Band-edge features in disordered systems

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Despite the complexity of real disordered materials, the electronic properties often have similar features in dissimilar materials, suggesting the presence of universal features, particularly near band edges. In the present paper, we demonstrate that under certain conditions, including weak disorder, band-edge features are universal for fewer than two dimensions. For higher dimensions, universality remains after a nonuniversal shift of the edge of the unperturbed band. The white-noise model proves very useful in the universality arguments.

I. INTRODUCTION

Real disordered materials can seem bewilderingly complex. Multiple single-site orbitals can be required to represent the wave functions;[1] there can be disorder in the single-site energies (diagonal disorder);[2] there can be disorder in the electron transfer-matrix elements (off-diagonal disorder);[3] the probability distributions of these matrix elements can be continuous and unbounded,[4] continuous and bounded,[2] or discrete;[5] and structural disorder can manifest itself both quantitatively and topologically in a variety of ways.[6] Yet the experimental data on the optical properties, for example, often show similar features in quite dissimilar material, e.g., tetrahedral amorphous semiconductors,[7] amorphous pnictides,[8] or amorphous chalcogenides.[9] One is tempted to speculate that there may be universal features in the electronic structures of disordered materials.[10]

In the present paper, we carry out a restricted search for such universal features. It seems clear that features which are sensitive to the full range of energies of an energy band or to distances on an atomic scale cannot be universal. The search should therefore be limited to relatively weak disorder and to energies relatively near band edges. Fortunately, disordered semiconductors are materials in which quantitative measures of the disorder are of order 10% of the valence or conduction band widths[6] and the band edges are of great significance, so our inquiry is not merely of academic interest.

We begin in Sec. II with a detailed discussion of the white-noise model (WNM), a generalization to disordered materials of the effective-mass model of crystals. We discuss briefly the conditions for applicability of the white-noise model and show that universality results if these conditions are met. We then show in Sec. III that the conditions can be met only for dimensions $d<2$. For higher dimensions, ultraviolet catastrophes occur in the WNM. Nevertheless, it is shown in Sec. IV that the continuum limit of the tight-binding model accurately retains its band-edge features for $2\leq d<4$, whereas that limit cannot be taken at all for $d>4$. Thus two marginal dimensions $d_l=2$ and $d_u=4$ emerge in the problem. It is then shown in Sec. V that the universal features of the white-noise model persist after a nonuniversal shift of the continuum edge is made. In Sec. VI, explicit results are given for the universal and, indeed, the nonuniversal features as well for all dimensions. We conclude in Sec. VII with a brief summary of our principal results and a listing of the extensions needed before the theory can be applied to real materials.

II. THE WHITE-NOISE MODEL AND UNIVERSALITY

States in the neighborhood of a band edge of a crystalline material can be accurately represented by use of a simple effective-mass model with effective Hamiltonian

$$H_{\text{eff}}=\frac{p^2}{2m^*} \tag{2.1}$$

under certain conditions.[11] First, the band edge must be nondegenerate (apart from spin). Second, attention is confined to energies in the immediate vicinity of the band edge, $(\Delta E)\ll B$, E_G, the bandwidth and band gap, respectively, and to lengths much larger than the lattice constant a. Perturbations added to (2.1) should not mix in energies or cause variations of the wave function on length scales which violate these conditions if effective mass theory is to be applicable.

A similarly simple continuum model can be used to represent the states near a band edge of a disordered material,

$$H_{\text{eff}}=\frac{p^2}{2m^*}+V(\mathbf{r})\ , \tag{2.2}$$

where $V(\mathbf{r})$ is a random potential, under a larger but related set of conditions. First, there must exist a suitable reference model for the material from which the disorder can be measured. Second, this model must possess a nondegenerate normal band edge.[12] At a normal band edge, the states are extended even in the presence of disorder, and the density of states (DOS) depends on energy as

$$n(E)=\begin{cases} a_d E^{d/2-1}, & E>0 \\ 0, & E<0\ , \end{cases} \tag{2.3}$$

where d is the dimension of the material. Equation (2.3) can readily be extended to fractal materials through the introduction of the spectral and fractal dimensions, but we shall leave such cases implicit here. Examples of normal band edges are provided by the bonding and antibonding bounds of the tight-binding, nearest-neighbor s-band model with fixed matrix element V in any bichromatic net, disordered or not. A bichromatic net is one that can be decomposed to two interpenetrating subnets, each point of which has all its nearest neighbors belonging to the other. Such a system can serve as a reference relative to which diagonal disorder, quantitative disorder in V (off-diagonal disorder), and further topological disorder caused by the introduction of odd rings can be measured. The first two are of comparable importance for both bounds; the last has a far greater effect on the antibonding bound, turning it from a normal band edge into a Lifshitz limit[13] while leaving the bonding bound a normal band edge. Third, a suitable measure w of the disorder must be much less than a suitable measure of the bandwidth B. Fourth, we are concerned with energy separations from the underlying band edge much smaller than B. Fifth, any characteristic lengths in the problem must be much larger than the interatomic spacing a, which in the present work we consider to be equal to the correlation length L of the random potential. If the correlation length L is larger than a, the conditions for the applicability of the WNM are violated in general. The degree of violation depends on many factors; the most important one is whether or not atomic scale potential fluctuations exist within the correlation length L. For example, if we have a binary random alloy A_xB_{1-x} with correlation favoring $ABAB$ configurations, then both a and L retain their physical relevance and thus the problem cannot be reduced to the single length WNM. On the other hand, for correlation favoring segregation of the components, the lattice spacing a loses its physical importance and L becomes the smaller relevant length; in this case the reduction to the WNM is possible. In any case, the question of the applicability of our conclusions for the case $L > a$ is a complicated one and will be discussed in a separate paper. The last condition for the applicability of the WNM is that the continuum model itself should contain no ultraviolet catastrophe, which implies no sensitivity to L, a, or B.

