Landauer equation in three-dimensional amorphous materials

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We use the Boltzmann transport equation to calculate the three-dimensional (3D) version of the Landauer equation for incoherent electrons diffusing in a slab of amorphous material. We use the P_1 approximation to calculate the multiple-scattering transmission coefficient as a function of the diffusion coefficient. The 3D transmission coefficient is, apart from numerical coefficients, similar to that for 1D. The result is valid only for positions far away from the boundaries and for slabs having a thickness much greater than one mean free path.

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I. INTRODUCTION

One of the problems that has most attracted the attention of solid state physicists in the past three decades is that of mesoscopic diffusion of electrons in nanostructures. This process, due to the multiple scattering of electrons within a solid, was first investigated by Landauer [1] who in 1957 obtained for conduction electrons in a one-dimensional (1D) solid his famous formula connecting the multiple-scattering transmission coefficient T and the diffusion coefficient D, namely,

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

where c is the Fermi velocity for the electrons and L is the length of the 1D solid. For mesoscopic materials the coefficient $T=1-R$ has all the fine coherent details of quantum theory.

The quantum derivation of Eq. (1) assumes that the potentials are measured some distance away from the scatterers and that this measurement is incoherent, which implies not taking into account the interference of the incident and reflected waves [2]. That the Landauer equation (1) is not a fully coherent result is a fact that has long been recognized by some authors [3–6].

What is striking is that the Landauer relation between T and D, which was originally quantum derived for mesoscopic materials, is also valid for bulk materials. Once the interference is neglected, the Landauer result (1) can also be derived with incoherent diffusive processes; as has been shown several times in the past [7–9]. The important difference is that in the macroscopic case the transmission coefficient T is a fully incoherent property.

One previous derivation of this Landauer result makes use of the Boltzmann transport equation free of external forces [9]:

$$\left[\frac{1}{c}\frac{\partial}{\partial t} + \hat{\Omega}\cdot \mathrm{grad}_{\mathbf{r}} + \Sigma_s\right] f(\mathbf{r},\Omega,t) = \int d\Omega' f(\mathbf{r},\Omega',t)\Sigma_s(\Omega'\to\Omega). \tag{2}$$

Here f is the distribution of independent, *monoenergetic* particles moving in a homogeneous and isotropic medium. Elastic collisions are only against fixed targets. The constant speed is denoted by c, and Ω is a unit vector in the direction of motion of the particles. $\Sigma_s(\Omega'\to\Omega)$ denotes the macroscopic scattering cross section which, for amorphous materials, is defined as the microscopic differential cross section multiplied by the density of target atoms. For isotropic scattering, $\Sigma_s(\Omega'\to\Omega)$ depends only on the deflection angle θ_0 between the Ω' and Ω directions, that is, $\cos\theta_0 \equiv \Omega\cdot\Omega'$. The quantity $\Sigma_s \equiv \int d\Omega\, \Sigma_s(\Omega'\to\Omega)$ denotes the total macroscopic scattering cross section and defines the inverse of the scattering mean free path, $\Sigma_s \equiv \lambda_s^{-1}$.

Particularized to the 1D case (x axis), this transport theory readily provides the *exact* two-stream theory in which the right- and left-moving densities, denoted by $f_1(x,t)$ and $f_2(x,t)$, respectively, satisfy the 1D transport equation

$$\left[\frac{1}{c}\frac{\partial}{\partial t} + \frac{\partial}{\partial x}\right] f_1 = \Sigma_s r(f_2 - f_1), \tag{3}$$

$$\left[\frac{1}{c}\frac{\partial}{\partial t} - \frac{\partial}{\partial x}\right] f_2 = \Sigma_s r(f_1 - f_2), \tag{4}$$

where r denotes the microscopic single-scattering backward probability: $r \equiv \Sigma_s(+\to-)/\Sigma_s = \Sigma_s(-\to+)/\Sigma_s$. If this 1D theory is used to calculate the multiple-scattering transmission coefficient T through a 1D solid of length L, the exact result becomes the Landauer equation (1)

$$T = \frac{2}{2 + cL/D}, \tag{5}$$

making clear that the Landauer result, for bulk materials, is both an incoherent and a 1D result. From this exact 1D case we learn that the Landauer equation describes a mesoscopic time diffusive regime (non-Markovian), which for long times correctly relaxes into the hydrodynamic regime.

Now if we take the three-dimensional (3D) case of the transport equation the question is, does the 3D transmission coefficient look similar to that in 1D (Landauer) or do we get something different? The purpose of the present work is to show that for an infinite slab of scattering material the 3D transmission coefficient looks, apart from numerical coeffi-

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cients, similar to that in 1D. We use the P_1 approximation to get the multiple-scattering coefficient. The result so obtained is valid only for points in the material far away from the boundaries. Another restriction for the validity of the result is that the length of the slab has to be much greater than one mean free path.

