Quantum percolation in a two-dimensional finite binary alloy: Interplay between the strength of disorder and alloy composition

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We address the rather controversial issue of wave propagation in two-dimensional disordered systems. We have followed the time evolution of wave packets in a binary alloy in a two-dimensional finite square lattice where the on-site energies ε_a and ε_b are randomly distributed. The parameter that measures the degree of disorder is $\eta=|(\varepsilon_b-\varepsilon_a)/W|$, where W is the hopping term. We were able to construct a phase diagram in the (η,x) plane characterizing the different kind of wave propagation, x being the concentration of type-a atoms.

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In this work we address the controversial and very important issue of wave propagation in two-dimensional (2D) disordered systems by solving the time-dependent Schrödinger equation, with the aim of contributing elements to elucidate this crucial question. For more than two decades the prevailing view has been that, based on results of scaling theory, there can be no metal-insulator transition in two dimensions for zero magnetic field.[1] This view was contradicted by experimental results reported in the last several years[2–4] done on dilute two-dimensional electron and hole systems, where a metallic behavior was observed down to the lowest accessible temperatures at electron or hole densities above some critical density n_c. It is worthwhile to state that experiments done with samples of Si metal-organic semiconductor field-effect transistors and with $GaAs/Al_xGa_{1-x}As$ heterostructures gave similar results.[2] On the other hand, previous theoretical work[5,6] predicted, among other results, for quantum percolation threshold in the case of diagonal disorder, the value 0.867 well above the classical one 0.5928, and different from unity as expected from scaling theory. All this motivates a renewed interest in the problem of the nature of the states in 2D disordered systems and consequently in their transport properties. While preparing this paper we came upon a recent review which presented the state of the art on the subject.[7] The conclusions of Ref. 7 can be summarized by saying that in the absence of magnetic field and in clean dilute 2D systems, a strong metallic temperature dependence $(d\rho/dt>0)$ is observed at carrier densities above some critical value, while an insulating behavior $(d\rho/dt<0)$ is seen at densities below the critical one, ρ being the resistivity. In other words, a good ideal of experimental work pointed to the existence of a metal-insulator transition for sufficient clean samples in 2D systems. The results presented in this work concerning a binary alloy show conclusively that propagation *is* possible even in the presence of random disorder, while the electrons are in 2D mesoscopic systems such as the ones realized in devices. This is close agreement with the theoretical founding by Odagaki and Chang[5,6] and the experimental results of Kravchenko *et al.*[2]

Contrary to the fact that in a crystalline solid the electron states (Bloch states) are extended through the system, the inclusion of disorder produces localized wave functions and, depending on the strength of the disorder, can inhibit propagation of wave packets. The pioneering work by Anderson[8] clarified the role disorder plays. He then concluded that for a sufficient degree of disorder all states should be localized.

In a classical entity the existence of a system-spanning cluster is a sufficient condition to percolate across the sample.[9] But simple classical connectivity does not assure a nonzero quantum transmittance. It could be that for large enough disorder carriers are localized in a definite region of the lattice even on connected spanning clusters. In the case of a binary alloy along a tight-binding model, *large* diagonal disorder means that on-site energies ε_a and ε_b are very different, thus any time the carrier is on site *a*, for example, it will find hopping to a neighboring *b* atom strongly inhibited and backscattering takes place.

Clearly it is not only the strength of the disorder but also the dimensionality of the system that contributes to the kind of propagation (localization) of wave packets. In 1D disordered random systems the picture was definitively established: it is impossible for a carrier to propagate through them. The exceptions belong to the class of *deterministic* aperiodic structures such as Fibonacci, Thue-Morse, and Harper[10–12] models, where one can even obtain superdiffusive propagation. But in a 2D system, such as the one we are analyzing in this work, due to the greater connectivity of the lattice we expect a different behavior from the 1D case.

Let us now briefly discuss the nature of the stationary solutions of the Schrödinger equation in disordered systems. The one-parameter scaling theory put forward by Abrahams *et al.*[1] implied that there are almost no extended states for carriers in a disordered layer. From works based on scaling theory it was widely believed that states are almost all exponentially localized with a localization length which varies with the energy of the state considered. Five years after the scaling theory prediction, Odagaki and Chang obtained theoretical evidence that such a prediction could be wrong. In spite of this, the prevailing view was that disorder in two dimensions implies localization.

A review work[13] analyzed in detail the nature of stationary states in systems such as the object of the present study.

They found the existence of transparent resonant states that give a transmittance near unity, though such states come are very few among several thousand.

