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Landauer diffusion coefficient: A classical result

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Using the classical version of the S-matrix scattering theory, we develop a stochastic process called persistent random walk. We show that the one-channel Landauer diffusion coefficient can be obtained from a purely incoherent classical theory. The time dependent mesoscopic diffusion current satisfies a Maxwell-Cattaneo relation. Therefore the time dependent mesoscopic diffusion process is described by the telegrapher's equation. [S1063-651X(97)05210-0]

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I. INTRODUCTION

Since the pioneering work by Landauer [1], who showed the relationship between the diffusion of a noninteracting quantum mechanical system and an associated scattering problem, several authors have given different quantum mechanical derivations of the mesoscopic diffusion coefficient [2,3]. Landauer's great insight, that diffusion (and conduction) in solids can be thought of as a scattering problem, has certainly been of great practical importance in guiding our intuition to an understanding of quantum transport in mesoscopic systems.

For a one-dimensional (1D) solid, the corresponding Landauer diffusion coefficient D can be written as

$$D = cL\,\frac{T}{2R}, \tag{1}$$

where c is the velocity of the particles, L is the length of the solid, and T and R are the transmission and reflection coefficients of the conductor treated as a single complex scattering center.

Lamentably, the transport community has failed to recognize that Eq. (1) is a purely incoherent *classical* result. Indeed, independently of the fact that the coefficients T and R in Eq. (1) may be given a classical interpretation (forward and backward transition probabilities), the algebraic structure $T/2R$ in the diffusion coefficient (1) is a very well-known consequence of a diffusion process described by a random walk with inertial memory. This stochastic process, called one-dimensional persistent random walk (1D-PRW) in the literature [4], is in fact an incoherent (classical) version of the quantum S-matrix scattering theory [5]. Next, we will show this.

II. THE CLASSICAL 1D-PRW PROCESS

The 1D-PRW is a random process which describes a succession of 1D elastic and *incoherent* scatterings in a crystal lattice. All particles, incident upon any arbitrary lattice potential barrier, are scattered with forward (transmission) and backward (reflection) classical probabilities (t,r), respectively. Conservation of particles demands $t+r=1$, and if absorption is requested then (t,r) can be substituted by $(t(1-\eta),r(1-\eta))$ where η is the probability of absorption at each potential barrier. Usually $t\neq r$ and this expresses the inertial memory of particles under scattering.

Assuming the particles to be described only at the midvalleys between potential barriers, the classical 1D-PRW equations may be written relating, at time t, the classical incoming probabilities $P_1(x,t)$ and $P_2(x+1,t)$ with the corresponding outgoing ones $P_1(x+1,t+1)$ and $P_2(x,t+1)$, at a later time $t+1$. The subscripts in the above probabilities denote the directions of motion (1 is right, 2 is left). Using the classical version of S-matrix scattering theory, the evolution of the 1D-PRW process becomes defined by the following pair of recurrence relations:

$$\begin{pmatrix} P_1(x+1,t+1) \\ P_2(x,t+1) \end{pmatrix} = \begin{pmatrix} t & r \\ r & t \end{pmatrix} \begin{pmatrix} P_1(x,t) \\ P_2(x+1,t) \end{pmatrix}. \tag{2}$$

Equation (2) describes a succession of elastic scattering events where all particles have the same average speed $c \equiv \Delta x/\Delta t$. In calculations of conductance in mesoscopic solids the speed c is chosen to be the Fermi velocity $c \equiv v_F$. Having constant energy in 1D, the velocity has only two values: $\pm c$. $P_1(x,t)$ and $P_2(x,t)$ describe the joint probability of finding the particle at a midvalley position x at time t with positive and negative velocities, respectively. Thus the 1D-PRW process (2) describes a classical Markov process with internal degrees of freedom.

Notice that inelastic collisions cannot be included in this model. The reason is that for describing diffusion in a crystal lattice, with the *recursive* PRW model (2), the jump time Δt has to be the same in every scattering process.

