Calculation of localization length in disordered chains

A. Peres, M. Revzen, and A. Ron
Department of Physics, Technion-Israel Institute of Technology, Haifa, Israel
(Received 30 September 1981)

The resistance of a random one-dimensional chain is calculated in a novel way. The electronic wave function is represented by a random walk on a hyperboloid, for which the hyperbolic angle χ is an additive scaling parameter. The resistance is $(\pi\hbar/e^2)\sinh^2(\chi/2)$. For strong disorder, χ is normally distributed and explicit expressions can be obtained for the localization length and its variance, in good agreement with the results of various computer experiments.

The problem of transmission by one-dimensional chains is beset by the following difficulty: The resistance ρ (in units of $\pi\hbar/e^2 = 12906\ \Omega$) has a probability distribution with a very long tail. Its average $\langle\rho\rangle$ and its dispersion $\Delta\rho$ increase exponentially with the length L of the chain[1] but the dispersion increases *faster*. Recently, a "scaling" theory of localization[2] was proposed, with the aim of finding a better characterization of the "typical" ρ. It was shown[3] that $\ln(1+\rho)$ is an appropriate variable with a normal distribution, provided that some assumptions about randomness of phases are valid.

In this Communication, we show how it is possible to *calculate explicitly* the localization length (not only to evaluate it by Monte Carlo simulations). We construct a vector $\vec{R}$ (bilinear in the electronic wave function ψ) which current conservation constrains to lie on a hyperboloid (see Fig. 1). For a random potential, $\vec{R}$ executes a random walk and the hyperbolic angle χ [related to ρ by $\rho = \sinh^2(\chi/2)$] *obeys a simple equation* similar to that for Brownian motion, making χ a natural, easily calculable, additive scaling parameter. Moreover, if χ is normally distributed (this again depends on the potential randomness) the parameters of its distribution can be obtained algebraically and give the localization length and its variance.

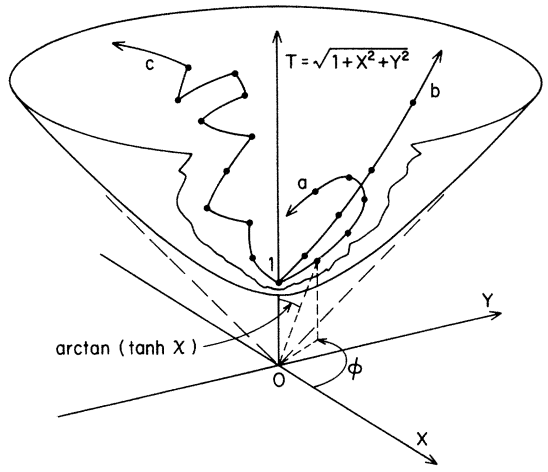

FIG. 1. Mapping of $\psi(x)$ into $\vec{R}(t)$. (a) In the conduction band of a periodic potential, the locus of $\vec{R}$ for consecutive sites is an ellipse. (b) In a forbidden band, it is a hyperbola and T grows exponentially. (c) For a random potential, the locus of $\vec{R}$ performs a random walk which almost always diverges exponentially.

Consider electrons of momentum $\hbar k$ impinging on a potential barrier $V(x)$. To solve the Schrödinger equation, it is convenient to start from the exit end of the barrier where $\psi = e^{ikx}$ and to progress in the negative x direction, till we finally obtain $\psi = Me^{ikx} + Ne^{-ikx}$ at the entrance. The transmission probability is $|M|^{-2}$ and the electric resistance is[3,4] $\rho = |M|^2 - 1 = |N|^2$. (The last equality follows from current conservation.)

It is convenient to introduce a nondimensional *length* parameter $t = -kx$ (the minus sign so that t *increases* as we proceed in the negative x direction) and to write $\dot{\psi} = d\psi/dt$. The Schrödinger equation becomes $-\ddot{\psi} + u\psi = \psi$, where $u = 2mV/\hbar^2k^2 = V/E$. We further define a "vector" $\vec{R} = (X, Y, T)$ by

$$X = (\bar{\psi}\psi - \dot{\bar{\psi}}\dot{\psi})/2 \ , \tag{1a}$$

$$Y = (\bar{\psi}\dot{\psi} + \dot{\bar{\psi}}\psi)/2 \ , \tag{1b}$$

$$T = (\bar{\psi}\psi + \dot{\bar{\psi}}\dot{\psi})/2 \ . \tag{1c}$$

Note that

$$T^2 - X^2 - Y^2 = [i(\bar{\psi}\dot{\psi} - \dot{\bar{\psi}}\psi)/2]^2 = 1 \ , \tag{2}$$

by current conservation, so that $\vec{R}$ lies on a unit hyperboloid. At the exit of the barrier, we have $\vec{R}_0 = (0, 0, 1)$ and at its entrance $T = |M|^2 + |N|^2$. Therefore the transmission probability is $2/(T+1)$ and the resistance is $\rho = (T-1)/2$.

