

Singular behavior of tight-binding chains with off-diagonal disorder

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We prove that the density of states of the one-dimensional tight-binding Hamiltonian with off-diagonal disorder is singular at the center of the band, $E = 0$, for every probability distribution of the hopping matrix elements V . The asymptotic form is $\rho(E) \simeq 2\sigma^2/|E(\ln E^2)|^3$, with $\sigma^2 \equiv \langle (\ln V^2)^2 \rangle - \langle \ln V^2 \rangle^2$. The localization length goes to infinity as $L(E) \simeq 2|\ln E^2|/\sigma^2$. We also give a procedure to handle the problem numerically near the singularity, and we present some sample calculations.

I. INTRODUCTION

In a recent paper, Theodorou and Cohen¹ studied the density of states and localization length of the following one-dimensional tight-binding Hamiltonian with off-diagonal disorder:

$$H = \sum_i V_i (|i\rangle\langle i+1| + |i+1\rangle\langle i|), \quad (1)$$

with the V_i -independent random variables having the same probability density $p(V)$.

For a generalized Poisson distribution

$$P_n(V) = 2 \frac{n^n}{(n-1)!} \left| \frac{V}{V_0} \right|^{2n-1} e^{-n(V/V_0)^2} \frac{1}{V_0}, \quad (2)$$

the problem can be reduced to a case solved exactly by Dyson² in his study of the normal modes of a disordered chain of oscillators. One obtains in this way an exact density of states for the Hamiltonian (1), which has the remarkable property of being singular at $E = 0$, the center of the band. The asymptotic form is

$$\rho(E) = 2\left(\frac{1}{8}\pi^2 - t_{n-1}\right)/|E(\ln E^2)^3|, \quad (3)$$

$$t_n \equiv \sum_{i=1}^n i^{-2}. \quad (4)$$

Theodorou and Cohen suggested that this singularity might be a general feature of Hamiltonian (1), not a consequence of the particular form (2) of $p(V)$. This idea is supported by the numerical work of Weissmann and Cohan³ using a square distribution for V : although the immediate neighborhood of $E = 0$ was not explored because of convergence problems, their results indicate a peak at the origin.

The purpose of this paper is to investigate the exact density of states of Hamiltonian (1) near $E = 0$ for an arbitrary distribution of the V 's. We show that the density of states behaves asymptotically as

$$\rho(E) \simeq 2\sigma^2/|E(\ln E^2)^3|, \quad (5)$$

with σ^2 the variance of $\ln V^2$. Thus, our result confirms the kind of singularity of $\rho(E)$ near $E = 0$ found by Theodorou and Cohen, and furthermore, gives the physical significance of the coefficient.

It should be noted that the existence of a singularity in $\rho(E)$ is far from being intuitively obvious. Consider, for example, a periodic chain in which all V 's are equal to V_0 [this of course gives a finite $\rho(E = 0)$]. Suppose next that a fraction c of the V 's is changed to $V_1 > V_0$ to form the binary chain with

$$p(V) = c\delta(V - V_1) + (1 - c)\delta(V - V_0).$$

On this basis of simple arguments like perturbation theory one would expect that all states be pushed away from the origin as the difference $V_1 - V_0$ is switched on. This can only decrease $\rho(E)$ at $E = 0$, never lead to a singularity. Our result (5) shows that such simple arguments break down near $E = 0$.

We also study the localization length,⁴ and show that it diverges as

$$L(E) \simeq 2|\ln E^2|/\sigma^2. \quad (6)$$

A similar result is established in Ref. 1 [for the particular $p(V)$ used there] through the Thouless equation⁵ which relates $L(E)$ directly to $\rho(E)$. We present here an alternative derivation of (6) based on the consideration of the self-energy as a stochastic process.