These conditions will be discussed in more detail in Secs. III–V, but let us now suppose that they hold and examine their consequences. Consider the autocorrelation function of the potential $C(\mathbf{r},\mathbf{r}')$, defined as

$$C(\mathbf{r},\mathbf{r}') \equiv \langle V(\mathbf{r})V(\mathbf{r}')\rangle - \langle V(\mathbf{r})\rangle\langle V(\mathbf{r}')\rangle \ . \tag{2.4}$$

Shift the underlying continuum edge to $\langle V\rangle$ and set the corresponding energy to zero. Reexpress $C(\mathbf{r},\mathbf{r}')$ in terms of the reduced correlation function $c(\mathbf{r},\mathbf{r}')$, which has unit spatial integral,

$$C(\mathbf{r},\mathbf{r}') = \gamma c(|\mathbf{r}-\mathbf{r}|) \ , \tag{2.5}$$

where we are supposing translational invariance and isotropy after the ensemble average indicated by the angular brackets in (2.4). The above conditions imply the applicability of the central limit theorem for the probability distribution of $V(\mathbf{r})$, which can therefore be taken as a delta-correlated Gaussian, with

$$\langle V(\mathbf{r})V(\mathbf{r}')\rangle = \gamma\delta(\mathbf{r}-\mathbf{r}') \ , \tag{2.6}$$

i.e., with $c(|\mathbf{r}-\mathbf{r}'|)$ replaced by a delta function. Given that L is the actual correlation length of the potential as expressed in $c(|\mathbf{r}-\mathbf{r}'|)$, γ can be interpreted as

$$\gamma = w^2 L^d \ , \tag{2.7}$$

where w is the appropriate measure of the strength of the disorder referred to above. Equations (2.2) and (2.6) and the Gaussian probability distribution constitute the white-noise model, or WNM, the simplest generalization to disordered materials of the effective-mass model of crystals.

The WNM contains only two parameters, $\hbar^2/2m^*$ and γ. These can be used to define natural units of energy ϵ_{0d} and length L_{0d}, which can be introduced for all d except four through

$$\gamma = \epsilon_{0d}^2 L_{0d}^d \ , \tag{2.8a}$$

$$\hbar^2/2m^* = \epsilon_{0d} L_{0d}^2 \ . \tag{2.8b}$$

The explicit solutions for L_{0d} and ϵ_{0d} are

$$\epsilon_{0d} = \left[\frac{2m^*}{\hbar^2}\right]^{d/4-d} \gamma^{2/4-d} \ , \tag{2.9a}$$

$$L_{0d} = \left[\frac{\hbar^2}{2m^*}\right]^{2/4-d} \gamma^{-(1/4-d)} \ , \tag{2.9b}$$

which become

d	ϵ_{0d}	L_{0d}
3	$\left[\frac{2m^*}{\hbar^2}\right]^3 \gamma^2$	$\left[\frac{\hbar^2}{2m^*}\right]^2 \gamma^{-1}$
2	$\left[\frac{2m^*}{\hbar^2}\right] \gamma$	$\left[\frac{\hbar^2}{2m^*}\right] \gamma^{-1/2}$
1	$\left[\frac{2m^*}{\hbar^2}\right]^{1/3} \gamma^{2/3}$	$\left[\frac{\hbar^2}{2m^*}\right]^{2/3} \gamma^{-1/3}$

for integral dimension <4.

When length and energy are expressed in units of ϵ_{0d} and L_{0d}, the Schrödinger equation and the correlation function of the potential, (2.6), become dimensionless and universal. All characteristic lengths L_{ad} and energies E_{ad} associated with specific features of the spectrum become universal pure numbers l_{ad}, ϵ_{ad}. Scaling relations can be written for such quantities of physical interest as the density of states, etc.:

$$n(E) = L_{0d}^{-d} \epsilon_{0d}^{-1} f_d(E/\epsilon_{0d}) \ . \tag{2.10}$$

Under the conditions posited at the beginning, the function $f_d(x)$ must have the limiting behaviors

$$f(x) \to a_d x^{[(d/2)-1]} \text{ as } x \to +\infty \ , \tag{2.11}$$

$$f(x) \to 0 \text{ as } x \to -\infty \ . \tag{2.12}$$

Upon substitution of (2.11) and (2.9) into (2.10), γ cancels and a_d can be related to the known quantities A_d by comparison with (2.3). At the underlying continuum edge (shifted to $\langle V\rangle$), $E=0$ and

$$n(0)=L_{0d}^{-d}\epsilon_{0d}^{-1}f_d(0)\ . \tag{2.13}$$

Because $f_d(0)$ is simply a number, Eq. (2.13) gives the explicit dependence of the density of states at the continuum edge upon disorder,

$$n(0)=f_d(0)\left[\frac{2m^*}{\hbar^2}\right]^{d/(4-d)}\gamma^{(d-2)/(4-d)}\ . \tag{2.14}$$

It is clear from the above dimensional analysis that the universality of the WNM is a significant characteristic of the model and a powerful tool for the analysis of physical phenomena. It is therefore important to examine the transition from the explicit microscopic description of the material to the WNM in order to establish the circumstances under which the conditions stated above for its validity are met. Before doing so, we shall catalogue the catastrophes inherent in the WNM in the next section. We should also point out that Freed has arrived at essentially identical scaling arguments from an entirely different point of view, although he did not exploit them in the manner done here and in what follows.[14]

III. ULTRAVIOLET CATASTROPHES IN THE WHITE-NOISE MODEL

The final condition imposed in the last section for the applicability of the WNM and therefore of universality and scaling in the energy and length dependences of physical quantities was that the WNM should not contain ultraviolet catastrophes.[15] Such catastrophes arise at lengths shorter than the lattice constant a or correlation length L and energies larger than the bandwidth B. When the catastrophes are removed by the introduction of discrete atomic structure, equivalent to the imposition of a length cutoff a or L and an energy cutoff B or $\hbar^2/2m^*L^2$, physical quantities become sensitive to the cutoffs and universality is destroyed or reduced.

