Phase averaging in one-dimensional random systems

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We calculate the resistance of a random sequence of scatterers and show that, in general, the phase uncertainty does *not* increase with the length of the wire. We elucidate the special circumstances under which phase averaging is appropriate.

In recent years, there has been considerable controversy surrounding the resistance of thin wires described by a random one-dimensional (1D) potential. It has been assumed that the phase of the wave function becomes random for a sufficiently long wire and that *phase averaging* occurs.[1-6] Although phase randomization can occur by phonon scattering and/or by variation in the local phase between scatterers, in the zero-temperature theory discussed by many authors, only the latter is relevant. In this Communication we examine this limit in some detail and show that phase averaging only occurs if the phase is randomized after scattering from each obstacle. Using longer segments will not, in general, increase the tendency to phase average. We illustrate these points with a simple example; a fuller account of the general case will be given in a forthcoming paper.[7]

The resistance of a one-dimensional wire may be written[1,8-10]

$$\mathcal{R} = \frac{h}{e^2} \frac{R}{T} \quad , \qquad (1)$$

where $h/e^2 \simeq 26 \text{ k}\Omega$, T and $R = 1 - T$ are the transmission and reflection coefficients. A one-dimensional potential can always be broken into a series of *segments*. There may be a natural way of doing this, as in Fig. 1, where each segment contains a single δ function, or it may be done more arbitrarily
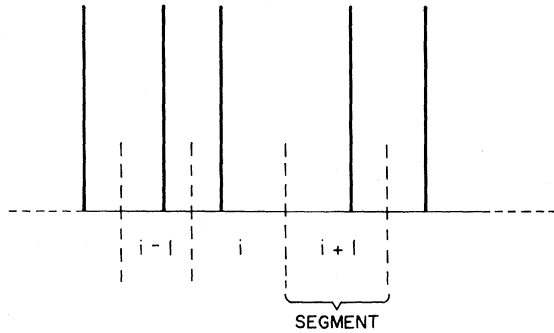

FIG. 1. Sequence of equal strength δ functions, with random spacings. The segments $i-1$, i, $i+1$, etc., are separated by dashed lines.

for a less structured potential. As scattering takes place at each segment, T gets smaller and the resistance $\mathcal{R}$ increases exponentially with length.

Thus the appropriate quantity to average is the logarithm of the resistance, as it is this which obeys the central limit theorem.[11]

In general, neglecting spin, the dimensionless resistance R/T for a sequence of n segments, written z_n, may be obtained from the transfer matrices $\vec{\mathsf{T}}_n$ that control the scattering of amplitudes at *single segments*.

$$\vec{\mathsf{T}}_n = \begin{pmatrix} (1+\rho_n)^{1/2} e^{-i\theta_n} & \rho_n^{1/2} e^{-i\phi_n} \\ \rho_n^{1/2} e^{i\phi_n} & (1+\rho_n)^{1/2} e^{i\theta_n} \end{pmatrix} , \qquad (2)$$

where the scattering is characterized by an amplitude ρ_n and phases θ_n and ϕ_n. A similar matrix $\vec{\mathsf{M}}_n$ describing the scattering by n segments is given by

$$\vec{\mathsf{M}}_n = \begin{pmatrix} (1+z_n)^{1/2} e^{-i\alpha_n} & z_n^{1/2} e^{-i\beta_n} \\ z_n^{1/2} e^{i\beta_n} & (1+z_n)^{1/2} e^{i\alpha_n} \end{pmatrix} . \qquad (3)$$

This satisfies

$$\vec{\mathsf{M}}_n = \vec{\mathsf{T}}_n \vec{\mathsf{M}}_{n-1} \quad , \qquad (4)$$

from which one obtains the following relations for z_n:

$$\ln(1+z_n) = \ln(1+z_{n-1}) + \ln(1+\rho_n)$$
$$+ \ln(1 + t_n + 2t_n^{1/2}\cos\epsilon_n) \quad , \qquad (5a)$$

$$r_n \exp[i(\epsilon_{n+1} - \theta_{n+1} - \theta_n + \phi_{n+1} - \phi_n)]$$
$$= \frac{s_n + r_{n-1}\exp(i\epsilon_n)}{1 + s_n r_{n-1}\exp(i\epsilon_n)} \quad , \qquad (5b)$$

$$r_n \exp[i(\beta_n - \alpha_n) - i(\beta_{n-1} - \alpha_{n-1})]$$
$$= \frac{s_n + r_{n-1}\exp(i\epsilon_n)}{\exp(i\epsilon_n) + s_n r_{n-1}} \quad , \qquad (5c)$$

where

$$\epsilon_n = \alpha_{n-1} + \beta_{n-1} + \theta_n - \phi_n$$

and

$$s_n = \left(\frac{\rho_n}{1+\rho_n}\right)^{1/2} , \quad r_n = \left(\frac{z_n}{1+z_n}\right)^{1/2} , \quad t_n^{1/2} = s_n r_{n-1} \quad . \qquad (6)$$

These equations are exact and completely general. They are in a convenient form, because in the thermodynamic limit $(n \to \infty)$, $r_n \to 1$ and all quantities are well behaved. The random-phase assumption suggests[12] that there is a "randomness length" at which the phases α_n and β_n become *independent* random variables uniformly distributed over 2π. However, in the thermodynamic limit it is clear from (5c) that $\alpha_n - \beta_n$ becomes independent of n. Thus, although they may individually be distributed over 2π, they are not mutually independent. The phase of interest, when one addresses questions concerning phase averaging, is the quantity ϵ_n on the right-hand side of (5a), and we now examine this in some detail.