In Sec. II, we show that the problem of the spectrum of Hamiltonian (1) near $E = 0$ can be reduced to the study of a certain diffusion process. Section III deals with this process in more detail, and we establish there the asymptotic form (5) of $\rho(E)$. Section IV contains our discussion of the localization length $L(E)$. In Sec. V, we show how to handle numerically the integral equation arising in the exact solution of the problem in the vicinity of the singularity. We also present sample calculations to verify and illustrate our analytic results. Our concluding remarks are presented in Sec. VI.

II. DIFFUSION EQUATION FOR THE SELF-ENERGY

We look for solutions of the Schrödinger equation $H|\psi\rangle = E|\psi\rangle$, with

$$|\psi\rangle = \sum_i c_i |i\rangle. \quad (7)$$

Using the explicit form (1) of the Hamiltonian one immediately obtains for the amplitudes c_i the equations

$$c_{i-1}V_{i-1} + c_{i+1}V_i = Ec_i. \quad (8)$$

It is convenient to introduce the "self-energies"⁶

$$\Delta_i \equiv c_{i-1}V_{i-1}/c_i, \quad (9)$$

so that (8) takes the form

$$\Delta_{i+1} = V_i^2/(E - \Delta_i). \quad (10)$$

It can be shown⁷ that the integrated density of states per site

$$N(E) = \int_{-\infty}^E \rho(E') dE'$$

equals the fraction of positive terms in the sequence $\{\Delta_i\}$ defined by (10). The recurrence relations (10) take a particularly simple form for $E=0$; in this case the signs of $\{\Delta_i\}$ follow the pattern $+-+--+\dots$, and therefore $N(E=0) = 0.5$. We shall concentrate our attention for the time being on the subsequence of positive Δ_i 's, and we assume that these correspond to even i 's:

$$\Delta_{2i} > 0, \quad \Delta_{2i+1} < 0. \quad (11)$$

Iterating (10) we find that

$$\Delta_{2i} = (V_{2i-1}/V_{2i-2})^2 \Delta_{2i-2} \quad (12)$$

or

$$u_{2i} \equiv \ln \Delta_{2i} = \ln(V_{2i-1}/V_{2i-2})^2 + u_{2i-2}. \quad (13)$$

Equation (13) shows that u_{2i} executes a *random walk*. The average displacement at each step is

$$\langle u_{2i} - u_{2i-2} \rangle = \langle \ln(V_{2i-1}/V_{2i-2})^2 \rangle = 0, \quad (14)$$

and the average square displacement is

$$\langle (u_{2i} - u_{2i-2})^2 \rangle = \langle [\ln(V_{2i-1}/V_{2i-2})^2]^2 \rangle = 2\sigma^2. \quad (15)$$

We have introduced here the variance of $\ln V^2$,

$$\sigma^2 = \langle (\ln V^2)^2 \rangle - \langle \ln V^2 \rangle^2. \quad (16)$$

It is well known that such random walks can be studied as diffusion processes.⁸ Let $\phi(n, u)$ be the probability density for u_n , then making the usual approximation of treating n as a continuous variable ϕ satisfies the diffusion equation

$$2 \frac{\partial \phi(n, u)}{\partial n} = \sigma^2 \frac{\partial^2 \phi(n, u)}{\partial u^2}. \quad (17)$$

[In our case it should be kept in mind that the solution of (17) is relevant only for $n = 2i$, the even integers.]

All this is strictly valid for $E=0$. Equation (17) has no well behaved steady-state solution; u_{2i} eventually drifts to $\pm\infty$.

