A microscopic Landauer diffusion coefficient

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Abstract. Using the methods of Correlated Walks and Quantum Scattering Theory in a perfect one-dimensional lattice we present a derivation of a microscopic Landauer diffusion formula. For a discrete-time formulation, an expression for the diffusion coefficient is obtained, depending on the scattering matrix S elements, which describes the quantum properties of the unitary cell. A similar result is obtained for a continuous-time correlated walk, for which the jump rate is characterized by a Poisson pausing-time distribution. In both cases the diffusion coefficient is a Landauer type of equation which depends only on the properties of the unitary cell such as the reflection coefficient and microscopic the energy of the incident particle. An example is given for the diffusion coefficient versus energy in a lattice described by a Kronig-Penny potential.

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1. Introduction

For a long time, the Landauer diffusion formula [1] has been known to be the correct result for a one-dimensional, non-interacting system of electrons on ordered and disordered metals. In this paper we present a rigorous derivation of the Landauer formula for a diffusion process described by a correlated walk.

Before going on, the argument of Landauer [1] which gives the correct result for the one-dimensional case would be worthwhile reviewing.

Landauer argued as follows. Consider particles incident from the left of an array of obstacles of length L, with a total reflection coefficient R. Averaging over several wavelengths, the density to the left is $1 + R$ and that to the right $1 - R$, giving a density gradient across the region, $\partial n/\partial x = -2R/L$. The total flux across the region is equal to the incident flux minus the reflected flux, $J = v(1 - R)$ where v

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is the velocity of the particle. Using the diffusion equation $J = -D\partial n/\partial x$, one gets

$$D = \frac{vL}{2}\left[\frac{1-R}{R}\right] \tag{1.1}$$

Eq. (1.1) is the Landauer formula, valid for a general one-dimensional system.

Attempts to derive (1.1) rigorously from linear response theory have produced some previous unsuccessful results [2], until Anderson *et al.* [3], and Stone [4] gave derivations using length an tedious quantum mechanical perturbation theories, proving that (1.1) is indeed correct, under the framework of quantum theory.

Eq. (1) was derived originally by Landauer having in mind a macroscopic disordered solid, where the reflection coefficient R belonged to a sample of size L. However a careful look at Landauer's derivation shows something that has so far escaped the attention of researchers, and is the fact that the of length L of the solid has no restrictions at all. As a consequence the derivation must also be valid even in the limit where the size L of the material becomes the size of a single atom!.

In other words, we claim that Eq. (1.1) may also be thought as the diffusion coefficient of a process where particles are incident upon potential barriers of single atoms at a time, and therefore R has to be the microscopic reflection coefficient of that potential barrier, and whose analytic expression is well predicted by the Quantum Theory. Not only that, we also claim that if our assumption is correct, then since the coefficient D becomes the microscopic coefficient of a diffusive transport process, therefore there must be possible to find, as a mathematical model, an appropriate stochastic walk such that the microscopic version of the Landauer coefficient (1.1) can be derived.

It is the purpose of this work to show that such stochastic walk exists and is given by a particular selection of a correlated walk in a one-dimentional lattice, and $1 - R$ will become the microscopic jumping probability between adjacent cells.

In Section 2 we show how the quantum theory of scattering gives a relation between the S-matrix elements and the jumping probabilities, next we show how these probabilities associated to a correlated walk can be expressed by the microscopic reflection coefficient. In Sections 3 and 4, from the correlated walk model we derive the Landauer equation as a function of the microscopic properties of the unitary cell. Finally in Section 5 we give an example where we apply the theory to a Kronig-Penney type of solid. Here we show explicitly how the Landauer coefficient depends on the microscopic properties of the particle and barrier.

2. Correlated walk and S-matrix

A standard starting point for the discussion of correlated walk in one dimension is

the following set of simultaneous difference equations [3,4]

$$\begin{aligned} P_1(X,N) &= \alpha P_1(X-1,N-1) + \beta P_2(X-1,N-1) \\ P_2(X,N) &= \beta P_1(X+1,N-1) + \alpha P_2(X+1,N-1) \end{aligned} \tag{2.1}$$

where $P_j(X,N)$ denotes the probability that the walker arrives at the lattice point X with a previous step-type j (right = 1, left = 2) at the N-th step. In this process the walker arrives at the lattices point located at a distance a_0X, where a_0 is the periodicity of the lattice, at regular time intervals τ so that the time t is measured in discrete units of τ: $t = N\tau$.