For purposes of illustration we restrict the discussion to the example of randomly spaced δ functions of equal scattering strength ρ. Initially, we divide the system into segments in the most natural way, with one δ function per segment as shown in Fig. 1. Iterating (5a) yields

$$\ln(1 + z_n) = n\alpha = n(\alpha_1 + \alpha_2) \ , \tag{7}$$

where

$$\alpha_1 = \frac{1}{n} \sum_{i=1}^{n} \ln(1 + \rho_i) \ , \tag{8}$$

and

$$\alpha_2 = \frac{1}{n} \sum_{i=2}^{n} \ln(1 + t_i + 2t_i^{1/2}\cos\epsilon_i) \ . \tag{9}$$

Since all segments now have equal scattering strength and in the thermodyamic limit terms of order n^{-1} and $n^{-1/2}$ can be neglected, we have

$$\alpha_1 = \ln(1 + \rho) \tag{8a}$$

and

$$\alpha_2 = \int d\epsilon P(\epsilon) \ln(1 + t + 2t^{1/2}\cos\epsilon) \ , \tag{9a}$$

where $P(\epsilon)$ is the distribution function of the cumulative phase ϵ and $t = [\rho/(1 + \rho)]^{1/2}$. The situation is particularly transparent in the large ρ limit,[13] where $t \to 1$, and from (5b),

$$\epsilon_{n+1} = \theta_{n+1} + \theta_n - \phi_{n+1} + \phi_n \ . \tag{10}$$

In this case, ϵ_n is determined entirely by the local phases and therefore averaging can only occur if the phase is randomized locally. *Phase uncertainty does not build up along the chain.* Indeed, it may even be useful to regard the phase ϵ_n as being *reset* at each scattering event.

In the present model,

$$\epsilon_{n+1} = 2\tan^{-1}\rho^{1/2} - 2k_0 y_n \ , \tag{10a}$$

where k_0 is the wave vector of the electron and y_n is the separation between the n and $n + 1$ δ functions. If these separations are distributed uniformly over

the interval $y_0 \pm \Delta y$, we have

$$P(\epsilon) = \begin{cases} \dfrac{1}{2\Delta\epsilon} & \text{for } \bar{\epsilon} + \Delta\epsilon \geq \epsilon \geq \bar{\epsilon} - \Delta\epsilon \\ 0 & \text{otherwise} \ , \end{cases} \tag{11}$$

where

$$\bar{\epsilon} = 2(\tan^{-1}\rho^{1/2} - k_0 y_0)$$

and

$$\Delta\epsilon = 2k_0\Delta y \ . \tag{12}$$

The integral for α_2 [Eq. (9a) with $t = 1$] can be obtained numerically. In Fig. 2, this is compared with
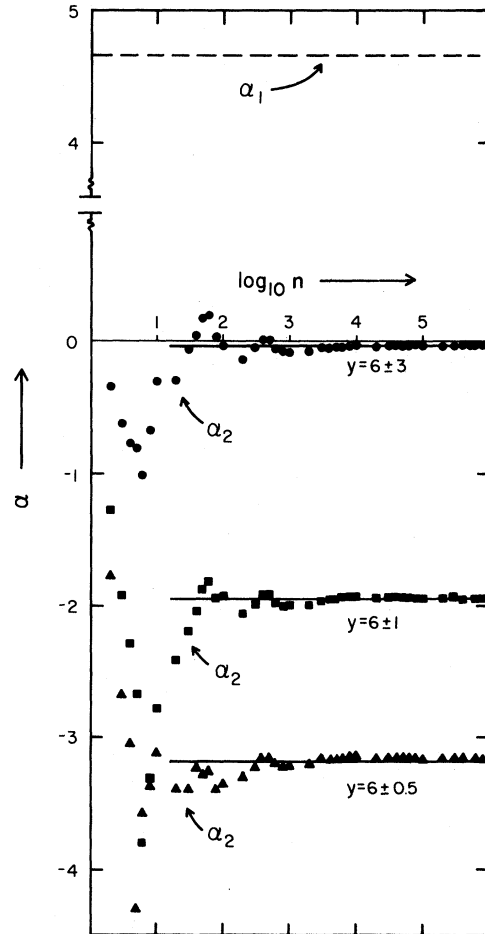