Next let us consider how the above changes when we take a small but nonzero E . Since the density of states is an even function of E , we assume without loss of generality that $E > 0$. Again using (10) we write

$$\Delta_{2i} = \left(\frac{V_{2i-1}}{V_{2i-2}} \right)^2 \Delta_{2i-1} \frac{1 - E/\Delta_{2i-2}}{1 + (E\Delta_{2i-2} - E^2)/V_{2i-2}^2}. \quad (18)$$

It is clear that as long as

$$E \ll \Delta_{2i-2} \ll V_{2i-2}^2/E, \quad (19)$$

the "correction terms" in (18) (exponentially small with respect to u) are irrelevant and we recapture (12). Thus, assuming again that $\Delta_0 > 0$, $u_{2i} \equiv \ln \Delta_{2i}$ executes a random walk as before, as long as it remains in the interval

$$\ln E \ll u \ll \ln(\tilde{V}^2/E). \quad (20)$$

Here we have indicated by \tilde{V} some typical V , its exact value will turn out to be irrelevant for the discussion that follows.

Our next goal is to see what happens to the random walk picture when u approaches the endpoints of the interval (20). For $\Delta_{2i-2} \approx \tilde{V}^2/E$, the effect of the denominator in (18) is to reduce Δ_{2i} , thus preventing it from growing too large. This situation can be approximately described by considering a random walk with a reflecting barrier at $u_{\max} = \ln(\tilde{V}^2/E)$.

At the low- Δ end, $\Delta \approx E$, the situation is somewhat more complicated. The term $1 - E/\Delta_{2i-2}$, which becomes relevant for $\Delta_{2i-2} \approx E$, favors a steady decrease in the sequence Δ_{2i} . Moreover, as soon as Δ_{2i} has reached a value slightly below E , the following things happen: (a) $\Delta_{2i+1} = V_{2i}^2/(E - \Delta_{2i}) > 0$. There is a break in the natural sign sequence since there appear two successive plus signs: $+-+--+\dots$; (b) from the point $++$ onwards the role of the even and odd sublattices is interchanged, it is now the Δ_{2i+1} which are positive; (c) the whole diffusion process starts again with the positive Δ 's, now on odd sites, of order \tilde{V}^2/E .

We conclude that the evolution of the Δ 's derived from (10) can be regarded as repetitions of the following cycle: the positive Δ 's start from a value of order \tilde{V}^2/E , diffuse down to the neighborhood of E (diffusion upwards is impossible because of the reflecting barrier of \tilde{V}^2/E), and are absorbed at E . After this, the next cycle starts.

Each time a cycle is completed, a ++ pair destroys the "natural" sign sequence + - + - + - ...

It is easily verified that it takes two of the above cycles to change a (-) of the natural sequence into a (+). Therefore calling \bar{n} the average number of sites required to complete one cycle, we have the following relation for the total number of states below E , $N(E)$:

$$N(E) - N(0) = N(E) - \frac{1}{2} = 1/2\bar{n}. \quad (21)$$

The determination of \bar{n} is the subject of Sec. III.

III. DENSITY OF STATES

To determine the quantity \bar{n} appearing in (21) we can use the diffusion equation (17) supplemented by the boundary conditions

$$\left. \frac{\partial \phi}{\partial u} \right|_{u=u_{\max}} = 0, \quad (22a)$$

$$\phi|_{u=u_{\min}} = 0, \quad (22b)$$

corresponding to a reflecting barrier of $u_{\max} = \ln(\bar{V}^2/E)$ and an absorbing barrier of $u_{\min} = \ln E$. We take the initial condition

$$\phi(u, 0) = \delta(u - u_{\max} - 0^+), \quad (23)$$

corresponding to a cycle started at $n = 0$. Let

$$P(n) = \int_{u_{\min}}^{u_{\max}} \phi(u, n) du \quad (24)$$

be the probability that u remains between u_{\min} and u_{\max} (i.e., has not been absorbed) after n steps. Clearly

$$\bar{n} = \int_0^{\infty} n \left(-\frac{dP}{dn} \right) dn = \int_0^{\infty} P(n) dn, \quad (25)$$

so that the calculation of \bar{n} reduces to solving (17) with the appropriate boundary conditions. This can be done by standard methods; the result is