Divergences such as ultraviolet catastrophes can be probed through study of the self-energy $\Sigma(x-y)$ and the vertex part Γ.[16] The former is defined via the average Green's function $\langle G(x,y)\rangle$, viz.,

$$\langle G(x,y)\rangle=G_0(x-y)+\int du\,dv\,G_0(x-u)\Sigma(u-v)\langle G(v,y)\rangle\ , \tag{3.1}$$

the latter is defined via the average of the product of two Green's functions $\langle G(x,y)G(x',y')\rangle$, viz.,

$$\langle G(x,y)G(x',y')\rangle=\langle G(x,y)\rangle\langle G(x',y')\rangle + \int du\,dv\,du'dv'\Gamma(u,v;u'v')\langle G(x,w)\rangle\langle G(x',u')\rangle\langle G(v,y)\rangle\langle G(v',y')\rangle\ . \tag{3.2}$$

The average in (3.1) and (3.2) is over the probability distribution of the potential, and G_0 is the Green's function of the unperturbed continuum for which $H_0=p^2/2m^*$.

One can construct the usual diagrammatic expansion[16] for Σ, which, for the WNM, has the structure shown in Fig. 1. Each dashed line in Fig. 1 connects two identical points because of (2.6) and contributes a factor γ to the term it enters. Each solid line between, e.g., the points z and x, contributes a factor $G_0(z-x)$. All disconnected parts of the diagrams can be summed, improving the convergence and replacing $G_0(z-x)$ by $\langle G(z,x)\rangle$, which must then be determined self-consistently.

Three divergences can appear in the above expansion:

(1) For $d<2$, G_0 is singular at $E=0$ in both its real and imaginary parts. For $d=2$, the singularity occurs only in the real part. This infrared singularity[15] disappears from $\langle G\rangle$ and does not present any problem in the final result for Σ or Γ. It simply requires the explicit use of the partial summation effected by replacing G_0 with $\langle G\rangle$. It is not necessary to introduce a cutoff for its removal. This removable singularity originates from the singularity of the continuum density of states (DOS) at the unperturbed band edge, a consequence of the phase space available to states of given energy: $n(E)\propto k^{d-1}dk/dE\propto k^{d-2}\propto E^{(d-2)/2}$.

(2) The second type of divergence arises from the fact that $G_0(x-y)$ behaves as $|x-y|^{-(d-2)}$ as $|x-y|\to 0$. This behavior is related to the structure of the differential equation obeyed by G_0:

$$\left[E+\frac{\hbar^2}{2m^*}\nabla_x^2\right]G_0(x,y)=\delta(x,y)\ . \tag{3.3}$$

As $x\to y$, the energy E can be ignored in (3.3), which reduces to the Poisson equation for a point source, the solution of which has the above singularity. The same singularity is present in the perturbed Green's function $G(x,y)$ in those neighborhoods in which $V(x)$ is finite because its differential equation

$$\left[E-V(x)+\frac{\hbar^2}{2m^*}\nabla_x^2\right]G(x,y)=\delta(x,y) \tag{3.4}$$

also reduces to the Poisson equation. It remains true for the averaged Green's function $\langle G(x,y)\rangle$ as long as the points at which $V(x)$ is singular have suitably small measures.

Thus we encounter here a nonremovable divergence in $\langle G(x,y)\rangle$ for $d\geq 2$ which leads to contributions to $\Sigma(x,y)$ which blow up in a nonintegrable way as $x\to y$. The resulting nonremovable divergence in $\Sigma(x,y)$ is already present in the second-order term, the first term in the ex-

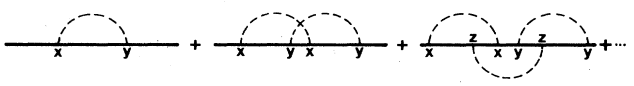

FIG. 1. Diagrammatic expansion for the self-energy Σ.

pansion of Fig. 1. The latter has the form

$$\Sigma^{(2)}(x,x)=\gamma^2\int dE'\frac{n(E')}{E-E'}\ , \tag{3.5}$$

where $n(E)$ is the averaged density of states, as expected from second-order perturbation theory. The DOS $n(E')$ does not vanish as $E'\to\infty$ for $d\geq 2$, behaving as $E'^{(d-2)/2}$. The integral (3.5) therefore diverges for $d\geq 2$. This ultraviolet divergence can be removed only by introducing the lattice constant a or the correlation length L as a distance cutoff or retaining a finite band with $B\propto\hbar^2/m^*a^2$ in those diagrams in which the divergence appears.

(3) The third type of divergence appears for $d\geq 4$ from integrals of the type $\int dz\langle G(x-z)\rangle^2$ which appear both in the self-energy (of the third diagram in Fig. 1) and in the vertex part shown in Fig. 2. This integral has an integrand of the form $|z-x|^{3-d}$ as $z\to x$ and therefore diverges for $d\geq 4$. Once again, this ultraviolet divergence can be removed only through the introduction of length or energy cutoffs associated with the actual atomic structure of the material.

At this point, we have discovered that the WNM has a lower marginal dimension $d_l=2$ and an upper marginal dimension $d_u=4$. We note that $d=4$ has already appeared as a special dimension in the dimensional analysis of Sec. II. Below the lower marginal dimension $d_l=2$, the WNM has no singularities and should accurately describe those systems obeying the remaining conditions of Sec. II. Thus, band-edge features are universal in the sense of Sec. II for $d<2$. In a later section, we give accurate numerical values for the universal function $f(x)$ entering the DOS and the corresponding function for the localization length for $d=1$. We examine in the next section the extent to which the WNM remains physically meaningful and retains universality above d_l.

IV. APPLICABILITY OF THE CONTINUUM MODEL

The presence of ultraviolet catastrophes in the WNM forces the explicit consideration of specific microscopic models for the one-electron Hamiltonian. We shall illustrate the removal of the divergences and the consequent breakdown of universality for the simplest model Hamiltonian, that of the tight-binding s band, which has matrix elements

$$H_{ij}=\epsilon_{i\delta ij}+V_{ij} \tag{4.1}$$

between sites i and j on a crystal lattice. We take the V_{ij} to be fixed and the ϵ_i to be random (diagonal disorder), with moments

$$\langle\epsilon_i\rangle=0\ , \tag{4.2}$$

$$\langle\epsilon_i\epsilon_j\rangle=C_{ij}\ . \tag{4.3}$$

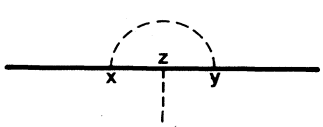

FIG. 2. Structure of the vertex part Γ.

