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. 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.\textsuperscript{7}

The resistance of a one-dimensional wire may be written\textsuperscript{1,8–10}

\[ R = \frac{h}{e^2} \frac{T}{T}, \]  

(1)

where \( h/e^2 \approx 26 \text{ k} \Omega \), \( T \) 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 \( \delta \) function, or it may be done more arbitrarily for a less structured potential. As scattering takes place at each segment, \( T \) gets smaller and the resistance \( R \) 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.\textsuperscript{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 \( T_n \) that control the scattering of amplitudes at single segments:

\[ T_n = \begin{pmatrix} 1 + \rho_n \frac{1}{2} e^{-i \theta_n} & \rho_n^{1/2} e^{-i \phi_n} \\ \rho_n^{1/2} e^{i \phi_n} & (1 + \rho_n) \frac{1}{2} e^{i \phi_n} \end{pmatrix}, \quad (2) \]

where the scattering is characterized by an amplitude \( \rho_n \) and phases \( \theta_n \) and \( \phi_n \). A similar matrix \( \tilde{M}_n \) describing the scattering by \( n \) segments is given by

\[ \tilde{M}_n = \begin{pmatrix} (1 + z_n) \frac{1}{2} e^{-i \alpha_n} & z_n^{1/2} e^{-i \beta_n} \\ z_n^{1/2} e^{i \beta_n} & (1 + z_n) \frac{1}{2} e^{i \alpha_n} \end{pmatrix}, \quad (3) \]

This satisfies

\[ \tilde{M}_n = T_n \tilde{M}_{n-1}, \quad (4) \]

from which one obtains the following relations for \( z_n \):

\[ \ln(1 + z_n) = \ln(1 + z_{n-1}) + \ln(1 + \rho_n) \]

\[ + \ln(1 + \epsilon_n + 2 \epsilon_n \cos \alpha_n), \quad (5a) \]

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

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

where

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

and

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

FIG. 1. Sequence of equal strength \( \delta \) functions, with random spacings. The segments \( i-1, i, i+1 \), etc., are separated by dashed lines.
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 \( \alpha_n \) and \( \beta_n \) become independent random variables uniformly distributed over \( 2\pi \). 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 \( 2\pi \), they are not mutually independent. The phase of interest, when one addresses questions concerning phase averaging, is the quantity \( \epsilon_n \) 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 \( \delta \) functions of equal scattering strength \( \rho \). Initially, we divide the system into segments in the most natural way, with one \( \delta \) function per segment as shown in Fig. 1.

Iterating (5a) yields

\[
\ln(1 + z_n) = n \alpha = n (\alpha_1 + \alpha_2) ,
\]

where

\[
\alpha_1 = \frac{1}{n} \sum_{i=1}^{n} \ln(1 + \rho_i) ,
\]

and

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

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

\[
\alpha_1 = \ln(1 + \rho)
\]

and

\[
\alpha_2 = \int d\epsilon P(\epsilon) \ln(1 + t + 2t^{1/2}\cos \epsilon) ,
\]

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

\[
\epsilon_{n+1} = \theta_{n+1} + \theta_n - \phi_{n+1} + \phi_n .
\]

In this case, \( \epsilon_n \) 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 \( \epsilon_n \) as being reset at each scattering event.

In the present model,

\[
\epsilon_{n+1} = 2\tan^{-1}p^{1/2} - 2k_0y_n ,
\]

where \( k_0 \) is the wave vector of the electron and \( y_n \) is the separation between the \( n \) and \( n + 1 \) \( \delta \) functions. If these separations are distributed uniformly over the interval \( y_0 \pm \Delta y \), we have

\[
P(\epsilon) = \begin{cases} \frac{1}{2\Delta \epsilon} & \text{for } \epsilon + \Delta \epsilon \geq \epsilon \geq \epsilon - \Delta \epsilon \\ 0 & \text{otherwise} \end{cases} ,
\]

where

\[
\epsilon = 2(\tan^{-1}p^{1/2} - k_0y_0) \]

and

\[
\Delta \epsilon = 2k_0\Delta y .
\]

The integral for \( \alpha_2 \) [Eq. (9a) with \( t = 1 \)] can be obtained numerically. In Fig. 2, this is compared with

![FIG. 2. Variation of \( \alpha \) with system size for \( \delta \) functions of strength \( \rho = 105 \) and spacing uniformly distributed in the ranges \( 6 \pm 0.5 \text{ Å} (\Delta), 6 \pm 1 \text{ Å} (\Box), \) and \( 6 \pm 3 \text{ Å} (\bullet) \). All results are for a wave vector \( k_0 \) corresponding to an electron with a kinetic energy of 1 eV. The value of \( \alpha_1 \) is the same for all three cases and is shown in the upper curve. The three lower curves are the results for \( \alpha_2 \). For large \( n \), \( \alpha_2 \) 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 $\Delta y = 0.5 \text{Å}$, $\alpha_2$ is almost the negative of $\alpha_1$, 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 $P(\varepsilon)$ increases, $\alpha_2$ becomes less negative until, for $\Delta y = 3 \text{Å}$, it is almost zero. This is approaching the situation in which the phase randomizes at each site, since $\Delta \varepsilon = \pi$ corresponds to $\Delta y = 3.07 \text{Å}$.

Choosing larger segments containing more scatterers does not increase the tendency to phase average. For example, dividing the system of $n = mL$ scattering 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

$$\alpha_2^* = \frac{\alpha_2}{L}.$$  \hspace{1cm} (13)

This result is obtained after noting that the new phases $\varepsilon_i^*$, which enter a relation for $\alpha_1^*$ analogous to Eq. (9), depend only on the phases associated with the first $L$ function of segment $i$ and those of the last $L$ function of segment $i - 1$. Thus, in the strong scattering limit considered here, the distribution function $P(\varepsilon^*|\varepsilon) = P(\varepsilon)$ 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 $\alpha_1^*$ could be obtained by ensemble averaging over chains of length $l$. Clearly, as $l$ gets large, $\alpha_1^*$ tends to the correct value $\alpha$ of Eq. (7). However, this is not because $\varepsilon_i^*$ randomizes over $2\pi$, 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.

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 $\rho$ limit, where the analysis is considerably simplified. Analytic results obtained in the small $\rho$ limit and numerical results in the intermediate regime yield a similar picture; $\varepsilon^*$ 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. 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.

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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.
11. This was pointed out by Anderson et al., (Ref. 1). For long chains in the thermodynamic limit it is irrelevant whether one considers $\ln(z_n)$, $\ln(1 + z_n)$, $\ln(1 + 2z_n)$, etc., all become well-behaved extensive quantities that obey the central limit theorem.
12. If the distribution of phases $\varepsilon$ is random over $2\pi$ then

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

Hence, for $\Delta y > 3 \text{Å}$, $\alpha_2 = 0$ 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 $\alpha$ in the thermodynamic limit can be obtained by ensemble averaging over short chains (Ref. 4) with a length $l \geq 100$. If the ensemble average is performed over a large number of chains, the result for $\alpha_1$ is correct to within $\alpha_2/l$. If $\alpha << |\alpha_2|$, this method would obviously fail unless $l$ were very large (i.e., $l >> |\alpha_1/\alpha|$).