

Density of states of one-dimensional random potentials

by Paul Erdős

Following an introduction to the early history of the theories of the density of electronic states in one-dimensional structures, pioneered, among others, by R. Landauer and J. C. Helland, a particular model, that of a multistep random potential, is discussed. It is shown that Kolmogorov-type equations can be obtained for the probability distribution of the phase of the wave function, and, by solving these equations, the density of states may be calculated. An analogy with the classical rotator in a random force field is worked out, and helps in visualizing the results.

1. Introduction

In historical perspective, it now seems quite natural that once the calculation of the electronic density of states in periodic potentials was mastered, theoreticians turned their attention to the density of electronic states in nonperiodic, disordered structures.

To cope with the complexity of nature, simple model systems were studied. Among these, a one-dimensional array of potentials localized at random positions was the first one investigated. This was done by H. M. James and A. S. Ginzburg [1] in 1953. The complications of this first

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analytical study revealed the need to apply numerical methods to obtain concrete and *transparent* results.

In 1954 R. Landauer and J. C. Helland [2] published for the first time their results for the density of states in random potentials obtained by an ingenious numerical simulation, thereby helping to lay the groundwork for the understanding of nonperiodic structures.

It is not my purpose here to describe the further development of this subject: This has been done in books [3] and reviews [4]. Rather, I would like to present a small contribution to the theory which is interesting from the point of view of the mathematical techniques used and also because it points out a relationship between the problem at hand and a problem of classical mechanics, that of the randomly driven rotator. In view of this relationship, I use the notation t instead of x for the coordinate, since the spatial coordinate of the random potential corresponds to the time coordinate of the rotator.

When a particle of mass m , restricted to move in one dimension in the interval $0 \leq t \leq L$, is subject to a potential $U(t)$, the Schrödinger equation for its wave function is

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dt^2} + [U(t) - E] \psi = 0. \quad (1)$$

According to Sturm's oscillation theorem, a real solution $\psi_m(t)$ of (1), obeying $\psi_m(0) = \psi_m(L) = 0$ with energy-eigenvalue E_m , has m zeros in the interval $(0, L)$, provided the eigenvalues are subscripted in increasing order. The integrated density of states $\mathcal{N}(E)$ is defined as the number of eigenvalues between $-\infty$ and E . Therefore, if

$$E_m < E < E_{m+1},$$

$$\mathcal{N}(E) = m. \quad (2)$$

It follows that if a real solution $\psi(t; E)$ of (1) for a given E is found, the number of its zeros within $(0, L)$ equals the integrated density of states $\mathcal{N}(E)$.

This fact provides the most powerful method to determine the average density of states for random potentials in one dimension, as was demonstrated by Frisch and Lloyd [5] and by Borland [6].

2. The phase evolution

It is practical to introduce

$$V(t) = 2m\hbar^{-2}U(t) \quad k = \hbar^{-1}(2mE)^{1/2}, \quad (3)$$

and a new function, $\Theta(t)$, henceforth referred to as the *phase*, defined by

$$\tan\Theta(t) = (d\psi/dt)/k\psi. \quad (4)$$

Elimination of $\psi(t)$ from (1) yields a first-order nonlinear differential equation for the phase

$$\dot{\Theta} = -k[1 - \beta(t)\cos^2\Theta(t)], \quad (5)$$

with

$$\dot{\Theta} = d\Theta/dt \quad \text{and} \quad \beta(t) = V(t)/k^2. \quad (6)$$

Equation (5) shows how the phase of the wave function varies along the t -axis. In particular, if the potential is zero, the phase varies linearly, as expected of a wave function of the form $\psi(t) = \cos kt$. If the potential is a nonzero constant, Equation (5) is easily solved, and this solution is used later in Equation (10). For a general potential, Equation (5) cannot be explicitly solved, but as we shall see, the knowledge of the differential equation (5) suffices for the calculation of the average density of states of an ensemble of random potentials.