The coefficients α and β denote step probabilities, such that α is the probability of stepping right (left) when the previous step was right (left), that is, α is the forward scattering probability on each lattice point; analogously β denotes the probability of stepping right (left) when the previous step was left (right), that means that β is the backward scattering probability on each lattice point. Clearly the coefficients α and β describe an isotropic (non-bias) diffusion process, and they are normalized in such a way that

$$\alpha + \beta = 1 \tag{2.2}$$

Since α and β are forward and backward scattering probabilities, they are related to the quantum properties of the lattice scattering points, in fact α and β can be interpreted as the transmission T and reflection R coefficients of the lattice points, respectively. The T and R coefficients are in turn described by the corresponding scattering matrix S of the unitary cell. From elementary quantum theory we know [7] that both coefficients are then given by

$$\begin{aligned} \alpha &\equiv T = |S_{12}|^2 \\ \beta &\equiv R = 1 - T = 1 - |S_{12}|^2. \end{aligned} \tag{2.3}$$

At it is well known [7], the S matrix does not depend on the particular structure of the incoming particle, it depends only on the dynamical nature of the interaction; the scattering potential parameters and the energy of the incoming particle.

3. Landauer equation in an infinite perfect lattice

Let us consider the set of equation (2.1) with constant coefficients α and β plus the initial condition that the walker arrives at the origin from the left at the initial time $N = 0$,

$$P_1(X, N=0) = \delta_{x,0} \qquad P_2(X, N=0) = 0. \tag{3.1}$$

The solution of these equations is obtained as follows:
Let us define the characteristic function $P_i(k, N)$ by

$$P_i(k, N) \equiv \sum_{x=-\infty}^{+\infty} e^{ikX} P_i(X, N) \qquad (i = 1, 2) \tag{3.2}$$

Fourier-transforming Eqs. (2.1), we obtain a vector Markov chain equation

$$\mathbf{P}(k, N+1) = T(k)\mathbf{P}(k, N), \tag{3.3}$$

where $\mathbf{P}$ is the column vector defined by

$$\mathbf{P}(k, N) \equiv \begin{pmatrix} P_1(k, N) \\ P_2(k, N) \end{pmatrix}, \tag{3.4}$$

and $T(k)$ is the transition matrix

$$T(k) \equiv \begin{pmatrix} Te^{ik} & Re^{ik} \\ Re^{-ik} & Te^{-ik} \end{pmatrix}. \tag{3.5}$$

The immediate formal solution of Eq. (3.3) is

$$\mathbf{P}(k, N) = T^N \mathbf{P}(k, N = 0). \tag{3.6}$$

Using the standard methods of linear algebra, we obtain

$$T^N = \frac{1}{\lambda_+ - \lambda_-} \times \begin{pmatrix} (Te^{ik} - \lambda_-)\lambda_+^N - (Te^{ik} - \lambda_+)\lambda_-^N & (\lambda_+^N - \lambda_-^N)Re^{ik} \\ Re^{-ik}(\lambda_+^N - \lambda_-^N) & (Te^{-ik} - \lambda_-)\lambda_+^N - (Te^{-ik} - \lambda_+)\lambda_-^N \end{pmatrix} \tag{3.7}$$

where λ_+ and λ_- are eigenvalues of the matrix, T, given by

$$\lambda_\pm(k) = T\cos k \pm \sqrt{R^2 - T^2 \sin^2 k} \tag{3.8}$$

The total characteristic function defined by

$$P(k, N) \equiv P_1(k, N) + P_2(k, N), \tag{3.9}$$

can now be obtained from (3.6) with the aid of (3.1) and (3.7) as follows

$$P(k, N) = \frac{1}{\lambda_+ - \lambda_-}\left[(Te^{ik} + Re^{-ik} - \lambda_-)\lambda_+^N - (Te^{ik} + Re^{-ik} - \lambda_+)\lambda_-^N\right]. \tag{3.10}$$

We note that all moments of the distribution can be obtained from the total characteristic function $P(k,N)$ through the formula

$$\langle X^n\rangle_N \equiv \sum_x X^n P(X,N) = (-i)^n \left[\frac{d^n}{dk^n}P(k,N)\right]_{k=0} \tag{3.11}$$

From Eqs. (3.10) and (3.11), after straightforward algebra we obtain

$$\langle X\rangle_N = \frac{T-R}{2R}\left[1-(CT-R)^N\right] \tag{3.12a}$$

$$\langle X^2\rangle_N = \frac{T}{R}N - \frac{T-R}{2R^2}\left[1-(T-R)^N\right] \tag{3.12b}$$

Eqs. (3.12) become, in the limit of weak correlation ($T = R = 1/2$)

$$\langle X\rangle_N \to 0, \qquad \langle X^2\rangle_N \to N. \tag{3.13}$$

analogously in the limit of strong correlation ($T \to 1, R \to 0$) we have

$$\langle X\rangle_N \to N, \qquad \langle X^2\rangle_N \to N^2. \tag{3.14}$$

Both limits are in total agreement with the physically expected behavior of the probability distribution.

