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Classical trajectories in quantum transport at the band center of bipartite lattices with or without vacancies

G. Chiappe,[1,2] E. Louis,[1] M. J. Sánchez,[2] and J. A. Vergés[3]

[1]*Departamento de Física Aplicada and Unidad Asociada del Consejo Superior de Investigaciones Científicas, Universidad de Alicante, San Vicente del Raspeig, Alicante 03690, Spain*

[2]*Departamento de Física J. J. Giambiagi, Facultad de Ciencias Exactas y Naturales, Universidad de Buenos Aires, Ciudad Universitaria, 1428 Buenos Aires, Argentina*

[3]*Departamento de Teoría de la Materia Condensada, Instituto de Ciencia de Materiales de Madrid (CSIC), Cantoblanco, Madrid 28049, Spain*

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Here we report on anomalies in quantum transport at the band center of a bipartite lattice with vacancies, namely: no weak localization effect shows up, and when leads have a single channel the transmission is either one or zero. We propose that both are a consequence of the chiral symmetry and the large number of states at the band center. The probability amplitude associated with the eigenstate that gives unit transmission resembles a classical trajectory both with or without vacancies. The large number of states allows one to build up trajectories that elude the blocking vacancies explaining the absence of weak localization.

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Bipartite lattices. The possibility that qualitative differences between models with pure diagonal or non-diagonal disorder may exist has attracted considerable interest since Dyson's work on a phonon model in one dimension.[1] For instance it has been reported that non-diagonal disorder promotes a delocalization transition at $E=0$.[2–4] Although this raised a controversy regarding the general statement saying that the particular type of disorder should not matter in a single parameter scaling theory,[5] in recent years a different view has emerged which ascribes that transition to the peculiar properties of bipartite lattices. A bipartite lattice is a lattice that can be divided into two sublattices such that a site in one of them is connected only with sites in the other lattice. A spectrum with electron-hole symmetry (also known as chiral symmetry) characterizes these lattices, and, while diagonal disorder efficiently breaks this symmetry, pure non-diagonal disorder[3] does not. More recently, however, it has been shown[6] that, at $E=0$, standard exponential localization occurs in a system with vacancies (a defect that also preserves chirality), proving that a naive diagonal versus non-diagonal classification of disorder loses subtle effects related to model details.

Here we report on anomalies in transport properties at the band center of bipartite lattices that are indeed related to chirality, namely: (i) the absence of weak localization,[7,8] and (ii) when single channels leads are connected to cavities with or without vacancies, the transmission is either zero or one. We show that these anomalies are associated with the existence of classical trajectories which are possible due to chiral symmetry and the large number of states at $E=0$. We illustrate these ideas on cavities of the square lattice with vacancies.

The Hamiltonian. We consider a tight-binding Hamiltonian in $L\times L$ clusters of the square lattice with a single atomic orbital per lattice site,

$$\hat{H}=\sum_{m,n}\epsilon_{m,n}|m,n\rangle\langle m,n|-\sum_{\langle mn;m'n'\rangle}t_{m,n;m'n'}|m,n\rangle\langle m',n'|, \tag{1}$$

where $|m,n\rangle$ represents an atomic orbital at site (m,n), and $\epsilon_{m,n}$ its energy (in the perfect system all were taken equal to zero). For zero magnetic field the hopping energies between nearest-neighbor sites (the symbol $\langle\ \rangle$ denotes that the sum is restricted to nearest-neighbors) were taken equal to 1. With this choice the spectrum of the square lattice covers the energy range $E\in[-4,4]$. A vacancy was introduced at site (m,n) by taking $\epsilon_{m,n}=\infty$. On the other hand, for a uniform magnetic field, and using Landau's gauge, the hopping energy from site (m,n) to site (m',n') is written as $t_{m,n;m'n'}=\exp\{2\pi i[m/(L-1)^2](\Phi/\Phi_0)\}$, where Φ is the magnetic flux through the $L\times L$ cluster and Φ_0 the magnetic flux quantum. In the absence of defects this system has L eigenstates at the band center with momentum $\mathbf{k}=(k_x,k_y)$ such that $k_x+k_y=\pi$ (the lattice constant is hereafter taken as the length unit). Once the cavity was connected to leads of width W, the conductance G was calculated by means of an efficient implementation of Kubo's formalism.[9]