$$\begin{aligned} \phi(u, n) = & \sum_{m=0}^{\infty} \frac{2}{\Delta u} (-1)^m \sin \left(\left(m + \frac{1}{2} \right) (u - u_{\min}) \frac{\pi}{\Delta u} \right) \\ & \times \exp \left(-\frac{\sigma^2}{2} \left(m + \frac{1}{2} \right)^2 \frac{\pi^2}{\Delta u^2} n \right), \end{aligned} \quad (26)$$

where Δu stands for $u_{\max} - u_{\min} = \ln(\bar{V}^2/E^2)$. Carrying out the integrations (24) and (25) we get

$$\bar{n} = \sum_{m=0}^{\infty} \frac{4(-1)^m (\Delta u)^2}{\sigma^2 (m + \frac{1}{2})^2 \pi^3} = \frac{(\Delta u)^2}{\sigma^2}. \quad (27)$$

To compute the above result we have used the equality⁹

$$\sum_{m=1}^{\infty} \frac{(-1)^{m+1}}{(2m-1)^3} = \frac{\pi^3}{32}.$$

Finally, using (21), we find for the integrated density of states

$$N(E) \simeq \frac{1}{2} \left(1 + \frac{\sigma^2}{[\ln(\bar{V}/E)^2]^2} \right). \quad (28)$$

Differentiating, we get

$$\rho(E) = \frac{dN}{dE} \simeq \frac{2\sigma^2}{E} \frac{1}{[\ln(\bar{V}/E)^2]^3} \simeq \frac{2\sigma^2}{E |\ln E^2|^3}. \quad (29)$$

The typical value \bar{V} simply adds a finite constant to the diverging denominator, and is therefore irrelevant as anticipated earlier.

For the generalized Poisson distribution (2) one finds by straightforward computation that $\sigma^2 = \frac{1}{6} \pi^2 - t_{m-1}$, so that our equation (29) reproduces the solution of Ref. 1.

IV. LOCALIZATION LENGTH

It was shown by Borland¹⁰ that the eigenstates of a one-dimensional Hamiltonian like (1) are always localized: each eigenfunction ψ_{α} is appreciable over some finite region (centered, say, at x_{α}) and decays exponentially $|\psi_{\alpha}| \sim \exp[-|x - x_{\alpha}|/L(E)]$ at great distances. Borland also showed that if one picks an arbitrary energy E and an arbitrary boundary condition at one end of a linear chain, the integration of the Schrödinger equation yields a function $\psi_E(x)$ which, with probability 1, grows exponentially $|\psi(x)| \sim \exp[x/L(E)]$ as one moves along the chain. Thus, to find the localization length $L(E)$, it is sufficient in our case to study the rate of growth of the $\{c_i\}$ generated by (8).

One technical detail must, however, be cleared up in order to compute $L(E)$ for $E \simeq 0$. Suppose we start at site 0 with the boundary condition $c_0 = 0$. It is then easy to see from (8) that for small even i , $c_i \simeq 0$. Therefore, near the starting point, the envelope of the wave function is determined by the amplitudes on odd sites. As we move along the chain, however, the situation is reversed. Near the end of the first cycle (in the sense defined in Sec. II) the amplitude has shifted from odd to even sites; it is now the c_{2i+1} which determine the envelope of the wave function. In order not to bother with this distinction and periodic interchange of the odd and even sublattices, and since all homogeneous forms of degree 1 in c grow at the same rate, we shall study the geometric mean $g_i \equiv |c_i c_{i+1}|^{1/2}$ of the amplitudes on two successive sites. This quantity increases more steadily, with the same average rate of growth of the $|c_i|$.

