

# Absence of Diffusion in Certain Random Lattices: Numerical Evidence\*

P. Markoš

Department of Physics, FEI STU, 812 99 Bratislava, Slovakia

**Abstract:** We demonstrate, by solving numerically the time-dependent Schrödinger equation, the physical character of electron localization in a disordered two-dimensional lattice. We show, in agreement with the prediction of P. W. Anderson, that the disorder prevents electron diffusion. The electron becomes spatially localized in a specific area of the system. Our numerical analysis confirms that the electron localization is a quantum effect caused by the wave character of electron propagation and has no analogy in classical mechanics.

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## 1. Introduction

The electron localization in disordered systems [1] is responsible for a broad variety of transport phenomena experimentally observed in mesoscopic systems: the non-Ohmic behavior of electron conductivity, weak localization, universal conductance fluctuations, and strong electron localization [2, 3].

The localization arises in systems with a random potential. Following the original work of Anderson [1], we consider a time evolution of a quantum particle located at a time  $t = 0$  in a certain small area of the sample. For  $t > 0$ , the electron wave function scatters spatial inhomogeneities (spatial fluctuation of the potential). Multiple reflected components of the wave function interfere with each other. Anderson proved that if the strength of the disorder increases over the critical value, the wave function will be non-zero only within a specific area, and decays exponentially as a function of the distance from the center of localization. The probability to find an electron in its initial position is non-zero for any time  $t$ , even when time increases to infinity,  $t \rightarrow \infty$ .

It is important to note that the localized state differs from the quantum bound state. The bound quantum particle is trapped in a potential well, if its energy is negative. Contrary, the localized quantum particle can be localized in any region of the disordered lattice. Also, there is no restriction to the eigenenergy of the localized state, which can exceed the highest potential barrier inside the sample. Another difference between the bound and localized state is that the spatial distribution of the localized state is highly sensitive to the realization of the random disorder. The localized state therefore represents, besides the extended and bound states, the third possible eigenstate of quantum Hamiltonian.

\*) Dedicated to Professor Viktor Bezák on the occasion of his 70th birthday.

Localized electrons cannot conduct electric current [4–7]. Consequently, the probability of electron transmission  $T$  through a disordered system decreases exponentially as a function of the system length  $L$ :  $T \sim \exp(-2L/\xi)$ . The length  $\xi$  is the localization length. Materials that do not conduct electric current due to the electron localization are called Anderson insulators.

In spite of significant theoretical efforts, our understanding of electron transport in disordered systems is still not complete. Rigorous analytical results were obtained only in the limit of weak randomness, where perturbation theories are applicable [8–11]. In the localized regime, we do not have any small parameter in the theory, so no perturbation analysis is possible. Also, the transmission of electrons is extremely sensitive to the change of sample properties. In particular, a small local change of random potential might cause a change of the transmission amplitude in many orders of magnitude [12–15]. Analytical description of localized systems is therefore extremely difficult. Fortunately, it is rather easy to simulate the transport properties numerically. In fact, many quantitative data about the electron localization was obtained numerically [7, 16–20].

In this paper we describe simple numerical experiments which demonstrate the key features of quantum localization. We solve the time-dependent Schrödinger equation for the electron in two-dimensional disordered lattice and investigate the time evolution of the spatial distribution of the electron wave function. This reproduces the Anderson's original problem [1] and proves that, indeed, the electron becomes spatially localized in a certain part of the disordered sample.

## 2. The model

We consider the two-dimensional tight binding Anderson model [6, 21]. The time evolution of the electron wave function is given by the Schrödinger equation

$$i\hbar \frac{\partial \psi(\vec{r}, t)}{\partial t} = W \sum_{\vec{r}'} \psi(\vec{r}', t) V_{\vec{r}\vec{r}'}(\vec{r}, t). \quad (1)$$

The electron propagates via hopping from the site  $\vec{r}$  into the nearest neighbor site  $\vec{r}'$ . Since sites are arranged on the two-dimensional lattice, we have  $|\vec{r}' - \vec{r}| = a$ , where  $a$  is the lattice spacing. The energies  $\epsilon(\vec{r})$  mimic random potential: we assume that  $\epsilon(\vec{r})$  are randomly distributed with the Box probability distribution,  $P(\epsilon) = 1$  if  $|\epsilon - E| < 1/2$ , and  $P(\epsilon) = 0$  otherwise. Also, random energies on different sites are statistically independent. The case of zero disorder,  $W = 0$ , corresponds to the tight binding Hamiltonian which describes the propagation of electron on the two-dimensional lattice. The eigenenergies create the conduction band,  $4V - E < E < 4V$  [21].