The correlation function C_{ij} has a range L, the correlation length, and can be written in terms of a normalized correlation function c_{ij} as

$$C_{ij}=w^2c_{ij},\quad \Sigma_i c_{ij}=1\ . \tag{4.4}$$

In the present work we assume $L=a$ so that $c_{ij}=\delta_{ij}$. The first diagram for $\Sigma(x,y)$ illustrated in Fig. 1 for the WNM goes over to

$$\Sigma^{(1)}_{ij}=w^2c_{ij}G^0_{ij} \tag{4.5}$$

in the present case. Provided the unperturbed wavelength corresponding to the energy E for which $\Sigma^{(1)}$ is being evaluated is much larger than a, the lattice constant, $\Sigma^{(1)}_{ij}$, can be treated as a continuous function of position in any equation involving it. That is, the limit $a\to 0$ can be taken without risk. In the particular case that $V_{ij}=V$ for i and j nearest neighbors and zero otherwise, $m^*=\hbar^2/2Va^2$. Thus to pass from the tight-binding model to the continuum model of Sec. II so that $\epsilon_i\to V(x)$, it is necessary to take the limits

$$a\to 0,\quad V\to\infty,\quad W\to\infty\ , \tag{4.6}$$

such that

$$w^2a^d=\gamma,\quad Va^2=\hbar^2/2m^* \tag{4.7}$$

remain finite, where a is defined so that a^d is the atomic volume. The bandwidth B is given by

$$B=2ZV\ , \tag{4.8}$$

where Z is the coordination number. We see from Eqs. (4.6)–(4.8) that in the limit $a\to 0$, we have

$$\frac{w}{B}\to 0,\quad d<4 \tag{4.9a}$$

$$\frac{w}{B}\to\infty,\quad d>4\ . \tag{4.9b}$$

Thus for $d<4$, the continuum model corresponds to the case of weak disorder in which both w and $|E|$ (with E measured from the unperturbed band edge) are much smaller than the bandwidth. On the other hand, for $d>4$ passing to the continuum limit cannot be done in an internally consistent way. We see from (4.9b) that the continuum limit implies that $w\gg B$. In that case, all states will be strongly localized to individual sites as long as c_{ij} has any appreciable variation from site to site, and the DOS is given simply by the probability distribution of the single-site energies ϵ_i enormously broadened relative to the original band. There is no universality whatsoever. The upper marginal dimension $d_u=4$ marks the limit of applicability of any continuum model, let alone the white-noise model. It is only between the two marginal dimensions, $2<d<4$, that one has mobility edges in the continuum limit.

V. THE NONUNIVERSAL CORRECTIONS TO THE WHITE-NOISE MODEL, $2\leq d<4$

Returning to Eq. (4.5), which reduces to

$$\Sigma^{(1)}_{ij}=w^2G^0_{ij}(E)\delta_{ij}\ , \tag{5.1}$$

and taking the Fourier transform of (5.1) shows that $\Sigma_{ij}^{(1)}$ corresponds to a k-independent shift of the entire energy band by $w^2 G_{ii}^0(E)$. Because the energy dependence of $G_{ii}^0(E)$ occurs on the scale of V and we are limiting ourselves to band-edge features so that $|E| \ll V$, we can set $E=0$ in $G_{ii}^0(E)$. Thus the contribution (5.1) to the self-energy simply corresponds to a rigid shift of the band in the energy range of interest.

$G_{ii}^0(E=0)$ has the form $-A_d/V$, where $A_3=0.253$ for a simple cubic lattice. There is another nonsingular but nonzero contribution to the energy shift which is not present in the WNM; it comes from the second diagram in Fig. 1. After Fourier transforming it adds

$$-(2w^4-\mu_4)[G_{ii}^0(E=0)]^3$$

to the energy shift, where μ_4 is the fourth moment of ϵ_i. All other extra contributions disappear in the limit $a \to 0$.

Putting all this together, we obtain that when the conditions of Sec. II are met the WNM can be used for $2 \le d < 4$ provided that the divergences are ignored and the unperturbed energy band is rigidly shifted by

$$E_B = -A_d \left[\frac{w^2}{V} - A_d^2 \frac{(2w^4-\mu_4)}{V^3} \right] \tag{5.2}$$

for $d=3$ with $A_d=0.253$.

The shift E_B is nonuniversal because of its dependence on crystal structure through its dependence on A_d, its dependence on w/V after being divided by ϵ_{0d}, and its dependence on the probability distribution of the disorder through the presence of the fourth moment μ_4. With regard to the latter point, $2w^4-\mu_4=\frac{1}{5}w^4$ for a rectangular distribution and $-w^4$ for a Gaussian. For $d=2$, Thouless and Elzain have shown that

$$E_B = -(w^2/4\pi V)[1+\ln(128\pi V^2/w^2)] \, . \tag{5.3}$$

VI. RESULTS FOR THE BAND-EDGE FEATURES

A. $d<2$

We have learned that the WNM is well behaved and needs no corrections for $d<2$. The simple results of the dimensional analysis of Sec. II stand without any qualifications. By specializing to the well studied 1D case, we obtain the DOS per unit length as

$$n(E) = \frac{1}{\epsilon_{01} L_{01}} f_1 \left[\frac{E}{\epsilon_{01}} \right] , \tag{6.1}$$

where $f_1(X)$ is a universal function. There is a closed analytic form[17] for f_1

$$f_1(x) = \left[\frac{2}{\pi} \right]^{1/2} \frac{N_+(x)}{N_-^2(x)} , \tag{6.2}$$

where

$$N_\pm(x) = \int_0^\infty dt \, t^{\pm 1/2} \exp(-t^3/6 - 2xt) \, . \tag{6.3}$$

In Fig. 3, we plot f_1 vs x, and in Table I, we tabulate its values. The localization length λ is given according to our simple dimensional arguments by