To find the number of zeros of $\psi(t; E)$ note that if for some t_0 : $\psi = 0$, $d\psi/dt \neq 0$, it follows from Equation (4) that the phase is

$$\theta(t_0) = \frac{\pi}{2} + n\pi \quad n = \text{integer}. \quad (7)$$

Therefore, the average (over a long interval L) density of states per unit length is equal to the average number of times $\Theta(t)$ passes through $\pi/2 \pmod{\pi}$ per unit length. Reflection shows that instead of observing a single random potential, we may observe a large ensemble of N random potentials created by some probabilistic law. If we then follow the evolution along the t -axis of the phase of the wave function with energy E in each of these potentials, the average density of states $\mathcal{N}(E)$ will be equal to the average number—divided by N —of wave functions whose phases pass through $\pi/2 \pmod{\pi}$ in any unit interval of the t -axis. (This assertion of ergodicity can be rigorously proven in the case here considered.)

3. The random potential

We choose a one-dimensional random potential which simulates a potential produced by a random distribution of different ionic species as follows: If in the interval $\Delta t = t_i - t_{i-1}$ the potential has the value V_n , then in the interval $\Delta t = t_{i+1} - t_i$ it may have the value V_m , and the probability of this change is given by a fixed number p_{nm} . In particular, we set $V_n - V_{n-1} = V$ for all n , and suppose that the stochastic matrix (p_{nm}) is such that it admits only the transitions $V_n \rightarrow V_n$ and $V_n \rightarrow V_{n\pm 1}$, hence (p_{nm}) is tridiagonal. Thus we have the relations

$$p_{n,n+1} + p_{n,n-1} + p_{n,n} = 1. \quad (8)$$

We further assume that there is a highest and lowest value of the potential, corresponding to $n = M$ and $n = -M$. The potential thus changes according to a Markov process which in probability theory is called a "one-dimensional random walk with reflecting barriers," the barriers being V_M and V_{-M} .

This random potential excludes arbitrarily large jumps of $V(t)$ between arbitrarily close points. Such jumps are a very unrealistic feature of white-noise-type potentials treated in the literature.

Note that for $L \gg \Delta t$ the Markov process becomes stationary. This and Equation (8) imply the detailed balance relation between the concentration c_n of segments of length Δt with potential V_n (i.e., ionic species of type n) and the stochastic matrix elements:

$$c_{n+1} = \frac{p_{n,n+1}}{p_{n+1,n}} c_n \quad n = -M, \dots, M-1,$$

where c_{-M} is determined by

$$\sum_{n=-M}^M c_n = 1.$$

4. The probability distribution of the phase

For the calculation of the average state density $\mathcal{N}(E)$ we need to know the average relative number of those wave functions of the statistical ensemble of random potentials the phase of which passes through $\pi/2 \pmod{\pi}$ per unit t -interval. This relative number is also equal to the probability that the phase of an individual wave function passes through $\pi/2 \pmod{\pi}$ in unit interval. To find the latter, we introduce the *conditional probability* $P_m(t, \Theta)d\Theta$, which gives the probability of finding, at the point t , the phase Θ in the interval $(\Theta, \Theta + d\Theta)$, provided that at the same point the potential has the value V_m .

The conditional probability $P_m(t, \Theta)d\Theta$ obeys a differential equation which is now derived. Suppose that during (t_{i-1}, t_i) the potential is V_m , and at t_{i-1} the phase was in the interval $(\Theta_{i-1}, \Theta_{i-1} + d\Theta_{i-1}^{(m)})$. Then the probability that at time t_i the phase is in the interval $(\Theta_i, \Theta_i + d\Theta_i^{(m)})$ is given by

$$P_m(t_i, \Theta_i)d\Theta_i^{(m)} = \sum_{n=-M}^M P_n(t_{i-1}, \Theta_{i-1})p_{nm}d\Theta_{i-1}^{(m)}. \quad (9)$$

