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Possibility of two types of localized states in a two-dimensional disordered lattice

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We report results of our numerical calculations, based on the equation of motion method, of dc electrical conductivity, and of density of states for up to 40×40 two-dimensional square lattices modeling a tight-binding Hamiltonian for a binary (AB) compound, disordered by randomly distributed B vacancies up to 10%. Our results indicate strongly localized states away from band centers separated from the relatively weakly localized states towards midband. This is in qualitative agreement with the idea of a "mobility edge" separating exponentially localized states from the power-law localized states as suggested by the two-parameter scaling theory of Kaveh in two dimensions. An alternative explanation, consistent with one-parameter scaling theory, is that the observed numerical effects may arise as a consequence of the variation of the localization length over the band.

While the absence of quantum diffusion on a two-dimensional (2D) random lattice, or a continuum, follows generally from the one-parameter scaling theory of localization of Abrahams *et al.*,[1] the spatial nature of the localized states still remains very much in question.[2–4] Thus the scaling theory predicts exponential localization of all eigenstates with the localization length ξ. This would imply that the resistance per square of a two-dimensional sample should increase exponentially with the sample's linear size L for $L > \xi$. (For $L < \xi$, of course, the growth is logarithmic.) This should be so independently of the Fermi level (or band filling). On the contrary, Kaveh[3] has argued for a two-parameter scaling theory giving a well-defined "mobility edge" separating two types of localized states—the exponentially localized states away from the band center and algebraically (power-law) localized states towards midband. This is in agreement with the experimentally determined β function of Davies, Pepper, and Kaveh.[2] Such a transition should show up when the size-dependent conductance is plotted as function of Fermi energy (band filling) for a given disorder. Of course, the non-self-averaging nature of conductance requires a reformulation of scaling as that of the full probability distribution of conductance.[5–8] Here, the validity of the one-parameter scaling hypothesis has been called into question,[5–7] notably by Altshuler, Kravtsov, and Lerner.[5] The present work, however, addresses numerically the limited question of the existence of the "mobility edge" in a model 2D disordered lattice, which would signal a two-parameter scaling.[3]

In this paper, we discuss numerical results obtained using the equation-of-motion (EOM) method, in which we calculated the conductivity $\sigma(E)$ (which is the same as conductance in two dimensions) for a finite two-dimensional square lattice up to size 40×40 as function of (Fermi) energy and sample size. For this we have chosen a tight-binding Hamiltonian modeling a binary compound AB, disordered by randomly distributed B vacancies up to 10 B at.%. We have also calculated the density of states (DOS) to ensure that any vanishing of conductivity is not simply due to absence of states at that energy. We would like to mention here, for the sake of completeness, that this model arose in a different context of our earlier study of electrical transport in the two-layer thick TiO_2, with the identification Ti≡A and O≡B [Fig. 1(a)]. A two-dimensional projection of this bilayer is shown in Fig. 1(b). The disorder corresponds to oxygen vacancies. This two-dimensional system shown schematically in Fig. 1(c) is now to be treated as the present model for a disordered binary alloy, independently of its original motivation.

The tight-binding Hamiltonian for our 2D two-sublattice (bipartite) model can be written in obvious notation,

$$H=\sum_{\sigma,i\in A} E_{Ai}a_{i\sigma}^{\dagger}a_{i\sigma}+\sum_{\sigma,l\in B} E_{Bl}b_{l\sigma}^{\dagger}b_{l\sigma}+\sum_{\langle i,j\rangle;\sigma,\sigma'} t_{AA}a_{j\sigma}^{\dagger}a_{i\sigma'} + \sum_{\langle l,m\rangle;\sigma,\sigma'} t_{BB}b_{m\sigma}^{\dagger}b_{l\sigma'} + \sum_{\langle i,l\rangle;\sigma,\sigma'} t_{AB}(a_{i\sigma}^{\dagger}b_{l\sigma'}+\text{H.c.})\,. \quad (1)$$

Here i,j run over the A sublattice; l,m run over the B sublattice and $\langle\ \rangle$ denotes nearest neighbors. (With respect to the original model, we can identify A≡Ti and B≡O.) The tight-binding parameters are chosen as follows.[9] The off-diagonal matrix elements are taken as ordered [see Fig. 1(c)] with

$t_{AA} \equiv t_2 = -0.2$ eV (nominally Ti:3d–Ti:3d hopping matrix element),

$t_{BB} \equiv t_3 = 1.5$ eV (nominally O:2p–O:2p hopping matrix element),

$t_{AB} \equiv t_1 = -2.3$ eV (nominally Ti:3d–O:2p hopping matrix element).

