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NATURE OF ELECTRONIC WAVE FUNCTIONS IN DISORDERED SYSTEMS

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ABSTRACT

The question of how to quantitatively characterize the wave functions in disordered systems is examined. We discuss the following relevant quantities: the phase coherence length ℓ, the localization length λ, the amplitude fluctuation length ξ, the participation ratio p and the fractal dimensionality D. Various techniques for calculating these quantities are mentioned and relevant results are presented.

INTRODUCTION

The electronic eigenfunctions in disordered systems are complicated objects. Recent explicit calculations by Soukoulis and Economou [1] show that the eigenfunctions have strong amplitude fluctuations of various spatial extents. This is clearly seen in figure 1 where we plot the probability density $|c_n|^2$ for a 2-d (squared) tight binding model of a disordered system with diagonal disorder of total width W. Even for weak disorder (W=1) the wave function has strong fluctuations and does not occupy the whole available space. For the 2-d case we have independent evidence that all eigenstates are exponentially localized but for weak disorder (W=1 for E=0) we expect the localization length to be $\lambda \sim 10^4$. Therefore the case shown in figure 1a is like any extended state but it has all these strong fluctuations. As disorder increases (figures 2b-2d) the wave function becomes localized within the size of the system studied. Of course, even for these strongly localized eigenstates there are strong fluctuations up to a length which is roughly equal to λ.

As a result of these fluctuations only a fraction of the available space is effectively utilized by the eigenfunctions.

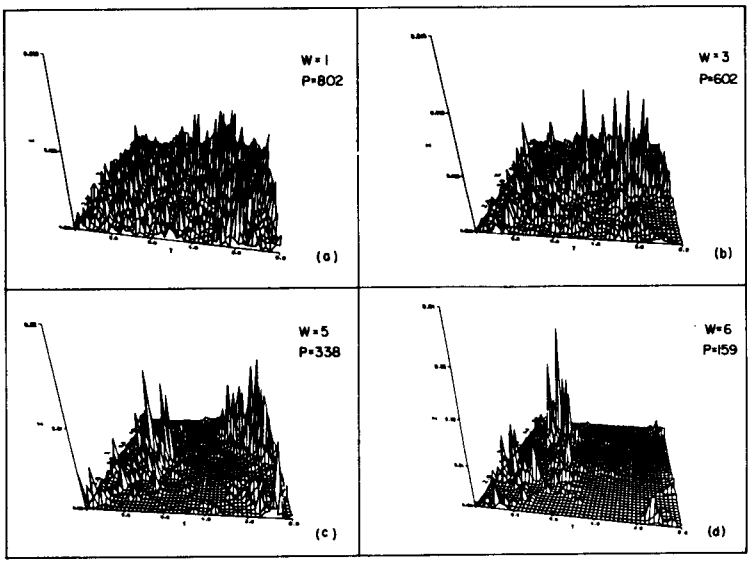

Fig. 1. Plot of the probability of finding a particle at site n, $|c_n|^2$, for a 50×50 square tight binding model with diagonal disorder of total width W. The energy E ≈ 0.45 and P is the participation ratio.

In contrast to these findings, ordinary transport theory is based upon the assumption that the amplitude of the eigenfunctions is essentially unaffected by the disorder, while the phase is randomized within a characteristic phase coherence length, the so called mean free path ℓ. The latter can be defined by the relation

$$< G\ (\underline{m},\underline{n}) > = G_0\ (\underline{m},\underline{n})\ \exp\ [-\frac{|\underline{m} - \underline{n}|}{2\ell}]\ , \qquad (1)$$

where $G_0(\underline{m},\underline{n})$ is the off-diagonal matrix element of the periodic Green's function between the points $\underline{m}$ and $\underline{n}$, and $< G\ (\underline{m},\underline{n}) >$ is the average value of the same matrix element for the disordered system. For weak disorder, ℓ is given by

