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Overview on Some Aspects of the Theory of Localization

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1. Introduction

Any improvement to the electronic properties and structure of disordered systems requires a proper theoretical understanding of certain fundamental questions, namely:

- the nature of the spectrum,
- the nature of the eigenstates with the possibility of disorder inducing localization,
- the existence and the nature of the mobility edge separating the localized from the extended states,
- the nature of the density of states,
- the nature of the quantum diffusion.

Most of our knowledge on the subject is probably coming from the one-band Anderson Hamiltonian [1] on a d -dimensional hypercubic lattice which is static in time but random in space. The conclusion obtained from this model is of universal validity: a critical value of the degree of disorder W , W_c may exist such that all the eigenstates are localized for $W \geq W_c$. This phenomenon known as Anderson localization is by now more than 30 years old but still alive.

In the sixties, Mott [2, 3] analyzed the consequence of localization putting forward the concept of the mobility edge E_c , originally suggested by Banyai [4], i.e. a sharp transition separating localized states in the band tails from extended states in the middle of the band, which applies when $W < W_c^*$. As a result generated by this work and because of the expansion of the range of technological applications (see Fig. 1), the beginning of the seventies saw a significant number of attempts for both the numerical value of the critical disorder and the phase diagram mobility edge E_c versus degree of disorder W . Obviously, in spite of the over-simplifications present in Anderson's model, various assumptions and approximations are needed to obtain solutions. Except the 1d case [5], it was assumed that

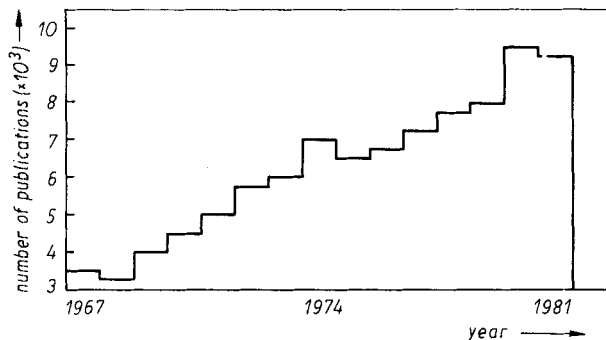


Fig. 1. Number of publications per year (source: Chemical Abstracts)

the localization depends only on the nature of disorder and the structure of the lattice. This period was somewhat troubled: quantitative discrepancies for W_c , dramatic surprises, and many hot debates have been reported. With the self-consistent theory [6, 7], an “exact approximate solution” has been provided and from 1974 begins the “era of belief” [8]. However, in the absence of a detailed picture of the localization transition and convincing experimental results at very low temperature, few predictions for physical quantities have been proposed, one of the exceptions is the concept of minimum metallic conductivity (σ_{\min}) suggested by Mott [9].

1979 is the year of the revolution. From this period the subject becomes quantitative and related to experiments. By now, a detailed picture of the localization phenomenon exists involving two fundamental mechanisms: the ideas of universal scale-dependent conductance and the singular backscattering [10]; and also a quantitative theory of weak localization [11] has been put forward. The main results obtained at $T = 0$ are that the conductivity goes to zero at the transition with a universal exponent and the effect of the dimension on the localization phenomenon, namely the existence of a lower critical dimension d^* such that for $d \leq d_c^* = 2$ there is no metallic disordered system. On the other hand, a number of spectacular novel effects such as magnetoresistance oscillation with half a flux quantum period and universal conductance fluctuations have been predicted and checked experimentally.

During this period, Altschuler and Aronov [12] analyzed the contribution of the electron–electron interaction in disordered metals and concluded on the existence of profound differences from the pure ones. These results are greatly appreciated in describing the metal–insulator transitions in doped semiconductors in which both the electron correlations and the disorder play a significant role.

Therefore, much progress has been achieved and the subject has matured, new questions have been also posed. The aim of this paper is to present an overview on the theory of localization through particular unresolved problems.

2. Electronic Properties

2.1 Electrons in crystals

Probably much of our understanding about electronic states in solid state physics is acquired from the picture of an independent electron moving in a periodic potential.

Mathematically, we refer to invariance under the translational operations of a lattice which in turn implies the condition of the validity of the Bloch theorem. Mainly the eigenstates are extended, and are distributed in energy bands separated by gaps where no solutions exist. The states are labelled by a band index and a quasi-momentum and the gaps arise from the destructive wave interference. All this is a standard theory for crystalline materials.

Deviations from periodicity, estimated as perturbation for the potential, introduce localized states with discrete energy levels lying within the gap. This is the situation for shallow donor states (e.g., Si slightly doped with phosphorus), surface states at any interface, and highly localized trap levels in semiconductors (e.g., Cu in Si). As the number of these levels increases, new effects appear. A typical case is the appearance of an impurity band when shallow impurity states in the semiconductor overlap and the system undergoes a transition from insulator to metallic behaviour.

2.2 Mott localization

It is well known for a long time that the above Bloch (or more properly the Bloch-Peierls-Wilson) theory of electrons in crystals fails qualitatively in describing NiO which is viewed as metal but is an antiferromagnetic insulator [13]. Mott [14] proposed a simple hypothetical model of a lattice of hydrogen atoms, with the lattice constant as the only variable, to isolate the qualitative effects of correlation. In the limit of small values of the lattice constant, the wave functions overlap considerably and the system, with one electron per atom, is a half-filled band metal. For large values of the lattice constant the same system is constituted by weakly interacting hydrogen atoms and becomes an insulator. To move an electron from one site to another one needs an activation energy $U = I - A$, where I denotes the energy required to ionize a hydrogen atom and A the electron affinity, respectively.

In this case, electrons are localized due to correlation. The nature of this transition occurring for a large class of systems is not yet understood in detail. In many of these systems disorder plays a significant role implying the low mobility of electrons on the metallic side of the metal-insulator transition.

2.3 Disorder system classification

Bloch theory fails also in describing disordered solids as long as the latter cannot be derived perturbatively from the perfect crystal and randomness cannot be treated in a finite order of perturbation. Thus we have to look for a theory of electronic and structure properties of disordered systems.

One would tend to think that crystals are all alike but every disordered system is disordered in its own way. As said by Brodsky [15]: "it is easier to define the amorphous state by starting what it is not than precisely specifying what it is". Therefore it appears relevant to define a certain class of disordered systems [16]. An example of classification of disordered systems is reproduced in Table 1.

2.4 Some universal features of disordered systems

Disordered solids lack the periodicity of the crystalline solids, i.e. the basic symmetry element. However, they also display certain universal characteristics which are clearly distinct from those of the crystals. These universal features are actually fairly well established experimentally and also predicted theoretically. Basing on the ideas originally due to Anderson [1], Mott [2], and Cohen et al. [17] have proposed the following simple model referred as the Mott-CFO model. Here the energy spectrum consists of bands which may overlap. Within each band there are two characteristic energies (see Fig. 2): the so-called "mobility edges", whose position depends on the degree of disorder. At these mobility edges the nature of the electronic states changes abruptly from being localized in band tails to being extended in the middle of the band. The sharpness of the mobility edge has however been a subject of controversy [16, 18, 19]. Thus the system should behave as a metal or an insulator (semiconductor) depending on whether the Fermi level lies in the region of the extended or the localized states. As the degree of disorder is increased the mobility edges move towards the centre of the band. For a critical disorder they coincide and the system undergoes a transition to an insulating phase termed "Anderson transition". We briefly mention the universal features predicted by the Mott-CFO model:

Table 1
Classification of disorder

material	system	kind of disorder
crystals	-ordered -periodic	
non-crystalline materials	-disordered -aperiodic -random	<ol style="list-style-type: none"> 1. cellular disorder → { -substitutional -compositional -quantitative 2. structural disorder → { -positional -qualitative } equilibrium → liquids non-equilibrium → { -glass -non-glassy amorphous solids 3. topological disorder 4. continuum disorder

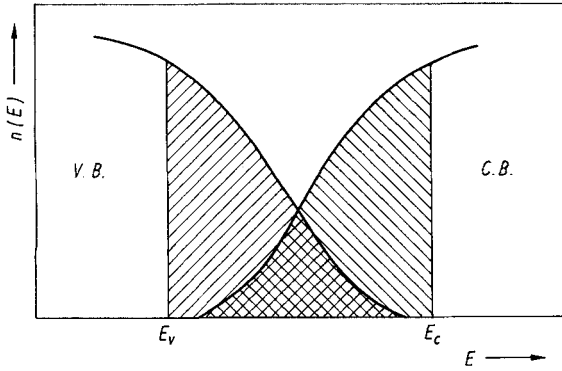


Fig. 2. Mott-CFO model for the density of states

– low temperature behaviour of dc conductivity,

$$\sigma(T) = \sigma(0) \exp\left(-\left(\frac{T_0}{T}\right)^{1/(1+d)}\right), \quad (1)$$

due to variable-range hopping [20] between localized states, where $\sigma(0)$ is the minimum metallic conductivity [21];

– low frequency ac conductivity,

$$\sigma(\omega) \sim \omega^2 \left[\ln\left(\frac{\omega}{\omega_0}\right) \right]^4, \quad (2)$$

due to exponential tailing of the envelope of the localized states [21]. This law is verified over several decades of temperature variation;

– exponential tailing [22] in the optical absorption similar to the Urbach tail, but due to nonvanishing density of states in the gap;

– fairly large concentration of the paramagnetic centres [23] (unpaired electrons due to large Coulomb correlation energy unfavouring double occupancy) in the localized states; also possibly a large diamagnetism associated with doubly-occupied states which are not too localized [24];

– it also predicts sharp change in the conductivity when E_F is made to sweep across the mobility edge as realized in inversion layers at the reverse-biased semiconductor–insulator interfaces [25, 26]. Experimental results do bear out these predictions to a great extent [3]. Some typical examples of electronically disordered systems include amorphous semiconductors, impurity band semiconductors, suitably doped covalent glasses, random binary alloys and metallic glasses, incommensurate charge-density-wave, liquid semiconductors, electron solvation [27].

In his pioneering and overquoted paper entitled “Absence of Diffusion in Certain Random Lattices”, Anderson [1] introduced the concept of disorder induced localization.

It is well established within Anderson’s model that a critical value of W , W_c^* , may exist such that all the eigenstates are localized for $W > W_c^*$. This disappearance of extended states has been referred to as Anderson transition. Most of the theoretical attention has been focussed on the Anderson model since the latter includes some universal properties characterizing disordered systems.

In spite of the oversimplifications present in Anderson’s model various assumptions and approximations are needed to obtain solutions. Although the approaches lead to the same qualitative conclusions, they differ appreciably in their quantitative results for the critical disorder W_c^* (see Table 2).

For a long time, the quantitative discrepancies in the numerical value of W_c^* have been given incidental attention. Since there was no way in checking experimentally the results. The exact value of W_c^* became a relevant quantity with the suggestion by Mott [21] that

Table 2
Critical disorder W_c^* from different models for a cubic lattice ($K = 4.68$) (in units of V) for a uniform distribution of site energies

model		W_c^*
Anderson	[1]	62
Ziman	[64]	32.6
Kikuchi	[106]	62
Economou and Cohen	[65]	32.4
Herbert and Jones	[55]	62
		41.9
		25.4
Khor and Smith	[107]	49.7
Economou et al.	[108]	24
Schönhammer and Brenig	[109]	24
Bishop	[67]	20.4
	[68]	≤ 25.2
Abou-Chacra and Thouless	[7]	62
Licciardello and Economou	[70]	22
		19.8
		14.5
Brouers and Kumar	[110]	18.5
Efros	[111]	14.4
Lukes	[112]	20.4
Domany and Sarker	[113]	24
Thouless	[114]	7.8
Pichard and Sarma	[115]	19 ± 0.5
Aoki	[116]	15
Prelovsek	[117]	10
Mac Kinnon and Kramer	[118]	16 ± 0.5
Kotov and Sadovski	[119]	13.91 to 19.67
Mc Kinnon and Kramer	[103]	16.5 ± 0.5
Elyutin et al.	[120]	19.2
Soukoulis and Economou	[40]	17 ± 2
Bulka et al.	[121]	16.5 ± 0.5
Pastawski et al.	[122]	16
Singh and Mc Millan	[123]	14.9 ± 0.4
Götze	[124]	15
Zekri and Brezini	[125]	19.9
Bulka et al.	[126]	16.3 ± 0.5
Schreiber et al.	[127]	16.5
Kroha et al.	[128]	15.8

a minimum metallic conductivity exists at $T = 0$ when the Fermi level E_F lies at the mobility edge. Using the Kubo-Greenwood formula, one can show [3] that

$$\sigma = \sigma_{\text{IR}} g^2, \quad (3)$$

where the factor g describes the reduction

$$\frac{1}{g} \left(\frac{N(E_F)}{N(E_F)|_{w=0}} \right)^{-1} = 1.74 \left(1 + \frac{W_c^{*2}}{2ZV} \right) \quad (4)$$

and $\sigma_{\text{IR}} \approx \frac{1}{3} e^2 / \hbar a$ [28]. When E_F lies at the mobility edge, (3) gives a conductivity σ_{min} where

$$\sigma_{\text{min}} = 0.03 e^2 / \hbar a. \quad (5)$$

Since σ_{min} , if it exists, is a measurable quantity, the exact value of W_c^* appears to be a relevant quantity.

