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A relation between the density of states and range of localization for one dimensional random systems

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Abstract. The formula of Herbert and Jones relating the distribution of eigenvalues to the range of localization of an eigenstate for the Anderson model in one dimension is discussed. An explicit formula for the localization distance is given for Lloyd's model in one dimension. The formula, which is essentially a dispersion relation, is generalized to the case of the Schrödinger equation in one dimension.

Herbert and Jones (1971) have shown that, for a particular model of an electron moving on a one dimensional array of sites, the range of localization of the eigenstates can be related to the distribution of the energy levels. Their argument can be applied to any system whose eigenstates are described by equations of the form

$$\mathscr{E}_i a_i^\alpha - V_{i,i+1} a_{i+1}^\alpha - V_{i-1,i} a_{i-1}^\alpha = E_\alpha a_i^\alpha \tag{1}$$

where i runs from 1 to N, and the a_i^α are amplitudes (which can be taken to be real) for the eigenstate with eigenvalue E_α. Since the chain runs from 1 to N, $V_{0,1}$ and $V_{N,N+1}$ can be taken to be zero. This equation represents the wave equation for an electron in the tight binding approximation, but, with a suitable modification, it can represent a normal mode of a chain of coupled harmonic oscillators.

The result is based on a study of the Green function (resolvent) for this system, defined by

$$(E - \mathscr{E}_i) G_{ij}(E) + V_{i,i+1} G_{i+1\,j}(E) + V_{i-1,i} G_{i-1\,j}(E) = \delta_{ij} \tag{2}$$

The quantities $G_{ij}(E)$ are the elements of a matrix which is the inverse of the tridiagonal matrix $E\mathbf{I} - \mathbf{H}$, where $\mathbf{I}$ is the unit matrix and $\mathbf{H}$ is the hamiltonian of the system whose matrix elements are defined in equation 1. The G_{1N} element is particularly easy to find, since the cofactor of the matrix element $(E\mathbf{I} - \mathbf{H})_{1N}$ is

$$\prod_{i=1}^{N-1} V_{i,i+1}$$

and so we have

$$G_{1N}(E) = \prod_{i=1}^{N-1} V_{i,i+1} \Big/ \det(E\mathbf{I} - \mathbf{H})$$

$$= \prod_{i=1}^{N-1} V_{i,i+1} \Big/ \prod_{\alpha=1}^{N} (E - E_\alpha) \tag{3}$$

There are two interesting interpretations of this result. Firstly, since G_{1N} has a pole of residue $a_1^\beta a_N^\beta$ at $E = E_\beta$, the value of $a_1^\beta a_N^\beta$ can be found from equation 3. Taking the logarithm we get

$$\ln |a_1^\beta a_N^\beta| = \sum_{i=1}^{N-1} \ln |V_{i,i+1}| - \sum_{\alpha \neq \beta} \ln |E_\beta - E_\alpha| \qquad (4)$$

The $(N-1)$th root of the product of the amplitudes at the two ends of the chain for a normalized eigenstate with eigenvalue E_β is therefore equal to the geometric mean of the matrix elements $V_{i,i+1}$ divided by the geometric mean of the differences between E_β and the other eigenvalues of the system. This can tell us whether or not the eigenstate is localized, since the $(N-1)$th root of this product of the amplitudes tends to unity as N tends to infinity for a nonlocalized eigenstate, whereas it tends to a constant less than unity, which we denote by $\exp(-\lambda_\beta)$, for a localized eigenstate; we expect that, if the eigenfunction has its maximum value at the site i, a_1 and a_N should be of order $\exp\{-\lambda_\beta(i-1)\}$ and $\exp\{-\lambda_\beta(N-i)\}$ respectively. It cannot be greater than unity. The quantity λ_β^{-1} is the fall-off distance for this eigenstate, and, from equation 4, it is given by

$$\lambda_\beta = \lim_{N \to \infty} \left\{ (N-1)^{-1} \sum_{\alpha \neq \beta} \ln |E_\beta - E_\alpha| - (N-1)^{-1} \sum_{i=1}^{N-1} \ln |V_{i,i+1}| \right\} \qquad (5)$$