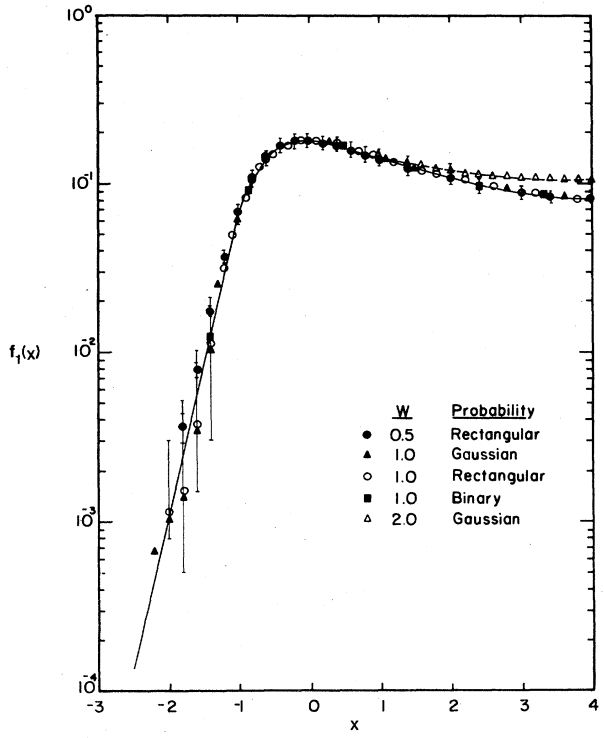

FIG. 3. Plot of the one-dimensional universal density of states (DOS) $f_1(x)$ versus the universal energy $x=E/\epsilon_{01}$. The solid line is the exact result [Eqs. (6.2) and (6.3)] for the white-noise limit. Numerical data for the DOS are also plotted for different amounts of disorder and different probability distributions. Note that the standard deviation $w=W/\sqrt{12}$, where W is shown in the figure (in units of V).

$$\lambda = L_{01} g_1 \left[\frac{E}{\epsilon_{01}} \right] , \tag{6.4}$$

where $g_1(x)$ is again a universal function. Sophisticated considerations[17] have led to a closed expression for $g_1(x)$

$$g_1(x) = \frac{1}{2} \frac{N_+(x)}{N_-(x)} \, . \tag{6.5}$$

In Fig. 4, we plot $g_1(x)$ vs x, and in Table I, we tabulate its values.

It is simply amazing, given the enormous amount of numerical work done on 1D systems, that this universality has not previously been recognized. In Figs. 3 and 4, we compare accurate numerical calculations of $n(E)$ and $\lambda(E)$ with the universal forms (6.1)–(6.5) for various probability distributions and various values of w/V. Within the numerical errors from Fig. 3, we see that universality holds for the density of states in the tail, and in the band up to a value of x which decreases with increasing disorder w/B, where B is the bandwidth. For example, for $w/B=0.14$, i.e., $W/V=2$, significant departures from universality occur at $x=1$ (i.e., at $E=0.48V$ above the unperturbed band edge), whereas no detectable departure from universality occurs up to $x=4$ (i.e., at $E=0.76V$ above the unperturbed band edge) for $w/B=0.072$. From Fig. 4 we see that universality holds

TABLE I. Density of states $f_1(x)$ and localization length $g_1(x)$ for different values of energy $x = E/\epsilon_{01}$. For a plot of these functions versus x see Figs. 3 and 4.