In our case, the behavior of $\{g_i\}$ is best studied by considering one of the cycles of Sec. II. Suppose a cycle starts at $i = 0$ and ends at $i = 2n$; this means $\Delta_0 \simeq \bar{V}^2/E$; $\Delta_1 \simeq -E$; $\Delta_2 \simeq \bar{V}^2/E$; ..., $\Delta_{2n} \simeq E$; $\Delta_{2n+1} \simeq \bar{V}^2/E$; $\Delta_{2n+2} \simeq -E$; ... It is more or less straightforward, using (9) and (10), to obtain

$$\ln\left(\frac{g_{2n+1}}{g_0}\right) = \frac{1}{2} \ln\left|\frac{V_0}{\Delta_1}\right| + \sum_{i=1}^n \left(\ln V_{2i-1} - \ln V_{2i} + \ln\left|1 - \frac{E}{\Delta_{2i}}\right|\right) + \frac{1}{2} \ln\left|\frac{V_{2n+1}}{\Delta_{2n}}\right|. \quad (30)$$

The first and last terms in the right-hand side of (30) are both of order $\frac{1}{2} \ln V/E$, and together make a contribution $\sim \ln(\tilde{V}/E)$. The sum

$$\sum_{i=1}^n (\ln V_{2i-1} - \ln V_{2i})$$

is zero on the average since any particular bond has equal probability of being the "even" or "odd" sublattice within the cycle to which it belongs.

The term

$$\sum_i \ln\left|1 - \frac{E}{\Delta_{2i}}\right|$$

gives at most a contribution of order 1 arising from the last Δ 's within the cycle. Thus, keeping only the leading contribution, the increase in $\ln(g)$ per cycle is

$$\ln(g_{2n+1}/g_0) \simeq \ln(\tilde{V}/E). \quad (31)$$

The inverse of the localization length is, by definition, the average increase of the wave function per site, thus

$$\frac{1}{L(E)} \simeq \frac{\ln(\tilde{V}/E)}{\bar{n}} \simeq \frac{\sigma^2 \ln(1/E)}{(\ln E^2)^2} = \frac{\sigma^2}{2|\ln E^2|}, \quad (32)$$

$$L(E) = 2|\ln E^2|/\sigma^2. \quad (33)$$

Again our result reproduces that of Theodorou and Cohen,¹ and gives physical insight for the parameter.

V. NUMERICAL TREATMENT NEAR THE SINGULARITY

We first explored the singularity in the density of states of Hamiltonian (1) near E equal zero by Monte Carlo techniques, i.e., the method of negative counts^{7,11} for the integrated density of states, or by direct method for the density of states,¹² computed by

$$\rho(E) = \left\langle \frac{1}{2} \left| \frac{E - \Delta}{E - \Delta'} \right|^{1/2} p(|(E - \Delta)(E - \Delta')|^{1/2}) \right\rangle. \quad (34)$$

However, a sufficient accuracy by these methods would require a prohibitive amount of computation; therefore, we solve numerically the integral equation for the probability density function $f(\Delta; E)$ [where Δ is defined in (12)] and for the associated distribution function

$$F(\Delta; E) = \int_{-\infty}^{\Delta} f(x; E) dx, \quad (35)$$

$f(\Delta, E) d\Delta$ is, for a given energy E , the probability that Δ belongs to the interval $(\Delta, \Delta + d\Delta)$; f is positive, normed to 1. F is nondecreasing, bounded by zero and one.

These functions satisfy the following integral equations³ (we omit the parameter E for brevity):

$$f(\Delta) = \frac{1}{\Delta^2} \int V^2 p(V) f\left(E - \frac{V^2}{\Delta}\right) dV \quad (36)$$

or, for F :

$$F(\Delta) = \int p(V) F\left(E - \frac{V^2}{\Delta}\right) dV - F(E) + \Theta(\Delta). \quad (37)$$

$p(V)$ is the probability density of the hopping integral V . $\Theta(\Delta)$ is the step function, valued to 1 for positive Δ , and 0 otherwise. These equations have been solved numerically by iteration in Ref. 3 for almost the whole spectrum; but the convergence of the procedure gets worse as $|E|$ approaches zero, so that the center of the band was inaccessible to this calculation. Our purpose is to study this central band region exactly.