$$\ell = |\underline{v}|\tau \qquad (2)$$

where $|\underline{v}|$ is the magnitude of the velocity $\underline{v} = \partial E(\underline{k})/\hbar\partial\underline{k}$ and τ is the relaxation time. In the weak scattering limit, where the assumption of a uniform amplitude is supposed to be valid, the mean free path ℓ is the quantity which controls the dc conductivity σ_0 [2,3]:

$$\sigma_0 = \frac{2}{(2\pi)^{d_d}}\ \frac{e^2}{\hbar}\ S_0\ell\ . \qquad (3)$$

In equation 3, d is the dimensionality of the space, and S_0 is the area of the Fermi surface (for d = 3), or the length of the Fermi line (for d = 2), or $S_0 = 2$ (for d = 1).

As the disorder increases, the amplitude of the eigenfunctions ceases to be uniform. As a result, the dc conductivity σ does not coincide anymore with the semiclassical expression σ_0 given by equation 3. One expects intuitively that $\sigma < \sigma_0$, and that the difference $\sigma_0 - \sigma$ would increase as the amplitude fluctuations become larger (in size and extent).

Characterization of the Amplitude

Localization length λ

It seems well established now that disorder may lead, if strong enough, to eigenfunctions whose amplitide decays to zero for large distances. Although there is no rigorous proof (except in 1-d), it is usually assumed that the decay is exponential on the average. The characteristic length λ, which determines this exponential decay is called the localization length, and is defined by the relation

$$\langle |\psi(r)| \rangle_g \sim \exp\left[-\frac{r}{\lambda}\right], \text{ as } r \to \infty \tag{4}$$

where the symbol $\langle\rangle_g$ indicates the geometric mean. The main effect of this disorder induced localization is to make the T=0, dc conductivity σ to approach zero as the linear dimension of the specimen L approaches infinity

$$\langle \sigma(L) \rangle_g \sim \exp\left[-\frac{2L}{\lambda}\right], \text{ as } L \to \infty . \tag{5}$$

It has been convincingly demonstrated that in 1-d disordered systems all eigenstates (except some special pathological cases [4]) are exponentially localized no matter how weak the disorder is [2,3]. It is widely believed that the same is true for 2-d disordered systems, although proposals for a power law localization have been advanced. On the other hand, for 3-d disordered systems the prevailing belief is that for not so strong disorder the spectrum is separated by critical energies termed mobility edges into alternating regions of extended ($\equiv$ non decaying) and localized eigenstates. As the disorder increases the regions of extended states may disappear altogether and the whole spectrum may consist of localized eigenstates.

Fluctuation length ξ

For extended states in 3-d disordered systems a length ξ has been introduced characterizing the spatial extent of the largest (in size) fluctuation. If the eigenfunction is averaged over length scales equal to or larger than ξ, it would look uniform. Obviously fluctuations are characterized not only by their extent but by their magnitude as well. The latter can possibly be defined as the ratio of an appropriately averaged maximum value of $|\psi(r)|$ over an appropriately averaged minimum value of $|\psi(r)|$. Very little attention has been given to the question of the magnitude and its possible correlation with ξ. Preliminary unpublished work by the authors of the present article based on the potential well analogy [5] indicates that the magnitude of the largest fluctuation equals ξ/a' where a' is comparable to the interatomic distance. This simple result leads to a reduction of the conductivity according to the formula

$$\sigma = \sigma_0 \frac{a'}{\xi} . \tag{6}$$

The ξ dependence of equation 6 coincides with the predictions of the scaling theory and the field theories (for a brief review see ref. [3]).

Since localized states exhibit considerable fluctuations before eventually their amplitude becomes negligible, a legitimate question to be raised is how to characterize these fluctations. Although this question has not been examined seriously, it is usually assumed that for localized states the role of ξ is played by λ. This assumption deserves more attention especially in the case of 2-d weakly disordered systems where λ can become very large.