3. Anderson Hamiltonian

Anderson [1] introduced the concept of localization which may be formulated in terms of the one-body, tight-binding one-band Anderson Hamiltonian on a d -dimensional hypercubic lattice (Fig. 3),

$$H^{\text{And}} = \sum_{i=1}^N \varepsilon_i |i\rangle \langle i| + \sum_{i \neq j}^N V_{ij} |i\rangle \langle j|. \quad (6)$$

Disorder is described in a particularly simple way, the static randomness is introduced through the site energies $\{\varepsilon_i\}$, i.e. the so-called diagonal disorder, and/or the transfer matrix elements $\{V_{ij}\}$, or off-diagonal disorder. Here the set $\{|i\rangle\}$ stands for the atomic "s"-like orbital centred at the lattice point "i". Indeed there are often many orbitals at each site.

It should be noticed here that the continuum analogue of this problem may be described by the Lorentz model,

$$H^{\text{Lor}} = -\frac{\hbar^2}{2m} \sum_{\alpha=1}^d \left(\frac{\partial^2}{\partial x_\alpha^2} \right) + \sum_{i=1}^N V(r - R_i). \quad (7)$$

The scatterers positioned at R_i are distributed at random. However, mathematically H^{And} and H^{Lor} are somewhat different in the sense that H^{Lor} is an unbounded operator in contrast

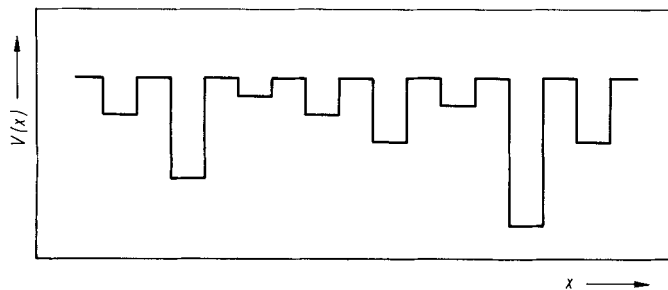


Fig. 3. Anderson random potential

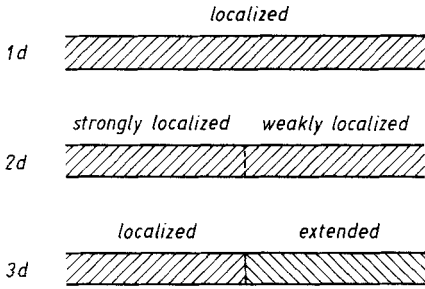


Fig. 4. Actual consensus on the Anderson transition for $d = 1, 2,$ and 3

to H^{And} . A possible model Hamiltonian that interpolates between H^{And} and H^{Lor} is the n -band Hamiltonian

$$H^{n\text{-band}} = \sum_{\nu, \mu} \sum_{i, j} V_{i\nu, j\mu} |i\nu\rangle \langle j\mu|. \tag{8}$$

The nice advantage is that $H^{n\text{-band}}$ may describe various situations:

- the statistical nuclear model of Wigner in the limit $d = 0$ and $n \rightarrow \infty$;
- the Anderson problem for $d \geq 1$ and $n = 1$;
- the Lorentz model for $d \geq 1$ and $n \rightarrow \infty$.

The following discussion will be limited, however, to the Anderson Hamiltonian. In this case the problem may be seen as a competition between the two terms of (6) which could in isolation create localized and extended states. According to recent developments on the subject, Fig. 4 presents the actual consensus on the Anderson transition in one, two, and three dimensions. The important remark is that the Anderson theorem has survived in three, but not in two dimensions.

4. Nature of the Spectrum

The spectral theory [29, 30] provides a formal description for the localization theory. The Hamiltonian H leads to a unique and invariant direct sum decomposition of Hilbert space \mathcal{H} , into three different orthogonal complements,

$$\mathcal{H} = \mathcal{H}_D \oplus \mathcal{H}_{SC} \oplus \mathcal{H}_{AC}; \tag{9}$$

here D means discrete, SC singularly continuous, and AC absolutely continuous, respectively. The state in which the electron is initially prepared may also be separated as

$$\psi = \psi_D + \psi_{SC} + \psi_{AC}. \tag{10}$$

This decomposition arises from the representation of the Hamiltonian H via its spectral measure S_M defined by

$$H = \int_{-\infty}^{\infty} E S_M(dE), \tag{11}$$

which yields

$$(\psi_i, H\psi_j) = \int_{-\infty}^{\infty} E (\psi_i, S_M(dE) \psi_j). \tag{12}$$

Since the term $(\psi_i, S_M(dE) \psi_j)$ displays the mathematical feature of a measure, it leads to a decomposition in three parts D, SC, and AC which in turn yields the corresponding decomposition of H .

Under the scheme of these three pure cases, it may be shown [30]:

- a discrete spectrum means localization, absence of diffusion, reality of the Green’s function for all the energies except a set of measure zero. This dense set corresponds to the Anderson localized states;
- a singularly continuous spectrum implies no “localization”, fast or slow diffusion, and reality of the Green’s function;
- an absolutely continuous spectrum implies no localization, fast diffusion, sometimes slow diffusion, and no reality of the Green’s function.

Thus one will associate the discrete spectrum with a truly bound-like state in the Lifshitz tail, the absolutely continuous spectrum with extended states in the middle of the band, and the singularly continuous spectrum with the disorder induced localized states.

Miller and Simon [31] have given an explicit example where such a spectral decomposition exists. Anderson [8] defined the localization “as an unrecognizable monster: e.g. singularly continuous spectra have no physical applications”. Indeed while some situations of SC spectra exist, its relation to the localization problem is still far from being achieved.

So far, we have discussed only the situation of pure cases. It is generally believed that localized and extended states with the same energy do not exist: the main argument is that admixture would delocalize the former but without any rigorous proof [32]. Recently, Srivastava [33] has cast doubt on this point by examining the possibility and the consequences of the presence of the poles of the Green’s function in the Riemann sheets of a cut z -plane. In particular, it is found that such poles lack the pure-point nature and are associated with states constituted by a “confluence” of degenerate extended and localized states. The nature of these states is shown to be different from the pure extended and localized states. They constitute a new regime of “slow” diffusion in the energy spectrum suggesting strongly the possibility of the existence of a new mobility edge separating the new regime from the absolutely continuous spectrum. Recalling the Anderson probability $P_0^\infty(t)$, the time-integral \mathcal{F} of $P_0^\infty(t)$ is given by

$$\mathcal{F} = \int_0^\infty P_0^\infty(t) dt \tag{13}$$

and the new spectrum is reported in Table 3.

In summary, a pole of the Green’s function describes a localized state in the Anderson picture only if it is isolated from the branch cut of the Green’s function. A pole can appear

Table 3
Nature of the eigenstates following the behaviour of the Anderson probability and its time-integral

$\lim_{t \rightarrow \infty} P_0^\infty(t)$	\mathcal{F}	nature of diffusion	nature of state
0	finite	fast	extended state
0	infinite	slow	confluence state
0	infinite	absence	localized state

in the branch cut losing therefore its discrete character. Such a pole cannot describe an extended state in the strict meaning since it still retains a property related with the pole representing a localized state, i.e. the divergence of \mathcal{F} . Such a particular localized state diluted in its nature from the coupling with the extended state may produce the “absence of diffusion” only in a weak sense.

Obviously, such a picture of the spectrum opens new questions:

- does the new regime, where the poles and the branch cut of the Green’s function coexist in the same energy domain, correspond to the singular continuous spectrum?

- is there any relationship between the confluence states and the power-law states [34]?

The analysis of Srivastava is particularly relevant for special types of disorder appearing in the quantum percolation model and in systems where the random potential can become infinite at some sites with a given probability. In such models, a special class of localized states has been reported: “the molecular states” which are not only localized but appear at energies which are dense in the spectrum [35].

5. Nature of the Eigenstates

The nature of the eigenstates indeed “approximate” eigenstates of disordered systems also permits a classification of the various possibilities.

5.1 Asymptotic spatial behaviour

If the energy E corresponds to the discrete spectrum, then the associated eigenstate $\psi(r)$ is normalizable, i.e. the integral

$$\int |\psi(r)|^2 d^d r \tag{14}$$

is finite. In most cases, $\psi(r)$ is known to behave exponentially [21],

$$\psi(r) \sim \exp(-r/\xi), \tag{15}$$

where ξ holds for the localization length. It should be noticed that the possibility of the existence of power-law localized states has been predicted in 2d systems [34, 36].

If the energy E belongs to the continuous spectrum, $\psi(r)$ is no longer normalizable and the integral

$$\int |\psi(r)|^2 d^d r \tag{16}$$

diverges. While the states in the case of an absolutely continuous spectrum appear to be extended over the whole system, the states corresponding to the singular spectrum tend to present some kind of self-invariant structure vanishing over very large regions and taking over again much further.

5.2 Asymptotic temporal behaviour

From time evolution, various classes of spectra and states correspond to different behaviour of an initially prepared wave function. In particular following the decay of the eigenstates different possibilities arise:

– exponential decay (or algebraic decay of rapid slope) implies normalizable, finite variance and the quadratic mean-square behaves like

$$\lim_{t \rightarrow \infty} \langle x^2(t) \rangle \sim O(t) \tag{17}$$

and therefore

$$\lim_{\omega \rightarrow 0} \sigma_{ac}(\omega) \sim \omega. \tag{18}$$

These states cannot escape to infinity;

– algebraic decay of slower descent implies normalizable and infinite variance. The limit

$$\lim_{t \rightarrow \infty} \langle x^2(t) \rangle \sim O(t^{\mu_1}) \tag{19}$$

with $0 < \mu_1 < 1$ yields:

$$\lim_{\omega \rightarrow 0} \sigma_{ac}(\omega) \sim \omega^{1-\mu_1}, \tag{20}$$

these states can escape to infinity;

– algebraic decay of still slower slope implies not normalizable and infinite variance.

Then the limit

$$\lim_{t \rightarrow \infty} \langle x^2(t) \rangle \sim O(t^{\mu_2}) \tag{21}$$

with $\mu_1 < \mu_2 < 1$ gives

$$\lim_{\omega \rightarrow 0} \sigma_{ac}(\omega) \sim \omega^{1-\mu_2} \tag{22}$$

and the states can again escape to infinity;

– no decay, i.e. extended states, implies not normalizable and infinite variance with the limit

$$\lim_{t \rightarrow \infty} \langle x^2(t) \rangle \sim O(t^{\mu_3}) \tag{23}$$

with presumably $\mu_3 \equiv 1$, hence a finite nonzero diffusion constant.

Table 4
Nature of the eigenstates from their asymptotic temporal behaviour

nature of the decay	$\lim_{t \rightarrow \infty} \langle x^2(t) \rangle$	normalization	variance	$\lim_{\omega \rightarrow 0} \sigma_{ac}(\omega)$
exponential	$\sim O(t)$	yes	finite	$\sim \omega$
algebraic	$\sim O(t^{\mu_1})$	yes	infinite	$\sim \omega^{1-\mu_1}$
	$0 < \mu_1 < 1$			
algebraic (of still slower slope)	$\sim O(t^{\mu_2})$	no	infinite	$\sim \omega^{1-\mu_2}$
	$\mu_1 < \mu_2 < 1$			
no decay	$\sim O(t^{\mu_3})$	no	infinite	$\sim \text{const} \neq 0$
	(with $\mu_3 \approx 1$)			

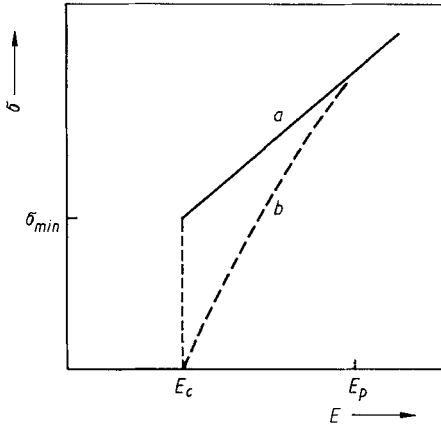


Fig. 5. Comparison of the possible behaviour of the conductivity as a function of the energy. σ_{min} denotes the minimum metallic conductivity, E_c and E_p the mobility edge and the pseudo-mobility edge. (a) Mott's prediction, (b) results of most of the experiments

While from the consensus (Fig. 4), power-law localized states may exist in 2d systems [17], they are not included in 3d systems and there is no general theorem proving their absence.

Comparison between Tables 3 and 4 seems to indicate the following correspondences:

- a) localized state → exponential decay,
- b) confluence state → algebraic decay (or power-law state),
- c) extended state → not decaying.

This remark suggests the possibility of the existence of two “pseudo”-mobility edges: one separating a) from b) and the other b) from c). A similar conclusion has been reached by Schreiber [37] giving a support to the analysis of Srivastava [33] (see Fig. 5). Probably the discrete nature of the one-band lattice Hamiltonian vis-a-vis the continuum (random potential) Hamiltonian is relevant here.

5.3 Fractal character

A new way in characterizing the wave functions of disordered systems is by their fractal dimensionality. It has been shown [38 to 42] that the localized eigenfunctions, in addition to their exponential decay, fluctuate widely with a fragmented character suggesting that they may be fractal objects. The fractal dimensionality D of such an object embedded in d -dimensional space has been determined by Mandelbrot [43] from the relation

$$\int_0^L \varrho(r) r^{d-1} dr \sim L^D, \tag{24}$$

where $\varrho(r)$ is the density and L the linear size of the object, respectively. Such a relation has no bearing in strongly disordered systems, mainly due to the strong dependence of the integral on the origin. Towards avoiding this difficulty, Soukoulis and Economou [44] proposed an alternative by averaging over all possible choices of origin, each weighted by the density itself, namely

$$A(L) \equiv \int \varrho(r_0) d^d r_0 \int_0^L \varrho(r + r_0) r^{d-1} dr \sim cL^D, \tag{25}$$

where c is a constant. The eigenfunctions are found to have a self-similar (fractal) behaviour up to length scales roughly equal to the localization length. Similar conclusions have been reported from an analysis of the inverse participation ratio in weakly disordered systems [37].

