INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS: CONDENSED MATTER

J. Phys.: Condens. Matter **17** (2005) L321–L327 doi:10.1088/0953-8984/17/30/L01

LETTER TO THE EDITOR

Universal features of localized eigenstates in disordered systems

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Received 26 May 2005
Published 15 July 2005
Online at stacks.iop.org/JPhysCM/17/L321

Abstract

Localization–delocalization transitions occur in problems ranging from semiconductor-device physics to propagation of disease in plants and viruses on the internet. Here, we report calculations of localized electronic and vibrational eigenstates for remarkably different, mostly realistic, disordered systems and point out similar characteristics in the cases studied. We show in each case that the eigenstates may be decomposed into exponentially localized islands which may appear in many different eigenstates. In all cases, the decay length of the islands increases only modestly near the localization–delocalization transition; the eigenstates become extended primarily by proliferation (growth in number) of islands near the transition. Recently, microphotoluminescence experiments (Guillet *et al* 2003 *Phys. Rev.* B **68** 045319) have imaged exciton states in disordered quantum wires, and these bear a strong qualitative resemblance to the island structure of eigenstates that we have studied theoretically.

In crystalline materials, electronic (and vibrational) eigenstates are extended (or delocalized) throughout the material. Since the 1950s [2], it has been recognized that disorder can cause some electron states to decay exponentially in space; such spatially confined states are called 'localized'. The earliest and simplest model of disorder for electrons is the celebrated 'Anderson model', in which the disorder is usually introduced in the electronic Hamiltonian by choosing the diagonal matrix elements (on-site energy terms) of the Hamiltonian from a uniform distribution. While important insights have accrued from this work, the relevance of these calculations to physical systems has not been certain, as Mott emphasized in his Nobel Lecture [3]. For this reason, our work employs disorder extracted from models which accurately reproduce experiments sensitive to the disorder. For example, the electronic case is best described by constructing the Hamiltonian matrix from a realistic topologically disordered model of a material. Structural disorder also leads to localization of vibrational normal modes [4], which we similarly explore with realistic models of two different amorphous materials. To enable comparison with conventional calculations, we analysed a simple three-

dimensional Anderson model [2]. Our work is also relevant to macroscopic vibrations, and the stability of structures [5].

For a particular disordered system, the character of vibrational or electronic states is determined by the corresponding eigenvalues (eigenenergy or eigenfrequency of the corresponding Hamiltonian or dynamical matrix, respectively), with a critical point, the 'mobility edge', separating extended from localized states. This localization–delocalization (LD) second-order phase transition has been the subject of intense research on toy models, and much is now known about the statistical properties of the states at, and around, the critical eigenvalue [6].

Localized eigenstates are characterized by an exponential spatial decay of the magnitude of the envelope of the wavefunction. The actual charge density or vibrational displacement at a particular point is understood to be a product of this exponentially decaying envelope with a rapidly spatially varying 'filling' function that ensures that the eigenstates remain orthogonal. The behaviour of the envelope function has been previously studied: it is now known that it changes from being exponentially decaying for localized eigenstates to being multifractal at the LD transition, and is spatially extended for delocalized states according to analytical considerations [6], accurate numerical analysis for simple lattice models [7] and numerical calculations on small realistic systems [8]. It has been established that the filling function is highly inhomogeneous and consists of 'lumps' of probability density, and Dong and Drabold introduced a 'resonant cluster proliferation model' to characterize the evolution of the states from localized to extended [9]. However, not much is known about the nature of such lumps, and possible spatial correlations between them, for different eigenstates. Our aim is to reveal such correlations and shed light on the origin of the localized states.

To achieve this aim, we use a numerical approach and investigate the spatial structure of localized states of different type (electronic and vibrational excitations) in a diverse range of models, starting from lattice models exemplified by the Anderson Hamiltonian and concluding with realistic models of amorphous Si and vitreous silica with long-range Coulomb interactions between atoms. Technically, we solve the eigenproblem for large random matrices (Hamiltonian and dynamical matrices for electronic and vibrational problems, respectively) using either direct diagonalization (for moderate sizes) or a Lanczos method for larger systems.

