From the quantum random walk to classical mesoscopic diffusion in crystalline solids

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We use a discrete approximation of quantum mechanics called the quantum random walk to study diffusion in one-dimensional crystalline nanostructures. There, intense fluctuations in the density are a consequence of quantum interference. As the size of the crystal increase, relative quantum fluctuations decrease and, if a coarse-grained averaging is taken, interference may be neglected. When this happens, we describe a far-from-equilibrium, classical, dynamic mesoscopic diffusion regime. In this regime, diffusion equations are given by a persistent-random-walk process. Density becomes a second-order Markov process, and in the continuum limit, the current satisfies the non-Fickian Maxwell-Cattaneo relationship. The generalized diffusion equation in the telegraphist's equation. [S1063-651X(96)10005-6]

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I. INTRODUCTION

An atomistic kinetic-theory approach to diffusion in a lattice is the stochastic process called the random-walk (RW) [1,2]. The traditional model of diffusion using RW is a *first-order* Markov process in configuration space. Let us interpret $P(x,t)$, as the probability distribution of the position x ($x \equiv 0, \pm l, \pm 2l, \dots$) for a diffusive particle at time t ($t \equiv 0, \tau, 2\tau, \dots$). Assuming a simple (nonbiased) RW in a lattice, the probability $P(x,t)$ satisfies the simple recurrence formula

$$P(x,t+\tau) = \frac{1}{2}P(x-l,t) + \frac{1}{2}P(x+l,t). \qquad (1.1)$$

Here, τ and l are the ''jump time'' and ''jump length,'' respectively. The factors $\frac{1}{2}$ in Eq. (1.1) are the isotropic jump probabilities for moving right or left. The continuum version of (1.1), called the Fokker-Planck equation is a parabolic differential equation

$$\frac{1}{D}\frac{\partial P}{\partial t} = \frac{\partial^2 P}{\partial x^2}, \qquad (1.2)$$

where $D \equiv l^2/2\tau = v_0^2\tau/2$ is the diffusion coefficient, and $v_0 \equiv l/\tau$ is the mean velocity of the particles.

From the point of view of kinetic theory, the most peculiar property of $P(x,t)$ in the above process is the fact that the probability *does not* depend on the momentum of the diffusive particles. This is due to the underlying condition that the diffusive particles described by Eq. (1.2) are assumed to be in *thermal equilibrium*. This assumption, called the hydrodynamic regime, implies that the one-body distribution function $f(x,p,t)$ must be written as

$$f(x,p,t) = \phi_{eq}(p)P(x,t) = \exp[-p^2/2Mk_BT]P(x,t). \qquad (1.3)$$

where M is the mass of the particles, k_B Boltzmann's constant, and T the temperature. In this near-equilibrium regime, the time scales associated with diffusion in a solid are enormous. For example, the time τ between jumps may be of the order of weeks or even months [3]. The distances l associated with this process are also much greater than the mean free path λ. In other words, Eq. (1.2) describes diffusion in a sample of *macroscopic size*.

Our main question is the following one. If we consider a diffusive regime in which the momentum variable p has not reached thermal equilibrium and, further, if the momentum variable has not even reached statistical independence from the position variable x, then what is the generalized diffusion equation? To answer this question, first we go as far away from the equilibrium regime as we can: the time-dependent quantum process. There, we know that the Schrödinger equation is the diffusion equation. In particular, for crystalline nanostructures, a discrete approximation of quantum mechanics, called quantum random walk (QRW), has been applied to study tunneling diffusion [4,5]. Second, using diffusive currents, we give an example where we show that for a large enough size of the crystal, quantum interference effects may be neglected. Third, after taking a coarse-grained averaging in the quantum probabilities, we can neglect quantum interference and, as a consequence, we destroy the time-reversal invariance of the original QRW process. We arrive at a classical, irreversible, mesoscopic diffusive process. Fourth, under this approximation the mesoscopic process is described by persistent-random-walk equations. Consequently, in this regime, the probability density becomes a *second-order* Markov process, and in the continuum limit the generalized diffusion equation becomes the telegraphist's equation [6].