III. LANDAUER'S DIFFUSION COEFFICIENT AND THE TELEGRAPHER EQUATION

To find the diffusion coefficient D we have to derive Fick's law. Let us keep constant the discrete values of $\Delta x \equiv l$ and $\Delta t \equiv \tau$, where l and τ are the lattice constant (mean free path) and jump time (mean collision time), respectively. The velocity $c \equiv \Delta x/\Delta t = l/\tau$ becomes a constant too. Next, consider the first row in Eq. (2) for all $P(x\pm\Delta x,\ t\pm\Delta t)$. After a first order Taylor series expansion in both variables around (x,t) we may rewrite such an equation as

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$$\frac{\partial P_1}{\partial t}+tc\,\frac{\partial P_1}{\partial x}=\frac{r}{\tau}\,(P_2-P_1). \tag{3}$$

Next, from Eq. (2), the second row can also be similarly expanded, namely,

$$\frac{\partial P_2}{\partial t}-tc\,\frac{\partial P_2}{\partial x}=\frac{r}{\tau}\,(P_1-P_2). \tag{4}$$

Subtracting Eq. (4) from Eq. (3) and substituting the probabilities (P_1,P_2) for a new set (ρ,J) where $\rho\equiv P_1+P_2$ is the mass concentration, and $J\equiv c(P_1-P_2)$ is the diffusion current, we get, after some simplifications, that

$$J=-c^2\tau\,\frac{t}{2r}\,\frac{\partial\rho}{\partial x}-\frac{\tau}{2r}\,\frac{\partial J}{\partial t}\equiv -D\,\frac{\partial\rho}{\partial x}-\theta\,\frac{\partial J}{\partial t}. \tag{5}$$

Equation (5), which describes a classical mesoscopic diffusion current, is called the Maxwell-Cattaneo relation in the literature [6,7]. The mathematical hallmark of mesoscopic diffusion is the substitution of Fick's law by the Maxwell-Cattaneo relation.

By inspection, the first term in the right hand side of Eq. (5) is just Fick's law, and the diffusion coefficient is given by

$$D=c^2\tau\,\frac{t}{2r}=cl\,\frac{t}{2r}. \tag{6}$$

Equation (6) looks very similar to the one reported by Landauer. The difference is that Eq. (6) is local, that is, it has *microscopic* scattering coefficients (t,r) due to scattering with individual atoms in the lattice, and Landauer's equation (1) has coefficients (T,R) of the whole solid. The ratio t/r (Landauer's resistance) has only a technical meaning and is not a physically accessible quantity. However, for an *incoherent* process (we add probabilities not amplitudes), the microscopic coefficients (t,r) are easily related to the mesoscopic coefficients (T,R) of a sample made of a sequence of N *incoherent* scatterers with a total length $L\equiv Nl$, by

$$T=\frac{t}{t+Nr},\quad R=\frac{Nr}{t+Nr}. \tag{7}$$

Taking the ratio of both equations (7), we get $NT/R=t/r$. Substituting this ratio into Eq. (6), we have

$$D=c(Nl)\,\frac{T}{2R}=cL\,\frac{T}{2R}, \tag{8}$$

Eq. (8) is the exact Landauer equation, and there was absolutely nothing quantum going on there.

Since the Maxwell-Cattaneo relation (5) substitutes Fick's law, it is very important to notice that mesoscopic diffusion is associated to a diffusion process which is described in a very small time regime (the mesoscopic regime). Indeed, Eq. (5) describes a diffusive current with a relaxation time $\theta\equiv\tau/2r$. In the long-time limit ($t\gg\theta$) the Maxwell-Cattaneo relation relaxes into Fick's law and we recover the hydrodynamic regime (in agreement with the central limit theorem). Therefore Landauer's diffusion coefficient (8) is associated to a classical mesoscopic diffusion process which is *not* described by the usual hydrodynamic diffusion equation $\partial\rho/\partial t=D\partial^2\rho/\partial x^2$. In fact, it can be proved that in the weak scattering limit $(t,r)\rightarrow(1,0)$, $(\tau,l)\rightarrow(0,0)$ keeping constants $l/\tau=c$ and $\tau/r=2\theta$, then the classical mesoscopic diffusion regime is described by the telegrapher equation [5].

$$\frac{1}{c^2}\,\frac{\partial^2\rho}{\partial t^2}+\frac{1}{D}\,\frac{\partial\rho}{\partial t}=\frac{\partial^2\rho}{\partial x^2},\quad D\equiv c^2\theta. \tag{9}$$

This equation can be obtained by combining the conservation of mass law with the Maxwell-Cattaneo relation. The hyperbolic diffusion equation (9) describes at all times a *finite-velocity* propagation of density signals, in striking contrast with the infinite speed of signals that the hydrodynamic solution allows.