For extended states, Aoki [45] argued that the wave function at the mobility edge, which occupies an infinitesimal fraction of the volume, should have a self-similar filamentary structure with a scale invariance. Therefore, it is expected that above the mobility edge, the extended states exhibit strong amplitude fluctuations up to a length χ and for a length scale above χ they look uniform. The existence of χ is a consequence of the scaling theory [10] and serves as a support of a continuous transition.

However, a recent analysis [46] of the fluctuations of localized wave functions in d has shown the following:

- the non-self-similarity of the fluctuations in space for a single wave function which disproves the claims of fractal character;
- the multifractal character of the fluctuations with respect to disorder configurations.

So, the situation on this point is still somewhat controversial and needs further investigations to be clarified.

Even if the above classification of both spectrum and nature of the eigenstate is complete and unambiguous, its relation to the physical problem of Anderson localization is still very remote. This is mainly because one still has to bring in the probabilistic element described in the random potential.

6. Definition

We consider a system at $T = 0$. For a classical particle in a random potential (Fig. 6), it is relatively easy to decide whether its motion is confined within finite portions of space. If the energy E of the particle is greater than E_c , it can move through the whole space. In the other case, if $E < E_c$ the motion is confined within finite intervals (x_1, x_2) , (x'_1, x'_2) , etc.

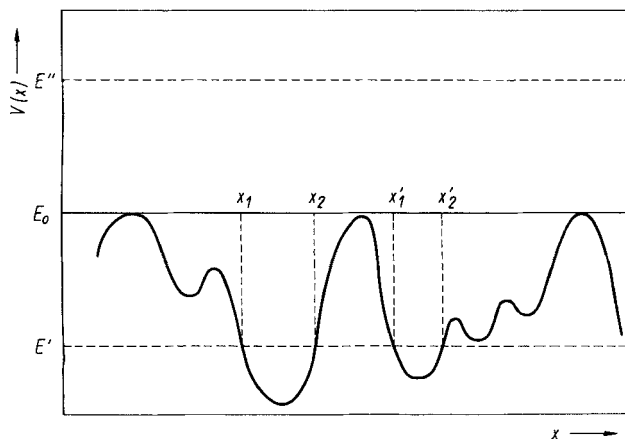


Fig. 6. Random potential

For the equivalent quantum mechanical situation, the problem is more complicated for two reasons:

- the tunnel effect which allows the particle to tunnel through the potential wells and contributes to delocalization of the particle for $E < E_c$;
- the interference effects within the wave functions scattered by the random potential which in turn may lead to the localization of the particle via destructive superposition for $E > E_c$.

Therefore, a difficulty arises in distinguishing localized from extended states and criteria of localization are needed in this context.

From a mathematical point of view: an eigenstate $\varphi(r)$ in the representation $\{|r\rangle\}$ of a Hamiltonian H is localized in a space \mathcal{R}^d if and only if a subspace Δ of \mathcal{R}^d exists with the property:

$$\int_{\mathcal{R}^d - \Delta} |\varphi(r)|^2 d^d r < \mathcal{E}, \tag{26}$$

where \mathcal{E} is a small positive quantity and $\mathcal{R}^d - \Delta$ the complement of Δ in \mathcal{R}^d , otherwise $\varphi(r)$ is extended.

In order to appreciate the localization criteria, we would like to precise the physical definition of the localized states which is based on normalization arguments. Towards this end, we consider a microscopically disordered, but macroscopically homogeneous, system of d -dimensional volume v and boundary surface S . Let $\Delta v \in v$, be a volume element, then we define

$$P_v(\Delta v \in v) = \frac{\int_{\Delta v} |\psi_v(r)|^2 d^d r}{\int_v |\psi_v(r)|^2 d^d r} \tag{27}$$

as the probability of finding the particle in the volume element Δv with the eigenstate $\psi_v(r)$ and eigenenergy E_v . Following the behaviour of P_v , we have

$$\lim_{\substack{v \rightarrow \infty \\ \Delta v \text{ fixed}}} P_v(\Delta v \in v) \rightarrow O\left(\frac{\Delta v}{v}\right) \Rightarrow \psi_v(r), \quad \text{extended state}, \tag{28}$$

$$\lim_{\substack{v \rightarrow \infty \\ \Delta v \text{ fixed}}} P_v(\Delta v \in v) \rightarrow O\left(\frac{\Delta v}{L^d}\right) \Rightarrow \psi_v(r), \quad \text{localized state}, \tag{29}$$

where L may be defined as the localization length. These statements stand also for the discrete analogue. Obviously $\psi_v(r)$ and E_v change in the limit $v \rightarrow \infty$, but we assume here that continuity allows one to keep the track of the given eigenstate. At this stage, one can make a comparison between the localized (extended) states induced by disorder and the negative (positive energy scattering) states of the well-known potential scattering theory. A deterministic potential tends to a well-defined value (vacuum level) asymptotically in the r infinite limit. Therefore, the negative energy state is bound and naturally localized. On the other hand, the random potential of a statistically disordered system does not tend to any reference value. Indeed the localized states in the Anderson sense are the “positive” energy bound states induced by interference effects.

7. Criteria of Localization

The problem of calculating the mobility edge systematically for the Anderson Hamiltonian requires some operationally well-defined and formally exact localization criterion. No wonder therefore, that diverse localization criteria have been proposed and are not necessarily equivalent in strict sense [29, 30]. In the following we briefly discuss some of the different localization criteria.

7.1 Criteria derived from the definition of the localization

These criteria are purely formal in the sense that no solution of the Schrödinger equation with random potential actually exists. In this light we examine here the problem of localization by presenting and comparing different localization criteria:

Criterion 1

The most intuitive definition of a localized state $\psi(r)$ requires the existence of the integral

$$\int |\psi(r)|^2 d^d r, \quad (30)$$

namely a localized state is normalizable.

Criterion 2

Demanding a more stringent test, one could use the existence of the integral

$$\int \psi^*(r) r^2 \psi(r) d^d r \quad (31)$$

as a definition of a localized eigenstate. This integral corresponds to the second-order moment of the wave function.

Criterion 3

Another definition of a localized eigenstate is the existence of the integral [47]

$$\int |\psi(r)|^4 d^d r. \quad (32)$$

Criterion 4

In cases where the wave function has been evaluated, i.e. usually in one dimension, $\psi(r)$ is known to behave exponentially,

$$\psi(r) \sim \exp\left(-\frac{\alpha r}{\xi}\right), \quad (33)$$

where ξ is the localization length, $\xi \sim E_c a_E / |E - E_c|^\nu$ [28]. The amplitude must also be modulated by a sinusoidal factor since different localized states are orthogonal to one another.

Criterion 5

For any point r and localized eigenstates, the spectral density

$$\int |\psi_v(r)|^2 \delta(E - E_v) dE \tag{34}$$

is discrete but dense. (For a review about these criteria see [48, 49]).

Criterion 6

One way of distinguishing between the localized and extended states is to examine the mean fourth power of the amplitude which is the reciprocal of the quantity introduced by Bell and Dean [50], the inverse participation ratio \mathcal{P}_v^N defined by

$$\mathcal{P}_v^N = \frac{\sum_{i=1}^N |\psi_i^v|^4}{\left(\sum_{i=1}^N |\psi_i^v|^2\right)^2} \leq 1 \quad \text{by Schwartz inequality,} \tag{35}$$

where ψ_i^v is the amplitude at the site i of the eigenstate ψ^v , i.e. $\langle i | \psi^v \rangle$, which measures the spread of the eigenstate. From the behaviour of $\langle i | \psi^v \rangle$, one derives

$$\lim_{N \rightarrow \infty} \mathcal{P}_v^N \rightarrow O(N^{-1}) \rightarrow \psi^v, \quad \text{extended state,} \tag{36}$$

$$\lim_{N \rightarrow \infty} \mathcal{P}_v^N \rightarrow O(N^0) \rightarrow \psi^v, \quad \text{localized state.} \tag{37}$$

For the wave equation, \mathcal{P}_v^N may also be written as

$$\mathcal{P}_v^N = \frac{\int |\psi^v(r)|^4 d^d r}{\left(\int |\psi^v(r)|^2 d^d r\right)^2} \leq 1. \tag{38}$$

\mathcal{P}_v^N has been used extensively in numerical work using computer simulation.

Weaire and Williams [51] showed how the equation-of-motion method in which quantities of interest are extracted from the time dependence of a random wave vector, could be applied. The quantity which converges most naturally from this approach is the “inverse participation ratio” which is, roughly speaking, the inverse of the number of sites over which a localized state has a significant amplitude. The average inverse participation ratio has been used for locating the mobility edge in the numerical work of Weaire and Williams [51], measuring the spread of the eigenstate.

Criterion 7

Another definition of the inverse participation ratio has been given by Kramer and Weaire [52],

$$\mathcal{P}_v^N = \sum_{i=1}^N |\psi_i^v|^4 \tag{39}$$

with

$$\lim_{N \rightarrow \infty} \mathcal{P}_v^N \rightarrow O(N^{-1}) \rightarrow \psi^v, \quad \text{extended state,} \tag{40}$$

$$\lim_{N \rightarrow \infty} \mathcal{P}_v^N \rightarrow O(N^0) \rightarrow \psi^v, \quad \text{localized state.} \tag{41}$$

A variant may also be defined as follows:

$$\mathcal{P}_v^N = N^{-1}(\mathcal{P}_v^N)^{-1} \tag{42}$$

implying

$$\lim_{N \rightarrow \infty} \mathcal{P}_v^N \rightarrow 1 \rightarrow \psi^v, \quad \text{extended state,} \tag{43}$$

$$\lim_{N \rightarrow \infty} \mathcal{P}_v^N \rightarrow 0 \rightarrow \psi^v, \quad \text{localized state.} \tag{44}$$

7.2 Absence of self-diffusion

The above statements are taken to require vanishing dc conductivity σ_{dc} at $T = 0$ which sometimes is used as a criterion of localization and appears to be a more realistic one since it may be checked experimentally.

7.2.1 Criterion based on absence of self-diffusion

As a direct consequence of the Kubo-Greenwood conductivity formula the contribution to conductivity is related to the variance of x for the eigenstate in question,

$$\int_0^\infty \omega^{-2} \sigma(\omega) d\omega = \frac{\pi e^2}{\Omega k T} \sum_v [\langle \psi^v | x^2 | \psi^v \rangle - |\langle \psi^v | x | \psi^v \rangle|^2]. \tag{45}$$

For exponential localized states, the variance is certainly finite and for a finite integral on the left $\sigma(\omega)$ must go to zero faster than ω in the limit $\omega \rightarrow 0$ and therefore $\sigma(0) = 0$. However, the possibility of weakly (algebraically) localized states makes the converse not true.

Mott argued that the main contribution to the right-hand side of (45) in the limit of small values of ω comes from coupling of states very closely together in energy such as the energy difference is much less than $\hbar\omega$ and for exponentially localized states the conductivity is of the form

$$\sigma_{ac} \sim \omega^2 (\ln \omega)^4. \tag{46}$$

7.2.2 Ioffe-Regel criterion

A well-known criterion is that of Ioffe and Regel [53]. In particular, Mott [21] made use extensively of this criterion. They argued that since the mean free path l corresponds to the distance over which the electron wave function loses its phase coherence 2π , a wavelength greater than l would be unphysical which in turn leads to the inequality

$$\lambda k > 1. \tag{47}$$

If this condition is not satisfied, the states are localized. From this criterion, Mott predicted the “minimum metallic conductivity” in two and three dimensions,

$$\sigma_{3d} > \frac{e^2 k_F}{3\pi^2 \hbar} \quad (48)$$

and

$$\sigma_{2d} > \frac{e^2}{2\pi \hbar}. \quad (49)$$

However, according to Souillard [54], the Ioffe-Regel criterion seems to be certainly not exact, but gives a qualitative rather than a quantitative picture of the phase diagram.

7.3 Criteria based on the analytic properties of the one-particle propagator

7.3.1 Criterion based on the dependence of the propagator on the distance

The question of localization has been examined by Herbert and Jones [55] via the dependence of the propagator

$$G_{ij}(z) = \langle i | (z - H)^{-1} | j \rangle \quad (50)$$

on the distance R_{ij} in the limit $R_{ij} \rightarrow \infty$. For extended states it is expected that

$$G_{ij} \sim R_{ij}^{-1} \quad (51)$$

as $R_{ij} \rightarrow \infty$, while for localized states exhibiting exponential decay

$$G_{ij} \sim \exp(-R_{ij}/R^d), \quad (52)$$

where R^d is defined as the localization length.

Such an approach, although more direct, has the disadvantage of dealing with a more complicated quantity like G_{ij} and requires additional approximations.

7.3.2 Criterion based on the analytic properties of the propagator

We consider a finite N -site system described by a complete set of local states $|i\rangle$, $i = 0, 1, 2, \dots, N$, each one associated with a given site i of the lattice. We examine the evolution of the electron wave packet $|\psi(t)\rangle$ prepared initially at the site 0, i.e.,

$$|\psi(t)\rangle = \exp\left(-\frac{iHt}{\hbar}\right) |0\rangle. \quad (53)$$

The propagator $G_{ij}^N(t)$ which measures the amplitude for the transition $i \rightarrow j$ is defined as

$$G_{ij}^N(t) = -\frac{i}{\hbar} \langle j | \exp\left(-\frac{iHt}{\hbar}\right) | i \rangle \quad \text{for } t \geq 0, \quad (54)$$

$$= 0 \quad \text{for } t < 0, \quad (55)$$

and its complex Fourier transform

$$G_{ij}^N(z) = \langle j | (z - H)^{-1} | i \rangle \quad (56)$$

is analytic for $\text{Im}(z) > 0$, i.e. in the upper half-plane. It is convenient to introduce the spectral representation

$$G_{ii}^N = \sum_{v=1}^N \frac{\langle i | v \rangle \langle v | i \rangle}{z - E_v^N} = \sum_{v=1}^N \frac{|\langle i | v \rangle|^2}{z - E_v^N}, \quad (57)$$

where E_v^N is the exact eigenenergy associated to the eigenstate $|v\rangle$.