Participation Ratio p

The participation ratio characterizes the fraction of space effectively occupied by an extended eigenfunction, i.e., $p = N_{eff}/N$; N_{eff} is the number of atomic sites where $\psi(r)$ is appreciable and N is the total number of sites. More precisely p is defined by

$$p^{-1} = N \sum_n |c_n|^4 \tag{7}$$

where $|c_n|^2$ is the probability of finding the particle at the site n. The participation ratio appears in phonon-mediated self energies and interactions, which in the static limit lead to an interaction part in the Hamiltonian of the form

$$H_{int} \sim \int |\psi(\underline{r})|^4 d\underline{r} \sim \frac{1}{Np} . \tag{8}$$

It is worthwhile to point out that preliminary results based on the potential well analogy [5] give for extended states that

$$p = \frac{a'}{\xi} \tag{9}$$

which combined with equation 8 lead to an enhancement of the lattice mediated interaction by a factor of ξ/a'. Equation 9 is consistent with numerical results for p.

Fractal Dimensionality D

The quantity D can be defined if the integral of the probability density $|\psi(r)|^2$ within a sphere of radius L is proportional to L^D with D independent of L. For a disordered eigenfunction the result depends strongly on where the center of the sphere is placed. To avoid this difficulty a weighted average over all positions of the center is taken; the weight is the probability density of finding the particle at each point. Thus the fractal dimensionality is defined as the L independent exponent in the relation

$$A(L) = \text{const } L^D \tag{10}$$

where A(L) is the density correlation function

$$A(L) = \int d\underline{r} \, |\psi(\underline{r})|^2 \int_0^L d\underline{r}' \, |\psi(\underline{r}'+\underline{r})|^2 . \tag{11}$$

For uniform extended states the fractal dimensionality coincides with the Euclidean dimensionality: D=d. Thus for extended states and $L > \xi$, D=d; as a result a non-trivial fractal dimensionality can be defined only in the range $a' \ll L \ll \xi$. For localized states a fractal dimensionality can only be defined for lengths less than the effective extent of the eigenfunction; beyond this length, A(L) saturates approaching asymptotically one.

Recently Soukoulis and Economou [1] have calculated numerically the density correlation function A(L) defined by equation 11 in order to check whether a fractal dimensionality could be defined for an eigenfunction in a disordered system. Their numerical results strongly suggests that D is well defined for length scales $a' \ll L \ll \lambda, \xi$ and that D is a continuous, decreasing function of the disorder. The most interesting case is for d=3 at the mobility edge, where both λ and ξ are infinite. The fractal dimensionality at the mobility edge was estimated [1] to be 1.7±0.3.

It is very interesting to check experimentally the fractal character of wave functions in disordered systems. A possible probe might be the frequency dependent conductivity $\sigma(\omega)$. In a 3-d disordered system where a mobility edge exists for low frequencies (long times) we are going to see a regular behavior of $\sigma(\omega)$ which is characteristic of uniform extended states. For high frequencies (short times) we are going to probe the local behavior of the states which are fractal like and therefore we will obtain a different frequency dependent of $\sigma(\omega)$. I want to emphasize that the ideas are very speculative in nature.

The quantity D in addition to its ability to characterize quantitatively the shape of the amplitude fluctuations may prove extremely important physically if it turns out that it can determine critical exponents for disordered systems, as the ordinary dimensionality does for ordered systems.

RESULTS

Quantities like the average density of states, the mean free path ℓ, the quasi-free carrier conductivity σ_0, etc., can be calculated rather successfully by mean field theories most notably by the so called Coherent Potential Approximation (CPA). The CPA has been employed both for simple model systems such as tight-binding Hamiltonians and for realistic systems such as amorphous semiconductors.