II. THE QUANTUM RANDOM WALK

In this section we show a summary of results above QRW that were obtained in previous papers [4,5]. Tunneling diffusion in a one-dimensional (1D) periodic lattice (Kronig-Penney model) has been studied using a microscopic, coherent (having interference), diffusive process called quantum random walk. In this quantum process, particles described by

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wave packets move freely in the potential valleys, and from each valley to the next by quantum scattering. In this model, let us denote cell m as the valley bounded by two potential barriers at positions $x = (m-1)l$ and $x = ml$ ($m = 0, \pm 1, \pm 2, \ldots$; l is the lattice constant). The QRW process defines at each cell m, and at each discrete time $t = n\tau$ (n is a positive integer and τ is a characteristic jump time), a wave function $\psi_m(x, t = n\tau)$ that describes a pair of modulated wave packets centered at the middle of the cell. The two wave packets have a sharp distribution of wave numbers around k_0 and an average momentum $\pm \hbar k_0$ that makes the packets move in opposite directions. The function $\psi_m(x, t = n\tau)$ is defined by

$$\Psi_m(x, t = n\tau) \equiv \Psi_m^+(x, n\tau) + \Psi_m^-(x, n\tau)$$

$$\equiv [A(ml, n\tau)e^{+ik_0 x} + B(ml, n\tau)e^{-ik_0 x}]$$

$$\times G\left[x - \left(m - \frac{1}{2}\right)l + v_0 n\tau, t = n\tau\right].$$

(2.1)

Here, $(ml, n\tau)$ denote the cell coordinate (ml) and discrete time $(n\tau)$ dependence of the amplitudes A and B for right- and left-moving wave packets, respectively. The modulating function G is defined by

$$G(x, t) \equiv \frac{1}{\sqrt{2\pi}} \int_0^\infty dk \, g(k) e^{-i\omega(k)t} e^{+i(k - k_0)x}, \quad (2.2)$$

where $\omega(k) \equiv \hbar k^2 / 2m$. We may assume the function $g(k)$ to be a real, peaked function at $k = k_0$ (the average wave number) with spreading Δk. Packets have velocities $v_0 = \pm \hbar k_0 / m$ and average energy $\varepsilon_0 = \hbar \omega(k_0)$. The $G(x, t)$ function depends on the particular form of $g(k)$, for example if $|g(k)|^2$ is a Gaussian, then $|G(x, t)|^2$ is also a spreading moving Gaussian centered at $x = v_0 t$ [7]. If $|G(k)|^2$ is normalized in k space, then $|G(x, t)|^2$ is also normalized in x space.

To facilitate the mathematics, QRW neglects more than one cell spreading of the packets. That is, at all times the wave packets are assumed to be bounded to a *single cell*. In other words, in the QRW model the time dispersion of the wave packets beyond a single cell is neglected. Under this assumption, every wave packet has no overlapping to neighboring cells. Normalization of $|g(k)|^2$ and nonoverlapping demand.

$$\int_{\text{cell}=m} |\Psi_m^+(x, n\tau)|^2 dx = |A(ml, n\tau)|^2,$$

$$\int_{\text{cell}\neq m} \Psi_m^+(x, n\tau) dx = 0, \quad (2.3a)$$

$$\int_{\text{cell}=m} |\Psi_m^-(x, n\tau)|^2 dx = |B(ml, n\tau)|^2,$$

$$\int_{\text{cell}\neq m} \Psi_m^-(x, n\tau) dx = 0. \quad (2.3b)$$

In conclusion, QRW assumes a total wave function $\Psi(x, t)$ for the whole crystal as a superposition of nonoverlapping cell waves:

$$\Psi(x, t = n\tau) \equiv \sum_{m=-\infty}^{+\infty} [\Psi_m^+(x, n\tau) + \Psi_m^-(x, n\tau)]. \quad (2.4)$$

In the QRW theory the amplitudes $A(ml, n\tau)$ and $B(ml, n\tau)$ in (2.1) are the only functions that describe the time evolution for both packets. The amplitudes A and B satisfy, for arbitrary lattice valley m, the recursive equations (for simplicity $l = \tau = 1$),

$$\begin{pmatrix} B[m, n+1] \\ A[m+1, n+1] \end{pmatrix} = \mathbf{s}(k_0, m) \begin{pmatrix} A[m, n] \\ B[m+1, n] \end{pmatrix}, \quad (2.5)$$

where $\mathbf{s}(k_0, m)$ denotes the scattering matrix associated with the potential barrier located at the boundary between the m and $m+1$ cells. If we demand for every scattering process (i) *conservation of probability*, (ii) *time-reversal invariance*, and we assume (iii) *symmetric potentials*, the $\mathbf{s}(k_0, 0)$ matrix has to be *unitary* and *symmetric* (with symmetry $S_{11} = S_{22}$). Since the matrix $\mathbf{s}(k_0, m)$ is shifted to position $x = ml$, it may be parametrized as [8]