Let us discuss the choice of a starting value $f_0(\Delta)$ and $F_0(\Delta)$.

We showed in Sec. II that if $E < \Delta < \tilde{V}^2/E$ the probability density function $\phi(u)$ of the random variable $u = \ln \Delta$ verifies the diffusion equation (17) with the following boundary conditions: (i) for the steady state, $\partial \phi / \partial n = 0$; and (ii) (22b), $\phi(\ln E) = 0$. Therefore, ϕ is the monomial

$$\phi(u) = A(u - \ln E). \quad (38)$$

Returning back to the variable Δ , one obtains from (38),

$$f_0(\Delta) = A \frac{\ln(\Delta/E)}{\Delta}, \quad E < \Delta < \tilde{V}^2/E. \quad (39a)$$

The extension to negative Δ , obtained from the integral equation (36) is

$$f_0(\Delta) = A \frac{\ln(\tilde{V}^2/E|\Delta|)}{|\Delta|}, \quad -\tilde{V}^2/E < \Delta < -E. \quad (39b)$$

We assume

$$f_0(\Delta) = 0 \quad \text{if } |\Delta| \in [E, \tilde{V}^2/E]. \quad (39c)$$

The constant A , determined from the normalization condition, is

$$A = [\ln(\tilde{V}^2/E)^2]^{-1}. \quad (39d)$$

By (35) the corresponding function $F_0(\Delta)$ is

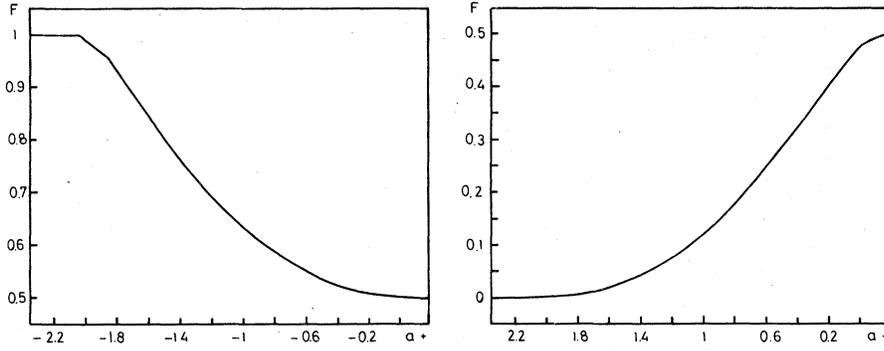


FIG. 1. For the energy $E = \sqrt{10} \times 10^{-6}$. $F(\Delta, E)$ curves vs

$$a^\pm = \frac{\ln(\pm\Delta) - \ln E}{\ln E - \ln \alpha}$$

The plus sign corresponds to positive Δ , the minus to negative one. The curve does not differ from F_0 on this scale, and the representation $F(a)$ is quite universal for the whole energy range explored $\sqrt{10} \times 10^{-6} \leq E \leq 10^{-1}$.

$$F_0(\Delta) = \begin{cases} 0, & \Delta \leq -\tilde{V}^2/E; \\ \frac{1}{2} \left(\frac{\ln(E|\Delta|/\tilde{V}^2)}{\ln(E^2/\tilde{V}^2)} \right)^2, & -\frac{V^2}{E} \leq \Delta < -E; \\ \frac{1}{2}, & -E \leq \Delta < E; \\ \frac{1}{2} \left[1 + \left(\frac{\ln(\Delta/E)}{\ln(E^2/\tilde{V}^2)} \right)^2 \right], & E \leq \Delta < \tilde{V}^2/E; \\ 1, & \Delta \geq \tilde{V}^2/E. \end{cases} \quad (40)$$