FIG. 2. Variation of α with system size for δ functions of strength $\rho = 105$ and spacing uniformly distributed in the ranges 6 ± 0.5 Å (▲), 6 ± 1 Å (■), and 6 ± 3 Å (●). All results are for a wave vector k_0 corresponding to an electron with a kinetic energy of 1 eV. The value of α_1 is the same for all three cases and is shown in the upper curve. The three lower curves are the results for α_2. For large n, α_2 is self-averaging and approaches the asymptotic value predicted by Eqs. (9a), (11), and (12) with $t = 1$.

results obtained for a single chain by evaluating Eqs. (5a) and (5b) for a particular sequence of up to 10^6 scatterers. It can be seen that for large n, the numerical results settle down to the expected asymptotic value. For $\Delta y = 0.5$ Å, α_2 is almost the negative of α_1, so the latter is very much greater than the sum $\alpha = \alpha_1 + \alpha_2$. In the limit of *no disorder*, $\alpha_1 + \alpha_2 = 0$, which corresponds to the *crystalline limit*. As the width of the distribution $P(\epsilon)$ increases, α_2 becomes less negative until, for $\Delta y = 3$ Å, it is almost zero. This is approaching the situation in which the phase randomizes at each site, since $\Delta \epsilon = \pi$ corresponds to $\Delta y \simeq 3.07$ Å.

Choosing larger segments containing more scatterers does *not* increase the tendency to phase average. For example, dividing the system of $n = ml$ δ functions into m segments each containing l scatterers yields $\alpha = \alpha_1' + \alpha_2'$, where

$$\alpha_1' = \alpha_1 + (1 - 1/l)\alpha_2$$

and

$$\alpha_2' = \alpha_2/l \quad . \tag{13}$$

This result is obtained after noting that the new phases ϵ_i', which enter a relation for α_2' analogous to Eq. (9), depend only on the phases associated with the *first* δ function of segment i and those of the *last* δ function of segment $i - 1$. Thus, in the strong scattering limit considered here, the distribution function $P(\epsilon') = P(\epsilon)$ and is *independent of the segment size*.

Our discussion in this Communication has centered on a single chain and ensemble averaging has not been considered. This is because, in the limit of large n, $\ln(1 + z_n)$ is self-averaging. It should be noted, however, that the inverse localization length α_1' could be obtained by ensemble averaging[4,5] over chains of length l. Clearly, as l gets large, α_1' tends to the correct value α of Eq. (7). However, this is not because ϵ' randomizes over 2π, rather it is because the *number* of terms neglected [there are m of these yielding a contribution $(m/n)\alpha_2 = \alpha_2'$] decreases while their magnitude remains roughly constant.[14]

The form of Eqs. (2) and (3) is determined by time-reversal symmetry, and so the problem of computing the resistance of a wire described by the 1D Anderson model, with diagonal and/or off-diagonal disorder, is readily mapped onto Eq. (4). Thus our conclusions apply equally well to tight-binding-type Hamiltonians.

For purposes of illustration we have restricted the discussion in this report to the strong scattering, large ρ limit, where the analysis is considerably simplified. Analytic results obtained in the small ρ limit and numerical results in the intermediate regime yield a similar picture; ϵ_n does not randomize for large n unless it randomizes at each site, and this feature cannot be circumvented by choosing large segments.

Assumptions about phase randomization are ubiquitous in theories of conduction in disordered systems.[1-5] The results presented here show that all phases are not necessarily sampled as the size of the system increases and that the neglect of this feature can lead to an incorrect result for the inverse localization length.

ACKNOWLEDGMENTS

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[9]There has recently been controversy as to whether R/T or $1/T$ should be used in Eq. (1) (Refs. 8 and 9). While this is of concern for finite chains, there is no difference in the thermodynamic limit $n \to \infty$ with which we are concerned in this report.

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[11]This was pointed out by Anderson *et al.* (Ref. 1). For long chains in the thermodynamic limit it is irrelevant whether $\ln(z_n)$, $\ln(1 + z_n)$, $\ln(1 + 2z_n)$, etc., as all become well-behaved extensive quantities that obey the central limit theorem.

[12]If the distribution of phases ϵ is random over 2π then

$$\alpha_2 = (1/2\pi) \int_0^{2\pi} d\epsilon \ln(1 + t + 2T^{1/2}\cos\epsilon) = 0 \quad .$$

Hence, for $\Delta y \gtrsim 3$ Å, $\alpha_2 \approx 0$ and the random-phase argument yields a reasonable approximation to the correct result.

[13]A more complete discussion of this limit will be presented elsewhere (Ref. 7).

[14]This is why reasonable results for α in the thermodynamic limit can be obtained by *ensemble* averaging over short chains (Ref. 4) with a length $l \gtrsim 100$. If the ensemble average is performed over a large number of chains, the result for α_1 is correct to within α_2/l. If $\alpha \ll |\alpha_2|$, this method would obviously fail unless l were very large (i.e., $l \gg |\alpha_1|/\alpha$).