The Schrödinger equation can now be written as $d\vec{R}/dt = \Omega\vec{R}$, where the "angular velocity" matrix Ω is

$$\Omega = \begin{pmatrix} 0 & 2-u & 0 \\ u-2 & 0 & u \\ 0 & u & 0 \end{pmatrix} \ . \tag{3}$$

It generates a pseudorotation (a rotation in a $2+1$ dimensional Minkowski space) $\vec{R}(t)=A(t)\vec{R}_0$, where the transfer matrix A belongs to the SO(2,1) group.[5,6]

If we have several consecutive barriers, we multiply the corresponding transfer matrices, in precisely the same order as the barriers. In particular, for n identical barriers, the transfer matrix is A^n and the resistance is $\rho=(T-1)/2=[(A^n)_{TT}-1]/2$. Now, the eigenvalues of a SO(2,1) matrix are 1 and either $e^{\pm i\theta}$ or $e^{\pm\lambda}$, depending on whether the invariant eigenvector (the one with eigenvalue 1) is timelike (Euclidean rotation) or spacelike (Lorentz boost). Therefore the eigenvalues of A^n are 1 and either $e^{\pm in\theta}$ (if $-1<\mathrm{Tr}A<3$ and we are in a conduction band) or $e^{\pm n\lambda}$ (in a forbidden band). The situation is described by Fig. 1.

If we have several types of sites randomly distributed, the locus of $\vec{R}$ performs a random walk on the hyperboloid, which almost always runs away exponentially, because all the points of the hyperboloid are equivalent (and thus equiprobable) under SO(2,1). This can be calculated as follows. First, suppose that we have just two kinds of sites, represented by a transfer matrix A occurring with probability a, and a matrix B, with probability $b=1-a$. If consecutive sites are uncorrelated, a chain such as $ABAAB\ldots$ has probability $abaab\ldots$. Then the average $\vec{R}$ after n sites simply is $\langle\vec{R}\rangle=(aA+bB)^n\vec{R}_0$, because expanding the parenthesis yields all the configurations, with each product of matrices multiplied by the corresponding probability. This result is readily generalized to more than two types of sites. For example, if there is a random parameter s such that the transfer matrix $A(s)$ occurs with probability $p(s)$, then, for n such transfer matrices, we have

$$\langle\vec{R}\rangle=\left(\int A(s)p(s)\,ds\right)^n\vec{R}_0\equiv\langle A\rangle^n\vec{R}_0 \quad . \tag{4}$$

Now, the average $\langle A\rangle$ of different SO(2,1) matrices is *not* a SO(2,1) matrix. It can be shown[6] that its largest eigenvalue Λ must be larger than 1 [except that $\Lambda=1$ if all the $A(s)$ are powers of the same matrix]. For large n, Eq. (4) will be dominated by Λ^n and $\langle\vec{R}\rangle$ will increase exponentially,[7] so that $\langle\rho\rangle\sim e^{\mu L}$.

Likewise, we can easily obtain $\langle\rho^m\rangle$, or $\langle T^m\rangle$, by considering tensor products of transfer matrices. For example, we may take as basis XY, XT, YT, $(X^2-Y^2)/2$, and $(3T^2-1)/2$ and construct new transfer matrices belonging to a five-dimensional representation of SO(2,1). All the preceding considerations apply without change, but with the $A(s)$ now being 5×5 matrices[8] and we get $\langle\rho^2\rangle\sim e^{\nu L}$. As $\langle\rho^2\rangle>\langle\rho\rangle^2$, we must have $\nu>2\mu$, i.e., the standard deviation increases faster than the mean.

It is therefore important[1,2] to find a better estimate for "typical" ρ. Since our problem is a random walk on the unit hyperboloid, let us parametrize it by $T=\cosh\chi$ and $X+iY=\sinh\chi e^{i\phi}$. The Schrödinger equation now becomes[9]

$$\dot{\chi}=u\sin\phi \quad , \tag{5}$$

and

$$\dot{\phi}=-2+u(1+\cos\phi\coth\chi) \quad . \tag{6}$$

These equations are remarkable. For *small* $\chi(\coth\chi\simeq\chi^{-1})$ we have $d(\chi\sin\phi)/dt\simeq u$, whence $\dot{\chi}\chi=u\chi\sin\phi\simeq u\int u\,dt$, or $\chi^2\simeq[\int_0^t u(t')\,dt']^2$. Thus on the average

$$4\langle\rho\rangle\simeq\langle\chi^2\rangle\simeq2\int_0^t\left[\int_0^{t-t'}\langle u(t')u(t'+\tau)\rangle\,d\tau\right]dt' \quad . \tag{7}$$

When t is much larger than the correlation length of u, the inner integral is independent of t' and $\langle\rho\rangle$ grows linearly with length.