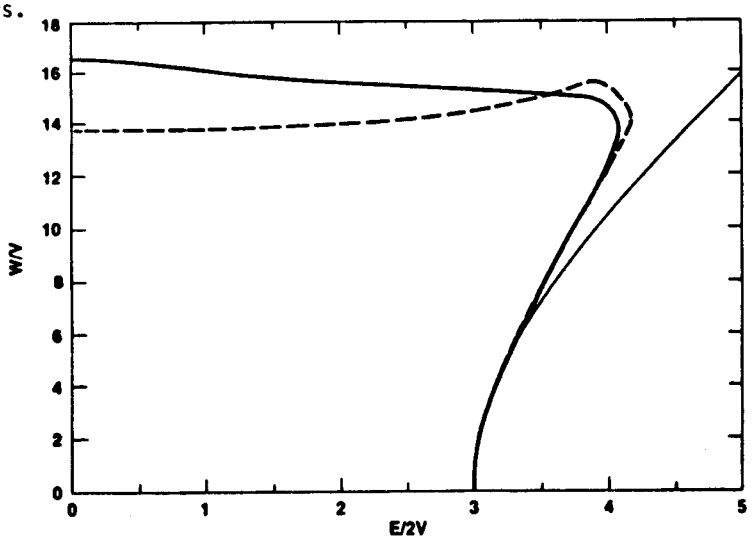

Fig. 2. Mobility edge trajectory for a simple cubic tight binding model with a diagonal disorder of rectangular shape and total width W. V is the off-diagonal nearest neighbor matrix element. The heavy solid line is based on equation 14 while the dashed line is based on the L(E)-method. The solid thin line is the CPA band edge.

Recently Economou et al. [5] have shown that the problem of localization in a disordered system can be approximately mapped into that of a bound level in a shallow single potential well. The extent a of the equivalent well has been taken as proportional to the mean free path ℓ

$$a \propto \ell \tag{12}$$

and the depth V_0 of the equivalent well is proportional to $1/\sigma_0 a^d$

$$V_0 \propto \frac{1}{\sigma_0 a^d} \sim \frac{1}{S\ell^{d+1}} . \tag{13}$$

For d=3, a bound level in a well appears only when the product $V_0 a^2$ exceeds a critical value. By analogy, in a 3-d disordered system, localized states appear only when the dimensionless quantity $S\ell^2$ is less than a critical value, which can be obtained by fitting the numerical value at the center of the band of a simple cubic tight binding model [6,7]. The final result is that the mobility edge in a 3-d disordered system is obtained from the simple relation

$$S\ell^2 \approx 9 . \tag{14}$$

It is worthwhile to point out that for an energy E well inside a band, S is proportional to a'^{-2} so that equation 14 gives $\ell \sim a'$ as the localization criterion in agreement with Mott's [2] proposal. On the other hand, for weak disorder, the mobility is close to the band edge and S there is much smaller than a'^{-2}. This means that for weak disorder the eigenstates can become localized while their mean free paths are considerably larger than the interatomic distance.

In figure 2 we show explicit results based on equation 14 for the trajectory of the mobility edge. The agreement with the results based on the L(E) - method (see ref. [3]) is very impressive especially in view of the fact that no adjustable parameters are present in the L(E) - method.

The single potential well analogy permits us to obtain the localization length as well. For a 3-d system the result is

$$\lambda \approx \frac{(20/S + A\ell^2)\ell}{\ell_c^2 - \ell^2} ; \quad \ell < \ell_c . \tag{15}$$

Explicit results are shown in figure 3 together with the numerical data of ref. [5]. The value of the constant A in equation 15 has been adjusted. The agreement is impressive.

For d < 2, a single potential well, no matter how shallow, always binds a particle. By analogy in d-dimensional disordered systems with d < 2 all eigenstates are localized; their localization lengths λ can be obtained by employing the analogy with the single potential well. For weak disorder in the 2-dimensional case we obtain

$$\lambda \approx \text{const } \ell \exp\left[\frac{S\ell}{4}\right] \tag{16}$$

where the constant, for E at the center of the band, is 2.72, and $S = 4\sqrt{2\pi}$ (in units of inverse lattice spacing). Explicit results are shown in figure 4 together with the numerical data of refs. [6] and [7]. Given that there is only one adjustable parameter in the theory the agreement is very good except for very weak disorder where the numerical data are systematically below the theoretical results.