We treated the problem of carrier percolation in a binary alloy $a_x b_{1-x}$ with diagonal disorder in a 2D underlying square lattice with on-site energies ($\varepsilon_{n,m}=\varepsilon_a$ or ε_b) randomly distributed. We solved the Schrödinger wave equation in the Wannier representation

$$i\frac{df_{n,m}}{d\tau}=(f_{n+1,m}+f_{n-1,m}+f_{n,m+1}+f_{n,m-1})+\zeta_{n,m}f_{n,m}, \tag{1}$$

where we introduced the dimensionless variables:

$$\tau=\frac{Wt}{\hbar}; \quad \zeta_{n,m}=\frac{\varepsilon_{n,m}}{W} \tag{2}$$

W is the hopping term considered to be *constant*, and a well-localized particle is taken as the initial condition:

$$f_{n,m}(t=0)=\delta_{n,o}\delta_{m,o} \tag{3}$$

We have considered lattices of $N_x\times N_y=N$ sites and avoided boundary effects. The maximum lattice size considered was one of 77×77 sites. In a previous work[14] we introduced a method to solve Eq. (1) based on a diagonalization of the dynamic matrix.

We have to deal with alloys of different concentrations, let us call x the concentration of type-a atoms. A crucial parameter that classifies the strength of disorder is the difference

$$\eta=\left|\frac{\varepsilon_b-\varepsilon_a}{W}\right| \tag{4}$$

It must be pointed out that this one-particle description remains valid for sufficiently long times such that the dephasing of the wave function due to interactions with phonons for instance is not appreciable.

A two-dimensional layer of electrons is obtained, for example, in experiments with metal-oxide-semiconductor devices where the carriers are trapped between the oxide and the semiconductor.[15] Also, at the interface between two perfectly matched crystals, as is the case of the semiconductors GaAs and $Ga_xAl_{1-x}As$, electrons donated by remote impurities are trapped there by the different chemical natures of the semiconductors.

A series of works was devoted to the problem of quantum percolation in 2D systems. Most of them dealt with the Kirkpatrick-Eggarter[16] model Hamiltonian, in which the site energies are constants independent of the site, while the hopping terms took the values 0 and 1 randomly distributed in the lattice.

While doing numerical calculations one is faced with the problem of the size of the sample. Thus it could happen that a particular state gives a transmittance close to 1 for a given lattice size, but when increasing the lattice size the transmittance falls to zero, which means that the localization length is larger than the former system size. In this case we are not in the presence of a true resonant state. The time limit taken in our calculations was 10^{-11} sec, much longer than any reasonable collision time in a sample. In order to avoid the problem associated with the finite size of samples which can mask the results, in the course of the calculations we increased the size until the outcome became size independent. The results reported here follow this criterion.

We proceed as follows. We start the calculations with an electron localized at a certain a site in the lattice when the concentration of a atoms is x. As stated above one important parameter that controls the type of propagation (localization) is η. Clearly when η is very small hopping is favored *even* between sites a and b. In these cases and independent of the concentrations of both types of atoms, we have a *ballistic* propagation of the initially localized wave packet: the mean square displacement to $C\,t^2$. Increasing η makes hopping between different species more difficult, so we reach several kinds of pictures which can be characterized as superdiffusive, diffusive, or subdiffusive propagations. Eventually for sufficient large η, the wave packet remains localized in a definite region of the lattice. But now all of this depends on the concentration x as opposed to the case of very small η.

The plotted curves are the results of an average done over several simulations performed for each alloy concentration x. In order to check our results we have done a number of tests. In particular, we have calculated for the crystalline monomer the mean-square displacement (MSD) obtaining the exact result,[14] a MSD of $4\tau^2$, while for the ordered ab dimer and for $\eta=1$ we obtained a MSD of $2.9\tau^2$. This is again ballistic, but with a smaller coefficient.

To analyze the different regimes of propagation (localization) we follow the temporal behavior of several functions. Following Anderson[8] we look at the amplitude of the wave function at the initial site, and assume that diffusion occurred if at $t\to\infty$ the amplitude goes to zero. Conversely, if the amplitude remains finite, decreasing rapidly with distance, we have a localized state. However, this is not so conclusive, so we also resort to an analysis of the following functions: (i) the Shannon (information) entropy[17] (which varies from 0 for a wave function confined to a single site, to $\ln N$ for a wave uniformly extended over the sites), (ii) the participation function[18] $P(t)=\{\Sigma_{n,m}|f_{n,m}(t)|^4\}^{-1}$ (which varies from 1 to N on both limits), and (iii) the mean-square displacement. At the same time we look at the three-dimensional plots of the wave function at different times. It is also illustrative to look at the site distribution for every configuration, since through this we can understand the way the wave packet travels through the structure.

Our results can be summarized in a phase diagram shown in Fig. 1, where the ballistic propagating regime is shown in the dotted region. In the white region lay the states that result in the propagation of different characteristics: superdiffusive, diffusive, and subdiffusive. In the dark area we show the region of localized regime.