Quantum transport anomalies in bipartite lattices with vacancies. In Fig. 1 we plot the results for the conductance versus magnetic flux in two cases. In the upper panel, results for a rather large cavity with leads of width $W=4$ are reported. It can be noted that while at an energy close to the band center the weak localization effect clearly shows up, just at the band center the conductance unambiguously decreases with the magnetic flux.[8] The lower panel of the figure provides further support to this result. It shows the results of a calculation on a rather small cluster which includes all possible configurations of disorder. Again at the band center no weak localization effect is present. At $E=-0.1$, instead, we observe a clean increase of G up to a flux in which an abrupt change of slope is noted. The latter is probably an effect of level crossing. In any case, this result confirms that obtained on the larger cluster. The conductance distribution obtained on 6×6 clusters with 6 vacancies and leads of width 1 connected at opposite corners of the cavity are shown in Fig. 2. All disorder realizations were included in

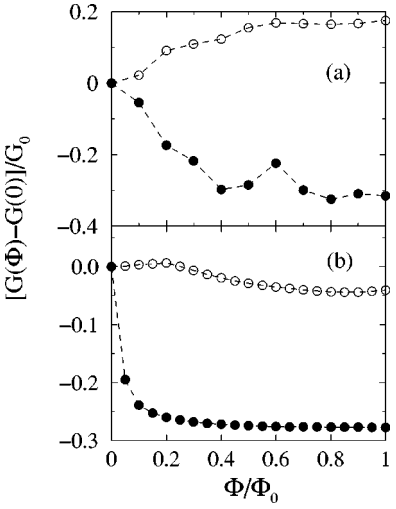

FIG. 1. Change in the conductance versus magnetic flux (both in units of their respective quanta) in: (a) 78×78 clusters with 78 vacancies (1200 realizations were included) and leads of width $W=4$ connected at opposite corners of the cavity, and (b) 6×6 clusters with 6 vacancies (all realizations were included in the calculation) and leads of width 1 connected at opposite corners of the cavity. The results correspond to $E=0$ (closed circles) and $E=-0.1$ (empty circles).

the calculation. At the band center the distribution is reduced to two δ-functions at $G=0$ and G_0, i.e., the cavity either does not conduct or behaves as a purely ballistic system with unit transmission. Similar behavior is obtained for other cluster sizes and averaging on different disorder configurations. This is no longer the case at a finite energy (still quite close to the band center) as shown in the lower panel of the figure. In fact the latter resembles the conductance distribution for a chaotic cavity with left-right symmetry and leads supporting a single channel.[10,11] Figure 3 illustrates how increasing the leads width and cavity size affect the rather odd result found

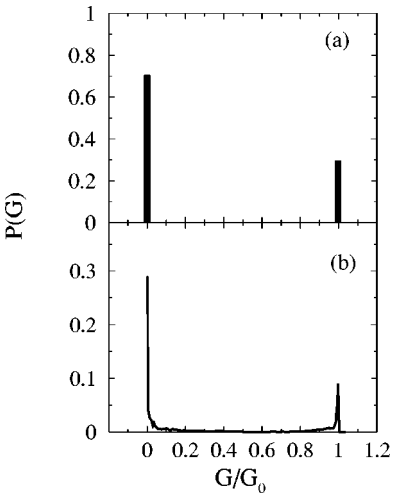

FIG. 2. Conductance distribution in 6×6 cavities with 6 vacancies (all realizations were included) and leads of width 1 connected at opposite corners of the cavity. The results correspond to $E=0$ (a) and $E=-0.1$ (b).