Disorder due originally to oxygen vacancies is now introduced by giving a fraction δ of B sites, chosen at random, different on-site energy values (depending on whether these correspond to oxygen vacancy or no vacancy). Thus $E_{Bl}=2.0$ eV (vacancy on the B sublattice), $E_{Bl}=-10.5$ eV (no vacancy on the B sublattice), $E_{Ai}=-6.4$ (A sublattice).

Simultaneous with the B sublattice on-site disorder, all site diagonal energies are also shifted depending on their distances from the B-site vacancy. (This is to be expected for the original model due to the Coulombic effects associated with O^{2-} vacancies.) Thus, due to a vacancy at a position $\mathbf{r}_o$, say, the diagonal elements of the other sites are shifted by

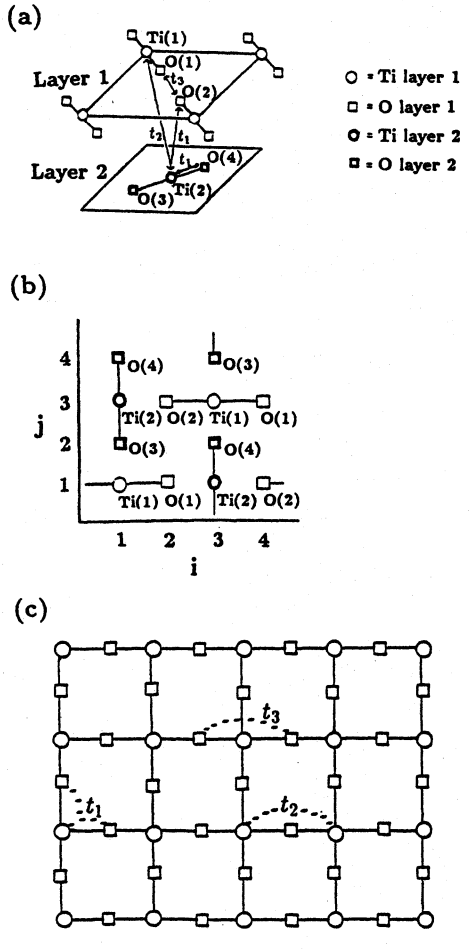

FIG. 1. (a) Rutile structure of TiO_2 showing the off-diagonal elements t_1, t_2, and t_3 in our model. (b) The projection of two layers of TiO_2. (c) Our present model of the binary alloy used in our work. A atoms (titanium) are in circles and B atoms (oxygen) are in squares.

$$E_{Ai} \rightarrow E_{Ai} \frac{-Qe^{-\beta|\mathbf{r}_i-\mathbf{r}_o|}}{\epsilon_\infty |\mathbf{r}_i-\mathbf{r}_o|}, \tag{2}$$

$$E_{Bl} \rightarrow E_{Bl} + \frac{-Qe^{-\beta|\mathbf{r}_l-\mathbf{r}_o|}}{\epsilon_\infty |\mathbf{r}_l-\mathbf{r}_o|}. \tag{3}$$

Here we choose[9] $Q=2|e|$, $\epsilon_\infty=6.7$, and the screening parameter $\beta=0.5$ A^{-1}. The pairwise Coulombic effects are, of course, superposed for a finite concentration of vacancies. The off-diagonal matrix elements to the vacancy are set to zero. This completes our description of the model. We again emphasize that this model arose in a different, realistic, context but our results have a bearing on the general questions concerning localization in two dimensions independently of the original context.

For the calculation of the density of states $N(E)$ and dc conductivity $\sigma(E)$ we use the EOM method. First we consider the DOS. For this, we have to evolve the initial state

$$|\Psi(t=0)\rangle = \sum_\nu e^{i\phi_\nu}|\nu\rangle \tag{4}$$

unitarily according to the Schrödinger evolution ($\hbar=1$)

$$|\Psi(t+\delta t)\rangle = e^{-iH\delta t}|\Psi(t)\rangle . \tag{5}$$

Here ν refers to all site orbitals and ϕ_ν are phases assigned uniformly to the orbitals ($0 \le \phi_\nu \le 2\pi$). Averaging over these phases, one gets the DOS,

$$\begin{aligned} N(E) &= \frac{Re}{\pi}\int_0^\infty dt\, e^{-(E+i\eta)t}\langle \Psi(t=0)|e^{-iHt}|\Psi(t=0)\rangle \\ &= \frac{Re}{\pi}\int_0^\infty dt\, e^{i(E+i\eta)t}\sum_{\mu,\nu} e^{i(\phi_\nu-\phi_\mu)}\langle \mu|e^{-iHt}|\nu\rangle \\ &= \frac{Re}{\pi}\sum_\nu \int_0^\infty dt \langle \nu|e^{i(E-H+i\eta)t}|\nu\rangle \\ &= \sum_\nu \langle \nu|\delta(E-H)|\nu\rangle = \sum_s \delta(E-E_s), \end{aligned} \tag{6}$$

where μ,ν denote orbitals and s denotes eigenstate. Here we have used for the random phase average $\langle e^{i(\phi_\nu-\phi_\mu)}\rangle = \delta_{\nu,\mu}$.