For structurally ordered systems (e.g. crystals), all the states (electronic, vibrational, spin) are spatially extended and their energies form bands, separated by gaps. For systems with disorder, 'band tails' appear at the edges of the bands, with possibly also states deep in a gap. First, we confirm that the localized (electronic) band-tail states consist of clumps or 'islands' (of charge density). This can be seen from figure 1, where a band-tail part of the calculated electronic density of states for a realistic model of amorphous (a-)Si is shown, together with representative eigenstates for selected eigenvalues in the tail. The number of such islands in a localized eigenstate increases on approaching the LD transition.

In order to demonstrate the strong spatial correlations between islands belonging to different eigenstates, we show, in figure 2(a), the charge density of three adjacent-energy localized electron eigenstates for a-Si, with each of the states depicted by a different colour (red, green and blue). Any departure of colour in the figure from these fundamental colours implies spatial overlap of states: the inset shows the secondary colours resulting from overlap of two islands, and regions of white indicate overlap of three islands. It is clear that the island structures in such localized eigenstates overlap spatially, very strongly so in certain regions, meaning that the same islands can participate in different eigenstates.

This fact leads us to conjecture on the existence of a bare-state (island) basis from which all the localized states can be constructed. Indeed, we were able to demonstrate numerically that the localized states in all the models studied can be decomposed into overlapping 'bare'

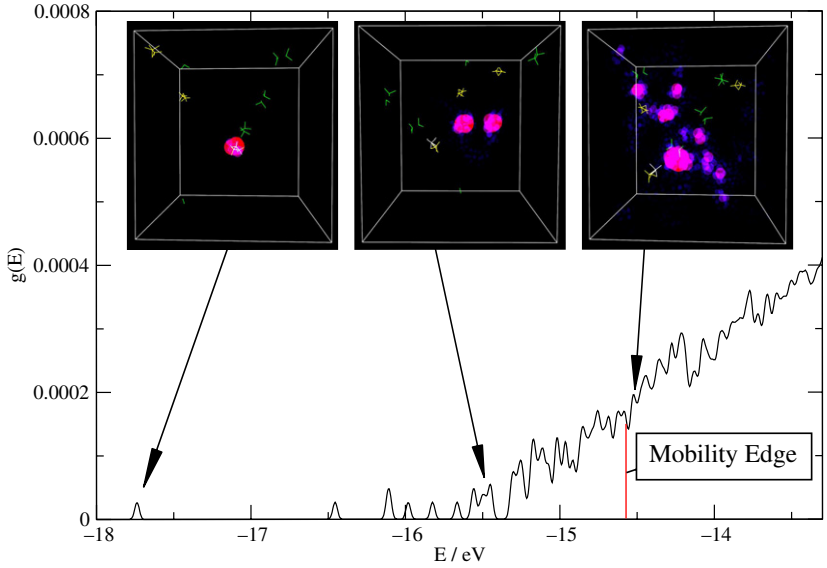

Figure 1. The electronic density of states in the lowest-energy band tail of the valence band for a 10 000-atom model of a-Si [10]. The indicated mobility-edge position was calculated using multifractal analysis [11]. Qualitatively similar behaviour is also found for the highest-energy valence-band tail (in the optical gap). Insets: charge densities of three selected eigenstates corresponding to the energies indicated, with a colour indicating the magnitude of the charge density (red maximum, blue minimum). The right-hand panel shows a multifractal critical eigenmode at the LD transition. Coordination-defect configurations in the model are shown by the stick diagrams. It can be seen that the most localized, single-island gap state is strongly associated with a coordination defect; this is not the case for multi-island localized band-tail states.