Here, p_{nm} is the stochastic matrix, which expresses the probability that at time t_{i-1} the potential changed from V_n to V_m . The phases $\Theta_i^{(m)}$ and $\Theta_{i-1}^{(m)}$ are related by the evolution equation (5). From Equation (5) one can derive a relation between the infinitesimal phase intervals,

$$d\Theta_{i-1}^{(m)} = \frac{1 - V_m k^{-2} \cos^2 \Theta_{i-1}}{1 - V_m k^{-2} \cos^2 \Theta_i} d\Theta_i^{(m)}, \quad (10)$$

and this relation permits the elimination of the infinitesimals $d\Theta_i^{(m)}$, $d\Theta_{i-1}^{(m)}$ from Equation (9). The evolution equation allows the elimination of Θ_{i-1} from Equation (9) as well. We are interested in the stationary probability distributions

$$P_m(\theta) = P_m(t \rightarrow \infty, \theta), \quad (11)$$

which (as can be rigorously proven) will develop if $t \gg \Delta t$. From Equation (9) we obtain after some algebra the Kolmogorov-type difference equations

$$P_m(\theta) = \sum_{n=-M}^M P_n(\theta - \Delta\theta^{(m)}) \cdot \frac{1 - V_m k^{-2} \cos^2(\theta - \Delta\theta^{(m)})}{1 - V_m k^{-2} \cos^2 \theta}, \quad (12)$$

with

$$\Delta\theta^{(m)} = \theta - \tan^{-1} \{a_m^{-1} \tan[a_m^{-1} k \Delta t + \tan^{-1}(a_m \tan \theta)]\} \quad (13)$$

and

$$a_m = (1 - V_m/k^2)^{-1/2}. \quad (14)$$

Once the functions $P_m(\theta)$ [which depend on the energy through the parameter k ; see Equations (12), (14)] are known, the density of states can be calculated. In fact, the probability per unit t -interval of the passage of the phase through any angle θ is given by the product of the probability density of that phase angle with the speed of phase change, summed over all possible values of the potential. Since the speed $|\dot{\theta}|$ of phase change equals k for all values of the potential if $\theta = \pi/2$ [see Equation (5)], it follows that

$$\mathcal{H}(E) = k \sum_{m=-M}^M P_m\left(\frac{\pi}{2}\right). \quad (15)$$

5. Differential equations for the stationary probability densities

To simplify the solution of Equation (12), we go from difference to differential equations by means of the transition $\Delta t \rightarrow 0$. Since p_{nm} is the probability that at the end of the interval Δt the potential changes from V_n to V_m , we have to require that p_{nm} scale linearly with Δt as follows:

$$p_{nm} = p_{nm}^{\circ} \Delta t, \quad (16)$$

and

$$p_{nn} = 1 - p_{nn}^{\circ} \Delta t, \quad (17)$$

where p_{nm}° are constants. According to Section 3, these constants must obey the relations

$$p_{-M-1,-M}^{\circ} = p_{-M,-M-1}^{\circ} = p_{M,M+1}^{\circ} = p_{M+1,M}^{\circ} = 0 \quad (18)$$

and

$$p_{m,m+1}^{\circ} - p_{mm}^{\circ} + p_{m,m-1}^{\circ} = 0 \quad m = -M, \dots, M. \quad (19)$$

In the limit $\Delta t \rightarrow 0$ we obtain the set of coupled differential equations

$$P_{m-1}(\theta) p_{m-1,m}^{\circ} - P_m(\theta) p_{mm}^{\circ} + P_{m+1}(\theta) p_{m+1,m}^{\circ} + \frac{d}{d\theta} [(1 - V_m k^{-2} \cos^2 \theta) P_m(\theta)] = 0$$

$$m = -M, \dots, M, \quad (20)$$

with the boundary conditions

$$P_m(\pi) = P_m(0) \quad m = -M, \dots, M, \quad (21)$$

and normalization

$$\sum_{m=-M}^M \int_0^{\pi} P_m(\theta) d\theta = 1. \quad (22)$$

It is easily seen from Equation (19) that the following expression is a "constant of motion":

$$\sum_{m=-M}^M P_m(\theta) (1 - V_m k^{-2} \cos^2 \theta) = c. \quad (23)$$

From Equation (15), it follows that

$$c = k^{-1} \mathcal{H}(E). \quad (24)$$

Therefore, the calculation of the density of states for a given energy E requires the knowledge of the functions $P_m(\theta)$, to be obtained by solving the differential equations (19). These functions depend, through the parameters $V_m k^{-2}$, on the energy $E = k^2/2m$. The set of $2M + 1$ differential equations, (19), can always be reduced to a single differential equation of order $2M$.