The problem defined by Eq. (1) has two parameters: the hopping amplitude  $V$  and disorder strength  $W$ . The last determines the maximal amplitude of the fluctuations of random energies  $\epsilon$ . Since  $V$  just defines the energy scale, we have in fact only one parameter: the ratio  $W/V$ , which we use as a measure of the strength of the disorder. We see from Eq. (1) that the time is measured in units of  $\hbar/V$ .

Consider first the zero disorder case,  $W = 0$ . The electron, located at time  $t = 0$  in a certain lattice site,

$$(\vec{r}, t = 0) = (\vec{r} = \vec{r}_0), \quad (2)$$

will diffuse to the neighboring sites. In the limit of infinite time,  $t \rightarrow \infty$ , the electron will occupy the entire lattice – it will be “everywhere”. Consequently, the probability to find it at the original site is zero (or, more accurate, of the order of  $1/\text{volume}$ ). We ask, whether the diffusion of the electron is possible also in the case of non-zero disorder. Intuitively, one expects that a very weak disorder will not affect the diffusion, while a sufficiently strong disorder stops the diffusion. Then, there should be a critical disorder  $W_c$  such that diffusion stops when  $W = W_c$ , and continues infinitely long when  $W > W_c$ . In the original paper [1] Anderson derived the equation for the critical disorder,

$$\frac{W_c}{V} = 2eK \ln(eK). \quad (3)$$

According to Eq. (3), the critical disorder depends only on the connectivity (the number of the nearest neighbor) of the lattice,  $K$ . Today, we know that the critical disorder depends on the dimension  $d$  of the lattice [22, 23]. In the absence of magnetic field and electron spin, all states are localized in the disordered systems with dimension  $d < d_c = 2$ . Therefore, the critical disorder  $W_c = 0$  for  $d < 2$  and is non-zero in systems with higher dimensionality  $d > 2$ .

### 3. Diffusion

For the numerical solution of the Schrödinger equation (1) we consider the finite size of the system  $L = L$ , where  $L = 2048a$  for weakly disordered samples and  $L = 1024a$  for systems with a stronger disorder  $W/V = 4$ .

First, we need to define the initial wave function  $(\vec{r}, t = 0)$ . A more suitable candidate than the  $\delta$ -function (2) is any eigenfunction of the Hamiltonian defined on a small sub lattice (typically the size of  $24a = 24a$ ) located in the center of the sample [24]. Usually we chose the eigenfunction which corresponds to the eigenenergy closest to  $E = 0$  (the middle of the conductance band).

We solve the Schrödinger equation (1) numerically and find the time evolution of the wave function  $(\vec{r}, t)$ . The numerical program is based on the alternating-direction implicit method [25, 26] used for the solution of elliptic partial differential equations.

The ability of an electron to diffuse through the sample is measured by a quadratic displacement, defined as

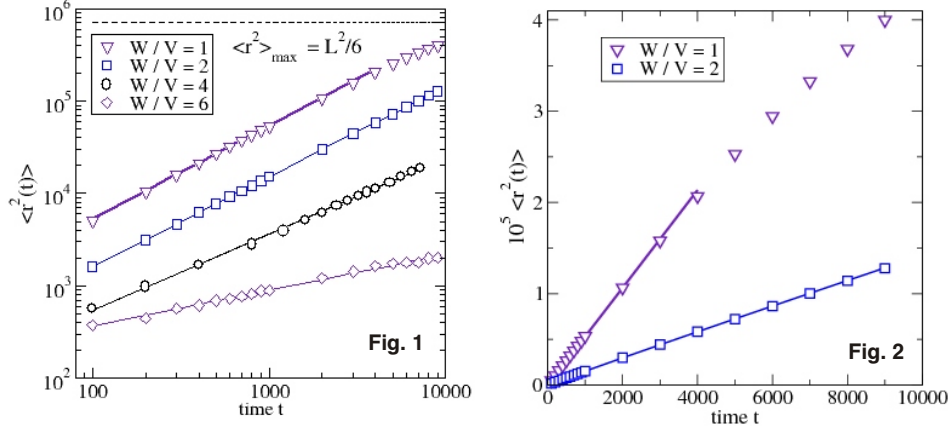
$$\langle r^2(t) \rangle = \int d\vec{r} r^2 |\psi(\vec{r}, t)|^2. \quad (4)$$