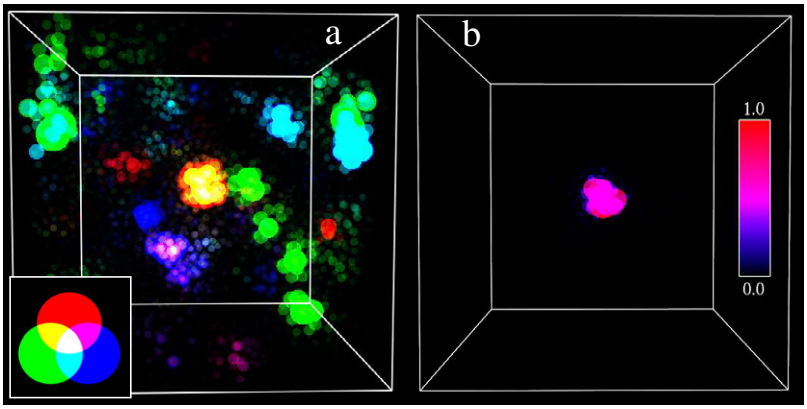

Figure 2. (a) Charge density of three adjacent-energy localized electron eigenstates in the lowest-energy tail of the valence band for the a-Si model (at energies $E = -14.630$, -14.628 and -14.623 eV), shown in red, green and blue, respectively. Regions where two islands overlap are shown with secondary colours according to the chart shown in the inset, and overlap between three islands is shown in white. These states are within the critical (LD) region. A linear mapping is used between charge and colour intensity. (b) An island extracted from the eigenstates shown in the left panel, corresponding to the (white) region of maximum overlap. Here, colour simply indicates charge density, according to the scale on the right.

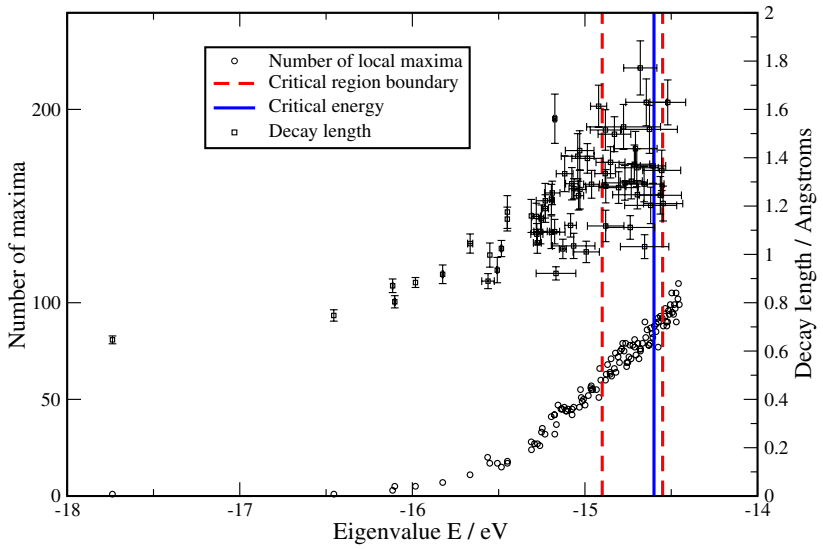

Figure 3. The island localization length (right vertical axis) and number of local maxima of the eigenstate amplitude (left vertical axis) versus eigenstate energy for the model of a-Si. The dashed vertical lines show the range of the critical (prelocalized) states found by a multifractal analysis (for a single size of model) using a method based on the investigation of the properties of the singularity spectrum. The blue line shows the localization–delocalization threshold obtained from multifractal analysis assuming universality of the singularity spectrum [12].

(This figure is in colour only in the electronic version)

islands. The problem of finding the bare-state (island) basis, given a collection of eigenstates in a certain energy range, is not computationally trivial. First, we assumed, and then proved, that the islands possess a fixed structure, independent of the eigenstates to which they contribute. Next, in order to extract the islands, we implemented a 'boot-strapping' procedure, in which we started with the most localized eigenstates (in the gap), essentially single islands, and then proceeded towards the LD threshold, extracting in each case the contributing islands (linear combinations of which form the eigenstates). This process required a metric for localization, since we needed to determine the most localized objects from which the states could be built. The localization gauge selected was the local inverse participation number, $p = \sum_{ieR} |y_i|^4$, where y_i is the wavefunction evaluated at atom i, and R is the set of atoms within a certain cut-off radius from the centre of an island. This value is minimal when there is least contribution to the eigenvector around the position of the island, and hence it is an ideal function for removing island states from an eigenvector. The method is computationally expensive, but powerful enough to allow island separation, for example, for a band tail involving 100 states for a model of a-Si with 10 000 atoms [10]. The utility of this procedure is demonstrated in figure 2(b), which shows an island, derived from the three eigenstates shown in figure 2(a), and corresponding to the most strongly overlapping part of the localized states involved.