With the help of Eqs. (3.12) we can now calculate the diffusion coefficient D in the usual way

$$D = \lim_{N\to\infty} \frac{a_0^2}{\tau}\frac{\langle X^2\rangle_N - \langle X\rangle_N^2}{2N} \tag{3.15}$$

$$= \frac{a_0^2}{2\tau}\frac{T}{R} = \frac{va_0}{2}\frac{T}{R}. \tag{3.16}$$

Eq. (3.16) is the Landauer equation for the particular case of an infinite lattice with perfect periodicity, see Figure 1. Notice that the parameters involved in our diffusion coefficient are just unitary cell properties. In this sense our diffusion coefficient is different from the one described by Landauer himself where he has the total reflection coefficient R of an array of obstacles of total length L. The general case of the Landauer formula may be used in a disordered metal, our result (3.16) may not. However our derivation shows how to generalize for disordered metals: we have to calculate Eq. (2.1) with stochastic $\alpha(X)$ and $\beta(X)$. This will be done in the future.

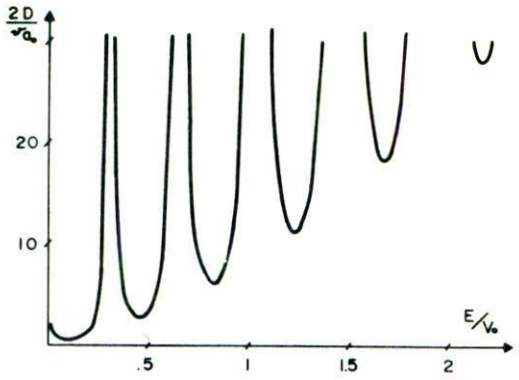

FIGURE 1. Diffusion coefficient versus energy of the incident particle. The example is for a Kronig-Penney potential where the unitary cell is a potential well given by Eq. (5.1): $V(x) = 0$, $0 \leq x < b$, $V(x) = -V_0$, $b \leq x \leq b + a$. Here $[2mV_0a^2/\hbar^2]^{1/2} = 11$.

4. Continuous-time correlated walk

In the discrete-time correlated walk the walker scatters a step right or left per unit time. We now make a generalization such that the time intervals between steps are regarded as random variables. We do this by introducing the pausing-time distribution [9] $\psi(t)$. Let us consider a walk in which the walker takes n steps at random times $t_1, t_2, \ldots, t_n$ where the n time intervals $T_1 \equiv t_1, T_2 \equiv t_2 - t_1, \ldots, T_n \equiv t_n - t_{n-1}$ are characterized by a common pausing-time distribution $\psi(T)$.

We can set up a general equation for the continuous-time correlated walk with the pausing time distribution $\psi(t)$ by a generalized vector master equation [10]:

$$\frac{\partial}{\partial t}\begin{pmatrix} P_1(X,t) \\ P_2(X,t) \end{pmatrix} = \int_0^t dt'\, \phi(t-t') \begin{pmatrix} TP_1(X-1,t') + RP_2(X-1,t') - P_1(X,t') \\ RP_1(X+1,t') + TP_2(X-1,t') - P_1(X,t') \end{pmatrix} \tag{4.1}$$

where the kernel $\phi(t)$ is given by

$$\phi(t) = \mathcal{L}^{-1}\left[\frac{s\tilde{\psi}(s)}{1-\tilde{\psi}(s)}\right]; \tag{4.2}$$

and $\mathcal{L}$ denotes the Laplace operator.

For on arbitrary pausing-time distribution $\psi(t)$, there is little hope for solving the set of Eqs. (4.1). However for the very important case of Poisson distribution

$$\psi(t) = \alpha e^{-\alpha t}, \qquad \tilde{\psi}(s) = \alpha(\alpha - s)^{-1}, \tag{4.3}$$

the problem can be handled in a simple manner [11], because only for this distribution the kernel $\phi(t)$ becomes

$$\phi(t) = \alpha\delta(t), \tag{4.4}$$

which, upon substitution into Eq. (4.1), generates a Markoffian master equation. The solution is already given in the literature [10], and we get for the diffusion coefficient

$$D = \frac{a_0^2\alpha}{2}\frac{T}{R}. \tag{4.5}$$

Since α^{-1} is the average time of the distribution, we see that our Eq. (4.5) reproduces the Landauer equation (3.16) for discrete times also.