G_{ii}^N is analytic everywhere on the complex z -plane except at the eigenvalues of the Hamiltonian H where a simple pole behaviour is exhibited. In the present situation the quantities E_v^N and $|\langle i | v \rangle|^2$ are random variables since they are functions of the random variables $H_{ii} = \langle i | H | i \rangle$. Thus the singularities of $G_{ii}^N(z)$ give the spectrum of H and the residues $|\langle i | v \rangle|^2$ evaluated at the poles of $G_{ii}^N(z)$ give the overlap of the state $|v\rangle$ with the site orbital $|i\rangle$. Obviously we are interested in the limit $N \rightarrow \infty$. In such a limit and for a given but compact disorder, the spectrum of H is bounded and therefore saturates to some finite energy interval. The number of states scales as N and then the set of poles becomes dense.

7.3.3 Criterion based on the residue

If the eigenstate $|v\rangle$ is extended as $N \rightarrow \infty$, i.e. the overlap $\langle i | v \rangle$ is relatively appreciable for an infinite number of states $|i\rangle$, the renormalization implies

$$|\langle i | v \rangle|^2 \sim O(N^{-1}) \quad (58)$$

for all states $|i\rangle$. Thus the dense set of poles of $G_{ii}(z)$ forms a fixed branch cut along the real axis.

On the other hand, for localized states $\langle i | v \rangle$ is appreciable only for a finite number of states $|i\rangle$ as $N \rightarrow \infty$ which defines the domain of localization and then

$$|\langle i | v \rangle|^2 \sim O(N^0). \quad (59)$$

Thus, only a finite number of sites i with residue $|\langle i | v \rangle|^2$ exceeds a preassigned quantity describing the domain of localization. The dense set of poles constitutes a natural boundary.

7.3.4 Criterion based on the line of singularities

As $N \rightarrow \infty$ the spectrum of the Hamiltonian turns to lines of singularities for $G_{ii}^\infty(z)$. In other words, the limit

$$\lim_{N \rightarrow \infty} \left[\lim_{s \rightarrow 0} \pm G_{ii}^N(z) \right] \quad (60)$$

does not exist, where $z = E + is$ and E belongs to the energy band. Because of the different behaviour of $|\langle i | v \rangle|^2$ as $N \rightarrow \infty$, the lines of singularities are of different nature.

In the case of extended states the parts of the spectrum become branch cut as $N \rightarrow \infty$. The limit

$$\lim_{s \rightarrow 0} \pm \left[\lim_{N \rightarrow \infty} G_{ii}^N(z) \right] \quad (61)$$

exists. On the other hand, the parts of the spectrum associated with localized eigenstates become natural boundaries as $N \rightarrow \infty$, because the limit

$$\lim_{s \rightarrow 0} \pm \left(\lim_{N \rightarrow \infty} G_{ii}^N(z) \right) \tag{62}$$

does not exist due to the fact that the residue $|\langle i | v \rangle|^2$ remains finite as $N \rightarrow \infty$.

In summary, the side limits

$$\lim_{s \rightarrow 0} \pm \text{Im} \left(\lim_{N \rightarrow \infty} G_{ii}^N(z) \right) \tag{63}$$

exist and are nonzero in the extended regime, while the side limits are zero almost everywhere in the localized regime, except if E corresponds to the eigenvalue where these do not exist.

7.3.5 Criterion based on absolute squared propagator

The above discussion on the overlaps $\langle i | v \rangle$ yields the following condition:

$$\lim_{N \rightarrow \infty} \left(\lim_{s \rightarrow 0} \pm \text{Im} z |G_{ij}^N(z)|^2 \right) = \pi \sum_v |\langle i | v \rangle|^2 |\langle j | v \rangle|^2 \delta(E - E_v) \tag{64}$$

if the limit vanishes as $O(N^{-1})$: $|v\rangle$ is an extended state and if the limit is a nontrivial function of the distance $|i - j|$, $|v\rangle$ is then a localized state [56].

7.3.6 Criterion based on absolute squared locator [1]

Localization implies a nonzero probability $P_{00}^N(t)$ of finding the particle where it was initially prepared ($t = 0$) after an infinite time ($t \rightarrow \infty$) has elapsed in the limit $N \rightarrow \infty$. It may be shown

$$\lim_{N \rightarrow \infty} \left(\lim_{t \rightarrow \infty} P_{00}^N(t) \right) = \lim_{N \rightarrow \infty} \left(\lim_{t \rightarrow \infty} \frac{1}{t} \int_0^t |G_{00}^N(t')|^2 dt' \right) = \int_0^\infty F_{00}^\infty(E) dE, \tag{65}$$

where

$$F_{00}^\infty(E) = \lim_{N \rightarrow \infty} \left(\lim_{s \rightarrow 0} \frac{s}{\pi} G_{00}^N(E + is) G_{00}^N(E - is) \right). \tag{66}$$

Therefore, one can deduce:

$$\begin{aligned} F_{00}^N(E) = 0 &\rightarrow \text{extended state at } E, \\ F_{00}^N(E) > 0 &\rightarrow \text{localized state at } E. \end{aligned} \tag{67}$$

7.4 Criteria based on convergence in probability of series

7.4.1 Criterion based on convergence of the diagonal matrix element $G_{ii}(z)$

Another way to distinguish between extended and localized states is to consider the convergence of $G_{ii}^N(z)$ in the limit $N \rightarrow \infty$ [57]. Since $|\langle i | v \rangle|^2$ and E_v^N are random variables, the convergence must be examined in terms of probability. The locator is given by

$$G_{ii}^N(z) = \sum_v \frac{|\langle i | v \rangle|^2}{z - E_v^N}. \tag{68}$$

Each term of the series $|\langle i | v \rangle|^2 / (z - E_v^N)$ becomes important in the limit $z \rightarrow E$, where E belongs to the spectrum only if

$$|E - E_v^N| \leq A |\langle i | v \rangle|^2, \tag{69}$$

namely if $E \in I_v$, where I_v is the interval

$$[E_v^N - A |\langle i | v \rangle|^2; E_v^N + A |\langle i | v \rangle|^2] \tag{70}$$

with $A \ll 1$. Within the interval I_v , one can define the union U_{v_0} of I_v such as the contribution of all the terms with $v > v_0$ is dominant.

$G_{ii}^N(z)$ may be developed such that the terms in the sum (68) are in the order of decreasing $|\langle i | v \rangle|^2$. For localized states, the extent of the integral I_v decreases exponentially in the limit $v \rightarrow \infty$ or equivalently $N \rightarrow \infty$. Consequently the extent of the union U_{v_0} goes to zero as $v_0 \rightarrow \infty$. Thus the probability of E belonging to U_{v_0} goes to zero as $v_0 \rightarrow \infty$ and the series for $G_{ii}^N(z)$ converges as $N \rightarrow \infty$ with probability distribution for $G_{ii}^N(z)$ which converges as $N \rightarrow \infty$.

For extended states, the union U_{v_0} goes to a nonzero value as $v_0 \rightarrow \infty$ implying that the series for $G_{ii}^N(z)$ diverges as $N \rightarrow \infty$ with probability unity, i.e. the probability distribution of $G_{ii}^N(z)$ diverges as $N \rightarrow \infty$.

7.4.2 Criterion based on convergence of the perturbation series for the self-energy

No review of localization is complete without a discussion of the approach based on the convergence in probability of the renormalized perturbation series (RPS) of the site-diagonal self-energy, due originally to Anderson.

The analytic properties of the diagonal matrix elements $G_{ii}^N(z)$ may be re-expressed in terms of the self-energy $S_i^N(z)$ defined by

$$G_{ii}^N(z) = \frac{1}{z - \varepsilon_i - S_i^N(z)} \tag{71}$$

with the property

$$\text{sgn Im} \{S_i^N(z)\} = -\text{sgn Im} \{z\}. \tag{72}$$

One verifies $S_i^N(z)$ to be analytic in the whole complex z -plane except for a possible cut on the real axis corresponding to the extended states. This implies nonconvergence of any series representation as the energy approaches the localized to delocalized transition, i.e. the mobility edge E_c .

The problem may be solved by expressing the self-energy $S_0(z)$ in the well-known Brillouin-Wigner perturbation series (PS),

$$S_0(z) = \sum_{i \neq 0} \frac{V_{0i}V_{i0}}{z - \varepsilon_i} + \sum_{\substack{i \neq 0 \\ i \neq j}} \sum_{j \neq 0} \frac{V_{0i}V_{ij}V_{j0}}{(z - \varepsilon_i)(z - \varepsilon_j)} + \dots \tag{73}$$

Since the PS contains random terms, i.e. the set $\{\varepsilon_i\}$, the convergence has to be treated in terms of probability. The PS may diverge apparently because of vanishing denominators

involving multiple scattering on a finite number of sites. From the Feenberg theory this simply shifts the energy levels and therefore the PS may be rearranged as a renormalized perturbation series (RPS),

$$S_0(z) = \sum_{i \neq 0} \frac{V_{0i} V_{i0}}{z - \varepsilon_i - S_i^{(0)}(z)} + \sum_{\substack{i \neq 0 \\ i \neq j}} \sum_{j \neq 0} \frac{V_{0i} V_{ij} V_{j0}}{(z - \varepsilon_i - S_j^{(0,i)}(z))(z - \varepsilon_j - S_i^{(0)}(z))} + \dots, \quad (74)$$

where the superscripts 0, i , ... denote that the corresponding quantity has been calculated for $\varepsilon_0 = \dots = \varepsilon_i = \dots = \infty$. The RPS can be represented by all paths which start and end at the site 0 without visiting the same site more than once, i.e. the self-avoiding walks. Now the RPS can diverge for two distinct reasons:

- as an infinite series;
- because a given term itself may diverge due to iterations implicit in the $S_i^{(\dots)}(z)$

occurring in the denominators.

The quantities $S_i^{(\dots)}(z)$ may be expressed through relations similar to (69). Iterating this procedure to eliminate all the unknown quantities yields an infinite continued fraction in each term of the RPS of the form

$$S_0(z) = \sum_{i \neq 0} V_{0i} \left[z - \varepsilon_i - \sum_{\substack{j \neq i \\ i \neq 0}} V_{ij} \left[z - \varepsilon_k - \sum_{l \neq k} \dots \right]^{-1} V_{ji} \right]^{-1} V_{i0}, \quad (75)$$

i.e. the renormalized perturbation expansion (RPE) (75) constitutes an explicit closed solution for the self-energy $S_0(z)$ for a finite system. For a finite system of N sites $S_0(z)$ may be written as

$$S_0^N = \sum_{p=2}^N S_{0(p)}^N(z), \quad (76)$$

where $S_{0(p)}^N(z)$ describes the sum of all diagrams visiting p sites. Following the nature of the eigenstates, the RPE and the RPS display different properties.

The absence of extended states implies that:

- the probability distribution of $S_{0(p)}^N(z)$ converges as $N \rightarrow \infty$;
- the contribution of all terms $S_{0(p)}^N(z)$ where $p > p_0$ are negligible as $p \rightarrow \infty$.

If both these two conditions are satisfied, the states at E are localized.

Divergence of the RPE implies divergence of the RPS but not the other way around. However, it is generally assumed that the convergence of the RPS is equivalent to the convergence of the RPE, in order to examine the convergence of the former and to eliminate mathematical complications, but without rigorous proof. Most model calculations on the statistical convergence in probability of the RPS must introduce additional approximations:

- omit altogether the self-energies in the propagators;
- assumption of statistical independence or strong correlations of the diagrams, etc.

At this stage, Anderson [1] suggested to study the self-energy itself rather than any series representation. This has been somewhat achieved through the self-consistent theory.

7.4.3 Criterion of Abou-Chacra et al.

In this self-consistent theory [6, 7], the RPS for the self-energy S_0 is truncated after its leading term

$$S_0(z) = \sum_{i \neq 0} \frac{|V_{i0}|^2}{z - \varepsilon_i - S_i^{(0)}(z)}. \quad (77)$$

In this analysis the equation is treated by a self-consistent method in the sense that a given probability distribution for ε_i and an assumed probability distribution for $S_i^{(0)}(z)$ must generate the same for S_0 , since S_0 and $S_i^{(0)}(z)$ are defined by similar equations.

S_0 may be used whether or not states are localized by separating real and imaginary parts, then

$$z = E + i\eta \quad (78)$$

implies

$$S_0(E + i\eta) = R_0 - i\Delta_0. \quad (79)$$

For extended states Δ_0 tends to a constant $\tilde{\Delta}$ as $\eta \rightarrow 0$, physically $\tilde{\Delta}$ is a measure of the rate at which a particle with energy E at the site 0 will escape. For localized states, Δ_0 is proportional to η and one can define the ratio

$$\lim_{\eta \rightarrow 0} \frac{\Delta_0}{\eta} = \sum_{i \neq 0} \frac{|\langle i | \varphi \rangle|^2}{|\langle 0 | \varphi \rangle|^2}, \quad (80)$$

which describes the extent of the localization domain of the eigenstate $|\varphi\rangle$.