On the other hand, for *large* $\chi(\coth\chi\simeq1)$ Eq. (6) is independent of χ and directly correlates ϕ to u, so that $\langle\dot{\chi}\rangle=\langle u\sin\phi\rangle$ tends to a positive constant[10] (unless u is periodic and $\langle\dot{\chi}\rangle=0$ in a conduction band). We thus write $\dot{\chi}=\langle\dot{\chi}\rangle+(u\sin\phi-\langle\dot{\chi}\rangle)$ so that the second term fluctuates around zero. This is a kind of Langevin equation and the corresponding Fokker-Planck equation is[11]

$$\dot{f}(\chi,t)\Delta t=-f'(\chi,t)\langle\Delta\chi\rangle+f''(\chi,t)\langle(\Delta\chi)^2\rangle/2-\cdots \quad , \tag{8}$$

where $f(\chi,t)\,d\chi$ is the number of representative points in $[\chi,\chi+d\chi]$ and f' means $\partial f/\partial\chi$. The ratio of consecutive terms in the right-hand side of (8) is of the order of t_{coh}, the coherence length of u, divided by the "mean free path" $t_{\mathrm{mfp}}\sim|u|^{-1}$. If we assume as usual[3] that this ratio is small, and if we take Δt such that $t_{\mathrm{coh}}\ll\Delta t\ll t_{\mathrm{mfp}}$, it is a good approximation to neglect $(\Delta t)^2$ and other higher terms in (8) which becomes

$$k\dot{f}=-\alpha f'+\beta f''/2 \quad , \tag{9}$$

where $\alpha=k\langle\Delta\chi\rangle/\Delta t=k\langle u\sin\phi\rangle$ is the inverse localization length, and

$$\beta=k\langle(\Delta\chi)^2\rangle/\Delta t=2k\int_0^\infty\langle\dot{\chi}(t')\dot{\chi}(t'+\tau)\rangle\,d\tau \quad .$$

(In the weak scattering limit, $|u|\ll1$, we get $\beta=2\alpha$ in agreement with Ref. 3.) The solution of (9), normalized to unity, is a Gaussian distribution

$$f=\exp[-(\chi-\alpha L)^2/2\beta L]/(2\pi\beta L)^{1/2} \quad , \tag{10}$$

where $L = t/k$ is the length of the chain.

The coefficients α and β are simply related to μ and ν which were defined earlier and are easily calculable (even though they have no apparent physical significance). Since $\rho \simeq e^{\chi}/4$, we have from (10)

$$\langle \rho^m \rangle = 4^{-m} \exp[(m\alpha + m^2\beta/2)L] \quad . \tag{11}$$

Comparing with $\langle \rho \rangle \sim e^{\mu L}$ and $\langle \rho^2 \rangle \sim e^{\nu L}$, we obtain $\mu = (\alpha + \beta/2)$ and $\nu = 2(\alpha + \beta)$, whence

$$\alpha = (4\mu - \nu)/2 \tag{12a}$$

and

$$\beta = \nu - 2\mu \quad . \tag{12b}$$

We have compared these predictions with the numerical experiments of Andereck and Abrahams,[12] who consider a potential $V(x) = \sum V_n \delta(x - n)$ with the V_n uniformly distributed between $-q/2$ and $q/2$. Between the delta functions, $u = 0$, and, therefore,

$$A = \exp\begin{pmatrix} 0 & 2k & 0 \\ -2k & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} = \begin{pmatrix} \cos 2k & \sin 2k & 0 \\ -\sin 2k & \cos 2k & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad . \tag{13}$$

At a delta function $u = v\delta(t)$, we have $\Delta\dot{\psi} = v\psi$ and Eqs. (1) give $\Delta\vec{R}$, corresponding to a transfer matrix

$$\begin{pmatrix} 1 - v^2/2 & -v & -v^2/2 \\ v & 1 & v \\ v^2/2 & v & 1 + v^2/2 \end{pmatrix} \quad . \tag{14}$$

[Note that $v_n = (2m/\hbar^2 k)\, V_n = 2V_n/k$ with the units of Ref. 12.] The complete transfer matrix for one site is the product of (13) and (14) and its average is easily obtained.[13] Next, we compute the direct product of each transfer matrix with itself and *then* take the average of these 9×9 matrices. The largest eigenvalues are obtained by standard methods.