5. An example of diffusion as a function of the energy

As an example of the usefulness of Eq. (3.16), let us calculate, the diffusion coefficient as a function of the energy E of the incoming particle, for the particular case of a Kronig-Penney potential with a unitary cell having a potential well given by

$$V(x) = \begin{cases} 0 & 0 \le x \le b, \\ -V_0 & b < x \le b + a. \end{cases} \tag{5.1}$$

For this case the S matrix elements of the unitary cell are straightforward to obtain [7] and we get

$$T = |S_{12}|^2 = \left[1 + \frac{1}{4}\left(\frac{k^2 - k'^2}{kk'}\right)^2 \sin^2 k'a\right]^{-1}, \tag{5.2}$$

where

$$\hbar k \equiv \sqrt{2mE}, \qquad \hbar k' \equiv \sqrt{2m(E + V_0)}. \tag{5.3}$$

Substituting Eq. (5.2) into Eq. (3.16) we obtain the diffusion coefficient D as a function of the energy E of the incident particle. In Fig. 1, we have a plot of D *versus* E for the particular case of $\sqrt{2mV_0a^2/h^2} = 11$. In Fig. 1, we see the fast oscillations the diffusion coefficient has, and the divergent behavior. This divergences are consequences of the resonances $T \sim 1$ involved in the transmission coefficient T.

In conclusion: it may be seen that a simple random process such as correlated walk can incorporate the quantum properties of the scattering lattice cells, giving

the same result as in a calculation made with full quantum density-matrix. In order to see that this is ideed so, we have to make two further calculations:

First, we need a macroscopic description of the Landauer equation (3.16). That is, we need to re-write it in terms of the total reflection $\mathcal{R}$ and transmission $\mathcal{T}$ coefficients of a macroscopic sample of length L. Since our theoretical description Eq. (2.1), is an incoherent superposition of probabilities, then it is an elementary problem of quantum mechanics to prove, that the total reflection and transmission coefficients of a sample made of M successive potential barriers, each one with individual coefficient T and R, is given (under the incoherent assumption) by

$$\mathcal{R} = \frac{MR}{1+(M-1)R} \qquad \mathcal{T} = \frac{T}{1+(M-1)R} \tag{5.4}$$

Substituting Eq. (5.4) into (3.16) we have

$$D = \frac{va_0}{2}\frac{T}{R} = \frac{v}{2}(Ma_0)\frac{\mathcal{T}}{\mathcal{R}} = \frac{v}{2}L\frac{\mathcal{T}}{\mathcal{R}} \tag{5.5}$$

Here $L = Ma_0$ is the total size of the macroscopic sample made of M microscopic cells of size a_0 each one.

Second, using the macroscopic description (5.5), we use the Einstein relation to calculate the electrical conductivity σ of a degenerate Fermi gas

$$\sigma = \frac{ne^2}{kT}D = \frac{e^2 L}{2\pi\hbar}\frac{\mathcal{T}}{\mathcal{R}} \tag{5.6}$$

And this is the correct one-chanel Landauer formula, derived by Douglas Stone (Eq. (2.27), reference [4]), for the more general case of disordered metals, using quantum linear response theory.

In conclusion, we have just given a particular example (crystalline solid) in which the Landauer equation can be derived using an incoherent stochastic process. In this case the microscopic properties of the diffusion equation are immediate.

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Resumen. Usando los métodos de caminos correlacionados y Teoría cuántica de dispersión en una red perfecta unidimensional, presentamos una derivación microscópica de la fórmula de difusión de Landauer. Para una formulación de tiempo discreto, se obtiene una expresión para el coeficiente de difusión que depende de los elementos de la matriz S de la celda unitaria. Un resultado semejante se obtiene para un camino correlacionado de tiempo continuo con una distribución de Poisson para el tiempo de espera. En ambos casos el coeficiente de difusión es un resultado tipo Landauer que depende de las propiedades microscópicas de la celda unitaria tales como los coeficientes de transmisión y reflexión y la energía de la partícula. Se da un ejemplo del coeficiente de difusión en un potencial de Kronig-Penney.