For the dc conductivity, we have adapted the EOM method to calculating $\sigma(E)$. The details of our calculations will appear elsewhere.[10] In the linear response theory, the dc conductivity of a noninteracting electron system is given by[11] the Kubo-Greenwood formula at $T=0$ K (with $E_F=E$) as

$$\sigma(E) = \frac{2\pi\hbar e^2}{m^2\Omega}\sum_{\mu,\nu} |\langle \mu|P^x|\nu\rangle|^2 \delta(E-E_\mu)\delta(E-E_\nu) . \tag{7}$$

Here the polarization is taken in the direction of the x axis, μ and ν label eigenstates, P^x is the momentum operator ($P^x/m = -(i/\hbar)[X,H]$), Ω is the volume of the sample, and H is the Hamiltonian of the system. To evaluate Eq. (7) using the EOM method, one must define two independent initial states as in Eq. (4) and make them evolve in time and finally average over phases in a fashion similar to the DOS case. We would like to note in passing here that averaging over the initial orbital phases, as-

sumed uniformly, randomly distributed over the 2π interval, is a purely mathematical artifice essential to our numerical technique for evaluating the trace involved in Eqs. (6) and (7). It is quite distinct from the usual ensemble averaging over the different realizations of the random potential. We may refer to these two as the "phase ensemble" and the "potential ensemble," respectively. Now, it is well known in the case of "potential ensemble" that an extensive self-averaging quantity like DOS obeys the central limit theorem and thus the iterations over the random sets converge fast. This is not so in the case of the dc conductance which is non-self-averaging. On general grounds, however, we expect this to be so with respect to averaging over the "phase ensemble" as well. Thus, the dc-conductivity calculation requires many iterations over random sets of phases because the fluctuations are not controlled only by the sample size as in the DOS case. We evaluated Eq. (7) for a sample of size 40×40 units (1200 sites) containing 1, 5, 8, 9, and 10 at. % of B (oxygen) vacancies.

Our results of the equation-of-motion calculations for the conductivity $\sigma(E)$ and the density of states $N(E)$ are presented in Figs. 2 and 3. Figure 2 shows $\sigma(E)$ and $N(E)$ for the defect concentration δ from 1% to 10% for the 40×40 square lattice (note the difference in conductivity scales). Several points can be noted: first, $\sigma(E)<e^2/\hbar$ in all cases suggesting that the sample is in the strong-disorder limit for this finite size. One clearly sees the expected decrease of conductivity with increasing disorder (δ). There are large fluctuations of the conductance as E varies over the band. These are presumed to be partly intrinsic due to disorder (the universal conductance fluctuation) and partly due to the finite size effects. It should be noted here that no ensemble averaging of the conductance or DOS for different realizations of disorder have been performed. Also, overall, the conductivity follows the density-of-states profile, but in Fig. 2 one sees that the conductivity vanishes sufficiently away from the centers of the nominally A and B subbands, where the DOS remains substantial. This may suggest a "mobility edge" separating two types of states; the inner states towards mid-band are more conducting and therefore less localized than the states on the outer sides of the "mobility edges."

To make this last point clearer we have presented our calculations for the $\sigma(E)$ and DOS on an expanded scale for three concentrations in Fig. 3. The range of energies presented spans the nominally A subband. One clearly sees an energy interval on either side of the main band where the conductance is essentially zero while the DOS is substantial. As a specific example for the case of $\delta=10\%$, the $\sigma(E)\sim0.1(e^2/\hbar)$, which is Mott's minimum metallic conductivity for E approximately the band center (about -3.5 eV). However, it becomes near zero for energies below about -6.5 eV and above -2.0 eV