II. MILNE'S PROBLEM

Consider the diffusion along the z axis of incoherent particles through an infinite slab (xy direction) of material. Assume that the incidence of particles is uniform over one surface of the slab (the $z=0$ plane, for instance). Then the distribution f is independent of x and y and depends only on z. This example, first studied by Milne in connection with the flow of light in a stellar atmosphere, is called Milne's problem [10,11]. Since the problem has azimuthal symmetry, the function f depends only on the angle θ between the velocity Ω and the z axis; we can write $f=f(z,\theta,t)$. Assuming the steady-state condition, the transport equation becomes

$$\cos\theta \frac{\partial}{\partial z} f(z,\theta) + \Sigma_s f(z,\theta) = \frac{\Sigma_s}{2}\int_0^\pi f(z,\theta')\sin\theta'\, d\theta'. \tag{6}$$

Measuring distances in units of the mean free path $\xi \equiv z/\lambda_s = z\Sigma_s$, this equation becomes

$$\cos\theta \frac{\partial}{\partial \xi} f(\xi,\theta) + f(\xi,\theta) = \tfrac{1}{2}\int_0^\pi f(\xi,\theta')\sin\theta'\, d\theta'. \tag{7}$$

The solution of this differential-integral equation will enable us to determine any required property of the diffusing particles.

Now suppose that the slab of scattering material is between the planes $z=0$ and $z=L\equiv\lambda_s\xi_0$. The incident distribution $f_0(\theta)$ on the surface $z=0$ penetrates into the slab, gradually disappearing as its constituent particles get scattered. The probability for such particles to survive a distance $z=\lambda_s\xi$ without suffering a collision is $f_0(\theta)e^{-\xi\sec\theta}$. The function $f_0(\theta)$ must be zero for $\pi/2\leqslant\theta\leqslant\pi$, for only this range of θ corresponds to flow out of the slab. Another contribution to $f(\xi,\theta)$, the diffuse part, comes from rescattering in the θ direction. Particles at distance ξ' having any another direction of motion, let us say θ', can be scattered into the θ direction and can travel freely from ξ' to ξ. The number scattered at distance ξ' will be proportional to the density $\rho(\xi')\equiv\int_0^\pi f(\xi',\theta')\sin\theta'\,d\theta'$, and the number of such particles arriving at depth ξ at angle θ will be proportional to

$$\rho(\xi')e^{-|\xi'-\xi|\sec\theta}, \tag{8}$$

where ξ' will be less than ξ if θ is less than $\pi/2$ (forward scattering) and greater than ξ for θ larger than $\pi/2$ (backward scattering). Consequently, the solution of Eq. (7) for $f(\xi,\theta)$ will have the general form $f(\xi,\theta)=f_{\rm inc}+f_{\rm dif}$, explicitly given by

$$f(\xi,\theta)=\begin{cases} f_0(\theta)e^{-\xi\sec\theta}+\frac{1}{2}\sec\theta\int_0^\xi \rho(\xi')e^{-(\xi-\xi')\sec\theta}dy', & 0\leqslant\theta<\dfrac{\pi}{2}\\[2ex] \frac{1}{2}\sec\theta\int_{\xi_0}^{\xi}\rho(\xi')e^{+(\xi'-\xi)\sec\theta}d\xi', & \dfrac{\pi}{2}<\theta\leqslant\pi. \end{cases} \tag{9}$$

Of course, this is not yet a solution, for we have not calculated the density ρ. However, this expression is *exact*. By direct integration we can reformulate the differential-integral Eq. (7) into Eq. (9), and show that the density $\rho(\xi)$ satisfies the integral equation

$$\rho(\xi)=\int_0^{\pi/2} f_0(\theta)e^{-\xi\sec\theta}\sin\theta\,d\theta+\tfrac{1}{2}\int_0^{\xi_0}d\xi'\rho(\xi') \times\left[\int_1^\infty \frac{dy}{y}e^{-|\xi-\xi'|y}\right]. \tag{10}$$

This is an integral equation of standard type. When ξ_0 is infinite, the equation is said to be of the Weiner-Hopf type [10]. The advantage of this integral formulation is that it shows explicitly the contribution of the incident distribution at the boundary. It also shows that the diffuse part of the distribution depends only on the density ρ, which is a simpler function than is f, for ρ depends only on ξ and not on θ.

III. THE P_1 APPROXIMATION

To derive the transmission coefficient from the exact integral equations (9) and (10) is a rather involved mathematical problem [12]. An easier and rather illuminating approximation to this problem is the so called P_1 approximation, which we describe next.