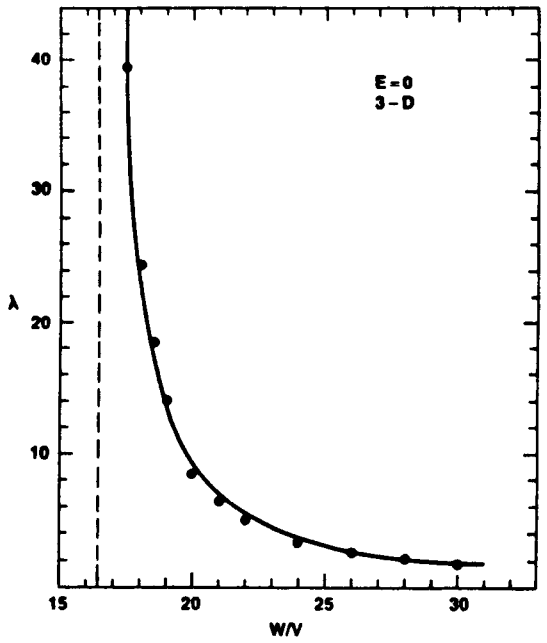

Fig. 3. Localization length λ (in units of lattice spacing) for the center of the band of a simple cubic tight binding model with diagonal disorder of total width W. V is the off-diagonal matrix element. The solid line is the result based on the single potential well analogy and the dots are numerical data of ref. [6].

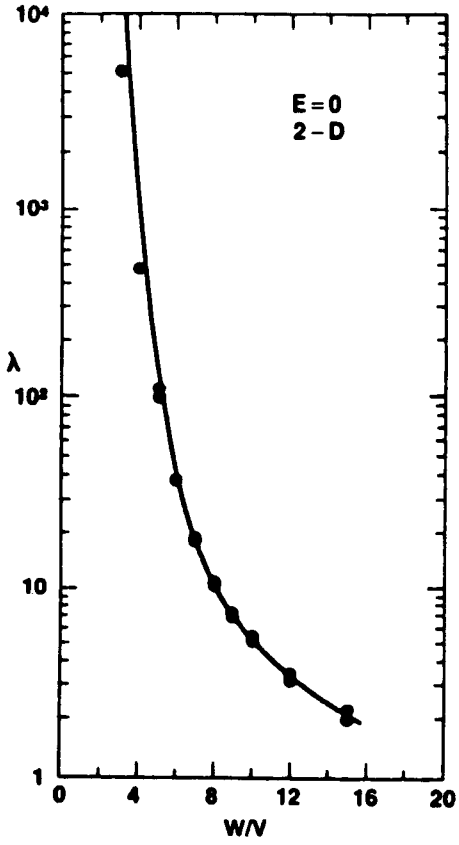

Fig. 4. Localization length λ (in units of lattice spacing) for the center of the band of a square tight binding model with diagonal disorder of total width W. V is the off-diagonal matrix element. The solid line is the result based on the single potential well analogy and the dots are numerical data of refs. [6,7].

In the 1-d case the final result based on the single potential well analogy is

$$\lambda = 2\ell \ . \qquad (17)$$

One may argue that ℓ in equation 17 must be obtained from the geometric mean of G (m,n) and not the arithmetic, because the former and not the latter is representative of the ensemble. With this interpretation of ℓ equation 17 becomes exact.

SOME CONSEQUENCES

We would like to conclude this brief presentation by pointing out two cases, where the previous considerations lead in an elegantly simple way to quite fundamental results.

The first case is that of small polaron formation, where the electron immobilizes itself by statically distorting the lattice. As it has been shown by Emin and Holstein [8], the formation or not of a small polaron is determined by the competition of two opposing physical factors. A "repulsive" kinetic energy term which scales as $1/L^2$ and favors delocalization and an "attractive" lattice mediated self-energy which is proportional to $\int|\psi|^4 dr$ and hence it scales as $1/L^3$ and favors shrinkage of the wave function into atomic size. The disorder reduces the "repulsive" term (by a factor of $a'/\min(L,\xi)$) and enhances the "attractive" term (by a factor of ξ/a' for $L > \xi$). These modifications can be understood physically as a result of the fact that the eigenfunction is not uniform, and it does not utilize all available space. Hence, the energy to compress it is lower, while the self-energy (being inversely proportional to the participation ratio) is higher. Thus the net effect of the disorder is to facilitate polaron formation; the larger the ξ, the easier it is to form polarons [9].

