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Localization and Spectral Singularities in Random Chains

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This paper reports consideration of the Hamiltonian for tight binding in one dimension with off-diagonal disorder of two forms, corresponding to Dyson's types I and II. The density of states and localization function at the center of the band are found by perturbation theory and a scaling argument. The distinction between the two types of disorder is clearly drawn, and new singularities in the Green's function pertinent to the problem of random classical diffusion are predicted.

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The dynamic properties of random chains have been of interest since Dyson[1] calculated the density of states for a model of phonons in a disordered chain. More recently there has been extensive work on the mathematically related problem of classical diffusion in a random chain.[2] Of particular interest is the fact that disorder leads to singularities in the density of states different from those of homogeneous systems. Dyson found such singularities for a soluble class of models with a form of disorder he dubbed "type I." Quite different singularities have recently been found by Alexander *et al.*[2] for a form of disorder (type II) superficially similar. Hitherto the reasons for such different behaviors have remained relatively obscure. I shall show how the singular behaviors found follow quite simply once the localization properties of the excitations are considered. In one dimension localization and spectral densities are closely related: Thouless[3] showed that the localization function $\lambda(E)$ and the integrated density of states are essentially real and imaginary parts of the same complex K vector. As well as illuminating the mechanism by which the singularities appear, such considerations lead to prediction of singular properties that have been neglected in the diffusion problem and are needed for a full understanding of the approach to asymptotic behavior.

I consider the eigenstates of the Hamiltonian for tight binding in one dimension with off diagonal-disorder,

$$H = -\sum_m J_m(|m+1\rangle\langle m| + |m\rangle\langle m+1|), \quad (1)$$

with two cases corresponding to Dyson's types I and II: Case I, "uncorrelated off-diagonal disorder." Each J_m is an independent identically distributed random variable. Case II, "spin wave symmetry." The J_m's come in identical pairs $J_{2n} = J_{2n+1}$. The J_{2n} are independent. The eigenstates satisfy

$$-Ea_m = J_m a_{m+1} + J_{m-1} a_{m-1}. \quad (2)$$

The significance of case II is clear if we eliminate odd sites in (2), finding for $b_n = a_{2n}(-1)^n$

$$(E^2 - J_{2n}^2 - J_{2(n-1)}^2) b_n = -J_{2n}^2 b_{n+1} - J_{2(n-1)}^2 b_{n-1}. \quad (3)$$

This is the equation for the amplitude of a single magnon in a random linear Heisenberg ferromagnet. Within the random-phase approximation these operators determine all the low-lying excitations. If we write $S = E^2$, $W_n = J_{2n}^2$, (3) can be rewritten

$$-s b_n = W_n(b_{n+1} - b_n) + W_{n-1}(b_{n-1} - b_n). \quad (4)$$

Equation (4) is the Laplace transform of the master equation for hopping over random barriers.[2] The equivalence of the model (1) to Dyson's model as well as to the random spin-$\frac{1}{2}$ XY model has been thoroughly discussed.[4]

It is useful to reformulate equations of the form (2) in terms of transfer matrices.[5] A theorem due to Ossedelec for the limiting properties of the resulting product of random matrices leads to the most rigorous statements of the scaling theory of localization.[6-8] For case I we have

$$\begin{pmatrix} a_{2n+2} \\ a_{2n+1} \end{pmatrix} = T_{2n} \begin{pmatrix} a_{2n} \\ a_{2n-1} \end{pmatrix}, \quad (5)$$

where

$$T_{2n}(E) = \begin{pmatrix} 1 - E^2/J_{2n}^2 & -J_{2n-1}E/J_{2n}^2 \\ EJ_{2n+1}/J_{2n}^2 & J_{2n+1}J_{2n-1}/J_{2n}^2 \end{pmatrix} \begin{pmatrix} -J_{2n}/J_{2n+1} & 0 \\ 0 & -J_{2n}/J_{2n+1} \end{pmatrix}; \quad (6)$$

for case II,

$$U_{2n}(E) = (-1) \begin{pmatrix} 1 - E^2/J_{2n}^2 & -EJ_{2(n-1)}/J_{2n} \\ E/J_{2n} & J_{2(n-1)}/J_{2n} \end{pmatrix}. \quad (7)$$

Let $K_{2N}(E)$ be the logarithm of the eigenvalue of the product $T_{2N}T_{2N-2} \cdots T_4 T_2$ (or the corresponding product of U's) whose modulus is greater than or equal to 1. The phase of the imaginary part must be determined by counting the number of sign changes of the sequence of amplitudes generated by the matrices.[9] The rate of exponential decrease of eigenfunctions $\lambda(E)$ and the integrated density of states are given by

$$\lambda(E) = \lim_{N\to\infty} \frac{1}{2N} \mathrm{Re}(K_{2n}(E)), \quad (8)$$

$$I(E) = \frac{1}{2\pi} \lim_{N\to\infty} \frac{1}{2N} \mathrm{Im}(K_{2n}(E)). \quad (9)$$