$$\mathbf{s}(k_0, m) = e^{i\alpha(k_0)} \begin{pmatrix} \sqrt{R} e^{+ik_0 2m} & i\sqrt{T} \\ i\sqrt{T} & \sqrt{R} e^{-ik_0 2m} \end{pmatrix}, \quad (2.6)$$

where $T(k_0)$ and $R(k_0)$ are the transmission and reflection coefficients, respectively ($T + R = 1$). The common phase $\alpha(k_0)$ may be neglected later on in the probability, as we will see in Sec. III.

Equation (2.5), which, for *complex* amplitudes (A, B), has the same time dependence as a *two-state* Markov random-walk process, defines the basic dynamic equations of the QRW model.

III. QUANTUM CONCENTRATION OF MASS

Next, we want the total probability $P(m, n)$ of finding at time $t = n$ a particle at an arbitrary lattice cell m. Since the packets do not overlap, we can integrate the probability density $|\Psi(x, n)|^2$ along a single cell m,

$$P(m, n) \equiv \int_{\text{cell}=m} |\Psi(x, n)|^2 dx$$

$$= \int_m |\Psi_m^+(x, n) + \Psi_m^-(x, n)|^2 dx. \quad (3.1)$$

Substituting from Eq. (2.1), we have

$$P(m, n) = |A(m, n)|^2 + |B(m, n)|^2$$

$$+ \left(\int_m \Psi_m^+(x, n) \Psi_m^-(x, n)^* dx + \text{c.c.} \right). \quad (3.2)$$

The last integral is an inference contribution produced by the total superposition, at the same cell m, of two wave packets

moving in *opposite* directions. After some elementary integrations the explicit value of this integral is given by

$$\int_m \Psi_m^+(x,n)\Psi_m^-(x,n)*dx$$

$$= AB^*\exp(i2\hbar k_0^2 n/m)$$

$$\times \int_{-\infty}^{\infty} dk \, g(k)g^*(k+2k_0)e^{i\hbar 2k_0 kn/m}. \quad (3.3)$$

The last integral has one function, $g(k)$, centered at k_0 and the other, $g(k+2k_0)$, centered at $-k_0$. Since by hypothesis we have a sharp distribution of momenta around k_0 so that $\Delta k \ll k_0$, the two g functions do not overlap and

the integral is negligible. As we will see, the only interference will come from packets superposing in the same valley and traveling in the *same* direction. The final result for (3.2) is that the total probability at each lattice cell is an incoherent superposition of two probabilities, one for each opposite moving wave packet:

$$P(m,n) \equiv P_+(m,n) + P_-(m,n) = |A(m,n)|^2 + |B(m,n)|^2. \quad (3.4)$$

So far, this looks like a classical result. However, notice that according to Eq. (2.5) both $A(m,n)$ and $B(m,n)$ are given by a coherent superposition of two amplitudes, currently traveling in the *same* direction, but evaluated at a previous time. This will produce a quantum interference, as we show next. Substituting Eq. (2.5) into Eq. (3.4), we find

$$P_+(m,n) \equiv |A(m,n)|^2 = TP_+(m-1,n-1) + RP_-(m,n-1) + \sqrt{TR}[iA(m-1,n-1)B^*(m,n-1)e^{+ik_0 2m} + \text{c.c.}], \quad (3.5a)$$

$$P_-(m,n) \equiv |B(m,n)|^2 = RP_+(m,n-1) + TP_-(m+1,n-1) + \sqrt{TR}[iA^*(m,n-1)B(m+1,n-1)e^{-ik_0 2(m+1)} + \text{c.c.}]. \quad (3.5b)$$