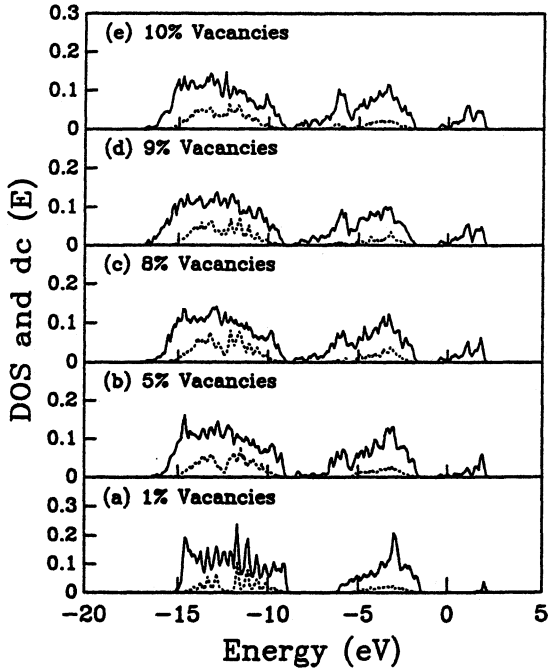

FIG. 2. DOS (solid curve) and dc conductivity (dotted curve) for a sample of 40×40 units containing B (oxygen) vacancies with various concentrations (1, 5, 8, 9, and 10 at. %). The scale shown is for the DOS in 1/eV units. However, the scales of conductivity in $e^2/\hbar$ are the shown times: (a) 30, (b) 7.5, (c) 4.5, (d) 4.5, and (e) 4.5.

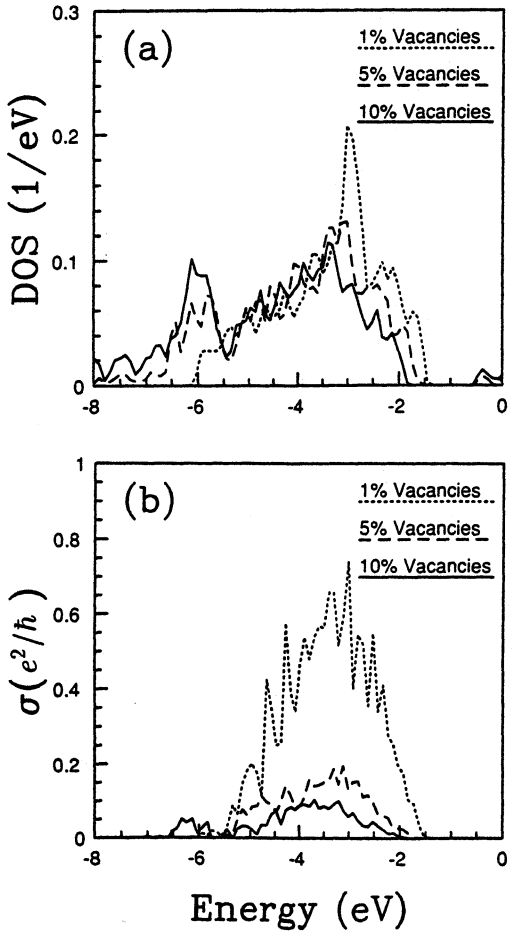

FIG. 3. (a) DOS in units of 1/eV per site for a sample of size 40×40 units containing 1, 5, and 10 at. % of B (oxygen) vacancies. (b) dc conductivity for the same samples of (a) displayed on the same energy scale to discriminate the nature of eigenstates of DOS.

where the DOS is quite substantial. Similar observations can be made for lower concentrations but the fluctuations are much too large to allow definitive conclusions. Preliminary studies of the scaling of conductance with finite lattice size (12×12, 20×20, and 40×40 units in Fig. 4) suggest that all states are localized, and that the conductance falls monotonically with increasing lattice size. (In two dimensions extended states would give conductance independent of system size.) However, the analysis also confirms that there is an energy interval outside of the main conducting band where the conductance remains nearly zero without the vanishing of the DOS. These observations are consistent with the idea that two types of localized states might exist as suggested by the two-parameter scaling theory of localization—weakly (power law) decaying states towards mid-band and strongly (exponentially) decaying states towards band edges. Our limited data of sample sizes do not permit us to make any quantitative estimates for the localization parameters. One remark about our lattice size. It should be noted that at least for the case of $\delta=10\%$, the conductance value is close to Mott's $\sigma_{\min}$ value, which may suggest that $k_F l_e \sim 1$ and, therefore, the 40×40 sample may not be too small. Despite the remarks of this paragraph, it should be emphasized that the numerical data do not exclude the possibility that the conductivity variation over the band might arise just as a consequence of the variation of the localization length ξ over the band, as in the one-parameter scaling theory.