The islands extracted from the localized eigenstates are also spatially localized, decaying exponentially away from the centre of the island, and their typical decay (localization) lengths can be found numerically and are shown in figure 3. Up to the critical LD-transition region, the island localization length smoothly increases from about 0.6 Å to about twice this value at the beginning of the critical region. The length scale of fluctuations of the filling function is therefore $\sim$1 Å. This is consistent with microphotoluminescence experiments [1] which show

little variation in island 'size' of localized exciton states for different levels of disorder and varying energies.

Thus, although the island decay lengths do *not* themselves diverge at the LD transition (figure 3), the islands proliferate in number (as suggested by Dong and Drabold [9]) as the transition is approached and the envelope of eigenstates becomes scale free. An estimate of the number of islands can be obtained by counting the number of local maxima in the eigenmodes. A local maximum is defined as the site on which the amplitude of the eigenfunction is greater than all others within a certain cut-off radius, R_c, for a particular model (e.g. R_c was chosen to be 5 Å in the case of the a-Si model). The number of local maxima gives an estimate of the number of islands and it smoothly increases up to the LD transition. Close to the critical point, the number of local maxima reaches the maximum possible value for finite-size models, thus fully filling the space in the limit of extended states, which is consistent with the conventional picture of the LD transition.

As we have emphasized, the LD transition appears in diverse contexts in disordered systems. In order to see how general is the picture of localized eigenstates comprised of bare island states that was found in the study of electron states in a-Si, we have also considered a simple-cubic-lattice Anderson electron model, atomic vibrations in a force-constant-disordered FCC lattice model [14] and in a realistic, topologically disordered model of a-Si and, to explore the role of long-range (Coulombic) interactions, in a 1650-atom realistic model of a-SiO_2 [13]. In figure 4(a), we show three superposed critical eigenstates, adjacent in energy, for the Anderson electron model. This figure illustrates that even critical eigenvectors are still clearly composed of islands. Three adjacent-energy localized vibrational eigenvectors showing island structures are shown for the model of a-SiO_2 in figure 4(b), of a force-constant-disordered FCC lattice in figure 4(c) and for the model of a-Si in figure 4(d). It is evident, therefore, that systems with highly distinct types of disorder possess qualitatively similar island-like internal structures of localized eigenstates. For all the model systems discussed in this paper, states in the gap, far from the band edge, are highly localized single-island states, while for energies in a band tail multi-island localized states appear; these eigenvectors may be decomposed into primitive islands, which may appear at the same position in several different adjacent-energy eigenvectors. The islands become more numerous, but only slightly spatially larger (see figure 3), as the energy approaches the critical LD energy. Moreover, these conclusions appear to hold for either long-range or short-range interactions, for electronic and vibrational eigenstates, and for diverse manifestations of disorder in both realistic and toy models.

The universal picture of the internal structure of localized eigenstates that emerges from this work leads to the conclusion that, contrary to naïve expectation, different localized states can be rather highly correlated with each other (especially for those with near-adjacent eigenvalues) as a result of the same islands of charge density or vibrational amplitude appearing in different eigenstates. Correlations between localized states (particularly in the vicinity of the critical LD region) had been anticipated [6], but this work is the first to demonstrate unambiguously the structural origin of such correlations and its occurrence for diverse realistic models. (Results of a quantitative analysis of auto- and cross-correlations for localized eigenvectors will be published elsewhere [15].) The existence of such (strong) correlations has a number of consequences for the physical behaviour associated with localized eigenstates. First, there will be a consequence on the form of the eigenvalue level-spacing statistics due to level-repelling effects associated with the correlations. A departure from the Poisson statistics characteristic of (uncorrelated) highly localized states is therefore expected [16] for localized states in band tails, particularly as the LD transition is approached; indeed, we have found evidence for such a departure, to 'semi-Poisson' level-spacing statistics [17], from a Bayesian analysis [9]. The picture of localized band-tail states as having an internal structure consisting

