \qquad (k = 1, 2)\,. \tag{9}$$

Multiplying equation (7) by $(\mathrm{e}^{-\mathrm{i}pm\delta}\delta)$ and summing gives

$$\begin{aligned} \begin{pmatrix} z_1(p, (s+1)\epsilon) \\ z_2(p, (s+1)\epsilon) \end{pmatrix} &= \frac{\alpha}{2} \begin{pmatrix} \mathrm{e}^{-\mathrm{i}p\delta} & \mathrm{e}^{\mathrm{i}p\delta} \\ \mathrm{e}^{-\mathrm{i}p\delta} & \mathrm{e}^{\mathrm{i}p\delta} \end{pmatrix} \begin{pmatrix} z_1(p, s\epsilon) \\ z_2(p, s\epsilon) \end{pmatrix} \\ &= T_z \begin{pmatrix} z_1(p, s\epsilon) \\ z_2(p, s\epsilon) \end{pmatrix} \end{aligned} \tag{10}$$

where T_z is the transfer matrix of the system. Thus, in vector notation

$$Z(p, s\epsilon) = T_z^s Z(p, 0)\,. \tag{11}$$

Now we shall want to find the limit of large powers of T_z as specified by (8). To do this we diagonalize T_z, calculate the large power, and then transform back. To this end note that the eigenvalues of T_z may be found to be 0 and $\alpha \cos p\delta$ and in the limit specified by (8)

$$(\alpha \cos p\delta)^s \to \mathrm{e}^{-p^2 Dt} \tag{12}$$

provided we choose $\alpha = 1$ as appropriate for probabilities normalized to 1. We then find, in the continuum limit

$$Z(p,t) = \tfrac{1}{2}\mathrm{e}^{-p^2Dt}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} Z(p,0)\,. \tag{13}$$

From equation (9) we can see that in this limit

$$Z_k(p,s\epsilon) \to \int_{-\infty}^{+\infty} Z_k(x,t)\mathrm{e}^{-\mathrm{i}px}\,\mathrm{d}x \tag{14}$$

which is the Fourier transform of Z in position space. If we assume

$$Z(p,0) = \frac{1}{2}\begin{pmatrix} 1 \\ 1 \end{pmatrix} \tag{15}$$

then

$$\begin{aligned} Z(x,t) &= \frac{1}{2}\begin{pmatrix} 1 \\ 1 \end{pmatrix}\frac{1}{2\pi}\int_{-\infty}^{+\infty}\mathrm{e}^{\mathrm{i}px}\mathrm{e}^{-p^2Dt}\,\mathrm{d}p \\ &= \frac{1}{2}\begin{pmatrix} 1 \\ 1 \end{pmatrix}\frac{1}{\sqrt{4\pi Dt}}\mathrm{e}^{-x^2/4Dt}\,. \end{aligned} \tag{16}$$

This is the usual solution of the diffusion equation except for the presence of two identical states. There are two identical direction states in the continuum limit because, although we have chosen to separately count left- and right-moving particles with z_1 and z_2, the walks are all symmetric and treat both directions equivalently.

The result (16) by itself is certainly not new. What is new is what is lost if we *only* analyse equation (7)! Returning to the extra information obtained by considering parity we consider solving equations (6). As in the previous case we define generating functions

$$\phi_k(p,s\epsilon) = \sum_{m=-\infty}^{+\infty}\phi_k(m\delta,s\epsilon)\mathrm{e}^{-\mathrm{i}pm\delta}\delta\,. \tag{17}$$

Equation (3) then becomes

$$\Phi(p,(s+1)\epsilon) = \begin{pmatrix} \phi_1(p,(s+1)\epsilon) \\ \phi_2(p,(s+1)\epsilon) \end{pmatrix} = T_\phi\Phi(p,s\epsilon) \tag{18}$$

where

$$T_\phi = \frac{\alpha}{2}\begin{pmatrix} \mathrm{e}^{-\mathrm{i}p\delta} & -\mathrm{e}^{\mathrm{i}p\delta} \\ \mathrm{e}^{-\mathrm{i}p\delta} & \mathrm{e}^{\mathrm{i}p\delta} \end{pmatrix}. \tag{19}$$

Now T_ϕ has two conjugate eigenvalues

$$\lambda_\pm = \frac{\alpha}{\sqrt{2}}\mathrm{e}^{\pm\mathrm{i}\pi/4}\left(1 \pm \mathrm{i}\frac{p^2\delta^2}{2} + \mathrm{O}(\delta^4)\right)$$

and the limit as $s \to \infty$ of T_ϕ^s is not well defined because of the phase factors $\mathrm{e}^{\pm\mathrm{i}\pi/4}$. The phase factors themselves express the symmetry of the walk in terms of the internal states. The expected state change of the walks is exactly one state for every *two* steps, making the walks statistically of period eight. For example, for a walker starting out in state 1, the expected number of steps to a first return to state 1 is eight.