For a long statistically homogeneous chain the sum over states can be replaced by an integral over the density of states, since no individual state contributes significantly to the average, unless two states happen to have an exponentially small spacing. Writing V for the geometric mean of the off-diagonal matrix elements and $\rho(x)$ for the density of states we get

$$\lambda_\beta = \int \rho(x) \ln |E_\beta - x| \, dx - \ln |V| \qquad (6)$$

A second interpretation of the Green function gives the same result. One can ask what would be the amplitude $a_N(E)$ if the set of equations (1), with the exception of the final one with $i = N$, were solved with E_α replaced by an arbitrary energy E, and with the initial condition $a_1 = 1$; the recurrence relations could be solved successively to get this amplitude. The answer is

$$a_N(E) = \frac{G_{NN}(E)}{G_{1N}(E)} \qquad (7)$$

Unless E is within a distance of order $\exp(-N)$ of an eigenvalue, in which case G_{NN} is very large, we get

$$\lambda_N(E) \equiv (N-1)^{-1} \ln a_N(E) \simeq \int \rho(x) \ln |E - x| \, dx - \ln |V| \qquad (8)$$

and so $a_N(E)$ is exponentially large unless the right side of this equation is zero. Comparison of equations 8 and 6 shows that the same exponent occurs in both cases.

For a regular chain the eigenstates are standing waves, and so $\lambda(E)$ must be zero within the band. This implies that the real part of the Green function must be zero within the band, since differentiation of the right side with respect to E gives the real part of the Green function.

This formula allows the localization distance to be determined if the energy spectrum

is known. For example, in the case of the Cauchy distribution, for which the Green function was determined by Lloyd (1969), an explicit algebraic expression for λ can be obtained. A reasonably compact expression of the result is

$$\cosh \lambda = (4V)^{-1} \left[\{(2V + E)^2 + \gamma^2\}^{1/2} + \{(2V - E)^2 + \gamma^2\}^{1/2} \right] \qquad (9)$$

from which it can immediately be seen that, when the width γ of the Cauchy distribution is nonzero, the value of λ is nonzero.

A relation similar to equations 6 and 8 can be obtained also for one dimensional systems satisfying the Schrödinger equation

$$-\frac{\hbar^2}{2m} \psi'' + V(x)\psi = E\psi \qquad (10)$$

in the interval from 0 to X, with the boundary condition that $\psi(x)$ vanishes for $x = 0$ and for $x = X$. For an arbitrary value of E we write $\phi_L(x,E)$ for the solution of the equation that vanishes and has derivative equal to unity at $x = 0$, and $\phi_R(x,E)$ for the solution that vanishes at $x = X$ and has derivative -1 there. The Green function can be written as

$$G(x,x';E) \begin{cases} = -\dfrac{\phi_R(x)\phi_L(x')}{(\hbar^2/2m)\phi_L(X)} & x > x' \\[4mm] = -\dfrac{\phi_L(x)\phi_R(x')}{(\hbar^2/2m)\phi_L(X)} & x < x' \end{cases} \qquad (11)$$

since $\phi_L(x) = \phi_R(0)$ is equal to the wronskian of the two solutions. It is convenient also to introduce another Green function

$$G_L(x,x;E) \begin{cases} = \dfrac{-\phi_R(x)\phi_L(x') + \phi_L(x)\phi_R(x')}{(\hbar^2/2m)\phi_L(X)} & x > x' \\[4mm] = 0 & x < x' \end{cases} \qquad (12)$$

which provides a solution of an inhomogeneous equation that vanishes and has zero derivative at $x = 0$. Differentiation with respect to E of the equation for ϕ_L gives

$$\left(E + \frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} - V(x) \right) \frac{\partial \phi_L}{\partial E} = -\phi_L \qquad (13)$$

which has the solution

$$\frac{\partial \phi_L(x)}{\partial E} = -\int G_L(x,x';E)\phi_L(x') \, \mathrm{d}x' \qquad (14)$$