In the limit of small η , we get for the localized states

$$R_0 = \sum_{i \neq 0} \frac{|V_{0i}|^2}{E - \varepsilon_i - R_i} \quad (81)$$

and

$$\frac{\Delta_0}{\eta} = \sum_{i \neq 0} \frac{|V_{0i}|^2 (1 + \Delta_i/\eta)}{(E - \varepsilon_i - R_i)^2}. \quad (82)$$

In this approximation the Laplace transform $f(s)$ of the probability distribution $P(\Delta/\eta)$ is given by

$$f(s) = \left[\int_{-\infty}^{\infty} P(E - x) f\left(\frac{sV^2}{x^2}\right) \exp\left(-\frac{sV^2}{x^2}\right) dx \right]^K, \quad (83)$$

where $P(x)$ is the probability distribution of $x_i = \varepsilon_i + R_i$. For extended states, one can expect to reach solutions of this equation by iteration collapsing to the trivial solution which is unity for $s = 0$ and zero otherwise, while for localized states there should be a nontrivial solution.

7.4.4 *Criterion of Logan and Wolynes*

In their model [58], the self-consistency conditions of Abou-Chacra et al. [6, 7] are simplified in such a way that they analyse algebraic equations rather than integral equations by demanding only the most probable value of the self-energy to be self-consistently determined instead of its probability distribution.

7.4.5 *Criterion of Kumar et al.*

A criterion for the existence of localized states overlapping with a given site 0 may be obtained by considering the diagonal element of the Green's function [59],

$$G_{00} = (E - \varepsilon_0 - S_0(E))^{-1}. \tag{84}$$

The pole $E_p = \varepsilon_0 + S_0(E)$ describes the energy of a localized state $|\varphi\rangle$ of the system and the residue

$$P_{00} = |\langle 0 | \varphi \rangle|^2 = \left(1 - \frac{dS_0(E)}{dE} \right)_{E=E_p}^{-1} \tag{85}$$

evaluated at this pole gives the overlap between the localized state $|\varphi\rangle$ and the site wave function $|0\rangle$. For extended states $|\varphi\rangle$, the residue $|\langle 0 | \varphi \rangle|^2$ with any site 0 vanishes as $O(N^{-1})$ and goes to $O(N^0)$ for localized states with probability. Therefore, the mobility edge E_c may be defined as the energy for which the derivative of the self-energy becomes infinite with probability unity. Defining $Y_0 = -dS_0/dE$ and differentiating $S_0(E)$ yields

$$Y_0 = \sum_{i \neq 0} \frac{V^2(1 + Y_i)}{(E - \varepsilon_i - S_i)^2}. \tag{86}$$

The problem is also treated by a self-consistent method in the sense that given probability distributions $P_S(S_i)$ and $P_Y(Y_i)$ must generate the same for $P_Y(Y_0)$. The Laplace transform of the self-consistent probability distribution $P_Y(Y)$ satisfies the general non-linear integral equation

$$P_Y(s) = \left[\int_{-0}^{\infty} P_z(x + E) \exp\left(-\frac{sV^2}{x^2}\right) P_Y\left(\frac{sV^2}{x^2}\right) \right]^K. \tag{87}$$

In comparing with the model of Abou-Chacra et al., one can conclude a perfect equivalence.

7.4.6 *Criterion of Heinrichs*

The model of Kumar et al. has been simplified by Heinrichs [60] by demanding only the average value of the derivative Y_0 to be self-consistently determined rather than the probability distribution at the cost presumably of loss of localization properties.

These models are exact for the Bethe lattice (Fig. 7) because of its particular topology: the only self-avoiding walk which returns to the initial point is the walk with two steps and both these theories may be viewed as the high-dimensional limit of the localization theory.

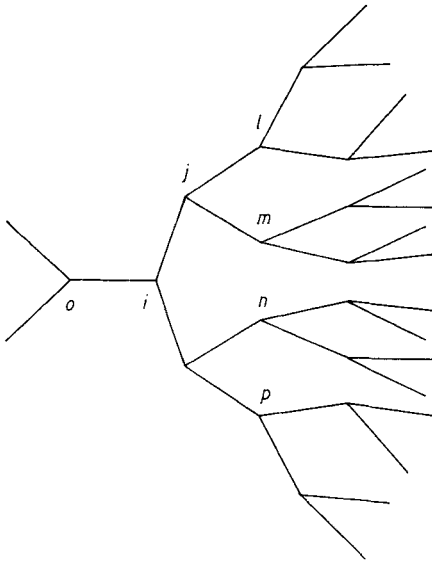


Fig. 7. Bethe lattice of connectivity $K = 3$

7.5 Sensitivities of eigenvalues to boundary variations

This criterion [61, 62] is also related to the normalized behaviour in the limit $N \rightarrow \infty$. As a matter of fact an extended state is spread out over the whole lattice and thus questions the boundaries. The change of boundary conditions, namely from periodic to antiperiodic to avoid surface effects, shifts the energy levels. More generally the convenient form of boundary conditions is the generalized periodic condition in a box of size L . The variation

$$\psi(x, y, z + L) = \exp(i\eta) \psi(x, y, z) \tag{88}$$

adds a term

$$\Delta H^N = \frac{\hbar\eta}{mL} \left(-i\hbar \frac{\partial}{\partial z} \right) + \frac{\hbar^2\eta^2}{2mL^2} \tag{89}$$

to the Hamiltonian. The result is that the energy shift ΔE_v^N will behave like

$$\Delta E_v^N \sim O(N^{-1}) \tag{90}$$

in the limit $N \rightarrow \infty$ for extended states and, on the other hand,

$$\Delta E_v^N \sim O(\exp(-aN^{1/d})) \tag{91}$$

for localized states, where a stands for the inverse localization length. This criterion has been shown powerful in numerical work. The main advantage is that the sensitivity to boundary conditions of the energy levels may be related to the conductance of the system at that energy which is in turn a measurable quantity and may be checked against experimental results.

7.6 Boundary conditions and resistance

In a hypothetical experiment [63] we assume an electron initially prepared ($t = 0$) in a wave packet at the centre of a system which is supposed to be many mean free paths large. Until it has reached the boundary at a distance $L_1/2$ from the centre its motion is insensitive to boundary conditions. Once it has reached the boundary, its motion will be perturbed. If $\Delta\tau$ is the time to travel through a distance L_1 and D the diffusion constant, we have from the uncertainty relation

$$\Delta E \sim \frac{\hbar}{\Delta\tau} = \frac{\hbar D}{L_1^2}. \tag{92}$$

Combining it with the Einstein relation yields the conductivity

$$\sigma = \frac{e^2}{2} D \frac{dn}{dE}, \tag{93}$$

here n stands for the density of states. The sensitivity of the energy levels to boundary conditions in a system defined by L_1 , L_2 , and L_3 is given by

$$\Delta E = \frac{2\hbar}{e^2} \frac{\sigma L_2 L_3}{L_1} \frac{1}{L_1 L_2 L_3} \frac{dE}{dn}, \tag{94}$$

$$\Delta E = \frac{2\hbar}{e^2 r} \frac{dE}{dn}, \tag{95}$$

where r is the resistance of the system and dE/dn the average spacing between energy levels. Thus the ratio of the spacing between energy levels to the sensitivity to the boundary conditions is linear to the resistance of the system.

If instead of changing periodic by antiperiodic boundary conditions, but the original cell being surrounded by statistically similar cells, the sensitivity to the boundary conditions ΔE gives the strength V' of a given level on one cell to its neighbours and the spacing dE/dn measures the amount W' by which a given energy level on one cell fails to match the nearest level on its neighbours (Fig. 8). Therefore, the original Anderson problem is rescaled:

$$\frac{W}{V} \rightarrow \frac{W'}{V'} = \frac{re^2}{2\hbar}. \tag{96}$$

This result may be viewed as a localization criterion, i.e. the resistance per cell determines whether or not states are localized:

- if $\Delta E/(dE/dn) = W'/V'$ is exponentially small, the eigenstate of the $(2(L_1, L_2, L_3))^d$ sample will be localized mainly in one of the $(L_1, L_2, L_3)^d$ samples.
- if $\Delta E/(dE/dn) = W'/V'$ is large, the eigenstate of the $(2(L_1, L_2, L_3))^d$ sample will be spread out over all the $(L_1, L_2, L_3)^d$ samples and thus be extended.

The essential point is that the resistance r or the conductance G are physically measurable quantities directly related to the ratio $\Delta E/(dE/dn)$ and appears to be the a simple parameter determining the behaviour of the localization properties of the system as it grows in size.

Assuming statistical independence of the K^L terms, Anderson showed that the sum of the K^L was dominated by the largest term which gave a factor $\ln(A/W)$ and hence the criterion becomes

$$W_c^* = 2ekV \ln(eK). \tag{101}$$

Herbert and Jones [55] and Economou and Cohen [65] argued that statistical independence was impossible and considered very strong statistical correlation such that the crude estimate was better.

Economou and Cohen [65] introduced an approximate theory of the mobility edge E_c by means of a localization function $L(E_c)$ such that $L(E) \neq 1$ indicates extended (localized) states at E_c and $L(E) = 1$. They find

$$L(E) = L_z(E) = ZV \exp(-\langle \ln|E - E_c| \rangle), \tag{102}$$

where the average is taken over the probability distribution of ε . L_z was firstly introduced by Ziman [64]. Within the framework of an effective medium theory [66] a more sophisticated approximation to $L(E)$ retains the self-energies in the denominators of (98), the localization function (102) is then replaced by

$$F(E) = \frac{ZV}{|E - \Sigma(E)|}, \tag{103}$$

where $\Sigma(E)$ is the effective medium site energy. This is referred to as an exact estimate of the region of localized eigenstates.

Their results, in the ordered limit, lead to extended states in the band and localized states outside the band, and in the general situation yields the same criterion in terms of the renormalized energy in the effective medium $E - \Sigma(E)$.

Bishop [67, 68] examined more carefully the Economou-Cohen criterion by using a more relevant approximation for $\Sigma(E)$ obtained for the CPA calculation.

Abou-Chakra et al. [6, 7] have developed a self-consistent localization criterion referred to as exact on the Cayley tree equivalent to the Anderson criterion in terms of the analyticity of the RPS for the self-energy. In particular this gives a qualitatively similar behaviour to Bishop's evaluation of the Economou-Cohen criterion, at least for a uniform distribution for site energies $\{\varepsilon\}$ (see Fig. 11).

Indeed, the Economou-Cohen criterion given by (102) is in fact a way to estimate whether localization exists from the average one-particle Green's function. Thouless [48, 69] suggested that (102) is not a localization criterion in the same sense as, say, the vanishing of the conductivity is, but it is an estimate of whether localization is likely.

Licciardello and Economou [70] have attempted to obtain a more sophisticated approximation to $L(E)$,

$$L(E) = \lim_{M \rightarrow \infty} (V^{n+1} \sum \tilde{G}_{n_1}^0 \tilde{G}_{n_2}^{0n_1} \dots \tilde{G}_{n_M}^{0n_1 \dots n_{M-1}}), \tag{104}$$

where the \sum indicates summation over all the indices n_1, n_2, \dots, n_M with the restrictions corresponding to all self-avoiding paths of order M starting and ending at the site 0 and at the same time estimated the errors introduced thereby. A general scheme for

evaluating the average in (102) is to introduce an effective Hamiltonian satisfying the relation

$$\begin{aligned} \ln \tilde{G}_{n_i}^{0\dots n_i-1}(E) &\equiv \langle \ln | \langle n_i | (E - H^{0\dots n_i-1})^{-1} | n_i \rangle \rangle_{\text{av}} \\ &\approx \ln | \langle n_i | (E - H^{0\dots n_i-1})^{-1} | n_i \rangle |. \end{aligned} \quad (105)$$

Using the single-site CPA [66] according to which H is determined by a single effective energy $\Sigma(E)$ and additional approximations leads to a new criterion,

$$L_l(E) = KV \left| G_n(E - \Sigma(E)) - \frac{G_{nm_i}(E - \Sigma(E)) G_{m,n}(E - \Sigma(E))}{G_n(E - \Sigma(E))} \right|. \quad (106)$$

The localization function $L_l(E)$ is referred and expected to be a definite improvement over the old localization criterion.

7.7.2 Numerical results

The first numerical attempts simply calculate eigenvectors of the Anderson Hamiltonian for some large array of sites. In the outstanding example, Yoshino and Okazaki [38] used a method of matrix diagonalization and obtained eigenvectors of a 2d system with $10^2 \times 10^2$ sites. Licciardello and Thouless [71, 72] used a more powerful approach, where only eigenvalues were calculated, the degree of localization being related to the sensitivity of the eigenvalues to changes in the boundary conditions.

Various attempts to develop still more refined methods have been proposed. Weaire and Williams [51] showed how the equation of motion method, in which the quantities of interest are extracted from the time dependence of a random wave vector, could be applied to the localization problem. The quantity which emerges most naturally from this approach is the “inverse partition ratio”. The recursion method has much in common with the equation of motion method [73].

However, difficult questions of interpretation [74] arise. The essence of the method is the transformation of the Hamiltonian into one which has the topological structure of a semi-infinite chain [75].

Prelovsek [76] has developed another simulation equivalent to the equation of motion in the sense that the time-dependent Schrödinger equation is to be integrated. However, he simply takes a wave packet which admits a Gaussian envelope in space and consists of eigenvectors from a particular energy range and looks at its spread with time. For extended states, it expands in the manner characteristic of diffusion ($r \sim t^{1/2}$), otherwise the wave packet remains localized.