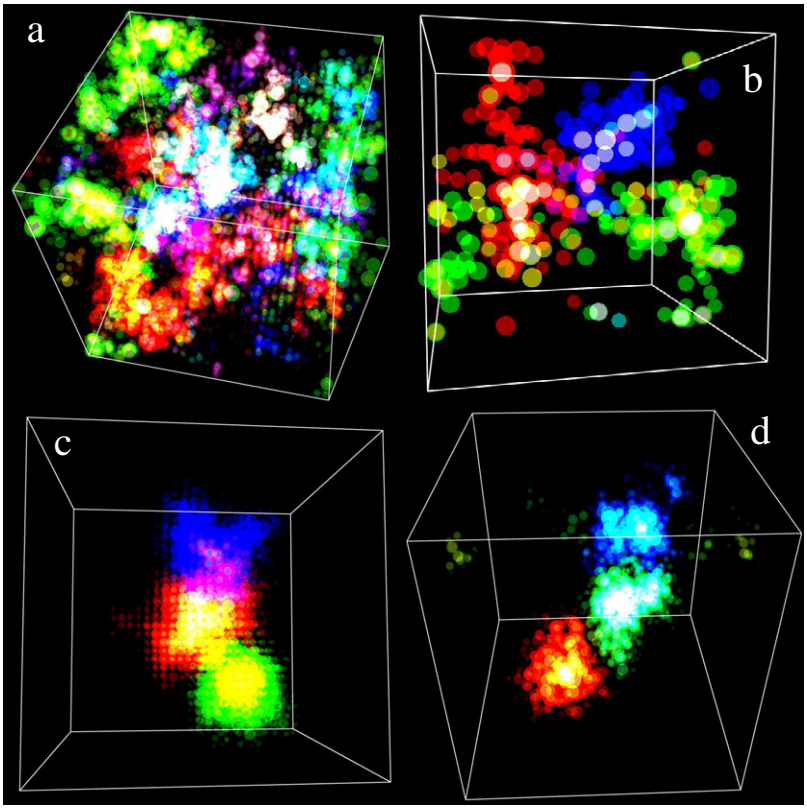

Figure 4. Universality of localized-eigenstate structure for sets of three localized eigenstates (red, green and blue) for various systems, showing spatial overlap of islands (the colour code indicating the overlap is the same as in figure 2(a). (a) Three adjacent-energy eigenvectors taken from the band centre for the electronic Anderson model on a simple cubic lattice with the critical ratio of the range of on-site disorder of width W to the off-diagonal interaction, V, i.e. $W/V = 16.5$, sufficient to localize all states in the band. These are critical eigenvectors of the model, and are clearly constructed from islands. The appearance of the same islands in consecutive eigenstates is clearly evident. (b) Three adjacent-energy vibrational eigenvectors of a 1650-atom vitreous silica model [13]. Three regions, that are mainly red, green and blue, can be seen, and each of these has a white centre, indicating overlap of the three eigenvectors at these points. (c) Three adjacent-energy vibrational eigenvectors on a 48-site [3] FCC lattice with force constants taken from a uniform distribution of width 2.0 and average value 1.0 (the crystal has a force-constant value of unity). The overlapping island states are less isotropic because of the underlying lattice. (d) Three adjacent-energy vibrational eigenvectors (red, green, blue) of a 10 000-atom model of a-Si, again showing strongly overlapping islands.

of overlapping islands also has implications for electron transport in band tails (e.g. in a-Si:H or conducting polymers) in photoconductivity or time-of-flight drift-mobility measurements, or in the thermalization of optically created carriers in band-tail states. The overlap between islands of charge density in localized band-tail states with similar energies means that a simple tunnelling picture for electron transport [18] between such correlated states may not be entirely correct.

In conclusion, we have shown that

(1) in a wide array of realistic physical models, localized eigenstates are composed of islands of 'charge' (electron probability density, vibrational displacement field);

(2) these individual islands spatially decay exponentially and their localization length does not change dramatically near the localization–delocalization transition;
(3) the number of islands reaches a value consistent with the space-filling nature of extended states around the localization–delocalization transition, thus producing a connectivity of the excitations (electronic or vibrational) through the system, being conceptually akin to a percolation model at criticality;
(4) we show, by construction, that consistent island extraction is possible for all these systems.

We are grateful to Dr G T Barkema for providing us with the model of a-Si, and thank Dr J C Phillips for pointing out recent experiments [1] on quantum wires and their significance and Professor Jianjun Dong for helpful discussions. DAD thanks the National Science Foundation for support under grant DMR 0310933 and DMR 0205858, and JJL the Engineering and Physical Sciences Research Council for the provision of a PhD studentship.

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