Figs. 1 and 2 show that, in weak disorders,  $W/V = 1$  and 2,  $\langle r^2(t) \rangle$  is a linear function of time  $t$ ,

$$\langle r^2(t) \rangle = 2Dt. \quad (5)$$

The parameter  $D$  is the diffusive constant which enters the Einstein formula for electric conductivity  $\sigma$ ,

$$\sigma = e^2 D. \quad (6)$$



**Fig. 1.** The quadratic displacement  $\langle r^2(t) \rangle$  (in units  $a^2$ ) as a function of time  $t$ . Time is measured in  $\hbar/V$ . The size of the system is  $L = 2048a$  ( $L = 1024a$  for  $W/V = 6$ ). Note the logarithmic scale of both axes. For weak disorder, we expect the electron to diffuse, so that  $\langle r^2(t) \rangle = 2Dt$ , in accordance with Eq. (5). Numerically, we find that  $\langle r^2(t) \rangle = 2Dt$  with  $D = 1.004$  for disorder  $W/V = 1$  and  $D = 0.98$  for  $W/V = 2$ . The corresponding diffusive constants are  $D = 25.7$  and  $9.1$  (in units  $a^2V/\hbar$ ). Only the data for time  $t = 4000\hbar/V$  were used for  $W/V = 1$ , the electron could reach the edge of the sample in longer time. The dashed line represents the limit  $\langle r^2 \rangle_{\max} = L^2/6$ , given by Eq. (7). For stronger disorders, the time evolution of the wave function is not diffusive. We find the exponent  $0.82$  ( $W/V = 4$ ) and  $0.39$  ( $W/V = 6$ ).

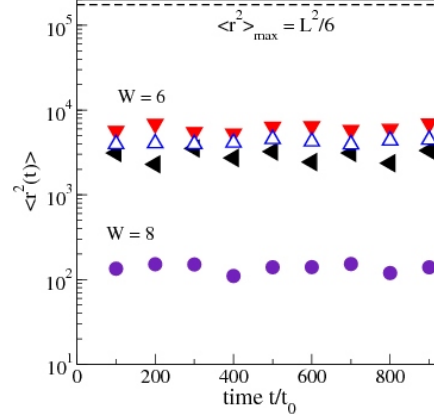
**Fig. 2.** The same data as in Fig. 1, but on a linear scale. Only the data for small disorder is shown. Note that for  $W/V = 1$ ,  $\langle r^2(t) \rangle$  is linear only when  $t = 4000\hbar/V$ . This is because the electron already reaches the edge of the sample.

Here  $e$  is the electron charge and  $\rho$  is the density of states [7].

Since we analyze only a lattice of a finite size, we have to take into account that the  $t$ -dependence of the electron wave function might be affected by the finiteness of our sample. In this case, we not only observe the diffusion, but also the refection of the electron from the edges. The diffusion (5) is observable only when  $\langle r^2(t) \rangle < \langle r^2 \rangle_{\max}$ , where  $\langle r^2 \rangle_{\max}$  corresponds to the homogeneously distributed wave function,  $|\psi(\vec{r})|^2 = \text{const} = 1/L^2$ :

$$\langle r^2 \rangle_{\max} = \frac{1}{L^2} \int_{-L/2}^{L/2} \int_{-L/2}^{L/2} (x^2 + y^2) dx dy = \frac{L^2}{6}, \quad (7)$$

It might seem that the diffusion of electrons shown in Figs. 1 and 2 contradicts the localization theory [23] which predicts that all electronic states must be localized in two-dimensional systems. However, this is not the case. The prediction of the localization theory concerns the limit of an infinite system size. Physically, localization occurs only when the size of the sample exceeds the localization length,  $L > \xi$ . Since  $\xi$  is very large in weak disorder ( $\xi \sim 10^6 a$  when  $W = 1$ ) [18], we observe metallic behavior and diffusion of electrons in Fig. 1. Of course, even in the case of  $W/V = 1$ , we would observe localization, if much larger systems are taken into account [7]. In general, we can observe the localization, if we either increase the size of the system or reduce the localization length. The latter is easier, as it requires only to increase the disorder strength  $W$ . We will do this in the next Section.



**Fig. 3.** Quadratic displacement  $\langle r^2(t) \rangle$  as a function of time  $t/t_0$ ,  $t_0 = 1000\hbar/V$  for three systems of the size  $L = 1024a$  and disorder  $W/V = 6$  (triangles). Although  $\langle r^2 \rangle$  does not increase when time increases, it fluctuates as a function of time. The limiting value,  $R^2$  (Eq. 8) depends on the actual realization of the random disorder  $(\vec{r})$  in the given sample. The dashed line shows  $\langle r^2 \rangle_{\max} = L^2/6 = 174762a^2$  which is 50 larger than actual values of  $\langle r^2 \rangle$ . For comparison, we also show the quadratic displacement for a system with stronger disorder,  $W/V = 8$ , which is typically  $130a^2$ .