All the above methods may be adapted to the calculation of the conductivity from the Kubo-Greenwood formula [77] except the method of Licciardello and Thouless which yields the conductivity rather directly.

8. Theories of Localization

A vast amount of literature has been accumulated during recent years on the approach to Anderson localization based on the analogy with the phase transition problem, even though no cooperative effects are involved here. We just briefly mention the underlying ideas of some of these not very successful approaches. It is well-known that the classical analogue

of the Anderson localization problem is the percolation [78 to 80], which can be treated as a particular case of magnetic phase transition [81]. The localization problem itself bears similarity to the problem of self-avoiding random walks on a lattice which in turn is equivalent to the excluded-volume problem of polymers. As pointed out by de Gennes [82] the latter may be mapped onto the problem of statistical mechanics of a nonrandom system of n -component classical fields in the limit $n \rightarrow 0$. This idea was further explored by Emery [83], Des Cloizeaux [84], and others within the framework of the renormalization group theory [85].

However, the failure of these approaches was essentially due to the fact that the sign of the quartic term in the effective free energy function was negative. Physically, the failure could be traced to the fact that the equivalence was based on the configurationally-averaged one-particle propagator which has no bearing on the localization problem. Motivated by this realization, Nitzan et al. [86] examined the renormalization group properties of the averaged absolute squared single propagator and found no fixed point. Similar conclusions have been obtained by Aharony et al. [87] who mapped the localization problem to a nonrandom nm spin model, where the effective Hamiltonian has n spins each having m components at each lattice site and the limit $n \rightarrow 0$ and $m = 1$ is to be taken at the end. Their negative results only showed that the localization problem is much more subtle [88]. Less controversial are the scaling theories which borrow only the general style of thinking associated with the renormalization group approach to the analysis of phase transitions [89 to 94].

Abrahams et al. [10] developed a scaling theory of localization in analogy with the scaling theories of critical phenomena. The first step is that a large disordered system can be divided into blocks large compared with the mean free path for electrons, but small compared with the size of the system.

8.1 Scaling theory

Let us consider an electron in a disordered medium. The phase of its wave function is modified at random. The length over which the fluctuation is about 2π defines the mean free path l . The averaged one-particle propagator is

$$\langle G(r) \rangle \sim \exp\left(-\frac{r}{l}\right). \quad (107)$$

For the localization problem, the microscopic length scale of interest is l . The conductance g_0 at this length scale is a signature of the amount of disorder.

In the limit $l \gg k_F^{-1}$, i.e. the Fermi wavelength, the conventional transport theory leads to a conductivity of the form

$$\sigma = \frac{ne^2\tau}{m} = \frac{ne^2l}{\hbar k_F}, \quad (108)$$

where n is the electron density and $\tau = l/k_F$ the relaxation time. The conductance for a hypercube of linear dimension $L \gg l$ in this "ohmic" regime is given by

$$g(L) = \sigma L^{d-2}. \quad (109)$$

On the other hand, for localized states the microscopic length scale is the localization length ξ which in general is greater than unity.

In this regime and for $L \gg \xi$, the conductance for exponentially localized states is

$$g(L) = g_c \exp(-L/\xi). \tag{110}$$

Abrahams et al. [10] argued that the Gell-Man-Low function

$$\beta(g) = \frac{d \ln g}{d \ln L} \tag{111}$$

is depending on only one parameter g which in turn leads to three regimes for β :

- large conductance $g \gg g_c$: $\beta = d - 2$,
- small conductance $g \ll g_c$: $\beta = \ln(g/g_c)$,
- perturbative regime: since a conduction in a disordered system is never quite ohmic, the perturbative theory yields in the limit of weak disorder, $\beta(g) = d - 2 - a/g$.

The scaling curve may be constructed (see Fig. 9) involving (110) and (111) under the assumptions that $\beta(g)$ is continuous and monotonic. Physically $\beta(g)$ has been assumed monotonic in g with respect to the fact that greater disorder means more localization. Therefore, the only singularities are the fixed points corresponding to $\beta = 0$. The consequences are the following:

- for $d \leq 2$ all the states are localized;
- for $d > 2$ near the transition the conductivity behaves as

$$\sigma \sim \left(\frac{g_0 - g_c}{g_c} \right)^{\nu(d-2)} \tag{112}$$

with $\nu < 1$.

The “revolution of the gang of IV” has pointed out two new features on the localization problem:

- the effect of the dimension;
- the conductivity vanishes continuously at the mobility edge with a universal exponent and the transition is thus a second-order transition in disagreement with the previous prediction of the Mott concept of σ_{min} .

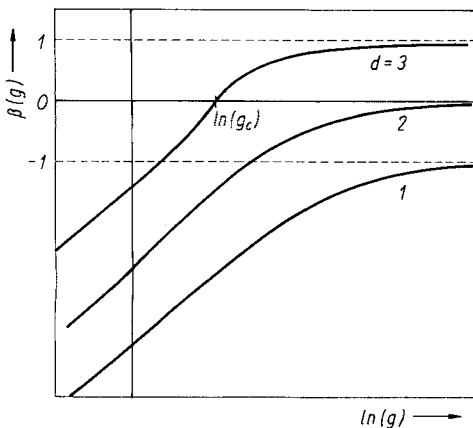


Fig. 9. Scaling curve of conductance $\beta(g)$ for different dimensions $d = 1, 2$, and 3

8.2 Scaling near the mobility edge

Earlier, Wegner [89] has considered the correlations of wave functions in an ensemble of disordered electronic systems. In this theory, the fundamental idea is to perform successive orthogonal transformations which mix nearby states in such a way that the transfer energies V decrease. For localized states, this procedure converges and the limit of convergency corresponds to the mobility edge. Additional to this elimination process, a transformation is needed to rescale both distances and energies. Two kinds of fixed point distributions are proposed: one homogeneous and the other one inhomogeneous.

The eigenstates of the Hamiltonian

$$H = \sum_r \varepsilon_r |r\rangle \langle r| + \sum_{r \neq r'} V_{rr'} |r\rangle \langle r'| \quad (113)$$

are obtained by iterating the orthogonal transformations

$$|r^{(l)}\rangle_l = \sum U_{r^{(l)} r^{(l-1)}}^{(l)} |r^{(l-1)}\rangle_{l-1} \quad (114)$$

with

$$|r^{(0)}\rangle_0 \equiv |r\rangle.$$

In this elimination procedure the transfer matrix elements $V^{(l)}$ in terms of the states $|r^{(l)}\rangle_l$ are weaker than the elements $V^{(l-1)}$. The matrices U are required to be localized, i.e. $U_{r^{(l)} r^{(l-1)}}^{(l)}$ for fixed $r^{(l)}$ decays faster than any power law in $r^{(l-1)}$ and reciprocally. With the help of a judicious choice of the matrix U , the localized states are reached as limit of $|r^{(l)}\rangle_l$ as $l \rightarrow \infty$. On the other hand, one cannot expect convergency for extended states.

8.2.1 Homogeneous fixed point ensemble

This ensemble is homogeneous in energy ε . During the elimination process, the matrix elements V connect smaller and smaller energy differences, on the opposite, the orthogonal transformation increases the matrix elements V connecting nearly degenerate states. Therefore, the scale transformation

$$r^{(l)} = b^{-1} r^{(l-1)} \quad (115)$$

implies

$$\varepsilon^{(l)} = b^d \varepsilon^{(l-1)}, \quad (116)$$

since the density of states has to be conserved during the renormalization group transformation. Thus V becomes smaller under the elimination process and has to be multiplied by a factor b^d as the energy. Therefore if for a given disorder, the increase of V being due to the elimination process, the fixed point ensemble is reached it is characterized by the dimensionless quantity

$$K = n \left\langle \sum_{r'} |V_{rr'}| |r - r'|^d \right\rangle \quad (117)$$

with fixed point value

$$K = K^* . \quad (118)$$

Now, let us consider a deviation from criticality

$$\tau = K - K^*, \quad (119)$$

i.e., V are slightly different from those of a fixed point ensemble. During one step of the renormalization group, τ grows as

$$\tau_l = b^y \tau_{l-1}. \quad (120)$$

Under the assumption of linear behaviour near the critical point, i.e. the mobility edge E_c , one has

$$\tau_l = c_l(\varepsilon^{(l)} - E_c^{(l)}), \quad (121)$$

and after one step

$$\tau_l = b^y \tau_{l-1} = b^y c_{l-1}(\varepsilon^{(l-1)} - E_c^{(l-1)}) = c_l(\varepsilon^{(l)} - E_c^{(l)}) \quad (122)$$

which determines

$$c_l = b^y c_{l-1}. \quad (123)$$

Therefore, if $y < d$ the gradient

$$\frac{d\tau_l}{d\varepsilon_l} = c_l \quad (124)$$

vanishes in the limit $l \rightarrow \infty$ implying that the iteration of the group renormalization leads to an ensemble more and more similar to the homogeneous one near the mobility edge. Otherwise if $y > d$, i.e. c diverging in the limit $l \rightarrow \infty$, there would be an abrupt transition from localized to extended states.

8.2.2 Inhomogeneous fixed point ensemble

The inhomogeneous fixed point ensemble differs from the homogeneous one in two points:

- the energy scale changes by a factor b^y ,
- the absence of a relevant perturbation and E_c is located at $E = 0$.

The main results from this theory are the power laws near the mobility edge for the density of states,

$$n_{\text{hom}} = \text{const}, \quad (125)$$

$$n_{\text{inhom}} = |\tau|^{(d-y)/y}, \quad (126)$$

and for the conductivity

$$\sigma_{\text{ac}}(\omega, 0) \sim \begin{cases} \omega^{(d-2)/d} & \text{(homogeneous),} \\ \omega^{(d-2)/y} & \text{(inhomogeneous),} \end{cases} \quad (127)$$

$$\sigma_{\text{dc}}(0, \tau) \sim \tau^{(d-2)/y}; \quad \tau > 0 \quad (128)$$

in the extended regime in agreement with other theories.

8.3 Field theory for localization

Wegner [92] was the first to develop the correct field theory mapping of the localization problem which has been achieved more precisely later [93]. In this context literature provides a large number of ways and most of them use n fields in the limit $n \rightarrow \infty$. Finally in order to eliminate physical processes related to closed electron loops, let us consider here Wegner's point of view.

The Green's function of an electron moving in a potential may be written in the configurational average as

$$G(r, r'; E \pm i\eta) = \mp i \langle \varphi_\alpha^p(r) \varphi_\alpha^{p*}(r') \rangle \quad (129)$$

in terms of the classical fields $\varphi_\alpha^1(r)$ and $\varphi_\alpha^2(r)$, with $p = 1, 2$, introduced for $E + i\eta$ and $E - i\eta$. Here the average is taken with respect to the Hamiltonian function, namely

$$\langle A \rangle = \frac{\int e^H A \{d\varphi\}}{\int e^H \{d\varphi\}}, \quad (130)$$

where

$$H = H_0 + H_1 \quad (131)$$

with

$$H_0 = -\frac{i}{2} \sum_{r,r'} (E\delta_{rr'} - v_{rr'}) \sum_\alpha [\varphi_\alpha^1(r^*) \varphi_\alpha^1(r') - \varphi_\alpha^2(r^*) \varphi_\alpha^2(r')] \quad (132)$$

and

$$H_1 = -\frac{\eta}{4} \sum_{\alpha,r} [\varphi_\alpha^{1*}(r) \varphi_\alpha^1(r) + \varphi_\alpha^{2*}(r) \varphi_\alpha^2(r)]. \quad (133)$$

$v_{rr'}$ is a nonlocal random potential and the configurational average has to be carried out. In this description there are n field replicas, i.e. $d = 1, 2, 3, \dots, n$. As a matter of fact the order of the limit $n \rightarrow 0$ and the configurational averaging may be inverted.

The density-density correlation function is given by

$$K(r, r') = \langle \Phi_\alpha^1(r) \Phi_\alpha^{1*}(r') \Phi_\beta^2(r) \Phi_\beta^{2*}(r') \rangle_{\mathcal{H}} \quad (134)$$

with Fourier transform in the limit of weak scattering

$$K(q, \eta) = \frac{1}{\eta + Dq^2}, \quad (135)$$

where D describes the constant diffusion: $D = h(lk_F)/(md)$.

These results may termed "classical" since known for some time. At this stage, the main contribution came from Wegner's analysis with the identification of the broken symmetry in the present context. In particular it has been shown that \mathcal{H}_0 is invariant under transformations leaving the term

$$\sum_\alpha (\varphi_\alpha^{1*} \varphi_\alpha^1 - \varphi_\alpha^{2*} \varphi_\alpha^2) \quad (136)$$

invariant, namely hyperbolic symmetry $O(n, n)$. On the other hand, the term \mathcal{H}_1 , invariant under $O(2n)$ transformations acts in breaking the symmetry. By analogy with the phase

transition where an external magnetic field breaks the rotational symmetry with magnetization as order parameter, η is identified with the symmetry breaking field. In this context, the conjugate variable is the local density of states,

$$n(E) = \frac{1}{2} \left\{ G_{rr} \left(E - \frac{i}{2} \eta \right) - G_{rr} \left(E + \frac{i}{2} \eta \right) \right\}, \quad (137)$$

i.e. the order parameter. The term $K(q, \eta)$ plays a role similar to the transverse magnetic susceptibility in a field η and D is the bare spin wave stiffness. Therefore, the basic field variable may be identified with

$$\varphi_{\alpha\beta}^{p\beta'}(r) = (S_p S_{p'})^{1/2} \varphi_{\alpha}^{p*}(r) \varphi_{\beta'}^{p'}(r) \quad (138)$$

with $S_1 = i$ and $S_2 = -i$. The components of φ correspond to those of spin. A given unit length system with components $S_{\lambda}(r)$ ($\lambda = 1, 2, \dots, n$) displays a transition in the limit of low temperatures to a broken symmetry phase where one of the components is unity, i.e. $S_0 = (1, 0, 0, \dots, 0)$. In particular, the low-energy fluctuations are associated with rotations slightly varying in space $S(r) = 0(r) S_0$. The effective free energy function describing these fluctuations is given by

$$H_{\text{eff}} = \int \left[\frac{K}{2} |\nabla S(r)|^2 + HS(r) \right] dr. \quad (139)$$

Here K is a measure of the resistance of the system to inhomogeneous tilting of the spin and always by analogy

$$\mathcal{H}_{\text{eff}} = \int \left[\frac{1}{2t} \nabla \varphi \nabla \varphi + i\eta \sum_{\alpha} (\varphi_{\alpha\alpha}^{11} - \varphi_{\alpha\alpha}^{22}) \right] dr, \quad (140)$$

where $t^{-1} = D_0$ denotes the bare diffusion constant.