Notice that $E = 0$ is a special point: The matrices all commute and the product is

$$\prod_{j=0}^{N-1} T_{2(N-j)}(E=0) = \begin{pmatrix} \pi_N & 0 \\ 0 & \pi_N^{-1} \end{pmatrix}, \quad (10)$$

where

$$\pi_N = \prod_{n=1}^{N} \left(\frac{-J_{2n}}{J_{2n+1}} \right). \quad (11)$$

For large N the central limit theorem implies that $K_{2N}(E)$ is given by[10]

$$K_{2N}(E=0) = (2N)^{1/2} \sigma_J \alpha + i\pi N, \quad (12)$$

where σ_J is the variance of the random variable $\ln J$, and α is distributed normally with mean zero and variance unity. Thus at $E = 0$, λ vanishes and the corresponding eigenstate should not be exponentially localized. From (12) it should decay as $e^{-\sigma J\sqrt{L}}$.[10] For case II, in contrast,

$$\prod_j U_{2(N-j)} = (-1)^N \begin{pmatrix} 1 & 0 \\ 0 & J_0/J_{2N} \end{pmatrix} . \tag{13}$$

In this case λ also vanishes but the solutions of the boundary-value problem do not increase at all. The eigenstate should be extended. We see, then, the first clear difference between the two types of disorder: In both cases the rate of exponential increase of solutions of (3) vanishes at $E=0$ but the nature of the products of the matrices and the corresponding eigenstates are quite different. The existence of such a "quasi-mobility edge" in the models can be traced back to a symmetry of the underlying physical model: invariance under uniform translations for Dyson's phonon model, and the existence of a uniform steady-state distribution for the hopping problem.

The question is now posed: At $E=0$ a sequence of random matrices commute; what is the effect of adding to each a small noncomuting part? There are two elements to the answer: the existence of limits (8) and (9) and a simple scaling hypothesis. Suppose that for $E\to\infty$, $N\to\infty$, the random variable $Z_{2N}=K_{2N}(E)-\pi Ni$ has a probability distribution function (PDF) p that depends on the two variables E and N through a single variable, for example, $Y=EN^{1/\varphi}$ where φ is to be determined. Furthermore suppose we have shown that for $Y=0$, i.e., $E=0$, Z_{2N} has a PDF independent of N. For E fixed and $N\to\infty$, i.e., $Y\to\infty$, Ossedelec's theorem guarantees that $\mathrm{Re}Z_{2N}/2N$ has a well-defined limit; we assume the same to be true for $\mathrm{Im}Z_{2N}/2N$, i.e., an average density of states exists:

$$\mathrm{Re}Z_{2N} \to 2\lambda(E)N + Z_N' , \tag{14}$$

$$\mathrm{Im}Z_{2N} \to \pi[I(E)-\tfrac{1}{2}]2N + Z_N'' , \tag{15}$$

where Z_N' and Z_N'' vanish with probability 1 as $N\to\infty$. Equations (14) and (15) follow if for $Y\to\infty$

$$\langle Z_{2N}\rangle = \alpha Y^{\varphi} = \alpha E^{\varphi} N , \tag{16}$$

with α a complex constant. Thus from the scaling hypothesis and identification of the scaling variable we would predict an inverse localization length and integrated density of states that vanish as E^{φ}.

The question remains: How do we identify the scaling variable? We do this by perturbation theory: by showing that the distribution of Z_{2N} is determined by a single variable y of the two variables E and N for small y. This will be demonstrated explicitly for case II. To simplify notation we take $J_0=J_{2N}$. The matrix product and logarithm are expanded in powers of E:

$$\ln\left[(-1)^N \prod_{j=0}^{N-1} U_{2(N-j)}(E)\right] = E\begin{pmatrix} 0 & -J_0\sum_n 1/J_n{}^2 \\ N/J_0 & 0 \end{pmatrix} - \frac{E^2}{2}\begin{pmatrix} \sum_n n/J_n{}^2 & 0 \\ 0 & \sum_n (N-n)/J_n{}^2 \end{pmatrix}, \tag{17}$$

$$K_{2N}(E)-\pi Ni = -\tfrac{1}{2}E^2N\sum_n J_n{}^{-2}\ \tfrac{1}{2}[(\tfrac{1}{2}E^2N\sum_n J_n{}^{-2})^2 - 4E^2N\sum_n J_n{}^{-2}]^{1/2} . \tag{18}$$

Thus to low order $K_{2N}(E)-\pi Ni$ is a function of $E^2N\sum_{n=1}^N J_n{}^{-2}$, whose asymptotic distribution depends on the distribution of variables J_n. Consider the following:

$$p(J) = (1-\alpha)/J^{\alpha} , \tag{19}$$

where $1>\alpha>-\infty$, $0<J<1$. By extension of the usual central limit theorem properties of the distribution of $\sum_{n=1}^N J_n{}^{-2}$ were proved. Three classes are distinguished.