First we assume, for simplicity, that the incident beam $f_0(\theta)$ on the surface $z=0$ is of constant intensity I/c (I is the incident flux) and is all directed in the positive z direction; that is, $f_0(\theta)\equiv(I/c)\delta(1-\cos\theta)$. Second, since the angular dependence of the function f is only on the angle θ we can have, for the diffuse distribution, a Legendre series representation as $f_{\rm dif}(\xi,\theta)=\Sigma_{l=0}^\infty f_l(\xi)P_l(\cos\theta)$. The P_1 approximation requires for the diffuse distribution that only $l=0$ and $l=1$ are taken into account, that is,

$$f(\xi,\theta)\simeq(I/c)e^{-\xi}\delta(1-\cos\theta)+\frac{1}{2}\rho_{\rm dif}(\xi)P_0+\frac{3}{2c}J_{\rm dif}(\xi)P_1 +\cdots, \tag{11}$$

where the diffuse density $\rho_{\rm dif}$ and flux $J_{\rm dif}$ are defined as

$$\rho_{\rm dif}(\xi)\equiv\int_0^{\pi}f_{\rm dif}(\xi,\theta)\sin\theta\,d\theta,$$
$$J_{\rm dif}(\xi)\equiv c\int_0^{\pi}f_{\rm dif}(\xi,\theta)\cos\theta\sin\theta\,d\theta. \tag{12}$$

Under this P_1 approximation the steady-state Boltzmann transport equation (7) becomes

$$\frac{1}{2c}\left(\frac{dJ_{\rm dif}}{d\xi}-Ie^{-\xi}\right)P_0+\frac{1}{2}\left(\frac{d\rho_{\rm dif}}{d\xi}+\frac{3}{c}J_{\rm dif}+\cdots\right)P_1+\cdots=0. \tag{13}$$

The orthogonality of the Legendre polynomials implies that the transport equation splits into a closed system of two equations for $\rho_{\rm dif}$ and $J_{\rm dif}$:

$$\frac{\partial J_{\rm dif}}{d\xi}=Ie^{-\xi},\quad J_{\rm dif}\simeq-\frac{c}{3}\frac{\partial\rho_{\rm dif}}{\partial\xi}+\cdots. \tag{14}$$

The first equation, which is exact, is just the steady-state continuity equation in the presence of a source distribution. As far as this part of the solution goes, the incident particles at $z=0$ appear inside the slab, at the point where they suffer their first collision, as though there were a source distribution of strength $Ie^{-\xi}$ inside the material. The second equation, which is only an approximation to the exact flow, is Fick's law and shows that the diffusion coefficient D is given by $D=c/(3\Sigma_s)$.

Both equations in (14) imply that the diffuse density $\rho_{\rm dif}$ satisfies the diffusion equation with sources,

$$\frac{d^2\rho_{\rm dif}}{d\xi^2}=-\frac{3I}{c}e^{-\xi}, \tag{15}$$

or, explicitly,

$$\rho_{\rm dif}(\xi)=\frac{3I}{c}(A\xi+B-e^{-\xi}), \tag{16}$$

where the constants (A, B) are adjusted to fit the boundary conditions at $\xi=0$ and $\xi_0\equiv L\Sigma_s$.

Therefore, in the P_1 approximation the distribution becomes

$$f(\xi,\theta)\simeq(I/c)e^{-\xi}\delta(1-\cos\theta)+\frac{1}{2}\rho_{\rm dif}-\frac{1}{2}\frac{d\rho_{\rm dif}}{d\xi}\cos\theta+\cdots, \tag{17}$$

where $\rho_{\rm dif}$ is given by Eq. (16).

Since the total macroscopic cross section Σ_s can be written in terms of the diffusion coefficient $\Sigma_s=c/3D$, then the dimensionless length ξ can also be rewritten in terms of the diffusion coefficient as

$$\xi=z\Sigma_s=\frac{c}{3D}z. \tag{18}$$

At this point we understand how we can generalize the Landauer result. We can have not only the transmission coefficient but the whole 3D distribution depending explicitly on the diffusion coefficient.

IV. TRANSMISSION COEFFICIENT

Notice that in the P_1 approximation $f(\xi,\theta)$ is nearly independent of the angle of direction of momentum; and for this approximation to be valid the magnitude of the flux $J_{\rm dif}$ has to be considerably smaller than the density $\rho_{\rm dif}$. These two requirements make the P_1 approximation valid as long as we do not require too much detail concerning the behavior of $\rho_{\rm dif}$ and $J_{\rm dif}$ within a few free paths of the boundary. Formula (17) is obviously inaccurate for f at the boundary surfaces.