x	$f_1(x)$	$g_1(x)$	x	$f_1(x)$	$g_1(x)$
−4.500	$0.491\,95\times10^{-10}$	0.477 89	0.300	0.177 31	4.827 9
−4.400	$0.111\,74\times10^{-9}$	0.483 52	0.400	0.173 00	5.354 2
−4.300	$0.251\,27\times10^{-9}$	0.489 37	0.500	0.168 24	5.911 8
−4.200	$0.559\,25\times10^{-9}$	0.495 43	0.600	0.163 28	6.497 8
−4.100	$0.123\,19\times10^{-8}$	0.501 73	0.700	0.158 29	7.109 7
−4.000	$0.268\,49\times10^{-8}$	0.508 29	0.800	0.153 37	7.744 6
−3.900	$0.578\,96\times10^{-8}$	0.515 11	1.900	0.112 72	$0.156\,46\times10^{2}$
−3.800	$0.123\,50\times10^{-7}$	0.522 22	1.000	0.144 03	9.072 9
−3.700	$0.260\,53\times10^{-7}$	0.529 64	1.100	0.139 68	9.761 8
−3.600	$0.543\,47\times10^{-7}$	0.537 39	1.200	0.135 56	$0.104\,65\times10^{2}$
−3.500	$0.112\,08\times10^{-6}$	0.545 51	1.300	0.131 67	$0.111\,80\times10^{2}$
−3.400	$0.228\,47\times10^{-6}$	0.554 01	1.400	0.128 02	$0.119\,04\times10^{2}$
−3.300	$0.460\,24\times10^{-6}$	0.562 93	1.500	0.124 58	$0.126\,38\times10^{2}$
−3.200	$0.915\,97\times10^{-6}$	0.572 32	1.600	0.121 35	$0.133\,80\times10^{2}$
−3.100	$0.180\,06\times10^{-5}$	0.582 20	1.700	0.118 26	$0.141\,32\times10^{2}$
−3.000	$0.349\,51\times10^{-5}$	0.592 64	1.800	0.115 41	$0.148\,87\times10^{2}$
−2.900	$0.669\,74\times10^{-5}$	0.603 67	1.900	0.112 72	$0.156\,46\times10^{2}$
−2.800	$0.126\,65\times10^{-4}$	0.615 38	2.000	0.110 20	$0.164\,10\times10^{2}$
−2.700	$0.236\,28\times10^{-4}$	0.627 82	2.100	0.107 83	$0.171\,76\times10^{2}$
−2.600	$0.434\,69\times10^{-4}$	0.641 10	2.200	0.105 56	$0.179\,49\times10^{2}$
−2.500	$0.788\,34\times10^{-4}$	0.655 30	2.300	0.103 43	$0.187\,23\times10^{2}$
−2.400	$0.140\,87\times10^{-3}$	0.670 56	2.400	0.101 41	$0.195\,00\times10^{2}$
−2.300	$0.247\,90\times10^{-3}$	0.687 00	2.500	$0.994\,94\times10^{-1}$	$0.202\,79\times10^{2}$
−2.200	$0.429\,37\times10^{-3}$	0.704 83	2.600	$0.976\,98\times10^{-1}$	$0.210\,58\times10^{2}$
−2.100	$0.731\,49\times10^{-3}$	0.724 25	2.700	$0.959\,52\times10^{-1}$	$0.218\,43\times10^{2}$
−2.000	$0.122\,48\times10^{-2}$	0.745 55	2.800	$0.943\,07\times10^{-1}$	$0.226\,28\times10^{2}$
−1.900	$0.201\,41\times10^{-2}$	0.769 05	2.900	$0.927\,41\times10^{-1}$	$0.234\,13\times10^{2}$
−1.800	$0.324\,90\times10^{-2}$	0.795 20	3.000	$0.912\,42\times10^{-1}$	$0.242\,01\times10^{2}$
−1.700	$0.513\,60\times10^{-2}$	0.824 53	3.100	$0.898\,34\times10^{-1}$	$0.249\,87\times10^{2}$
−1.600	$0.794\,53\times10^{-2}$	0.857 76	3.200	$0.884\,49\times10^{-1}$	$0.257\,79\times10^{2}$
−1.500	$0.120\,10\times10^{-1}$	0.895 75	3.300	$0.871\,43\times10^{-1}$	$0.265\,68\times10^{2}$
−1.400	$0.177\,12\times10^{-1}$	0.939 59	3.400	$0.858\,90\times10^{-1}$	$0.273\,59\times10^{2}$
−1.300	$0.254\,34\times10^{-1}$	0.990 70	3.500	$0.846\,86\times10^{-1}$	$0.281\,50\times10^{2}$
−1.200	$0.355\,01\times10^{-1}$	1.050 7	3.600	$0.835\,50\times10^{-1}$	$0.289\,39\times10^{2}$
−1.100	$0.480\,80\times10^{-1}$	1.121 8	3.700	$0.824\,21\times10^{-1}$	$0.297\,35\times10^{2}$
−1.000	$0.630\,84\times10^{-1}$	1.206 2	3.800	$0.813\,52\times10^{-1}$	$0.305\,29\times10^{2}$
−0.900	$0.800\,98\times10^{-1}$	1.306 8	3.900	$0.803\,24\times10^{-1}$	$0.313\,22\times10^{2}$
−0.800	$0.983\,70\times10^{-1}$	1.426 6	4.000	$0.793\,31\times10^{-1}$	$0.321\,17\times10^{2}$
−0.700	0.116 41	1.572 3	4.100	$0.783\,92\times10^{-1}$	$0.329\,08\times10^{2}$
−0.600	0.134 50	1.737 7	4.200	$0.774\,51\times10^{-1}$	$0.337\,06\times10^{2}$
−0.500	0.150 21	1.935 6	4.300	$0.765\,57\times10^{-1}$	$0.345\,02\times10^{2}$
−0.400	0.162 69	2.169 5	4.400	$0.756\,96\times10^{-1}$	$0.352\,97\times10^{2}$
−0.300	0.172 64	2.434 9	4.500	$0.748\,60\times10^{-1}$	$0.360\,93\times10^{2}$
−0.200	0.179 77	2.734 5	4.600	$0.740\,69\times10^{-1}$	$0.368\,85\times10^{2}$
−0.100	0.183 46	3.076 0	4.700	$0.732\,69\times10^{-1}$	$0.376\,86\times10^{2}$
0.000	0.184 58	3.456 5	4.800	$0.725\,09\times10^{-1}$	$0.384\,83\times10^{2}$
0.100	0.183 63	3.875 8	4.900	$0.717\,74\times10^{-1}$	$0.392\,79\times10^{2}$
0.200	0.181 12	4.332 7	5.000	$0.710\,58\times10^{-1}$	$0.400\,77\times10^{2}$

for the localization length $g_1(x)$ for $-3 \le x \le 4$ with disorder up to $w/B = 0.072$ For strong enough disorder, $w/B = 0.29$, we see from Fig. 4 that universality breaks down for $x \gtrsim 0.5$ but still holds for negative x, up to $x = -3$. Note that for this strong disorder, $x = 1.5$ corresponds to the center of the unperturbed band, where in $d = 1$, we know that localization length has its maximum value.

B. $2 < d < 4$

For $2 < d < 4$, the situation is as follows. There is a shift of the unperturbed band which depends on the disorder in a way which violates the universality given by the simple dimensional analysis. If the energy is measured from this new band edge E_B, the WNM behaves well, and the dimensional analysis based on it becomes valid. Thus

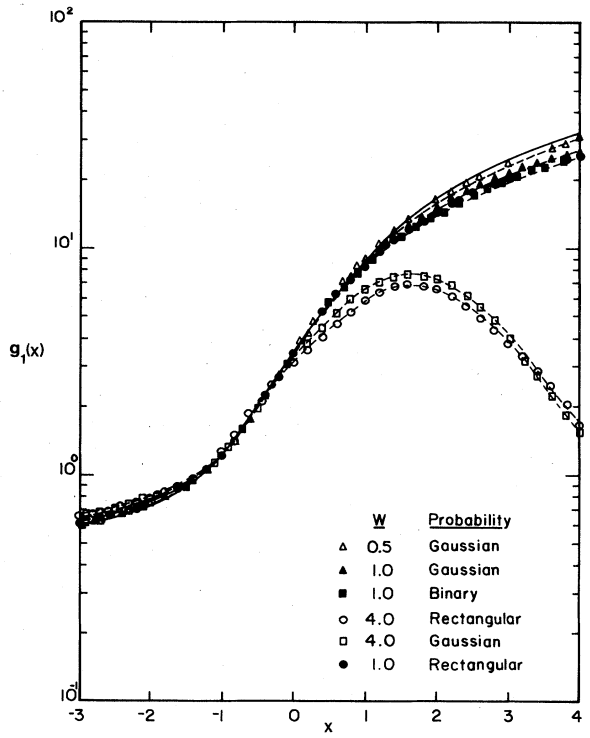

FIG. 4. Plot of the one-dimensional universal localization length $g_1(x)$ versus the universal energy $x=E/\epsilon_{01}$. The solid line is the exact result [Eqs. (6.5) and (6.3)] for the white-noise limit. Numerical data for the localization length are also plotted for different amounts of disorder and different probability distributions. Note that the standard deviation $w=W/\sqrt{12}$, where W is shown in the figure (in units of V).

we can reach the following conclusions. We have for the mobility edge

$$E_c-E_B=C_{1d}\epsilon_{0d}\ , \tag{6.6}$$

where C_{1d} is a universal number. In three dimensions,[18] C_{13} is 4.5×10^{-3}. The apparent continuum band edge E_B has as its leading term a contribution of order w^2, but the separation of E_B and E_C increases only as w^4 in $d=3$. Thus the mobility edge remains very close to the band edge for small disorders, even as the band edge itself shifts.