6. Two-step random potential

As an example [7], we consider a potential which may take the values 0 and v , i.e., $M = 1/2$. The stochastic matrix p_{nm}° depends now on two parameters, q_0 and q_1 , defined by

$$q_0 = p_{-1/2,-1/2}^{\circ} = p_{-1/2,1/2}^{\circ}, \quad q_1 = p_{1/2,1/2}^{\circ} = p_{1/2,-1/2}^{\circ}. \quad (25)$$

This potential may be thought of as being produced by two sorts of ions with concentrations

$$c_0 = \frac{q_1}{q_0 + q_1}, \quad c_1 = \frac{q_0}{q_0 + q_1}, \quad (26)$$

respectively, c_0 being the concentration of the atoms producing zero potential. The probability $\pi_i(t)$ per unit length of finding a segment of length l of constant potential is

$$\pi_i(t) = q_i \exp(-q_i t) \quad i = 0, 1. \quad (27)$$

Giving q_0 and q_1 specifies more than just the concentration of the two species: It also specifies the correlations between adjacent ions.

The solution of Equation (20) is given by

$$P_{1/2}(\theta) = -cq_0k^{-1} \left[\int_0^\theta \exp[-f(\varphi)]d\varphi + d \right] \cdot \exp f(\theta) [1 - (1 - a^{-2})\cos^2\theta]^{-1}, \quad (28)$$

with the abbreviations

$$f(\varphi) = k^{-1}[q_0\varphi + aq_1 \tan^{-1}(a \tan \varphi)], \quad (29)$$

$$d = [\exp k^{-1}\pi(-q_0 - q_1a) - 1]^{-1} \int_0^\pi \exp[-f(\varphi)]d\varphi \quad (30)$$

and

$$a = (1 - vk^{-2})^{-1/2}. \quad (31)$$

From Equation (23) it follows that

$$P_{-1/2}(\theta) = c - (1 - vk^{-2}\cos^2\theta)P_{1/2}(\theta), \quad (32)$$

and from Equations (22)–(24) the density of states is

$$\mathcal{N}(E) = k\pi^{-1} \left[1 + vk^{-2} \int_0^\pi P_{1/2}(\theta)\cos^2\theta d\theta \right]^{-1}. \quad (33)$$

To restrict the discussion, let us consider two limiting cases only, $k^2 \gg v$ and $k^2 \ll v$.

When $k^2 \gg v$, a simple power series expansion in vk^{-2} yields

$$\mathcal{N}(E) \cong \frac{\sqrt{2mE}}{\pi\hbar} \left(1 - \frac{1}{4} \frac{v\hbar^2}{mE} c_1 \right), \quad (34)$$

where c_1 is the concentration of ions producing the potential v . This formula shows the change in the free-electron density of states $N_0 = k\pi^{-1}$ due to a weak random potential.

When $k^2 \ll v$,

$$\mathcal{N}(E) = \frac{q_0q_1}{q_0 + q_1} \exp\left(-\frac{q_0\hbar\pi}{\sqrt{2mE}}\right). \quad (35)$$

This result may be understood by a simple physical argument, due to Luttinger and Sy [8]: When the particle energy is very much smaller than the height of the potential v , the particle may be thought of as being localized in the wells of zero potential which exist between the subsequent segments of potential v . The lengths of these wells are statistically distributed according to the probability law given by Equation (27). According to quantum mechanics, the energy levels of a particle in a deep well of length l are given by

$$E_j(l) = (A_j/l)^2, \quad A^2 = \hbar^2\pi^2/2m, \quad j = \text{integer}. \quad (36)$$

The average number of wells of length l per unit length is, from Equations (26) and (27), $n_0(l) = \pi_0(l)/(q_0 + q_1)$. Hence, the average number of energy levels below E per unit length is obtained by averaging with respect to the distribution

$n_0(l)$. Thus, using the step function $\theta(x) = 1$ for $x > 0$, $\theta(x) = 0$ for $x < 0$:

$$\begin{aligned} \mathcal{N}(E) &\cong \int_0^\infty \sum_{j=1}^\infty \theta[E - E_j(l)]n_0(l)dl \\ &= \frac{q_0q_1}{q_0 + q_1} \sum_{j=1}^\infty \exp(-Aq_0jE^{-1/2}) \\ &= \frac{q_0q_1}{q_0 + q_1} [\exp(Aq_0E^{-1/2}) - 1]^{-1}. \end{aligned} \quad (37)$$

For small E we obtain the exponentially decreasing density of states given in Equation (35).