Another case where the length scaling of the kinetic energy is very important is that of the tailing of the density of states N(E). Halperin and Lax [10] have shown that N(E) behaves as

$$N(E) \propto \exp\left[-\left|\frac{E}{E_0}\right|^{2-\frac{d}{2}}\right] . \tag{18}$$

The factor 2 that divides the dimensionality d in the exponent is the same as the exponent in the length scaling of the kinetic energy: $1/L^2$. In three and higher dimensionality and for $L < \xi$ the kinetic energy scales [11] as $1/L^d$. Hence the exponent $|E/E_0|$ in equation 18 must become $2-(d/d)=1$ and the DOS must be given by

$$N(E) \propto \exp\left[-\left|\frac{E}{E_0}\right|\right] \; ; \; d > 2 . \tag{19}$$

This naturally resulting exponential tail in the DOS may provide a convincing interpretation of the exponential absorption edge appearing almost universally in disordered systems.

On the other hand, one can argue [12] that in 1-d we are almost always in the regime, where the kinetic energy scales as $1/L^2$ so that

$$N(E) \propto \exp\left[-\left|\frac{E}{E_0}\right|^{3/2}\right] \; ; \; d = 1 \tag{20}$$

which is the exact result in 1-d.

REFERENCES

1) Soukoulis, C. M. and Economou, E. N.: Phys. Rev. Lett. (1984) 52, 565 and unpublished.

2) Mott, N. F. and Davis, E. A.: Electronic Processes in Non-Crystalline Materials, 2nd Ed. (Clarendon, Oxford, 1979).

3) Economou, E. N.: Green's Functions in Quantum Physics, 2nd Ed. (Springer, Heidelberg, 1983).

4) Soukoulis, C. M. and Economou, E. N.: Phys. Rev. (1981) B24, 5698.

5) Economou, E. N. and Soukoulis, C. M.: Phys. Rev. (1983) B28, 1093 and Economou, E. N., Soukoulis, C. M. and Zdetsis, A. D.: Phys. Rev (1984) B30, 1686.

6) MacKinnon, A. and Kramer, B.: Z. Phys. (1983) B53, 1.

7) MacKinnon, A. and Kramer, B.; Phys. Rev. Lett. (1982) 49, 695.

8) Emin, D. and Holstein, T.: Phys. Rev. Lett. (1976) 36, 323.

9) Cohen, M. H., Economou, E. N. and Soukoulis, C. M.: Phys. Rev. Lett. (1983) 51, 1202.

10) Halperin, B. I. and Lax, M.: Phys. Rev. (1966) B14, 722 and Phys. Rev. (1967) 153, 802.

11) One argument to understand the different length scaling of the kinetic energy is the following: For a random walker in a regular periodic system after time t the square of the average displacement $< r^2 >$ from its starting point goes proportional to t. Therefore by an uncertainty principle argument ($(\Delta E)(\Delta t) \sim h$) one obtains that energy scales as $1/L^2$ in any dimension. Now if the random walker moves in a fractal space or in a highly non uniform space after time t, $\langle r^2 \rangle \sim t^x$ where $x < 1$. This is so, because the random walker spends most of its time wandering around its starting point. Using $(\Delta E)(\Delta t) \sim h$ one obtains that energy scales as $1/L^{2/x}$, $x < 1$. There is a lot of numerical evidence that $x = 2/d$ for disordered systems.

12) Soukoulis, C. M., Cohen, M. H. and Economou, E. N.: Phys. Rev. Lett. (1984) 53, 616.