The DOS is given by

$$n(E)=\frac{1}{\epsilon_{0d}L_{0d}^d}f_d\left[\frac{E-E_B}{\epsilon_{0d}}\right], \tag{6.7}$$

where $f_d(x)$ is a universal function. Somewhat above E_B, it is quite accurately given by the coherent potential approximation (CPA).[18] Somewhat below E_B, it is accurately given by a function in which the dominant variation is an exponential of the form[19]

$$n(E)\propto\exp(E/E_{0d}) \tag{6.8}$$

in which

$$E_{0d}=C_{2d}\epsilon_{0d} \tag{6.9}$$

must hold with C_{2d} a universal number [$C_{22}=0.0855$ (Ref. 20) and $C_{23}=0.0095$].[18] Numerical and analytical work done by Thouless and Elzain for 2D show these features explicitly; they did not, however, test for universality.[21]

All relevant lengths such as the localization length λ, the mean-free-path l, and the correlation length ξ of the extended states have the universal form

$$\lambda=L_{0d}g_d\left[\frac{E-E_B}{\epsilon_{0d}}\right], \tag{6.10a}$$

$$l=L_{0d}p_d\left[\frac{E-E_B}{\epsilon_{0d}}\right], \tag{6.10b}$$

$$\xi=L_{0d}q_d\left[\frac{E-E_B}{\epsilon_{0d}}\right], \tag{6.10c}$$

where g_d, p_d, and q_d are universal functions of their argument. Finally, the conductivity σ has the form

$$\sigma(E)=\frac{e^2}{\hbar L_{0d}^{d-2}}S_d\left[\frac{E-E_B}{\epsilon_{0d}}\right], \tag{6.11}$$

where S_d is a universal function. The limiting forms of these functions can easily be obtained from perturbation theory for large and positive argument. In particular, one finds for the conductivity that

$$S_d(x)\propto x,\quad x\gg1 \tag{6.12}$$

for all dimensions d. $S_d(x)$ goes to zero as $E\to E_c$

$$S_d(x)\propto(x-x_c)^s\ , \tag{6.13}$$

where s is unity in various mean-field theories[22] and to fifth order in the ϵ expansion of renormalization group theory.[23] The ratio of the two slopes in (6.12) and (6.13) is 6.

Use of the CPA,[18] the potential well analogy,[24] and numerical transfer matrix methods[25] allows us approximate determination of all of these universal functions for all relevant values of x in 2D and 3D. Some of these results have been quoted above. Further details and more results will be published separately.

The universality we have discussed in such detail breaks down as the energy moves up into the band because of the presence of critical points in the unperturbed band structure.[18] It also breaks down as the energy moves more deeply into the tail.[18] The details of the breakdown are different for unbounded probability distributions such as the Gaussian on the one hand, and bounded such as the rectangular or the binary alloy on the other. In the former case, potential fluctuations on a single site can be strong enough to localize a state. In the latter case, one finds, in addition, nonuniversal behavior as the Lifshitz limit is approached. The Lifshitz limit is displaced from the unperturbed continuum edge by an amount proportional to w. Thus, we have identified nonuniversal behaviors which scale individually as w, w^2/B, and w^4/B^3

C. $d>4$

We have shown that we cannot pass to the white-noise limit for $d\geq4$. Nevertheless, we shall show here that

universal features remain after the nonuniversal features are extracted at finite a, just as for the $2 \leq d < 4$ case. For weak disorder and $a \neq 0$, the leading contribution to the self-energy Σ is the first diagram of Fig. 1 in its partially resummed form. Moreover, we shall simply state without giving the details that Σ is local in coordinate space and constant in k space for the relevant energy region. Thus, the first diagram becomes

$$\Sigma = w^2 G_0(E-\Sigma) , \tag{6.14}$$

where $G_0(E)$ is the diagonal element of the unperturbed Green's function. For $d > 4$, the unperturbed Green's function has the energy dependence[16]

$$G_0(E) = G_0(0) + AE + B(-E)^{(d-2)/2} \tag{6.15}$$

for $E \ll B$. In (6.15), A and B are constants except that when d is even, B includes a factor proportional to $\ln(-E)$. Combining the above equations, it follows that

$$\Sigma = E_B + \delta\Sigma , \tag{6.16}$$

where $\delta\Sigma$ satisfies the equation

$$\delta\Sigma = w^2 A(E - E_B - \delta\Sigma) + w^2 B(E_B - E + \delta\Sigma)^{(d-2)/2} , \tag{6.17}$$

Eq. (6.17) gives to leading order

$$\delta\Sigma = \frac{w^2 A(E-E_B)}{1+w^2 A} \approx w^2 A(E-E_B) , \tag{6.18}$$

and E_B is given by the leading term in Eq. (5.2),

$$E_B = w^2 G_0(0) . \tag{6.19}$$

Equation (6.18) implies that there is no further shift of the band edge beyond E_B as $E \to E_B$.