Notice that the interference contributions become directly responsible for intense quantum fluctuations in the probability. These fluctuations can be readily appreciated from Fig. 1, where numerical values were obtained from the analytic solution for $A(m,n)$ and $B(m,n)$ given in Ref. [5]. The amplitudes AB^* of the interference terms are of the same order of magnitude as the probabilities P_+ and P_-. Both interference and probabilities oscillate in space. Probabilities oscillate between positive values, but interference terms oscillate between positive and negative values. Therefore, for a large enough solid, if we define a coarse-grained distribution $P_\pm(x,t)$ by averaging the quantum distribution $P_\pm$ for a small number of cells Δm in coordinate space,

$$P_\pm(x,t) \equiv \frac{1}{\Delta m}\sum_{m=(x-1)\Delta m}^{x\Delta m} P_\pm(m,t),$$

$$x = \text{integer number}$$

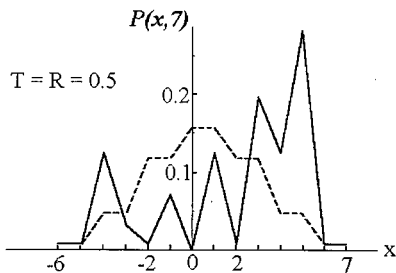then, after a coarse-grained averaging, the interference terms

FIG. 1. Total probability $P(x,t)$ for quantum QRW (solid) and classical PRW (broken). Quantum and classical initial conditions: $A(x,0)=\delta_{x,0}$, $B(x,0)=0$, $P_+(x,0)=\delta_{x,0}$ and $P_-(x,0)=0$. Numerical results are obtained from Ref. [4].

may be neglected from the probabilities (3.5). Consequently, we arrive at a classical (incoherent) persistent-random-walk (PRW) equation [6], namely,

$$P_+(x,t) = TP_+(x-1,t-1) + RP_-(x,t-1), \quad (3.6a)$$

$$P_-(x,t) = RP_+(x,t-1) + TP_-(x+1,t-1). \quad (3.6b)$$

We will return to these classical equations later on.

Notice that time reversal was a built-in condition in our QRW process (**s**-matrix was unitary and symmetric). We had initially, in Eqs. (3.5) for QRW probabilities, a fully reversible quantum process [12]. However, Eqs. (3.6) for PRW are *irreversible*. That is, by eliminating the interference terms, we introduced irreversibility in the microscopic diffusive process.

IV. THE DIFFUSION CURRENTS

In the next two sections, we show with a particular example, using diffusive currents, that if the size of a solid is great enough, then the effects of quantum interferences may be neglected.

Let us now calculate the quantum probability current density $J(m,n)$ at each lattice cell m.

$$J(m,n) = \int_{\text{cell } m} \frac{\hbar}{2Mi}\left(\Psi^*(x,n)\frac{d\Psi(x,n)}{dx}\right.$$

$$\left. - \Psi(x,n)\frac{d\Psi^*(x,n)}{dx}\right)dx. \quad (4.1)$$

Substituting from Eq. (2.1) and following the same procedure we used to calculate the probability $P(m,n)$, after some elementary algebra we obtain

$$J(m,n) = \frac{\hbar k_0}{M}[|A(m,n)|^2 - |B(m,n)|^2]$$

$$= v_0[P_+(m,n) - P_-(m,n)]. \qquad (4.2)$$

As expected, the probability current density at each cell is just the current density moving right minus the current density moving left. Substituting from the QRW probability (3.5) into (4.2), we have

$$J(m,n)/v_0 = \{T[P_+(m-1,n-1) - P_-(m+1,n-1)] + R[P_-(m,n-1) - P_+(m,n-1)]\}$$

$$+ i\sqrt{TR}\{A(m-1,n-1)B^*(m,n-1)e^{+i2k_0 m} - A^*(m,n-1)B(m+1,n-1)e^{-ik_0 2(m+1)} - \text{c.c.}\}. \qquad (4.3)$$

By inspection, we can separate the total current $J(m,n)$ into an incoherent $J_{\text{inc}}(m,n)$ and a coherent $J_{\text{coh}}(m,n)$ component:

$$J(m,n) \equiv J_{\text{inc}}(m,n) + J_{\text{coh}}(m,n), \qquad (4.4)$$

where

$$J_{\text{inc}}(m,n) \equiv v_0\{T[P_+(m-1,n-1) - P_-(m+1,n-1)] + R[P_-(m,n-1) - P_+(m,n-1)]\}, \qquad (4.5a)$$

and

$$J_{\text{coh}}(m,n) \equiv iv_0\sqrt{TR}\{A(m-1,n-1)B^*(m,n-1)e^{+i2k_0 m} - A^*(m,n-1)B(m+1,n-1)e^{-i2k_0(m+1)} - \text{c.c.}\}. \qquad (4.5b)$$

Notice that the coherent current J_{coh} in Eq. (4.5b) is made of nothing but pure quantum interference contributions in the probabilities. In other words, J_{coh} contains the source of quantum fluctuations as we have discussed previously in Eqs. (3.5). On the other hand, the incoherent current J_{inc} contains only the incoherent addition of probabilities without interference terms. The incoherent current (4.5a) could also be derived from a classical theory such as the PRW Eq. (3.6) and the result would be *the same*.