The singular behavior of f_0 appears clearly on formula (39). We solve the integral equation (37) for the difference $\chi(\Delta) = F(\Delta) - F_0(\Delta)$ which measures the precision of our approximate asymptotic solution to the exact one, by iteration $\chi(\Delta)$ satisfies

$$\chi(\Delta) = \int p(V)\chi\left(E - \frac{V^2}{\Delta}\right) dV - \chi(E) + Q(\Delta), \quad (41)$$

where

$$Q(\Delta) = \int p(V)F_0\left(E - \frac{V^2}{\Delta}\right) dV - F_0(E) + \Theta(\Delta) - F_0(\Delta) \quad (42)$$

is computed once for the mesh Δ used. The initial value of χ is zero. As probability density function $p(V)$ for the hopping integral V , we chose a Bernoulli law; this is one of the most critical distribution functions from the numerical point of view [the kernel of integral equation (36) is not bounded].

As mesh for Δ , we use an equidistant logarithmic scale, i.e.,

$$a = (\ln|\Delta| - \ln E) / (\ln E - \ln \alpha),$$

where $\alpha = \langle V^2 \rangle^{1/2}$. Such a choice is adequate, since a low value of $|\Delta| \ll E$ generates a high value at next iteration $\sim 1/|\Delta|$. The values of $F(\Delta)$ are linearly interpolated from this mesh.

As convergence criterion we required that

$$\frac{1}{N_j} \sum_j [\chi^{(i)}(\Delta_j) - \chi^{(i-1)}(\Delta_j)]^2 < 10^{-10}.$$

N_j is the number of Δ points; i denotes the iteration rank. The uniform convergence (over the whole interval) is achieved in about 100 iterations.

We present in Fig. 1 a set of $F(\Delta, E)$ which coincide quite well with F_0 , and in Fig. 2 a typical

$$\chi(\Delta) = F(\Delta) - F_0(\Delta).$$

It can also be shown that the distribution function $F(\Delta, E)$ for the particular value $\Delta = E$ is the total number of states below E , $N(E)$ (7).

In Table I we report the values of $F(E, E) - 0.5$, and the asymptotic value $N(E) - N(0)$. The agreement is good. It can be noted that the correct value for $F(E)$ is obtained at the first iteration of (41) and (42). These results are obtained for the set of parameters given in Table II.

VI. CONCLUDING REMARKS

The tendency of the eigenstates to pile up at the center of the band seems to be an interference effect, related to the fact that the lattice constant is exactly $\frac{1}{4}$ of a wavelength at $E = 0$. This fact has already led to puzzling consequences in other situations.¹³

To get some physical insight into the origin of the singularity, it is instructive to consider a dis-

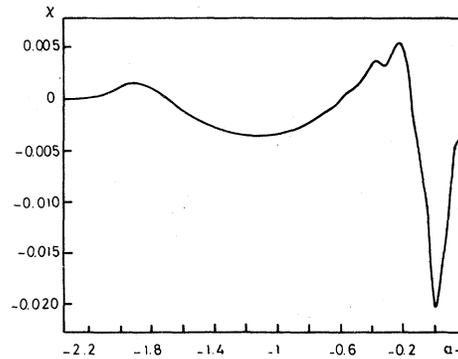


FIG. 2. Correction $\chi = F - F_0$ in the negative Δ range and energy $E = \sqrt{10} \times 10^{-6}$; for definition of a see Fig. 1.

TABLE I. Comparison of the asymptotic and the computed value of the total number of states between E and 0.