The time evolution of the wave packet could be explained as follows: we start with a strongly localized packet on a given a site. It can therefore easily propagate through a sea of degenerate sites (a connected region with no b sites in it). This indicates the ''easy'' route to the packet. It could happen that this sea is surrounded by b sites which cause backscattering; if the strength of disorder is sufficiently large, it

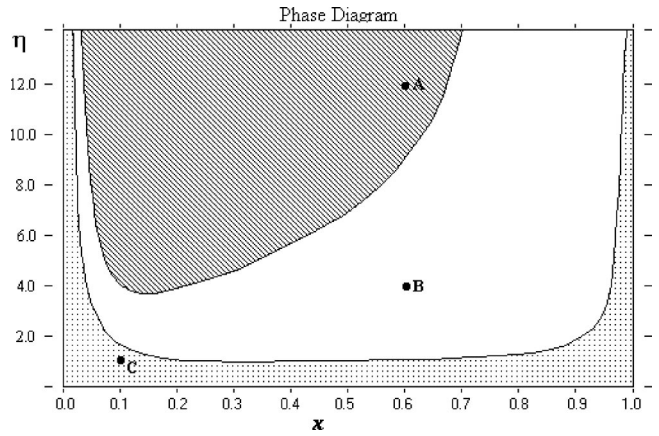

FIG. 1. The dotted area corresponds to the ballistic behavior of the wave packet. The superdiffusive, diffusive, and subdiffusive regimes are shown in white, and in the dark region we show the localized states.

will prevent the wave for entering this unfavorable region of the lattice. In this situation we are in the presence of a localized state.

We can infer from our calculations that in the limit of very strong tunneling, that is, when the difference of the on-site energies is small as compared with the bandwidth ($\eta \ll 1$), the initially localized wave packet tends to propagate ballistically through the lattice independent of the alloy composition, because hopping is favorable even between different atomic species. When increasing η, the alloy composition begins to determine the kind of propagation, which we explain as follows: if we start with a small η, such that for every concentration ballistic propagation takes place, when η increases hopping becomes more difficult between atoms *a* and *b*, in this way, the concentration plays important role, the more so the larger the disorder. This explains the asymmetry of the upper curve in the phase diagram by remembering that the packet is initially localized on an *a* site.

Note that for very low concentrations of *a* atoms ($x \ll 1$) we still have a ballistic behavior, even for large η. The reason for this is that the wave, which is initially on an *a* site, once it diffuses to a neighboring *b* site, will find a great facility to propagate to the other *b* sites that are the large majority. At the other extreme ($x \simeq 1$) it is clear that the wave will propagate ballistically independent of the intensity of disorder, since there exist a very few *b* sites that could prevent hopping.

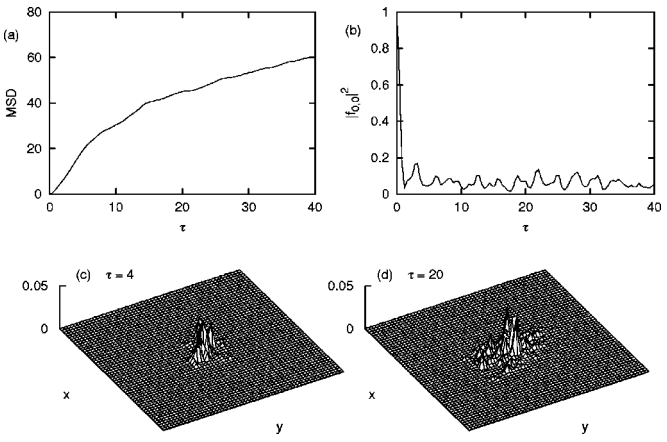

FIG. 2. Case A ($x=0.6, \eta=12$) shows the localized regime. (a) MSD. (b) Amplitude probability at the origin. (c) and (d) Wave function for different times.

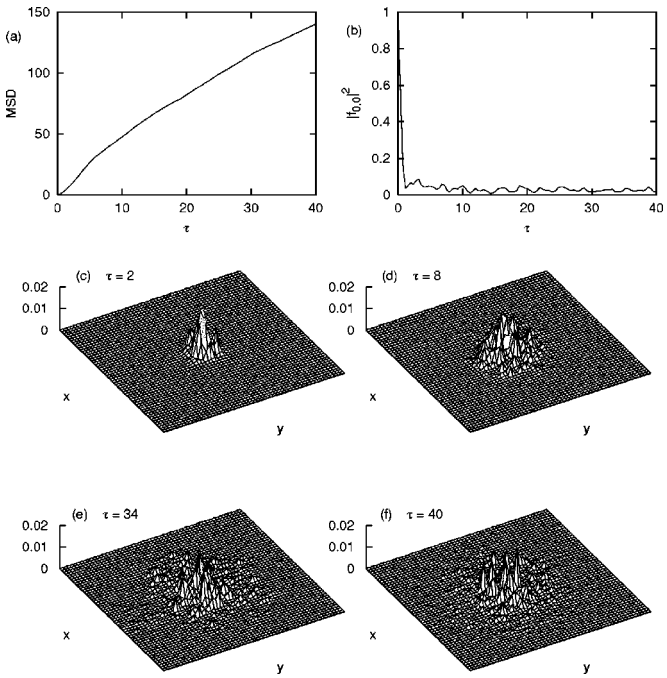

FIG. 3. Case B ($x=0.6, \eta=4$) shows the diffusive propagation regime. (a) MSD. (b) Amplitude probability at the origin. (c)–(f) Wave functions for different times.