One way to find the dynamic microscopic diffusion coefficient is to take a continuum approximation. First, we assume the distance l between adjacent lattice cells to be very small; then we can make a first-order Taylor expansion around the position m of the functions $P(m\pm l,n)$, $A(m\pm l,n)$, and $B(m\pm l,n)$. While keeping the interference terms, this expansion breaks the *time-reversal* invariance of the microscopic current and introduces irreversibility in the resulting equations. Second, to make things easy, we may assume a long time; here we assume that a quasistationary state has been reached $P^*(m,n) \cong (m,n-\tau) \equiv P(m)$, which we may write independent of time. Under these two assumptions, we obtain, after a first-order Taylor expansion,

$$J_{\text{inc}}(m)/v_0 \cong (T-R)[P_+(m) - P_-(m)] - T\frac{d}{dm}[P_+(m) + P_-(m)]$$

$$= (T-R)J(m)/v_0 - T\frac{d}{dm}P(m), \qquad (4.6)$$

and

$$J_{\text{coh}}(m)/v_0 \cong -\sqrt{TR}\,ie^{+i2k_0 m}\left(A^*(m)\frac{d}{dm}B(m) + B^*(m)\frac{d}{dm}A(m) - \text{c.c.}\right)$$

$$+ i\sqrt{TR}\,2\{e^{+i2k_0 m}A(m)B^*(m) - \text{c.c.}\}. \qquad (4.7)$$

Substituting these two results into Eq. (4.4), we have, after some algebraic simplifications, the following irreversible current:

$$J(m) \cong -v_0\frac{T}{2R}\frac{d}{dm}P(m) - \frac{v_0}{2}\left(\frac{T}{R}\right)^{1/2}i\left(e^{-2ik_0 m}A^*(m)\frac{d}{dm}B(m) + e^{+i2k_0 m}B^*(m)\frac{d}{dm}A(m) - \text{c.c.}\right)$$

$$+ v_0\left(\frac{T}{R}\right)^{1/2}i\{e^{+i2k_0 m}A(m)B^*(m) - \text{c.c.}\}. \qquad (4.8)$$

By inspection, we can now identify the microscopic diffusion coefficients. The results for the linear density current are as follows (for clarity we rewrite $l \neq 1$).

(1) We have an incoherent current

$$J_{\text{inc}}(m) \equiv -v_0 l \frac{T}{2R} \frac{d}{dm} P(m). \tag{4.9}$$

As expected, this diffusive current is nothing but the dynamic microscopic version of Fick's law. QRW shows that the dynamic diffusion coefficient is given by the microscopic Landauer result [9]:

$$D = v_0 l \frac{T}{2R} = v_0^2 \tau \frac{T}{2R}, \quad \frac{l}{\tau} \equiv v_0. \tag{4.10}$$

We stress the fact that (4.9) was obtained using the pure incoherent current (4.6). However, if, instead of using the quantum equations (2.5), we had taken the classical persistent-random-walk equations (3.6), we would have obtained *the same result*. This suggests that Fick's law is a classical result (incoherent). It seems that we do not need a quantum theory to obtain Landauer's result. A suitable incoherent theory such as the Boltzmann or Fokker-Planck equations will get the same result with painless mathematics [10].

(2) We have a coherent current contribution:

$$J_{\text{coh}}(m) = -v_0 l \left(\frac{T}{R} \right)^{1/2} \frac{i}{2} \left(e^{-i2k_0 m} A^*(m) \frac{d}{dm} B(m) \right.$$
$$\left. + e^{+i2k_0 m} B^*(m) \frac{d}{dm} A(m) - \text{c.c.} \right). \tag{4.11}$$

This diffusive current has a pure quantum origin: the interference contributions in probability. It depends on the gradients of *complex amplitudes*. There is no way we can obtain this contribution from a classical theory. The associated coefficient that depends on the microscopic properties of the lattice will be called the *coherent diffusion coefficient C*,

$$C \equiv v_0 l \left(\frac{T}{R} \right)^{1/2}. \tag{4.12}$$

As we will show in next section, the root square in C will make this coefficient vanish as the size of the material increases.