To find the imaginary part of $\delta\Sigma$ to leading order, we notice that

$$E_B - E + \delta\Sigma = (E_B - E)\frac{1-w^2 A}{1+w^2 A} \tag{6.20}$$

plus terms of higher order. Thus we have

$$\mathrm{Im}\delta\Sigma = \mathrm{Im}\Sigma \approx w^2 B(E_B - E)^{(d-2)/2} \tag{6.21a}$$

and

$$\mathrm{Im}G_0(E - E_B - \delta\Sigma) = B(E-E_B)^{(d-2)/2} . \tag{6.21b}$$

The physical meaning of these results is the following. For $d > 4$ there is a rigid shift of the band by E_B. This effect is not properly described by the WNM; it is heralded by the divergence of the second-order diagram for Σ. All other effects such as a further shift of energy in the DOS or in the conductivity, etc., vanish linearly with $E - E_B$. Consequently, the mobility edge coincides with the band edge, and the results of mean-field theory become exact in the limit $E \to E_B$. This is indeed what one obtains by applying the dimensional analysis of the WNM using the variable $E - E_B$. More explicitly, the dimensional analysis gives results identical in form to (6.7), (6.10), and (6.11).

However, for $d > 4$,

$$\epsilon_{0d} \propto w^{-4/(d-4)} \underset{w \to 0}{\to} \infty ,$$

while

$$L_{0d} \propto w^{2/(d-4)} \underset{w \to 0}{\to} 0 .$$

Because $\epsilon_{0d} \to \infty$ in the weak-disorder limit, only the immediate neighborhood of the point $E = E_B$ matters. In that neighborhood, all three functions f_d, l_d, and S_d have power-law behavior with the critical exponents u, v, and s, respectively. Thus we obtain

$$n(E) = \frac{1}{\epsilon_{0d}^{1+u} L_{0d}^{d}} (E - E_B)^u . \tag{6.22}$$

Because $n(E)$ must have a finite, nonzero limit as $w \to 0$, the exponent u must be such that

$$\frac{4(1+u)}{d-4} = \frac{2d}{d-4} \quad \text{or} \quad u = \frac{d-2}{2} , \tag{6.23}$$

which lead to

$$n(E) = \frac{B}{\pi}(E - E_B)^{(d-2)/2} , \tag{6.24}$$

the unperturbed result simply shifted by E_B. For the mean-free-path we have

$$l = \frac{L_{0d}}{\epsilon_{0d}^{v}} (E - E_B)^v . \tag{6.25}$$

In the limit that $w \to 0$, l can be determined from perturbation theory which yields the requirements that $l \propto w^{-2}$ or $l \propto$ velocity divided by density of states or $\propto E^{1/2}/E^{(d-2)/2} = E^{(3-d)/2}$. Both requirements lead to the result

$$v = (3-d)/2 \tag{6.26}$$

and

$$l \propto \frac{1}{w^2}(E - E_B)^{(3-d)/2} . \tag{6.27}$$

Finally, the conductivity is

$$\sigma(E) = \frac{e^2}{\hbar L_{0d}^{d-2} \epsilon_{0d}^{s}} (E - E_B)^s . \tag{6.28}$$

Once again, perturbation theory can be used in the limit $w \to 0$ and σ must be $\propto w^{-2}$. Imposing this on (6.28) yields the results

$$s = 1 \tag{6.29}$$

and

$$\sigma \propto (E - E_B)/w^2 . \tag{6.30}$$

Equation (6.30) shows that the mobility edge E_c coincides with the apparent band edge E_B, and that the scaling arguments yield the mean-field value of the critical exponent, (6.29).

The arguments given thus far are incomplete. They yield correct answers only above the mobility edge $E_c = E_B$. Just as for the case $2 \leq d < 4$, E_B is only an apparent band edge. For a terminating probability distribution, there is a Lifshitz limit $E_L \propto w$ down to which the

density of states remains finite, whereas the apparent band edge $E_B \propto w^2$. $n(E-E_B)$ retains the universal form (6.7), but f_d is only given by (6.22) above a crossover region around E_B. Below that crossover region, it is given by (6.8) or (6.9). The universal form holds until states bound to single or few sites occur or the Lifshiftz limit is approached. Similar considerations hold for nonterminating probability distributions. The most significant result of the present analysis for $d>4$ is that (6.6) still holds but with

$$C_{1d}=0, \quad d>4 . \tag{6.31}$$

VII. CONCLUSIONS

The white-noise model of a disordered, nondegenerate band edge has been shown to apply to systems of dimension $d<2$, when the conditions of Sec. II are met. As a consequence, all physical properties of such systems can be expressed in terms of disorder-dependent units of length L_{0d} and energy E_{0d} and universal functions of reduced energy. The power of this seemingly simple conclusion is displayed in Figs. 3 and 4 in which the density of states and localization length are shown for different disorders and different probability distributions to collapse into the universal form for $d=1$.

The white-noise model loses its universality for $2 \leq d <4$ because cutoffs in length and/or energy must be introduced through explicit reference to the atomic structure to avoid divergences. When this is done correctly, it is found that the band shifts rigidly to a new apparent edge of the continuum. When energy is measured relative to this new, nonuniversal edge, the universal features are restored and the method regains its power. The energy range within which universality occurs is bounded on the one side by the effect of internal critical points or other finite bandwidth effects in the continuum and on the other side by the presence of states localized to one or a few sites or through the effect of a Lifshitz limit. The latter occurs at an energy $\propto w$ below the unperturbed band edge.

Above $d=4$, the white-noise model cannot be used to represent the band edge of a disordered system because in it all states are infinitely localized. On the other hand, the dimensional analysis which emerges from the WNM remains valid after energies are measured relative to the shifted, nonuniversal continuum edge. The difference between $d \geq 4$ and $2 \leq d <4$ is that the mobility edge remains at the shifted band edge and, as is usual at and above an upper marginal dimension, the mean-field exponents become exact, e.g., the conductivity exponent is $s=1$.

Before these results can be used with confidence for real materials, it will be necessary to generalize the arguments to include such effects as off-diagonal disorder, more than one orbital per site, and topological disorder. While these extensions are not difficult in any essential way, they are sufficiently intricate and complex as not to warrant developing them here. For example, we have found that the presence of off-diagonal disorder violates in principle the universality; however, the degree of violation under certain rather common circumstances is small so that our conclusions remain approximately valid. Finally, electron-phonon interactions play a fundamentally important role in the vicinity of the band edge of disordered materials and must be included as well.

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