To overcome the problem of an ill-defined limit we can either redefine $\phi_k(p,s\epsilon)$ depending on s, or we can simply require that we take the limit $s \to \infty$ through integer values of s which are 0(mod 8) in which case $(\mathrm{e}^{\pm\mathrm{i}\pi/4})^s = 1$. Furthermore, we see that to converge to a normalizable propagator we must have $\alpha = \sqrt{2}$. With these choices we have

$$\lim_{\delta\to 0}\lambda_\pm^s = \mathrm{e}^{\pm\mathrm{i}p^2Dt} \tag{20}$$

and in the limit as $s \to \infty$ (0 mod 8)

$$\lim_{s\to\infty} \Phi(p, s\epsilon) = \left(e^{i p^2 Dt} \frac{1}{2} \begin{pmatrix} 1 & i \\ -i & 1 \end{pmatrix} + e^{-ip^2 Dt} \frac{1}{2} \begin{pmatrix} 1 & -i \\ i & 1 \end{pmatrix} \right) \Phi(p, 0)$$
$$= \begin{pmatrix} \cos(p^2 Dt) & -\sin(p^2 Dt) \\ \sin(p^2 Dt) & \cos(p^2 Dt) \end{pmatrix} \Phi(p, 0)\,. \tag{21}$$

Finally, if we write

$$\psi_+(p, t) = \tfrac{1}{2} i\phi_1(p, t) + \tfrac{1}{2}\phi_2(p, t)$$
$$\psi_-(p, t) = -\tfrac{1}{2} i\phi_1(p, t) + \tfrac{1}{2}\phi_2(p, t) \tag{22}$$

equation (23) becomes

$$\begin{pmatrix} \psi_+(p, t) \\ \psi_-(p, t) \end{pmatrix} = \begin{pmatrix} e^{-ip^2 Dt} & 0 \\ 0 & e^{ip^2 Dt} \end{pmatrix} \begin{pmatrix} \psi_+(p, 0) \\ \psi_-(p, 0) \end{pmatrix}. \tag{23}$$

Taking $\Psi(p, 0) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$ and transforming back to position space we have

$$\Psi(x, t) = \begin{pmatrix} \frac{e^{ix^2/4Dt}}{\sqrt{4\pi i Dt}} & 0 \\ 0 & \frac{e^{-ix^2/4Dt}}{\sqrt{-4\pi i Dt}} \end{pmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}. \tag{24}$$

There are several things to note about equation (24) and its derivation.

- Replacing the real positive constant D by the real positive constant $\hbar/2m$ in equation (24), we see that both components of Ψ satisfy a Schrödinger equation for a 'free particle' in one dimension.
- There is *no formal analytic continuation* involved in the derivation of (24). Ψ is a result of counting arguments only, and its real and imaginary parts are *observable* in the lattice system.
- The factoring of the original difference equation (4) is a result of the fact that at any lattice resolution, ϕ_i and z_i exist on separate orthogonal eigenspaces and both objects correspond to *projections* from the full four dimensional space. It is for this reason that the Feynman path integral which pertains to the $\psi_\pm$ shares the same composition law as the Wiener Integral pertaining to the z_i [8]. Both systems inherit this law from the parent probabilistic system (2) which contains them both.
- The choice of $\alpha = \sqrt{2}$ for the system involving the ϕ_i is dictated by the path statistics for the underlying symmetric random walk. The total number of such N-step walks is 2^N and so the probabilistic weight of each step is $\frac{1}{2}(\alpha = 1)$. However, the difference between the number of N-step paths of different parity grows as $(\sqrt{2})^N$ so the appropriate weight is $(1/\sqrt{2})^N$ $(\alpha = \sqrt{2})$ for the correlations [9].
- If one chooses $\alpha = \sqrt{2}$ so that the ϕ_i have the usual normalization in the continuum, the z_i diverge. However, if one chooses $\alpha = 1$ then the ϕ_i go to zero in the continuum limit since the correlations are a second order effect. This simply means that on a lattice ϕ_i is a small difference between two large numbers and in practice, with finite precision one would have to decide either to store the differences alone (giving ϕ_i but not z_i) or the sums (giving z_i but not ϕ_i). This incompatability of observation in the continuum does not mean that the correlations described by ϕ_i do not exist (they are easily seen by counting paths on a lattice and forming the required differences, see figure 1), but the incompatability does emphasize that the Schrödinger equation acquires a fair amount of its mystery from the continuum limit itself. It is this continuum limit which hides its

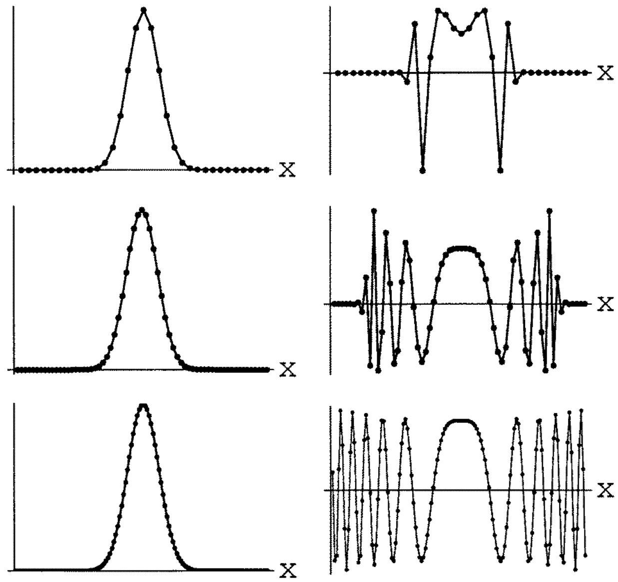

Figure 1. The quantities z_1 and ϕ_2 at fixed t as the lattice is refined. z_1 approaches the Gaussian in equation (6). ϕ_2 approaches the real part of the Feynman propagator in equation (24) (cf [10] figure (3.1)). The plotted values were calculated by counting exactly the number of paths to the respective spacetime points. The curves are smooth interpolations between the calculated points.

simple relation to diffusion on a lattice. Since the diffusive continuum limit is in any case artificial, the above calculation suggests that difference equations may provide an interesting alternative description of non-relativistic quantum mechanics.

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