(3) Finally, we have another coherent contribution:

$$J(m) = v_0 l \left(\frac{T}{R} \right)^{1/2} i \{ e^{+i2k_0 m} A(m) B^*(m) - \text{c.c.} \}. \tag{4.13}$$

This quantum interference current comes from the ballistic motion of the amplitudes in our model. Since this is not a diffusive current, we may forget about it in the present context of transport theory.

V. THE BULK LIMIT

The present QRW, so far, represents a microscopic diffusion theory. However, the ratio R/T (Landauer's resistance) [9] has only a technical meaning and is not a physically accessible quantity. Next, we proceed to show how the microscopic coefficients T and R are related to the corresponding measurable coefficients $\mathscr{T}$ and $\mathscr{R}$ of a *whole sample* of total length $L = Nl$ made of N identical successive cells.

Assuming a unitary incoming probability upon a sample of total length $L = Nl$, and adding *incoherently* (the waves arrive at different times) the infinite series of partial reflecting and transmitting outgoing probabilities, we easily arrive, after straightforward algebra, at the well known results [5]:

$$\mathscr{T} = \frac{T}{1 + (N-1)R}, \quad \mathscr{R} = \frac{NR}{1 + (N-1)R}. \tag{5.1}$$

Next, taking the ratio of both macroscopic coefficients in (5.1), we have

$$\frac{T}{R} = N \frac{\mathscr{T}}{\mathscr{R}}. \tag{5.2}$$

Substituting (5.2) into the diffusion coefficients D in (4.10) and C in (4.12), we have

$$D = v_0 l N \frac{\mathscr{T}}{2\mathscr{R}} = v_0 L \frac{\mathscr{T}}{2\mathscr{R}}, \tag{5.3}$$

$$C = v_0 l \left(\frac{N\mathscr{T}}{\mathscr{R}} \right)^{1/2} = v_0 L \frac{1}{\sqrt{N}} \left(\frac{\mathscr{T}}{\mathscr{R}} \right)^{1/2}. \tag{5.4}$$

In the bulk limit, where $l \ll 1$, $N \gg 1$ such that $Nl = L \rightarrow$ constant, we see that the incoherent Landauer diffusion coefficient D in (5.3) remains unchanged. However, the coherent diffusion coefficient C in (5.4) goes to zero like $(N)^{-1/2}$. This dependence is the same for relative fluctuations of any additive quantity in equilibrium statistical mechanics [13].

This is a key result. As the size of the crystal increases, quantum diffusion tends to decrease the quantum fluctuation effects. We use this property to move from the reversible quantum regime to the irreversible classical mesoscopic regime of diffusion.

VI. CLASSICAL MESOSCOPIC DIFFUSION

As we saw in the preceding sections, as we keep increasing the size L of any nanostructure sample, the quantum interference effects keep decreasing monotonically. If we have a microscopic material, and we increase its size to the point where we can confidently neglect quantum fluctuations, we call such a material a *classical mesoscopic* sample. A classical mesoscopic sample is then, by definition, an incoherent system, but a very small one. So small, in fact, that the times involved in diffusing through such materials are not long enough for the momentum variable p to reach statistical independence from the position variable x, even less to reach thermal equilibrium.

Diffusion in classical mesoscopic materials can be described with any incoherent kinetic theory. The only condition is that the one-body distribution function must be a joint distribution function $f(x, p, t)$ of position and momentum. Both variables (x, p) will depend on time and will be correlated. QRW predicts in the coarse-grained distributions Eqs.

(3.6) one discrete stochastic process model PRW which can be satisfied by the one-body distribution function $f(x,p,t)$ in a 1D mesoscopic system:

$$P_+(x,t)=TP_+(x-1,t-1)+RP_-(x,t-1), \quad (6.1a)$$

$$P_-(x,t)=RP_+(x,t-1)+TP_-(x+1,t-1). \quad (6.1b)$$

Equations (6.1) describe a classical system where all particles have the same average speed $v_0 \equiv l/\tau$. The effect of elastic collisions is simply to change their directions of motion. In a 1D lattice, the momentum will have only two values: $p = \pm|p_0|$. For simplicity we have defined $P_+(x,t) \equiv f(x,+|p_0|,t)$ and $P_-(x,t) \equiv f(x,-|p_0|,t)$, respectively. P_+ and P_- describe the joint probability of finding the particle at position x at time t with positive and negative velocities. The constants T and R denote, classically, the forward and backward scattering probabilities, respectively. Usually $T > R$, and they express the inertia of particles under scattering. The condition $T+R=1$ guarantees the conservation of particles in every scattering process.