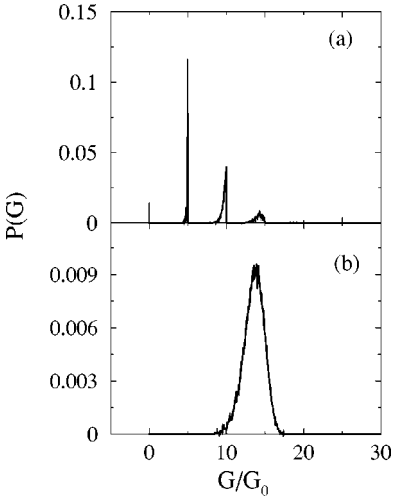

FIG. 3. Conductance distribution in $L\times L$ cavities with L vacancies connected to leads of width L. The results correspond to $L=6$ (a) and $L=30$ (b). For $L=6$ all realizations were included while for $L=30$ the distribution was calculated with 300000 realizations. The x axis in the upper panel should be divided by 5.

at $E=0$.[6] The conductance distribution for the 6×6 cavity with $W=6$ leads and 6 vacancies, although still showing peaks at $G=G_0,2G_0,\ldots$ they are no longer δ-functions. Increasing the system size shows the expected tendency toward a Gaussian distribution. The probable causes of these results are discussed below.

Classical trajectories. At this stage we wish to identify the nature of the state that, at zero magnetic field, contributes to the current with exactly one conductance quantum in the case of leads of width $W=1$ (see below). Working within the Green functions formalism does not allow one to single out a given state as Green functions contain information of all states at a particular energy. As it is evident that only one of the states at $E=0$ is participating in the current, we should look for an alternative procedure. In the following we try to derive directly from the Hamiltonian the relevant information changing the boundary conditions. In order to center the discussion let us focus on a defect free $L\times L$ cluster with leads of width 1 connected at opposite corners of the cavity. Diagonalizing such a cluster with two negative imaginary parts added to the diagonal energies of the sites at which the leads are connected, gives $L-1$ eigenstates with real energy at $E=0$. None of the probability densities associated with these states seem to be related to the unit transmission found in this case. What actually happens is that, in order to build up an eigenstate which travels from one lead to the other, one should diagonalize a Hamiltonian which includes a large portion of the leads. When this is done, the eigenstate missing from the L set shows up. Now, to establish a current we have added to the diagonal energies at the two lead ends a positive and a negative imaginary part, respectively, which is a practical way to introduce the source and sink required to produce a current. This procedure splits an eigenstate from the L degenerate set at $E=0$ which is precisely the one that contributes to the current. The result obtained on a 30×30 defect free cluster connected to leads of length 100 is shown in the