#### 4. Absence of diffusion localization

The data in Fig. 1 indicate that the time evolution of the wave function is not diffusive when the disorder  $W$  increases. The linear increase of  $\langle r^2(t) \rangle$  is observable only for short initial time interval. For longer time, the increase of the spatial extent of the electron is slower and finally ceases (Fig. 3).

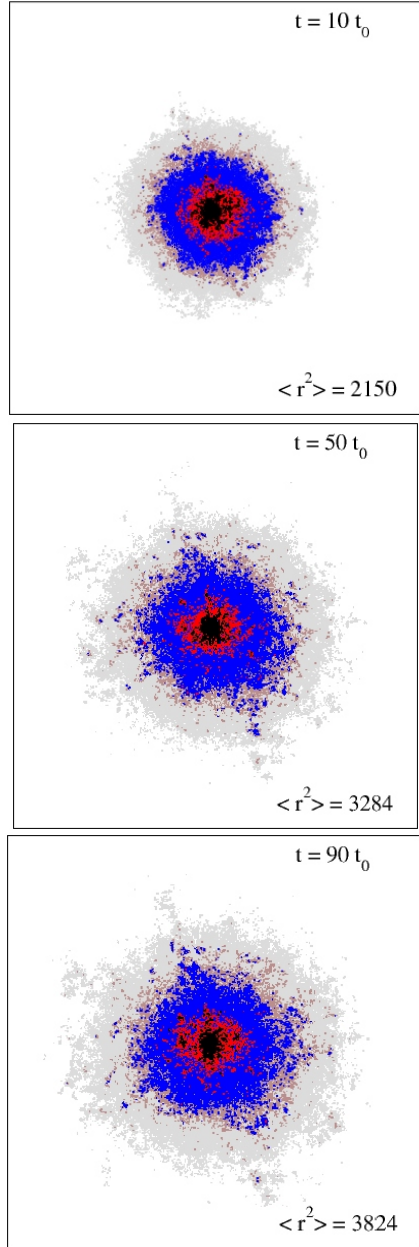
To demonstrate the electron localization more explicitly, we repeat the experiment in Section 3 with a stronger disorder  $W/V = 6$ . Similarly to the previous experiment, the initial wave function is non-zero in the small area  $24a \times 24a$  located at the center of the sample. For shorter times, we observe that the spatial extent of the wave function increases. Then, after a while,  $\langle r^2(t) \rangle$  saturates:

$$\lim_{t \rightarrow \infty} \langle r^2(t) \rangle = R^2 = \langle r^2 \rangle_{\max}. \quad (8)$$

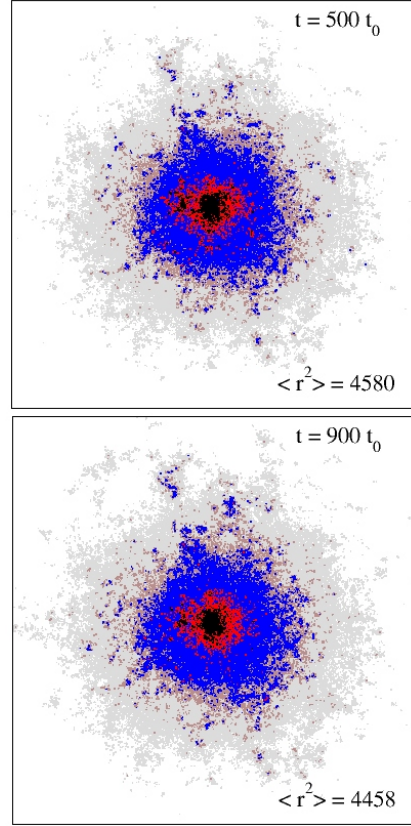
Although the spatial distribution of the electron varies in time,  $\langle r^2(t) \rangle$  does not increase any more even if the time  $t$  increases ten and more times.

Figs. 4 and 5 show the spatial distribution of the wave function,  $|\psi(\vec{r}, t)|^2$ . They represent the lattice sites with  $|\psi(\vec{r})|^2 = 10^{-4}$ . This means that the probability to find the electron in any other lattice site is less than  $10^{-8}$ .