The PRW process (6.1) describes in phase space a Markovian random walk with *internal degrees of freedom* [11]. Each individual probability P_+ and P_- in Eq. (6.1) is a *second-order Markov process* [6].

Starting from a reversible quantum process QRW and moving toward the irreversible direction, our classical PRW process lands in a region long before the hydrodynamic regime. Since PRW is a classical Markov process, a dynamical microscopic H theorem is satisfied [13], and eventually, for long enough times, the system must evolve toward the hydrodynamic Gaussian solution (central limit theorem) [12].

Finally we ask: In configuration space, what is the generalized diffusion equation (continuum) associated with a PRW process? The answer is well known in the literature [6]. For arbitrary values of the coefficients (R,T) the continuum limit $(l,\tau) \to (0,0)$ of a PRW process (6.1) *does not exist!* However, if the coefficients R and T satisfy the particular relations

$$R \equiv \frac{\tau}{2\theta} \sim 0, \quad T=1-R \sim 1, \quad (6.2)$$

where θ is a characteristic time, only in this particular case will PRW give the following continuum equations relating the total probability $P(x,t) \equiv P_+ + P_-$ and current $J(x,t)/v_0 \equiv P_+ - P_-$ [6]: (i) local conservation of mass:

$$\frac{\partial P(x,t)}{\partial t} = -\frac{\partial J(x,t)}{\partial x}; \quad (6.3)$$

(ii) the dynamic non-Fickian Maxwell-Cattaneo relationship [14–16]:

$$J(x,t)=-D\frac{\partial P(x,t)}{\partial x}-\theta\frac{\partial J(x,t)}{\partial t}, \quad (6.4)$$

where, as we expected, $D \equiv v_0^2 \tau T/2R \sim v_0^2 \theta$ is the Landauer diffusion coefficient derived in Eq. (4.10) and associated with the incoherent part of the QRW process. Combining Eqs. (6.3) and (6.4), we have the generalized mesoscopic diffusion equation for PRW: the hyperbolic *telegraphist's equation* [6,17]:

$$\frac{1}{v_0^2}\frac{\partial^2 P(x,t)}{\partial t^2}+\frac{1}{D}\frac{\partial P(x,t)}{\partial t}=\frac{\partial^2 P(x,t)}{\partial x^2}. \quad (6.5)$$

The velocity $v_0 \equiv l/\tau$ is the mean velocity of the particles, *not the speed of sound*. Sound is a macroscopic concept that does not occur in very small materials and very small times. Equation (6.5) describes diffusion where density wave signals are propagated with finite velocity [6,18,19].

To better understand the origin of the second-order time derivative in the telegraphist's equation (6.5), we show next how the total probability density $P(x,t)$ is described by a *second-order Markov* process. Using straightforward algebra, from Eqs. (6.1) the following property can easily be proved: The total probability $P(x,t)$ satisfies, for *arbitrary* values of (R,T), the recursion equation

$$P(x,t+2)=T[P(x-1,t+1)+P(x+1,t+1)]$$

$$+(R-T)P(x,t). \quad (6.6)$$

Equation (6.6) shows clearly that if $T=R=\frac{1}{2}$ (isotropic scattering), we recover a *first-order* random walk given by Eq. (1.1). But, as long as we keep some record of inertia (memory) in scattering processes ($T \neq R$), $P(x,t)$ satisfies a *second-order* Markov equation. Assuming ($T \neq R$), the probability $P(x,t)$ defines a process that relates probabilities at *three* consecutive times. Therefore, time derivatives only up to a *second-order* are allowed in the Taylor series expansion associated with the continuous time. Clearly, the Maxwell-Cattaneo relationship (6.4) and the second-order time derivative in the telegraphist's equation (6.5) are a consequence of this *second-order Markov* property of the diffusion process in configuration space.

Since for arbitrary values of (R,T), the discrete equation (6.6) *does not* have any continuous equivalent, this gives us an additional clue to the range of applicability of PRW equations. The size of the solid and times of diffusion are still so small that a continuum description is not even allowed.

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