The main results may be summarized as follow:

– the field theory is renormalizable with only one effective coupling constant t . The scaling function $\beta(g)$ measures the variation of t as a function of the upper scale cut-off b of the field theory and in particular

$$\frac{d \ln t}{d \ln b} = -\varepsilon + 2t + O(t^4) \quad (141)$$

with $\varepsilon = d - 2$. Hikami [95] has demonstrated the absence of the term of order t^3 ;

– the correlation function is of the form

$$K(q) \sim q^{n-2} \sim q^{-d} \sim [D(q) q^2]^{-1} \quad (142)$$

or equivalently,

$$D(q) \sim q, \quad \text{i.e.,} \quad D(L) \sim L^{-1}, \quad (143)$$

exhibiting a slow diffusion at the mobility edge;

– the wave function near the mobility edge presents strong fluctuations measured by

$$e_k = \sum_{\nu} |\psi(r)|^{2k} \delta(E - E_{\nu}) \sim (E - E_c)^{\nu k}. \quad (144)$$

The critical exponent has been found [92] to be

$$\pi_k = (k - 1)(2e^{-1} - k) \quad (145)$$

in $2 + \varepsilon$ dimension.

8.4 The self-consistent theory

In a different theoretical approach, Vollhardt and Wolfle [96, 97] have described the conductivity behaviour as well as the transition and critical properties. The novelty of this theory lies in the fact it does not rely on scaling assumptions but on self-consistency. The spirit of this technique was first suggested by Götze [98]. Within this method one attempts to express the frequency dependent conductivity, or the diffusion coefficient $D(\omega)$, in terms of a nontrivial, generally approximate, relation involving the same quantity.

The equation of interest is, therefore,

$$D(\omega) = \mathcal{F}[D(\omega)] \quad (146)$$

whose solution yields $D(\omega)$ for all values of ω and disorder parameters W . Since $D(\omega)$ vanishes at the transition, the inverse $D_0/D(\omega)$ diverges. Using a diagrammatic theory Vollhardt and Wolfle performed a self-consistent calculation of the quantity $D_0/D(\omega)$ by summing up the largest contributions of perturbation theory. The self-consistent equation has the structure

$$\frac{D_0}{D(\omega)} = 1 + \frac{1}{\pi n_F} \int \frac{d\mathbf{k}}{(2\pi)^d} \frac{1}{D(\omega) k^2 - i\omega}, \quad (147)$$

where n_F is the density of states at the Fermi level and the integral goes over a diffusion pole involving the diffusion coefficient itself rather than the diffusion constant D_0 .

We mention here some of the results obtained from the solution of (133):

– for $d \leq 2$ the dc conductivity $\sigma(0)$ is always zero, no matter how small the disorder is. However, for $d = 2$, the localization length is exponentially large for $W \ll 1$

$$\xi \sim \exp((2W)^{-1}); \quad (148)$$

– for $d > 2$, there exists a critical value of the degree of disorder W_c below which $\sigma(0)$ is finite, i.e. a metallic regime and for larger values it vanishes corresponding to the insulating regime. In this formulation, the challenging point is the limit $\omega \rightarrow 0$ which can be explicitly performed. Therefore, the results obtained go beyond the domain of validity of the scaling theory of Abrahams et al. [10] while one obtains complete agreement with the latter. Equation (147) itself displays scaling properties and thus leads in a natural way to a scaling theory. In particular, integration of (147) with appropriate units leads to a “scaling equation”

$$\frac{d-2}{r_d} G = \pm Z^{\frac{2-d}{d}} + G^{\frac{2-d}{2}}. \quad (149)$$

Here G and Z are dimensionless quantities instead of D and ω , the plus (minus) corresponds to the metallic (insulating) phase and r_d is a dimension-dependent constant. This equation describes a universal dependence of the conductivity on frequency whose solution determines a complete and smooth curve for the β -function.

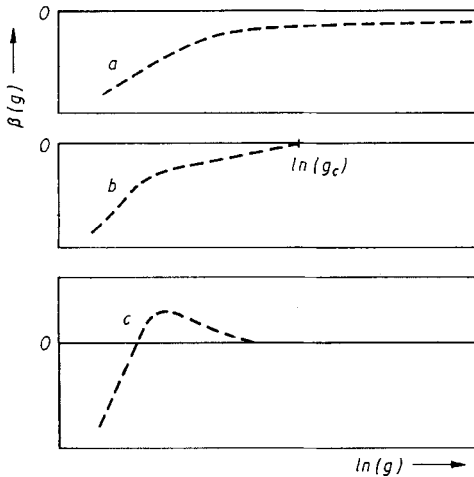


Fig. 10. The possible types of the β -function for a 2d system

8.5 Discussion

In summary, metal-insulator transition in 3d and its absence in 1d seemed well established a long time ago, whereas the marginal 2d case remains still controversial [99]. Recent developments on the subject include:

- the first numerical studies in the orthogonal case (zero magnetic field) by Pichard [100] suggest a Kosterlitz-Thouless transition corresponding to an algebraic zero of the β -function supported by an analogy with the XY model [101];
- the field theory of Wegner [102] for both the orthogonal and the unitary ($B \neq 0$) ensembles implies complete localization in either situation. However, it predicts a breakdown of one-parameter scaling close to transitions occurring in $2 + \varepsilon$ dimensions;
- the self-consistent theory of Vollhardt and Wolfe [96, 97] leads to the same conclusions for the orthogonal case;
- the numerical proof of Mc Kinnon and Kramer [103] shows that the critical dimension is $d \leq 2$ for zero field. However, recent indications suggesting that some usual transition might take place in 2d remained persistent [104].

Following the typical nature of the eigenstate as defined previously three types of β -function may be proposed for $d = 2$ (Fig. 10). Curve a stands for the “classical” exponential eigenstates deduced from the scaling theory which, however, is lacking a serious proof. The β -function, curve b displays an algebraic zero but without support, curve c describes a standard transition to “quasi-extended”, “power-law localized”, and probably multifractal states [43] occurring at W_c . The region $\beta > 0$ corresponds to extended states which are assumed to show up in the symplectic (spin-orbit) case [105].

9. Phase Diagram and Critical Behaviour

9.1 Mott-Anderson transition

Disordered systems with dimension larger than two display a transition from localized to extended states, i.e. the so-called mobility edge E_c or the Mott-Anderson transition. A challenging point is the phase diagram E_c versus the degree of disorder W . As a matter of

fact, the approximate position of the mobility edge is strongly dependent on the model considered, i.e. both criteria of localization and additional approximations. This is clearly shown in Table 2 where the critical disorder W_c has been reported from different theories for a uniform distribution of site energies. The amusing remark is that as the subject has matured, the famous ratio W_c^*/ZV seems to go to e (see Fig. 8)!

The two overquoted models for which E_c has been examined analytically to some extent are the Anderson model on a Bethe lattice [6, 7] and the sophisticated treatment of Licciardello and Economou [70] using CPA-like partial summation techniques for the one-particle Green's function. The results of the former referred to as an "exact solution" correspond to a translation of the Anderson model to an infinite-dimensional space. The authors have shown the existence of localized states for all values of the disorder parameter W . Fig. 11 summarizes universal characters in the case of a uniform probability distribution of site energies for the trajectory of E_c as a function of disorder:

- the existence of extended states outside the unperturbed band $B(W = 0)$;
- in the limit of small disorder, E_c behaves like

$$E_c = B(W = 0) + \frac{W^2}{2(B(W = 0))}; \tag{150}$$

- the number of extended states increases up to a disorder W' near to W_c .

These results underline and measure the competition between quantum tunneling and quantum interference in inducing localization. In the limit or weak disorder, the states are firstly localized in the band tails due to a broadening of the band, the perturbed band edge behaves like

$$E_b = B(W = 0) + \frac{W}{2} \tag{151}$$

which in turn implies an increase of the density of states at a given energy. Therefore, spatially the states come closer such that the tunneling probability is enhanced and quantum tunneling can act in delocalizing the states near the band edge. While quantum tunneling

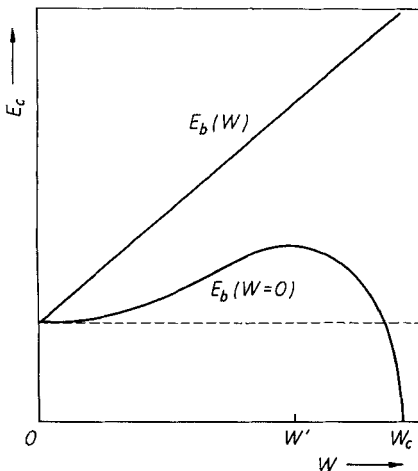


Fig. 11. Mobility edge trajectory as a function of the disorder parameter W . Case of a uniform distribution of site energies

seems to be the essential mechanism near the band edge, quantum interference is the dominant process for energies near the centre of the band.

From this phase diagram, two domains appear delimited by $W < W'$. It is not yet clear how this picture can be compatible with the one-parameter scaling hypothesis which asserts that “the function $\beta(g)$ is monotonic in the conductance g since greater disorder surely always means more localization”. This point has to be related to the magnitude of critical exponents near the transition which is subject obviously to some controversies both theoretically and experimentally (see Table 3 and 4).

9.2 Critical exponents

Similarly to the study of critical points in phase transition theory, critical exponents may be defined:

- for localized states, the characteristic length, i.e. the localization length, diverges like

$$\xi(E) \sim |E - E_c|^{-\nu} \quad (152)$$

near the mobility edge;

- polarizability α , being related to the square of the localization length, near E_c in a disordered insulator goes as

$$\alpha \sim |(\varepsilon_F - E_c)/E_c|^{-2\nu} \quad (153)$$

implying the same behaviour for the dielectric constant ε ;

- for extended states, the dc conductivity at $T = 0$ at the Fermi level vanishes as

$$\sigma(E) \sim |E - E_c|^s, \quad (154)$$

the inverse participation ratio defines a critical exponent near E_c

$$P(E) \sim |E - E_c|^p. \quad (155)$$

As usual, relations exist between these exponents. In particular, linearizing the β -function near the critical point yields a hyperscaling relation

$$s = (d - 2)\nu, \quad (156)$$

firstly outlined by Wegner [92].

The best-quoted exponents are predicted from the field-theory approach using an expansion in the parameter $\varepsilon = d - 2$ in the limit of small ε (see Fig. 12) and lead to the following values:

$$\nu = \varepsilon^{-1} + O(\varepsilon^2), \quad (157)$$

$$s = 1 + O(\varepsilon^3), \quad (158)$$

$$p = 2\varepsilon^{-1} - 1 + O(\varepsilon). \quad (159)$$

For the three exponents the first correction in the expansion has been found to vanish. The self-consistent theories agree with these predictions. The challenging numerical results have been performed through finite size scaling arguments [103] for the exponent ν .

More information on the critical exponents is of great interest. Indeed a proper understanding requires an expansion of the exponent near the upper critical dimension which is suspected to be $d_c^* = 4$. In the localization problem, this has still to be achieved.