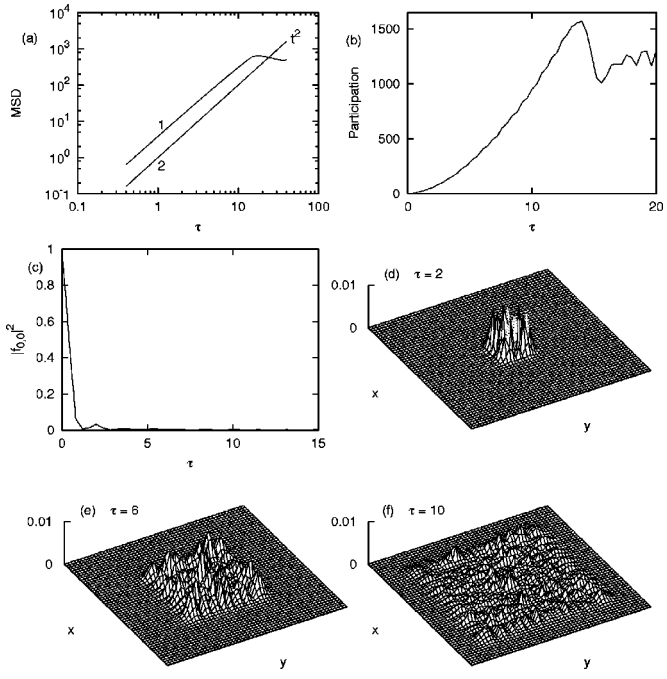

FIG. 4. Case C ($x=0.1, \eta=1$) shows the ballistic propagation of the wave packet. (a) MSD. (b) Participation function. (c) Amplitude probability at the origin. (d)–(f) Wave functions for different times.

In order to exemplify three different types of behavior of the wave packet, we show the averaged values of the MSD, the participation function, and the probability amplitude at the origin as function of time for three indicated points. A, B, and C in the phase diagram. We also show the evolution of the wave packet for different times in these three cases.

In case A ($x=0.6, \eta=12$), in Fig. 2 we show the MSD (a) and the amplitude probability (b) at the origin as function of time. Note that in this case $x>x_c$, which would imply a classical percolation. In Figs. 2(c) and 2(d) we show the wave function for different times, making it evident that the confinement of the wave in a finite region is the *localization* regime.

In case B ($x=0.6, \eta=4$) the MSD grows linearly in time clearly, indicating a *diffusive* behavior; see Fig. 3(a). In Fig. 3(b) the probability amplitude at the origin as a function of time is reported. We also show the time evolution of the wave packet at four different times, where we can step the spread of the wave.

In case C ($x=0.1, \eta=1$) the ballistic regime is evident. In fact in Fig. 4(a) we plot the MSD in curve 1, and a quadratic function for comparison in curve 2. The decrease in the MSD is because at that time the wave have reached the boundary. In Fig. 4(b) we also show the participation function, which on average grows linearly in time until the wave reaches the boundary. In Fig. 4(c) we show the amplitude probability at the origin which decreases very rapidly in time. Note the rapidly spreading of the wave function as shown in Figs. 4(d)–4(f).

We have estimated the quantum percolation threshold to be 0.76, by considering the limiting case $\eta \gg 1$, which can be compared with the value 0.867 obtained by Odagaki and Chang.[5] As can be seen, both estimates are well above the classical value and below the scaling prediction theory of unity. Another conclusion drawn from our calculations is that for $\eta<4$ localization does not take place (see Fig. 1). This should be compared with the estimate of 5.17 by Chang and Odagaki,[6] who used the coherent potential approximation in their work.

In this report we have presented results that show the time evolution of wave packets in two-dimensional disordered systems for different degrees of disorder strength as well as for different compositions of a binary alloy. Our main conclusion is that in a mesoscopic system such as that produced in devices, it is possible for a carrier to propagate, provided that a compromising situation is reached between the alloy composition and disorder strength. This is shown in a compact form in the phase diagram, which makes the different regimes of propagation evident. Finally, a metal-insulator transition for $B=0$ is expected to exist in 2D systems.

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