(i) $1>\alpha>-1$: $\langle J^{-2}\rangle$ does not exist and asymptotically

$$\sum_1^N J_n{}^{-2} = N^{2/(1-\alpha)} y , \tag{20}$$

where y is a random variable independent of N. {Its PDF is the Laplace transform of $\exp[-\Gamma(\frac{1}{2}(1+\alpha)s^{(1-\alpha)/2}]$}.

(ii) $-1>\alpha>-3$: $\langle J^2\rangle$ exists but $\langle J^4\rangle$ does not, and

$$\sum_1^N J_n{}^{-2} = N\langle J^{-2}\rangle + N^{2/(1-\alpha)} y' , \tag{21}$$

where y' has a distribution independent of N.

(iii) $\alpha<-3$, or more generally any distribution for which $\langle J^2\rangle$ and $\langle J^4\rangle$ exist: The usual central limit theorem applies, and

$$\sum_1^N J_n{}^{-2} = N\langle J^{-2}\rangle + N^{1/2} y'' , \tag{22}$$

where y'' is normally distributed. For $K_{2N}(E)$ we find

(i) $K_{2N}(E) = \pi Ni + EN^{(1/2)[1+2/(1-\alpha)]} i\sqrt{y} + \dots$,

(ii) $K_{2N}(E)$

$$= \pi Ni + iEN\langle J^{-2}\rangle + EN^{2/(1-\alpha)} \tfrac{1}{2} iy' + \dots , \tag{23}$$

(iii) $K_{2N}(E) = \pi Ni + iEN\langle J^{-2}\rangle + EN^{1/2}\tfrac{1}{2} iy'' + \dots$.

This identifies the three scaling variables as $EN^{(1/2)[1+2/(1-\alpha)]}$, $EN^{2/(1-\alpha)}$, and $EN^{1/2}$, respectively. (Nonfluctuating terms are absorbed into the definition of Z_{2N} to make the scaling hypothesis valid.) Proceeding as outlined above we predict that $\lambda(E)$ vanishes as E^{φ} where

$$\begin{aligned}\varphi &= \frac{2(1-\alpha)}{3-\alpha}, && \text{(i) } -1<\alpha<1, \\ &= \tfrac{1}{2}(1-\alpha), && \text{(ii) } -3<\alpha<-1, \\ &= 2, && \text{(iii) } \alpha<-3.\end{aligned} \tag{24}$$

The result (24) is new but for case (iii) is expected by comparison to the results for weak diagonal disorder.[11] For the integrated density of states the constant imaginary part dominates for (ii) and (iii); the prediction is then that $I(E) - \frac{1}{2}$ is proportional to E^{φ} for (i) and to E for (ii) and (iii). For case I a similar argument identifies the scaling variable as $N^{1/2}\sigma_J/\ln(E^2)$. Combined with (12) and a scaling hypothesis we find

$$\begin{aligned}\lambda(E) &\sim \sigma_J^{\,2}/\ln(1/E^2), \\ I(E) - \tfrac{1}{2} &\sim \sigma_J^{\,2}/[\ln(1/E^2)]^2.\end{aligned} \tag{25}$$

Singularities (25) agree with those found by Eggarter and Riedinger[9] by arguments more detailed but similar in spirit, as well as Dyson's solutions.

In conclusion I have demonstrated how a perturbation approach combined with a hypothesis of scaling leads to definite predictions of the singular spectra of the Hamiltonian (1) and clear distinction of types I and II of disorder. The singular forms have been verified by multiplying chains of up to 10 000 random matrices and determining $\lambda(E)$ and $I(E)$ numerically. A detailed comparison will be presented elsewhere with a fuller exposition of the present work. For the uncorrelated case the results (25) agree with previous work.[1,9] It is straightforward to extend the argument to cases where σ_J does not exist for which the singularities (25) will be modified. For the "spin-wave" case the singularities in the density of states agree with those of Alexander *et al.*[2] In fact with the change of variables $S \leftrightarrow E^2$, $W \leftrightarrow J^2$ and PDF $p(W) = (1-\gamma)W^{-\gamma}$, the density of states $\rho(s)$ diverges as

$$\begin{aligned}\rho(s) &\sim s^{-1/(2-\gamma)}, && \text{(i) } 0<\gamma<1, \\ &\sim s^{-1/2}, && \text{(ii), (iii) } \gamma<0.\end{aligned} \tag{26}$$

In addition it is predicted from (24) that eigenstates of (4) will be exponentially localized with inverse localization length $\lambda(s) \sim s^{\omega}$ where

$$\begin{aligned}\omega &= (1-\gamma)/(2-\gamma), && \text{(i) } 0<\gamma<1, \\ &= \tfrac{1}{2}(1-\gamma), && \text{(ii) } -1<\gamma<1, \\ &= 1, && \text{(iii) } \gamma<-1.\end{aligned}$$

This is a new and important qualification to the statement that for negative γ the asymptotic spectral properties of the random chain are essentially as for a uniform chain. Effective-medium theories generally neglect such localization effects. Note that localization properties here do not imply the absence of diffusion in the classical process as they do in the equivalent quantum problem, but they are necessary for a full understanding of the approach to the infinite-time limit, a subject of current debate.[12]

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