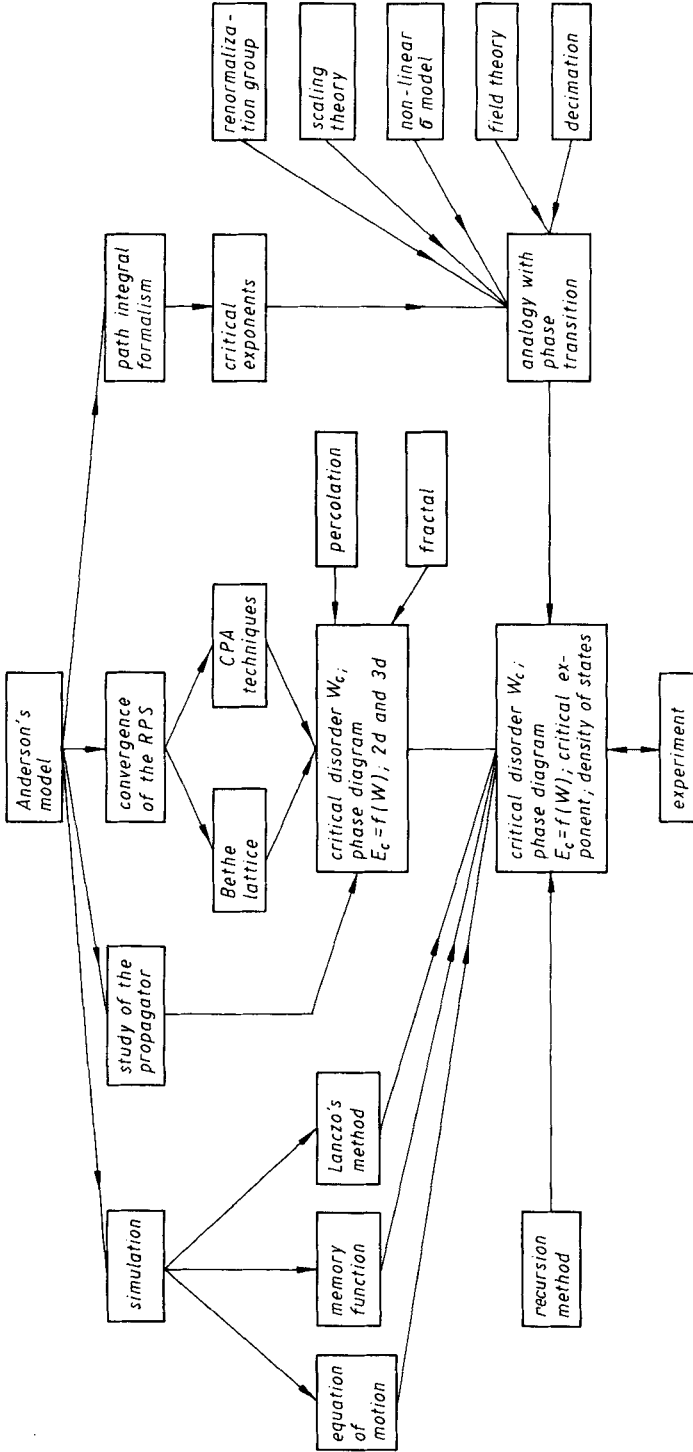


Fig. 12. Anderson model from different theories

In this context, exact results have been reported only on the Bethe lattice which may be viewed as a lattice with an infinite dimensionality (see Table 7). In particular one finds

$$\nu = 1, \quad (160)$$

which has to be reinterpreted as

$$\nu = 0.5. \quad (161)$$

Table 5
Critical exponent ν from different models

model		ν
Cohen	[129]	1.6
Freed	[130]	2/3
Lukes	[131]	0.6
Abram and Edwards	[132]	$d = 2: 0.75$ $d = 3: 0.6$
Anderson	[133]	0.6
Mott	[134]	$> 2/3$
Wegner	[89]	a) $0 > 1/\nu > d$ b) $1/\nu < d$
Licciardello and Thouless	[135]	$d = 2: 1$
Weaire and Srivastava	[136]	$d = 2: \nu_M = 1$
Yoshino and Okazaki	[38]	$d = 2: \nu_M = \begin{cases} 0.8 \\ 1 \end{cases}$
Aharony and Imry	[137]	0.59
Götze	[98]	0.5
Schuster	[101]	$d = 2: 1$
Domany and Sarker	[113]	$1.25 \leq \nu \leq 1.75$
Oppermann and Wegner	[91]	$d > 2^+ : \frac{1}{d-2}$
Wegner	[92]	$d = 2^+ : 0.5$ $d = 3 : 1$
Abrahams et al.	[10]	< 1
Stein and Kray	[138]	$d = 2: \nu_M = 0.80 \pm 0.05$ $\nu_E = 1.30 \pm 0.10$ $d = 3: \nu_M = 0.66 \pm 0.05$ $\nu_E = 1.25 \pm 0.10$
Allen	[139]	$d > 4: 0.5$ $d_c < d \leq 4: 1/(d-2)$
Hikami	[140]	0.5 $\nu(O) = 1$ orth. case $\nu(H) = 0.5$ unit. case
Brezin et al.	[141]	1
Vollhardt and Wolffe	[96, 97]	1
Pichard and Sarma	[115]	$d = 2: \nu_M = 0.5 \pm 0.1$ $d = 3: \nu = 0.66 \pm 0.02$
Prelovsek	[117]	$d > 4: \nu_M = 0.5$ $d < 2 \leq 4: \nu_M = 1/(d-2)$
Mc Millan	[142]	0.96
Mott	[143]	1
Kotov and Sadovski	[119]	$d > 2: \nu_M = 1/(d-2)$

Table 5 (continued)

model		ν
Mc Kinnon and Kramer	[103]	$\nu_M = 1.2 \pm 0.3$ estimation $\nu_M = 1.50 \pm 0.05$ calculation
Kunz and Souillard	[144]	$d > 2: \nu = 1/(d - 2)$
Frölich and Spencer	[145]	$d > d_c^* = 0.5$
Singh and Mc Millan	[123]	$\nu_M = 1.78 \pm 0.15$
Chayes et al.	[146]	$d = 1: \nu = 2$ $d > 1: \nu_d \geq 2$
Bernreuther and Wegner	[147]	$\varepsilon/2 - 3/4 + O(\varepsilon)$ $\varepsilon = 4 - d$

Shapiro [167] has proposed from an approximate model an exponent (also found by Souillard [54])

$$p = 0. \tag{162}$$

Finally, Chayes et al. [146] have demonstrated the existence of a constraint for the exponent ν which has to satisfy the inequality

$$d\nu \geq 2. \tag{163}$$

However, the numerical values for the critical exponents are difficult to evaluate. Such a remark holds both for theory as well as for experiments. The main difficulty is that the power-law behaviour can only be expected in the real limit of phase transition. Most of

Table 6
Critical exponent ν from different experimental data and different materials

authors		material	ν
Pepper et al.	[148]	Si/SiO ₂	0.75
Sayer et al.	[149]	La _{1-x} Sn _x VO ₃	0.6 or 2/3
Pollit	[150]	Si/SiO ₂	0.75
Rosenbaum et al.	[151]	Si: P	0.5
Dodson et al.	[152]	a-GeAu	1
Thomas et al.	[153]	GeSb	0.5
Nishida et al.	[154]	a-Au _x Si _{1-x}	1
Ionov et al.	[155]	Si: As	0.5
Hertel et al.	[156]	a-Nb _x Si _{1-x}	1
Epstein et al.	[157]	Xc-Hg	0.6
Yamagushi et al.	[158]	a-SiAu	1
Bishop et al.	[159]	a-SiAu	1
Ludwig and Micklitz	[160]	a-Bi _x Kr _{1-x}	1.07 ± 0.1
Yoshizumi	[161]	a-GeMo	1
Morita et al.	[162]	Ga: As/In: Sb	1
Long and Pepper	[163]	Si: Sb	0.5
Shafarman et al.	[164]	Si: As	≈ 1

Table 7
Critical exponent ν for the Bethe lattice

model		ν
Mookerjee and Choudry	[165]	1
Srivastava et al.	[166]	1
Shapiro	[167]	1
Kunz and Souillard	[144]	1
Brezini	[168]	1

analytical theories work only in the asymptotic regime: weak and/or strong scattering. They are not necessarily correct in the regime of the transition. Numerical estimates are confronted with the problem of accuracy. Difficulties arise also in experimental work; the critical exponent is comprised between 0.5 and 1.7 (see Table 6). On the other hand, the interaction effects (Table 8) and/or external fields complicate seriously the critical behaviour. There are two essential questions on this point:

- why does $\nu = 1$ work so well in most cases?
- why does $\nu = 0.5$ work so well for Si:P?

These questions are actually the challenge in the localization problem.

9.3 Metal–insulator transition

Several fundamental mechanisms play a significant role in the metal–insulator transition: disorder, short-range correlation, excitonic effects, electron–lattice interaction, etc. In a real situation all these effects are present to different degrees.

In the present paper we have been concerned with the metal–insulator transition induced by increasing disorder. This transition is continuous, characterized by transport anomalies and by the divergence of the dielectric constant from the insulating side. Experimentally, one of the best examples is the transition in phosphorus-doped silicon, Si:P.

Table 8
Critical exponent ν in the presence of electron–electron interaction

model		ν
Mc Millan	[142]	1
Finkelstein	[169]	1 interaction at infinite order
Kaveh	[171]	1 exchange term 0.5 Hartree term
Anderson	[172]	0.5 fluctuation of spin
Lee and Ramakrishnan	[99]	1

Si:P presents a continuous zero temperature transition from insulator to metal in the impurity band due to overlap of hydrogen donor wave functions for phosphorus concentrations $n \geq 3.7 \times 10^{18} \text{ cm}^{-3}$. The donor wave functions being large $\approx 3 \text{ nm}$ compared to the lattice parameter ($\approx 0.25 \text{ nm}$) the electron–lattice interaction may be neglected. Si:P is an intrinsically disordered system since phosphorus and thus the effects of disorder are assumed to be important. On the other hand, in uncompensated Si:P there is one electron per impurity site and the Mott-Hubbard correlation effects are relevant.

Many high-quality experimental results are available in the close vicinity of the metal–insulator transition at very low temperature ($\approx \text{mK}$). In the following, we summarize some of them [173]:

9.3.1 *dc conductivity*

The dc conductivity transition is continuous. The extrapolated zero-temperature conductivity $\sigma(0)$, as a function of the dopant density n , goes to zero as

$$\sigma(0) \approx \sigma_c \left| \frac{n - n_c}{n_c} \right|^{1/2}, \tag{164}$$

where σ_c is about $20\sigma_{\text{min}}$. The exponent 1/2 is quite different from the value 1 expected from the theory of localization of a noninteracting electron system (Fig. 13). Actually there is no theory leading to this value. Anderson [8] suggested that this exponent is due to the development of magnetic moments. For such situation the transition takes its origin from a random potential inducing localization with adding magnetic impurities and the Gell-Man-Low function transforms as

$$\beta(g) = d - 2 - bg^{-2}, \tag{165}$$

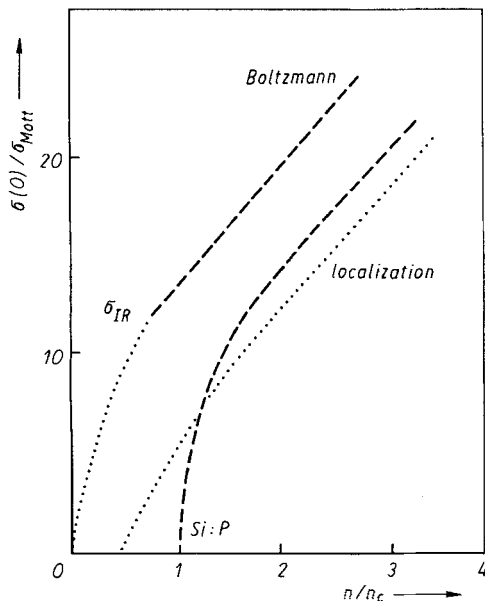


Fig. 13. Discrepancy between experiment and theory; Si:P

which implies a conductivity exponent 1/2 [174]. While the exponent is 1/2 for uncompensated doped semiconductors, it crosses over to unity with compensation [175], i.e. if correlation effects are not crucial.

9.3.2 *ac conductivity*

The ac conductivity $\sigma(\omega)$ of Si:P has been measured on the insulating side [176]. In particular, it has been observed that at very low temperature and near the critical concentration

$$\sigma(\omega) = A\omega^s, \quad (166)$$

where $s \approx 1$ and the factor A diverges similarly to the static dielectric constant $\varepsilon(0)$.

The ac conductivity from the Anderson model has been calculated by Mott (41) predicting a term proportional to $\omega^2 (\ln \omega)^4$ and another one like $\omega k_B T (\ln \omega)^4$. Unfortunately such results do not fit the experimental data: the prefactor is temperature independent. The prefactor in the Mott formula goes as $\xi_{\text{loc}}^5 n$ as $\varepsilon(0)^{5/2}$ while experiment predicts a different behaviour.

Shklovski and Efros [177] have suggested that Coulomb interaction qualitatively changes the ac conductivity. $\sigma(\omega)$ depends on the number of electronic pair states in such a way that one is occupied and the other one not, energetically the difference being $\hbar\omega$. In the absence of interaction, this number is proportional to $\hbar\omega N(E_F)$ leading to the Mott formula. In the presence of Coulomb interaction the number of pair states singly occupied increases, since double occupancy requires an extra Coulomb energy e^2/Kr_ω . The density of such states behaves as $(e^2/Kr_\omega) N(E_F)$ leading to an ac conductivity going as $\omega |\ln(\omega)|^3$. Bhatt and Ramakrishnan [178] have shown that this mechanism is continuous to be operative even near the divergence of ξ_{loc} , the ratio corresponding to the Mott criterion $n^{1/3} a_H \approx 0.25$.

9.3.3 *Dielectric constant*

The static dielectric constant $\varepsilon(0)$ has been also measured on the insulating side [176]. It diverges as $n \rightarrow n_c$ with an exponent of value near unity, i.e. twice the conductivity exponent. The one-parameter scaling theory predicts this ratio by identifying $\varepsilon(0) = \xi_{\text{loc}}^2$ but the exponents are different.

10. Conclusion

It is apparent from bits and pieces of experimental finding and theoretical understanding that disorder, long-range Coulomb interaction, as well as spin correlation effects are of great importance in metal-insulator transitions. Obviously there are again rather large subjects such as amorphous semiconductors [179, 180] where short-range disorder acting on electron near the band-edge leads to the Meyer-Neldel rule [179] and to a density of states depending exponentially on energy [180].

In summary we have presented here the onset of electron localization and its consequences studied during the last three decades. Our understanding on this area has developed considerably. During the eighties it has become quantitative since experimental data are available and the theoretical model may be checked. In this context for the nineties the field seems still promising in presenting nice extensions in different domains such as quasiperiodic systems (for a review see [181], quantum chaos [182, 183], metal-insulator transitions [99], non-electrical analogues such as propagation of light and sound in random media [184]). Our feeling is that the best has still to come.

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