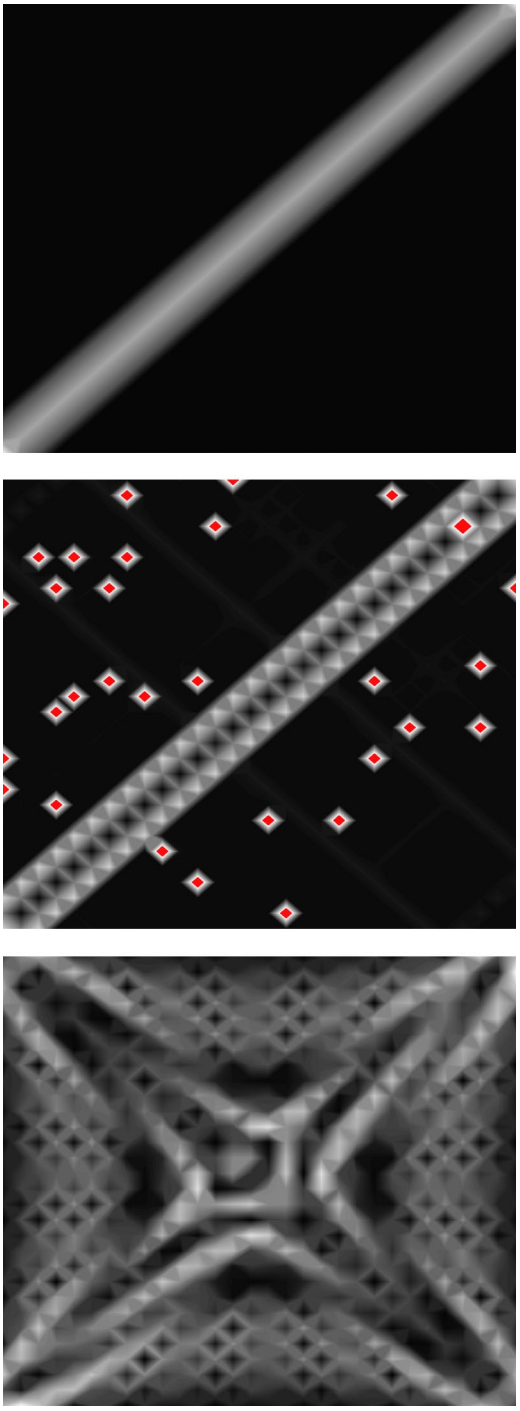

FIG. 4. (Color online) Probability density associated with the eigenfunction that gives unit transmission in a 30×30 cluster connected to leads of width $W=1$ at opposite corners of the cavity. Upper panel: zero magnetic flux and no vacancies. Middle panel: zero magnetic flux and 30 vacancies (also shown in the figure by means of rhombi). Lower panel: same as upper panel with a magnetic flux $\Phi=0.1\Phi_0$ (in this case transmission is no longer 1, see the text).

upper panel of Fig. 4. The figure shows the probability density associated with the just mentioned eigenstate. Interestingly enough it is noted that the image is much like a classic ray. We have checked that all of the rest of the $L-1$ eigenstates remain localized within the cavity. Introducing vacancies slightly distorts this straight trajectory but still keeping the classical picture. The results for the same cavity with 30 vacancies are shown in the middle panel of Fig. 4. The system has enough degrees of freedom (see below) to build up a trajectory that eludes the blocking vacancies. Of course, as this is not always possible, the average conductance is reduced by the presence of vacancies (see below). Nonetheless, the classical picture of Fig. 4 offers an explanation to the odd conductance distribution of Fig. 2 reduced to just two peaks at 0 and G_0. As shown in the lower panel of Fig. 4, a magnetic field destroys the classical picture and, as a consequence, transmission is reduced. The conductance histogram (not shown here) is no longer similar to that of Fig. 2.

How are these results related to the absence of the weak localization effect shown in Fig. 1? As already observed in Ref. 12, the change in G for small magnetic fields is negligibly small unless a ''stopper'' is placed on the cavity to prevent direct transmission. On semiclassical grounds, the magnitude of the weak-localization correction was derived to be[13] $G(\Phi)-G(0)\propto T_{cl}R_{cl}$ where T_{cl} and R_{cl} are the classical transmission and reflection probabilities respectively. Therefore if a trajectory eludes the vacancies (as in Fig. 4), $R_{cl}\sim0$ and the weak localization correction is suppressed. This explains the absence of the weak localization effect. Besides, the spreading of the probability amplitude shown in Fig. 4 is the cause of the decrease in conductance as the field is switched on.

Discussion. Now the question is how can the system manage to build up a wave function that avoids scattering with vacancies. Building up a wave function localized along lines requires combinations of a sufficiently large number of momenta. This is actually possible due to the L available momenta with $k_x+k_y=\pi$ that, in the defect free cavity, are associated with the eigenstates at $E=0$. By combining the wave functions of this linear space in the reciprocal lattice, and others with energy positive *and* negative very close to zero, it is possible to construct trajectories in real space which are straight lines parallel or perpendicular to that space. States with energies positive and negative participate with the same weight, to guarantee that the total energy is zero. This has been verified by projecting the wave functions of Fig. 4 (upper and middle panel) onto the eigenstates of the isolated cavity. When leads of width $W=1$ are attached to the cavity, there is a set of lead positions (in fact those couples that preserve inversion symmetry) for which there is a perfect matching between the wave functions of the cavity and those of the semi-infinite leads and, thus, perfect transmission. This occurs more rarely as the leads width increases. For other energies, the manifold of constant energy corresponds to an arbitrary curve in **k** space. In addition, the energies in its vicinity are not symmetrically distributed. This does not allow, in general, to construct a well-defined curve in real space. It is the chiral symmetry of the lattice which guarantees that this manifold is a straight line just at $E=0$. In three dimensions (a cubic lattice) a similar effect shows up. If leads of width $W=1$ are connected to opposite corners of a cube of side L the conductance is exactly one quantum. It can be easily checked that in such a cube there are $3L$