The evaluation of the density of states for the multistep potential, obtained by numerical integration of Equation (20) will be published elsewhere.

7. The rotator model

We may interpret $\Theta(t)$ as the angle between the positive x -axis and the radius vector of a point moving around the unit circle [9]. The evolution equation [see Equation (5)]

$$\dot{\Theta}_n(t) = -k + V_n k^{-1} \cos^2 \Theta_n(t) \quad k = \text{constant}, \quad (38)$$

shows, that except for $V_n = 0$, the angular velocity varies with time. One may regard the rotator as being subject to a random force. For the multistep potential V_n , the functions $P_n(t; \Theta)$ represent the probability density (per unit angle) that if the potential has the value V_n at time t , the rotator is found at the angle Θ . If one thinks of many points starting their rotation simultaneously at $\Theta(t=0) = 0$, the motion of each point being governed by another realization of the random potential $V(t)$, the function $P_n(\Theta)$ may be thought of as the stationary density distribution around the unit circle of those points which at the angle Θ happen to be subject to the particular value V_n of the potential ($n = -M, \dots, M$). The stationary distribution develops after a sufficiently long time. Since the total number of circling points is conserved, it follows that the total number of points traversing at any given angle has to be a constant of the motion, and is given by

$$\sum_{n=-M}^M P_n(\Theta) \dot{\Theta}_n = c, \quad (39)$$

in accordance with Equation (23). Since $\dot{\Theta} = -k$ for $\Theta = \pi/2, 3\pi/2$, at these particular angles all points have the same angular velocity, hence the simple expression, Equation (15).

This equation may be understood with reference to the rotator model as follows: Proceeding from left to right every "time" the wave function crosses the t -axis, the corresponding rotator passes through $\Theta = \pi/2$ (since $\tan \Theta = \dot{\psi}/k\psi$). Since the average number of zeros per unit length is proportional to the density of states, the latter becomes proportional to the average number of rotators crossing $\Theta = \pi/2$, i.e., to the flux c of rotators.

As a consequence of the Schrödinger equation, the wave function does not cross the t -axis along an interval where the potential is higher than the kinetic energy of the particle. In these intervals the phase approaches a limiting angle, which for the two-step potential is

$$\theta_c = \cos^{-1}(kv^{-1/2}). \quad (40)$$

The rotator corresponding to this wave function slows down, but never reaches this limiting angle. Eventually, at some further point of the axis the potential changes to a lower value, and the rotator moves on. I do not treat this case in detail here, except to remark that the calculation of $\mathcal{N}(E)$ proceeds the same way as indicated above.

The density distribution of the rotators around the circle is by no means uniform. Even the first approximation in terms of vk^{-2} leads, for the two-step potential treated in Section 6, to

$$P_{1/2}(\theta) \cong \mathcal{N}(E)k^{-1}c_1(1 - vk^{-2}c_0)(1 - vk^{-2}\cos^2\theta)^{-1}. \quad (41)$$

This result is in accord with the intuitive idea that the density of the rotators is less at those angles where they are moving faster.

An interesting case which can also be treated by the method here described is the one where the random potential consists of an array of delta-functions. Integrating Equation (5) between a point preceding and a point following a δ -potential shows that θ changes discontinuously across this type of potential. This corresponds to a jump of rotator by a finite angle (the "kicked rotator"). One has to take into account the fact that the flux of rotators consists of two components: the flux due to the uniform motion with speed k between potentials, and the flux due to the jumps. In this case, there is only one probability density distribution function $P(\theta)$ instead of the $2M + 1$ functions discussed above, so that $\mathcal{N}(E)$ is easy to find.

This paper is dedicated to Dr. Rolf Landauer on the occasion of his sixtieth birthday.

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9. B. U. Felderhof, "Transmission and Reflection of Waves in a One-Dimensional Disordered Array," *J. Stat. Phys.* **43**, 267-279 (1986) uses another interesting analogy with a harmonic oscillator, introduced by James and Ginzburg [1].

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