To find the transmission coefficient in a slab, the following boundary conditions are required: (i) we have an incident beam at the bottom surface $\xi=0$, and (ii) we require no incoming beam at the top opposite surface $\xi_0=cL/3D$. Since in the P_1 distribution $f(\xi,\theta)$ is inaccurate at the boundary surfaces, we will satisfy our requirements by asking the average of $\Omega_z=\cos\theta$ to satisfy the above boundary conditions. So, using the P_1 distribution $f(\xi,\theta)$ given by Eq. (17), we define the up- and down-moving fluxes (J_+,J_-) as follows. The up-moving flux is given by

$$J_+(\xi)\equiv c\int_0^{\pi/2}f(\xi,\theta)\cos\theta\sin\theta\,d\theta$$
$$=Ie^{-\xi}+\frac{c}{4}\left(\rho_{\rm dif}(\xi)-\frac{2}{3}\frac{d\rho_{\rm dif}(\xi)}{d\xi}\right). \tag{19}$$

Similarly, the down-moving flux becomes

$$J_-(\xi)\equiv c\int_{\pi/2}^{\pi}f(\xi,\theta)\cos\theta\sin\theta\,d\theta$$
$$=-\frac{c}{4}\left(\rho_{\rm dif}(\xi)+\frac{2}{3}\frac{d\rho_{\rm dif}(\xi)}{d\xi}\right), \tag{20}$$

Now the boundary conditions for our multiple-scattering transmission problem become

$$J_+(0)=I,\quad J_-(\xi_0)=0. \tag{21}$$

These two boundary conditions allow us to find the two constants (A, B) found in the diffuse density, Eq. (16). We obtain

$$A=\frac{1}{3\xi_0+4}(e^{-\xi_0}-5), \tag{22}$$

$$B=\frac{1}{3}\frac{1}{3\xi_0+4}(2e^{-\xi_0}+15\xi_0+10). \tag{23}$$

Substituting these two constants into Eqs. (19) and (20), we get an explicit expression for both fluxes in the range ($0\leqslant\xi\leqslant\xi_0$):

$$J_+(\xi)(4/I)=-e^{-\xi}-\frac{15-3e^{-\xi_0}}{3\xi_0+4}\xi+\frac{20+15\xi_0}{3\xi_0+4}, \tag{24}$$

$$J_-(\xi)(4/I)=+e^{-\xi}+\frac{15-3e^{-\xi_0}}{3\xi_0+4}\xi-\frac{15\xi_0+4e^{-\xi_0}}{3\xi_0+4}. \tag{25}$$

Notice that $J_+(\xi)$ is positive and $J_-(\xi)$ is negative, as they should be.

Now we can get the 3D multiple-scattering transmission coefficient, which is defined as $T \equiv J_+(\xi_0)/I$. We obtain (in the P_1 approximation)

$$T = \frac{5 - e^{-\xi_0}}{3\xi_0 + 4} = \frac{5 - e^{-cL/3D}}{4 + cL/D}. \tag{26}$$

Similarly for the reflection coefficient $R \equiv |J_-(0)|/I$, we get

$$R = 1 - T, \tag{27}$$

showing that the conservation of mass is well satisfied. We can verify this in another way: from both fluxes (24) and (25) we have

$$J_+(\xi) + J_-(\xi) = I \frac{5 - e^{-\xi_0}}{3\xi_0 + 4} = IT, \tag{28}$$

verifying that the total flux is indeed a constant. The total flux must be the same either at the top (IT) or at the bottom $[I(1-R)]$ boundary.

Equation (26) is, in the P_1 approximation, the 3D equivalent of the Landauer equation we have been looking for.

V. CONCLUSIONS

Why is that we have an exponential contribution exp $(-\xi_0)$ in the transmission coefficient (26)? This exponential has its origin in the incident contribution in the exact integral Eq. (9). However, as we can clearly see in the exact 1D theory (5), the exponential should not appear at all in the final result. In the exact 1D approach, the diffuse contribution cancels the exponential of the incident contribution. The exponential is then a mathematical consequence of the P_1 approximation. However, as we can immediately see, it has no physical consequences.

We must understand that, since the P_1 distribution f is inaccurate at the boundary surfaces, any results we get from this approximation can be reliable only in space coordinates far from the boundaries. The P_1 approximation makes sense only if the thickness of the slab L is much greater than one mean free path $3D/c$. The opposite implies that both boundaries are very close to each other, invalidating the P_1 results at any intermediate position. Therefore, an implicit physical restriction of the P_1 approximation is that $\xi_0 \gg 1$. In this case, the exponential decay is negligible and we arrive at a similar equation as for the 1D case,

$$T \simeq \frac{5}{4 + cL/D}, \quad L \gg 3D/c, \tag{29}$$

or equivalently

$$D \simeq cL \frac{T}{4R + 1}, \quad T < 1. \tag{30}$$

This last restricted equation is the 3D result predicted by the P_1 approximation. As expected, for the same value of the transmission coefficient T, the numerical value of the 3D diffusion coefficient is less than the 1D (Landauer) one.

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