Our limited numerical data are consistent with, but do not prove, the following scenario: In one dimension, all (but zero measure) states are well known to be localized exponentially. In two dimensions there is a pseudomobility edge $E_{c'}$ separating the outer exponentially localized states from the inner power-law localized states. In this picture, the latter would be *normalizable* and expected to give anomalous "subdiffusion"; i.e., mean-squared displacement growing with time t as t^{η} with $\eta<1$, and hence zero conductivity in the $L\rightarrow\infty$ limit. In three dimensions, in this scenario, there is a genuine mobility edge E_c separating the outer exponentially localized states from the *non-normalizable* "resonant states" up to $E_{c'}>E_c$ when $\sigma(E_{c'})\simeq\sigma_{\min}$ in the $L\rightarrow\infty$ limit. Beyond this ($E_c>E_{c'}$) the states are extended and diffusive, albeit with small weak-localization corrections. In other words, this picture supposes that in three dimensions, the weak-localization corrections to $\sigma>\sigma_{\min}$ (due to coherent backscattering) develop into *non-normalizable* and therefore conducting "resonances" for $0<\sigma\leq\sigma_{\min}$. In two dimensions, on the other hand, these resonances remain *normalizable* giving merely anomalous "subdiffusion" and, therefore, zero conductivity in the $L\rightarrow\infty$ limit. To definitively establish the existence of such resonance states (normalizable in two dimensions and non-normalizable in three dimensions) would obviously require deeper numerical analysis.

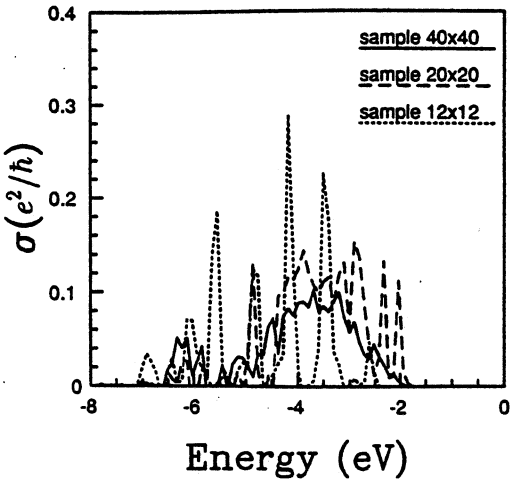

FIG. 4. Scaling of conductance with sample size. The sample sizes displayed are of dimensional 40×40, 20×20, and 12×12 units. Each sample contains 10 at. % of *B* (oxygen) vacancies. The energy scale displayed includes the *A* (titanium) subband region.

In conclusion, we have presented some numerical indications possibly consistent with exponentially localized states at the band tails and power-law localized states at the band centers separated, presumably by a pseudomobility edge in agreement with the prediction of Kaveh. Such power-law localized states may be normalizable resonances caused by the coherent backscattering, which, in such a picture, become non-normalizable in three dimensions and dominate the critical regime $0<\sigma\leq\sigma_{\min}$. On the other hand, our numerical data may also be consistent with the conventional one-parameter scaling theory. If the first interpretation is correct, an understanding of why no evidence of such two-parameter behavior appears to arise in recent two-dimensional simulations of the Anderson model[12] is also required.

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[1]E. Abrahams, P. W. Anderson, D. C. Licciardello, and T. V. Ramakrishnan, Phys. Rev. Lett. **42**, 693 (1979).

[2]R. Davies, M. Pepper, and M. Kaveh, J. Phys. C **16**, L285 (1983).

[3]M. Kaveh, J. Phys. C **17**, L79 (1985).

[4]N. F. Mott and M. Kaveh, Adv. Phys. **34**, 329 (1985).

[5]See, e.g., B. L. Altshuler, V. E. Kravtsov, and I. V. Lerner, in *Anderson Localization*, edited by T. Ando and H. Fukuyama, Springer Proceedings in Physics Vol. 28 (Springer, Berlin, 1988), p. 300.

[6]V. E. Kravtsov and I. V. Lerner, Zh. Eksp. Teor. Fiz. **88**, 1281 (1985) [Sov. Phys. JETP **61**, 758 (1985)]; Solid State Commun. **52**, 593 (1984).

[7]N. Kumar and A. M. Jayannavar, J. Phys C **19**, L85 (1986).

[8]B. Shapiro, Phys. Rev. Lett. **65**, 1510 (1990).

[9]J. W. Halley and H. B. Shore, Phys. Rev. B **36**, 6640 (1987).

[10]J. W. Halley, H. B. Shore, and N. Tit (unpublished).

[11]R. J. Elliott, J. A. Krumhansl, and P. L. Leath, Rev. Mod. Phys. **46**, 465 (1974).

[12]B. I. Shklovskii, B. Shapiro, B. Sears, P. Lambrianides, and H. B. Shore (unpublished).