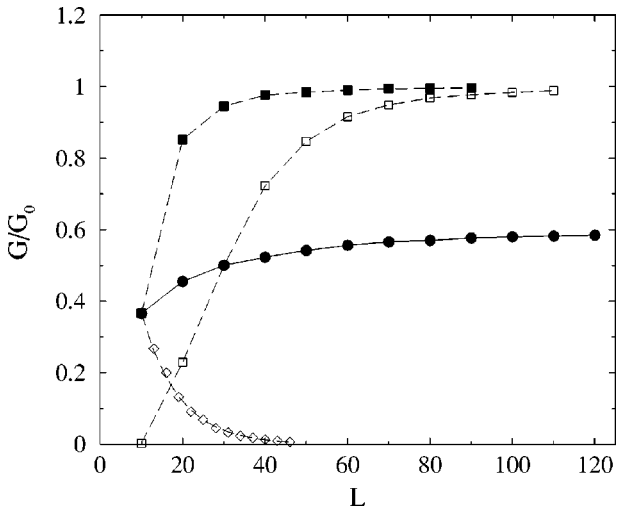

FIG. 5. Average conductance at the band center in $L\times L$ clusters of the square lattice with leads of width 1 connected at opposite corners, vs cluster size. The results correspond to: a fixed number of vacancies N_v ($N_v=10$ closed squares, and $N_v=30$ open squares) $N_v=L$ (closed circles) and $N_v=0.1*L^2$ (open diamonds). Lines are guide to the eye but in the latter case where it corresponds to an exponential fitting to the data. The number of disorder realizations included in the calculations was $10L^2$.

-2 eigenstates with zero energy contained in the plane $k_x+k_y+k_z=3\pi/2$. However, this only holds for L odd.

Scaling. It is interesting to investigate how the above results scale with the system size. As shown in Fig. 5, when the number of vacancies is constant the conductance increases with L reaching 1 at a size which depends on the actual number of vacancies. This shows that as far as the number of eigenstates at $E=0$ removed by the defects remains finite, the fraction of disorder realizations for which the conductance is zero will vanish. If the number of vacancies is proportional to the linear size of the system (in the figure we show results for L vacancies), G again increases with L although our results do not elucidate the precise limit value (between 0 and 1) for large systems. However, we have checked that the conductance distribution remains as in Fig. 2(a), reinforcing our assessment concerning the rather odd behavior of the system here investigated. Finally, for a constant defect concentration the conductance goes exponentially to zero as in the case of leads of width $W=L$.[6]

Experimental implementation. Is it possible to detect this effect? In recent years quantum corrals have been assembled by depositing a closed line of atoms or molecules on noble metal surfaces.[14–17] In these systems the local density of states (DOS) reveals patterns that remind the wave functions of two-dimensional non-interacting electrons under the corresponding confinement potential. These systems could be candidates in order to detect the effect here described. The transport must be done now in the plane of the surface, not orthogonal to it. Also, Co atoms can be inserted into the quantum corral. When this atom is in the Kondo regime it produces a local depletion in the density of states which can simulate the effect of vacancies in our model, allowing to made up arbitrary distributions (in number and location) of them. Another possibility is to build up a dot array[18] on a square lattice with a number of electrons that exactly half fill one of the bands of the array. Controlling the gate potential applied to a particular dot, it can be put into or out of resonance, simulating in this way the existence of vacancies in the array.

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