For example, with $k = 1.4$ and $q = 1.0$, we obtained $\mu = 0.084\,927\,2$ and $\nu = 0.257\,568$, whence $\alpha = 0.041\,07$ and $\beta = 0.087\,71$, in excellent agreement with the numerical experiments of Ref. 12 [in their Fig. 2, $L = 700$ and we expect $\Delta\alpha = \sqrt{(\beta/L)} = 0.0112$]. Agreement was also achieved with other parameters and with numerical experiments on random models of our own.

However, *not* every model gave a Gaussian distribution for χ. For example, for an "alloy" (two equiprobable strongly scattering sites) we obtained $\alpha = \langle \chi \rangle / L = 0.20$, $\beta = \langle (\chi - \alpha L)^2 \rangle / L = 0.36$, $\mu = 0.335$, and $\nu = 0.810$, so that Eqs. (12) are not satisfied.[14] For the same alloy in a 1:15 ratio, the discrepancy was even larger: $\alpha = 0.060$, $\beta = 0.127$, $\mu = 0.088$, and $\nu = 0.402$. The distributions were markedly non-Gaussian, well beyond the statistical fluctuations of our numerical simulations. (The latter involved thousands of random chains, with up to 4096 sites.) Obviously, a single dichotomic random variable is not enough for the central limit theorem to be valid.

In summary, we have shown that the moments $\langle \rho^m \rangle$ can be obtained explicitly from the eigenvalues of averaged transfer matrices of order $(2m + 1)$. In the strong disorder limit $t_{\text{coh}} << t_{\text{mfp}}$, these $\langle \rho^m \rangle$ satisfy Eq. (11) and the scaling parameter χ is normally distributed. The localization length and its variance can then be obtained explicitly from (12). For weak disorder ($t_{\text{coh}} \gtrsim t_{\text{mfp}}$) χ is not normally distributed but still is additive, by Eq. (5).

This work was partly supported by the Israel Academy of Sciences, the U.S.-Israel Binational Science Foundation, the Gerard Swope Fund, and the Fund for encouragement of Research at Technion. This paper benefited from comments by P..W. Anderson during a visit of one of us (A.P.) at Bell Laboratories.

---

[1]R. Landauer, Philos. Mag. 21, 863 (1970).

[2]E. Abrahams, P. W. Anderson, D. C. Licciardello, and T. V. Ramakrishan, Phys. Rev. Lett. 42, 673 (1979).

[3]P. W. Anderson, D. J. Thouless, E. Abrahams, and D. S. Fisher, Phys. Rev. B 22, 3519 (1980).

[4]E. N. Economou and C. M. Soukoulis, Phys. Rev. Lett. 46, 618 (1981).

[5]A. O. Barut and C. Fronsdal, Proc. R. Soc. London Ser. A 287, 532 (1965). We shall henceforth freely borrow the Lorentz group terminology, although our problem is of course not relativistic.

[6]These 3×3 transfer matrices are locally isomorphic to the 2×2 matrices used by E. Abrahams and M. J. Stephens, J. Phys. C 13, L377 (1980). The latter belong to the SU(1,1) group. Detailed mathematical proofs are planned to be published separately.

[7]Explicitly, $\langle \rho \rangle \rightarrow \Lambda^n P_{TT}/2$, where P_{KL} is the projection matrix corresponding to the eigenvalue Λ.

[8]In practice, it is more expendient to take the 9×9 matrices of the direct product. The latter are reducible into 1, 3×3, and 5×5 matrices and the largest eigenvalue must come from the 5×5 part.

[9]χ is analogous to the "rapidity" which is the additive parameter for Lorentz boosts: J.-M. Lévy-Leblond, Am.

J. Phys. 48, 345 (1980).
[10]We can always assume $\chi > 0$ because Eqs. (5) and (6) are invariant under $\chi \rightarrow -\chi$ and $\phi \rightarrow \phi + \pi$.
[11]A. Isihara, *Statistical Physics* (Academic, New York, 1971), p. 206.
[12]B. S. Andereck and E. Abrahams, J. Phys. C 13, L383 (1980).
[13]This average is the same as Eq. (18) of Ref. 12, except for rearranging rows and columns.
[14]The values of μ and ν were obtained from the highest eigenvalues of $\langle A \rangle$ and those of α and β by numerical simulation of the resistance of a large number of random chains of different lengths.