IV. COMMENTS

The origin of the confusion about the quantum nature of Landauer's diffusion coefficient has at least two sources: first, in Landauer's original derivation in Ref. [1] explicit mention of the word *wave function* for the reflected and transmitted densities is made. What is more, Landauer explicitly states that those densities are calculated at a distance of several *wavelengths* of the solid to avoid *interference* effects. So, a casual reader may get the wrong impression that a quantum calculation was carried out, and the derived diffusion coefficient D in Eq. (1) has to be a quantum result. Second, and more important, is Landauer's brilliant calculation of the single-channel conductance

$$g=\frac{e^2}{\pi\hbar}\,\frac{T}{R}. \tag{10}$$

To get Eq. (10) Landauer used the Einstein relation between conductivity and diffusion [1],

$$\sigma=\frac{ne^2}{k_BT}\,D, \tag{11}$$

where ne^2/k_BT was derived, for conduction electrons, with a full quantum theory, and the diffusion coefficient D was just substituted from the classical Eq. (1). The validity of Eq. (10) has been independently confirmed several times using quantum linear response theory [8–10]. The confusion comes, then, from the fact that if Eq. (10) is a valid quantum result, therefore, the diffusion coefficient D used in Eq. (11) has to be also a valid coherent quantum result. One clear example of this confusion can be seen in the excellent review article of Beenakker and van Houten [11]. Describing ballistic transport and the Landauer formula they mention ''We will discuss corrections to the classical Drude conductivity that follow from correlations in the diffusion process due to quantum interference'' (p. 22, Ref. [11]).

On the other hand, the knowledge that Landauer's diffusion coefficient, given by Eq. (1), is a classical result is not entirely new in the literature. Beginning with Landauer's original discussion presented in Ref. [1], where the incoherence of his derivation is self-evident, this subject has been repeatedly suggested several times: (i) The Landauer and Büttiker revision of the problem of a sequence of N incoherent barriers [12]. They calculated a classical transmission and reflection diffusion probabilities (T,R) using a classical technique similar to persistent random walk presented in our Sec. II. They used the steady state $P_1(i,t)=P_1(i)$ and $P_2(i,t)=P_2(i)$, with emphasis on the case $r=t=0.5$, to calculate the electrical resistance $\mathcal{R}=(\pi\hbar/e^2)R/T$ and the diffusive traversal time $\tau_T=(L/3c)R/T$. (ii) The same classical ideas are used by Landauer to calculate the resistance of planar barriers [13]. (iii) Laikhtman and Luryi made use of the Boltzmann equation to calculate the resistance, due to quantum reflection, of a planar heterostructure interface in three-dimensional bulk systems [14]. In fact, the interface boundary condition they used [Eq. (10) of Ref. [14]] is just, once again, the steady-state case of our PRW. (iv) Kunze treats the transport problem through a planar barrier using classical kinetic equations [15].

V. CONCLUSIONS

Both classical and quantum mechanical approaches lead to the same 1D Landauer diffusion coefficient Eq. (6) with the well-known $t/2r$ expression. This suggests that, in a time dependent quantum diffusion current, Fick's law must be an *incoherent* contribution. In fact, it can be proved that the whole Maxwell-Cattaneo relation Eq. (5) is the incoherent contribution [16]. Clearly, the time dependent quantum diffusion current also has an interference term which is intrinsic to the quantum wave description

$$J_{\text{quan}}(x,t)=J_{\text{inco}}(x,t)+J_{\text{inter}}(x,t)$$
$$=-D\,\frac{\partial|\psi|^2}{\partial x}-\theta\,\frac{\partial J_{\text{quan}}}{\partial t}+J_{\text{inter}}(\psi,\partial\psi/\partial x). \tag{12}$$

Therefore as far as Fick's law is concerned, being an incoherent result, any suitable incoherent (classical) theory such as a Boltzmann or a master equation will give the same diffusion coefficient without the burden of quantum calculations.

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