Note that there is no potential well in the center of the sample where the electron is localized. The only reason why the electron is localized in the lattice center is that the initial wave function,  $|\psi(\vec{r}, t=0)|^2$ , was non-zero only in the center of the lattice. Starting with the initial wave function localized in any other area of the sample, we would observe electron localization in that area. This is demonstrated in Fig. 6 showing the time development



**Fig. 4.** Spatial distribution of an electron in sample with disorder  $W/V = 6$ . The size of the lattice is  $1024a \times 1024a$ . Time is given in units of  $t_0 = 1000\hbar/V$ . The different colors show sites where  $|\psi(r)|^2 \times 10^4$  (gray),  $5 \times 10^4$  (brown),  $10^3$  (blue),  $5 \times 10^3$  (red), and  $5 \times 10^3$  (black). The probability to find an electron on any other site is less than  $10^{-8}$ .



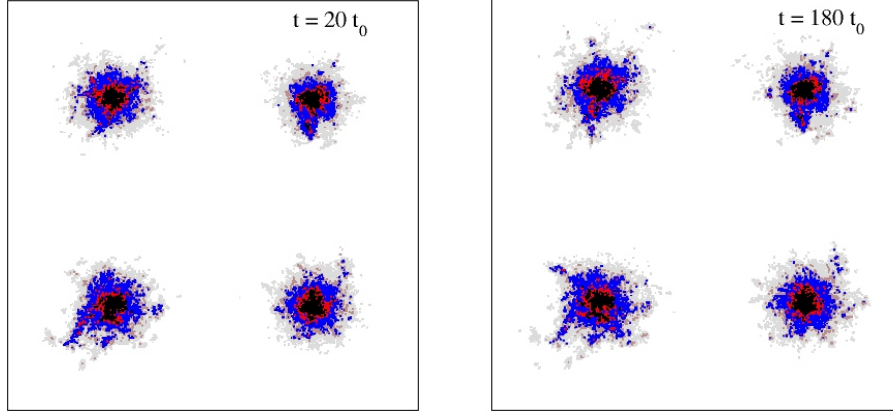
**Fig. 5.** The same as in Fig. 4 only the time is  $t = 500t_0$  and  $900t_0$  ( $t_0 = 1000\hbar/V$ ).

of the wave functions of four electrons in the same lattice. The initial position of the electrons is centered around four points

$$x = L/2 \pm L/4, y = L/2 \pm L/4. \quad (9)$$

We see that each electron is localized around its initial position in time  $t = 0$ . This proves that localization is indeed the result of interference of wave functions. The electron is not trapped in any potential well. The localized state is not a bound state.

Fig. 6 also shows that the localized states are very sensitive to the realization of the random potential. The spatial distribution of each electron reflects the local distribution



**Fig. 6.** The time development of four electrons located in time  $t = 0$  in four different areas of the same lattice. The electrons do not leave the initial areas. The size of the sample is  $L = 1024a$ . Disorder  $W/V = 8$ . Again, time is measured in units of  $t_0 = 1000\hbar/V$ .

bution of random energies  $\langle \bar{\epsilon} \rangle$ . This was already shown in Fig. 3, where we plot  $\langle r^2(t) \rangle$  as a function of time for three different realizations of the random disorder. We see that although all three samples have the same macroscopic parameter  $W/V = 6$ , the limiting value  $R^2 = \lim_t \langle r^2(t) \rangle$  is not universal but depends on the actual distribution of random energies in the given sample. Moreover,  $\langle r^2(t) \rangle$  fluctuates as a function of time.

## 5. Conclusion

We demonstrated numerically that the diffusion of the quantum particle through randomly fluctuating potential ceases after certain time. Owing to the scattering of the wave function on randomly distributed impurities (fluctuations of the random potential), the particle becomes spatially localized.

The key condition for the electron localization is the quantum coherence of the wave function. This is generally not fulfilled in the experiment, where the incoherent scattering - for instance the scattering of electrons with phonons - plays a crucial role. As any incoherent scattering destroys quantum coherence, the electron localization can be observed experimentally only if the mean free path of incoherent scattering is larger or comparable than the size of the sample. This happens at a very low temperature. Of course, localization can affect the electron transport also at higher temperatures [27]. These effects are, however, above the scope of present discussion.

With localization being a wave phenomenon, we expect similarity of quantum propagation with classical wave phenomena [28]. That enables us to observe localization in many other instances. In particular, classical waves - electromagnetic or acoustic - can also be localized in a disordered medium [29]. The localization of microwave electromagnetic waves [30], ultrasound waves [32] and weak localization of seismic waves [31] were recently observed experimentally.

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