Energy	$N(E) - 0.5$	$F(E, E) - 0.5$
0.1×10^{-4}	0.001 14	0.001 24
$\sqrt{10} \times 10^{-5}$	0.001 41	0.001 55
0.1×10^{-3}	0.001 78	0.001 99
$\sqrt{10} \times 10^{-4}$	0.002 32	0.002 67
0.1×10^{-2}	0.003 16	0.003 63
$\sqrt{10} \times 10^{-3}$	0.004 55	0.005 33
0.1×10^{-1}	0.007 11	0.008 67
$\sqrt{10} \times 10^{-2}$	0.012 64	0.014 65

ordered segment imbedded in an otherwise perfect chain. Suppose V_i random for $-2N < i < 2N - 1$, and constant outside. In other words, take $2N$ random V 's to each side of the origin, and perfect order outside. It is an easy matter to calculate the local density of states of the central site $\rho_0(E)$ if $E = 0$; we simply sketch the procedure. The pure crystal self-energy has some imaginary value $\Delta_{\text{pure crystal}} = -i\delta$. Using the recurrence relation (10) to compute the self-energies inside the disordered region and expressing the Green's function in terms of Δ 's one finds

$$G_{00}(E=0) = i/\delta(\pi^+ + \pi^-), \quad (43)$$

where

$$\pi^+ = \prod_{i=0}^n \left(\frac{V_{2i+1}}{V_{2i}} \right)^2, \quad (44)$$

and a similar relation gives π^- in terms of the V 's to the left of the origin. Since the local density of states is $\rho_0(E) = (1/\pi) \text{Im}G_{00}(E+i0)$, we get

$$\rho_0(E=0) = \rho_{\text{pure crystal}} 2/(\pi^+ + \pi^-) \quad (45)$$

The π 's are random variables which, according to (44), have the property that π and $1/\pi$ are identically distributed. To see the implication of this, let us make the most drastic approximation which conserves this symmetry: suppose each π takes

TABLE II. Bernoulli distribution for the hopping integral V .

i	1	2
V_i^2	0.2	1.8
p_i	$\frac{1}{2}$	$\frac{1}{2}$

only two values, a and $1/a$, with probabilities $\frac{1}{2}$ and $\frac{1}{2}$. The resulting density of states has the average value

$$\begin{aligned} \langle \rho_0 \rangle &= \frac{\rho_{\text{pure crystal}}}{4} \left(\frac{2}{a+a} + \frac{2}{1/a+1/a} + \frac{4}{a+1/a} \right) \\ &= \rho_{\text{pure crystal}} \frac{1}{2} \left[\frac{1}{2} \left(a + \frac{1}{a} \right) + \frac{1}{\frac{1}{2}(a+1/a)} \right] \\ &\geq \rho_{\text{pure crystal}} \end{aligned} \quad (46)$$

(The inequality follows from $\xi + 1/\xi \geq 2$, $\xi > 0$.) Only in the ordered case $a = 1$ is $\langle \rho_0 \rangle = \rho_{\text{pure crystal}}$; any spread in π causes $\langle \rho_0 \rangle$ to increase. Physically, what happens is the following: certain configurations will be repulsive for $E = 0$ states, push these states out, and depress ρ_0 by a certain factor; others will be attractive, pull states in, and enhance ρ_0 by a similar factor. Since $\frac{1}{2}(\xi + \xi^{-1}) > 1$, the next result of this is to increase $\langle \rho_0 \rangle$.

Always assuming the $a, 1/a$ behavior, let us now choose an a that reasonably reproduces the spread in π . Since $\ln \pi$ is a random walk, the natural choice is $a \approx \exp[\sigma(2N)^{1/2}]$. Inserting this in (45) and assuming N large, we find

$$\langle \rho_0 \rangle \approx \rho_{\text{pure crystal}} \frac{e^{\sigma(2N)^{1/2}}}{4}, \quad (47)$$

which diverges for $N \rightarrow \infty$, this is the reason for the singularity in $g(E)$. Random walks have strange recurrence properties¹⁴: each point is visited infinitely many times for dimensionality ≤ 2 , but the average number of steps between successive visits is infinite. For this reason we expect states near $E = 0$ to exhibit huge fluctuations around the asymptotic behavior $|\psi(x)| \sim \exp[-|x|/L(E)]$.

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