In the special case $x = X$ we get

$$\begin{aligned} \frac{\partial \phi_L(X)}{\partial E} &= -\frac{2m}{\hbar^2} \int_0^X \phi_R(x')\phi_L(x') \, \mathrm{d}x' \\[3mm] &= \phi_L(X) \int_0^X G(x',x';E) \, \mathrm{d}x' \\[3mm] &= \phi_L(X) \sum_\alpha (E - E_\alpha)^{-1} \end{aligned} \qquad (15)$$

This equation cannot immediately be integrated to give a result of the form of equation 8, because the density of eigenvalues E_α is too great at high energies—it falls off only as $E_\alpha^{-1/2}$. We can divide equation 15 by $\phi_L(X)$ and subtract from it the corresponding equation in the case of zero potential, and then integrate so that we get

$$\ln|\phi_L(X)/\phi_L^0(X)| = \int [\rho(z) - \rho_0(z)] \ln|E - z| \, dz \tag{16}$$

where ϕ_L^0 is the solution of the Schrödinger equation for a free particle and ρ_0 is the corresponding density of states. This is the formula equivalent to equation 8. An equation equivalent to equation 6 can be obtained by subtracting $\ln|E - E_\beta|$ from both sides of equation 16 and taking the limit $E = E_\beta$. On the left side this gives $\ln\{(\partial\phi_L/\partial E)/\phi_L^0\}$, which can be evaluated by use of the first line of equation 15. Since E_β is an eigenvalue, ϕ_L and ϕ_R are both proportional to the normalized eigenfunction ϕ_β, with constants of proportionality determined by the derivatives at the end points. The result is

$$-\ln\left\{\frac{\hbar^2}{2m}|\phi_\beta'(0)\phi_\beta'(X)\phi_L^0(X)|\right\} = \int \{\rho(z) - \delta(z - E_\beta) - \rho_0(z)\} \ln|E_\beta - z| \, dz \tag{17}$$

A formula such as equation 16 or 17 can be used to find an explicit formula for the localization length for a system whose energy spectrum is known, such as the 'gaussian white noise' system which was solved by Frisch and Lloyd (1960). As was shown by Halperin (1965), the integrated density of states for this system is given by

$$N(E) = X\pi^{-2}[\{Ai(-2Em/\hbar^2)\}^2 + \{Bi(-2Em/\hbar)\}^2]^{-1} \tag{18}$$

Equation 16 can be integrated by parts to give

$$\ln\left|\frac{\phi_L(X)}{\phi_L^0(X)}\right| = \int \frac{N(z) - N_0(z)}{E - z} \, dz \tag{19}$$

and substitution of equation 18 in this gives, for large positive E

$$\lambda \sim (EX)^{-1} \int \{N(z) - N_0(z)\} \, dz = \frac{\hbar^2}{8mE} \tag{20}$$

where λ is the reciprocal of the localization distance. This formula was evaluated by using the properties of the modulus and phase of the Airy function given by Abramowitz and Stegun (1964). Several more terms of this expansion of λ in powers of E^{-1} have been given by Borland (1963).

Again it should be noted that in the energy bands of any regular chain the right sides of equations 16, 17 and 19 divided by X should vanish in the limit of infinite X, and this implies that the density of states satisfies a dispersion relation, and that the real part of the Green function is zero in the energy band.

A simple explanation can be given of the existence of these dispersion relations connecting the exponential fall-off rate with the density of states. Since the number of states with energy less than E can be found by counting the number of nodes of the wavefunction with energy E, the wavenumber $k(E)$ gives the integrated density of states per unit length. It is possible to define a complex wavenumber, analytic except on the real axis, whose real part gives the integrated density of states and whose imaginary

part gives the fall-off rate. One possible definition for this wavenumber for a statistically homogeneous system is

$$k(E) = \lim_{x \to \infty} \frac{i}{x} \ln \phi_{\mathrm{L}}(x) \tag{21}$$

where ϕ_{L} is the wavefunction which vanishes and whose derivative is unity at the origin. This function is an analytic function of E, proportional to $E^{1/2}$ for large E for a continuous system, and therefore satisfies the dispersion relations given in this paper.

Some very similar results have been obtained by Hirota and Ishii (1971).

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