Localization of electronic wave functions due to local topology

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(Received 20 January 1986)

We present a simple two-dimensional hopping model for independent electrons which has strictly localized states in addition to the extended states. These localized states can exist either in a band gap or within the continuum. The localized states persist if the lattice periodicity is destroyed. Finally, the effect is shown to hold for a much more general class of systems.

I. INTRODUCTION AND DESCRIPTION OF THE MODEL

During an investigation of the effect of lattice quasiperiodicity on the localization of the electronic wave function,[1] we were surprised to find localized states both within the bands and within the band gaps, but for reasons which apparently had nothing directly to do with the lack of periodicity in the model. Instead, the existence of these states—either strictly localized about a point or localized in all but one dimension to a line—seem to depend only on the local topology.

This observation is not new,[2–7] but in this paper we wish to understand it better so that we can separate the effects of local topology from those of the global aspect of quasiperiodicity or nonperiodicity. For this reason we have constructed a very simple two-dimensional hopping model for noninteracting electrons which illustrates very clearly all of these effects: (i) First, the model has strictly localized states, and thus the spectrum is highly degenerate so that the density of states has a δ-function peak whose height is proportional to the number of sites in the crystal. (ii) Second, the model also has extended states. (iii) Third, the model may be made random, so that the strict periodicity is destroyed, yet the localized states persist. (iv) Fourth, the localized states may either be within the band or within the band gap of extended states.

The usual mechanisms of localization are several:[8,9] localization due to impurities, Anderson localization due to a disordered lattice,[10] localization due to the electron-electron Coulomb repulsion as in the Mott transition,[11] and probably others. The mechanism we study in this paper might best be termed topological localization, since it depends only on the local topology of a finite portion of the lattice. Wherever this particular lattice configuration occurs locally in the lattice, there we will find a localized state.

Since the states are strictly localized on identical lattice configurations, they are degenerate in energy. If we wished, we could thus take superpositions with a suitable phase and create Bloch wave functions. More importantly, if a small perturbation is added to the Hamiltonian so that our previous states are no longer exact, the band of states can be expected to acquire a finite width. For a periodic lattice, the new states would be extended, although with a very large effective mass. For other lattices, such as quasiperiodic or random, the nature of the states is an open question.

We begin with a triangular lattice. The electrons can sit on the sites of the lattice, and where there are bonds between sites, there are nonzero hopping matrix elements in the Hamiltonian. There are no other nonzero hopping matrix elements, and the on-site diagonal energies are all the same, which we take to be the zero of energy. Finally, we ignore spin by treating each spin component independently.

Now we modify the lattice by removing one-third of the bonds; this means that we set the corresponding hopping matrix elements of the Hamiltonian equal to zero. The result is shown in Fig. 1. This is the dice and decorated dice lattice studied by Morita and Horiguchi.[7] (At this point ignore the distinction between circle and square sites.) We shall speak of pairs of sites connected by a bond as nearest neighbors; this is what we mean by the topology of the lattice. In Fig. 1, the unit cell is indicated by the rhombus; it contains 9 sites and 18 bonds. We take the distance between nearest-neighbor sites to be 1, so the repeat distance is 3.

Now, with Fig. 1 in mind, let us make some observations about the lattice. The lattice divides into two types of sites indicated by circles and squares, which we call "rim" and "hub" sites, respectively, so that a nearest-neighbor pair consists of one rim and one hub site. The electrons hop back and forth from rim to hub. The lattice is thus bipartite, and consequently the energy spectrum is symmetric if we reflect about the origin. The ratio of rim

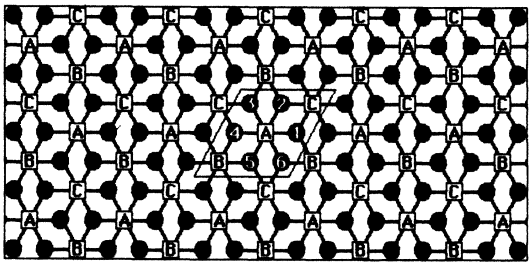

FIG. 1. A portion of the lattice; all symbols are described in the text.

to hub sites is 2:1, and the rim sites have coordination number 3, while the hub sites have coordination number 6. The average coordination number is 4. The rim sites form a hexagonal or honeycomb lattice, and the hub sites a larger triangular lattice.

II. LOCALIZED STATES

Let us now assume that all nonzero matrix elements—represented by a bond in Fig. 1—have the same value which we take to be 1. Then the Schrödinger equation is a matrix equation, and if we now restrict ourselves to the eigenvalues with zero energy, it says that the sum of the wave function of the electron on all nearest-neighbor sites about every site is zero.

Consider now the six rim sites numbered 1 to 6 in Fig. 1. They form a wheel about a hub site centered in the unit cell. We claim that an eigenstate of the Hamiltonian with zero energy is given by a wave function which vanishes everywhere *except* on the rim of six sites, and there the (unnormalized) wave function is $\Psi(n)=(-1)^n$. To verify, the sum of this wave function on rim sites nearest-neighbor to each of the seven surrounding hub sites must vanish, or $\Psi(n)+\Psi(n+1)=0$. [$\Psi(n+6)=\Psi(n)$.] This is obviously so.

Thus we have an eigenstate with zero energy. It is certainly localized or bound, since it vanishes everywhere off the rim. Furthermore, we could have centered such a state on *any* of the equivalent hub states; the states are highly degenerate.

III. THE BAND STRUCTURE

Let us go on and identify the complete spectrum, by determining the band structure. Since the lattice is periodic, and hence invariant under translations by 3 in directions parallel to the sides of the unit cell, we can classify the states by the irreducible representations of this translation group. This is the Bloch or Floquet theorem.

Let $\mathbf{w}_1,\mathbf{w}_2,\mathbf{w}_3$ be three unit vectors in the plane of the crystal, where $\mathbf{w}_1=(1,0)$, $\mathbf{w}_2=(-\frac{1}{2},\sqrt{3}/2)$, and $\mathbf{w}_3=(-\frac{1}{2},-\sqrt{3}/2)$. Then the sites of the crystal are given by $n_1\mathbf{w}_1-n_2\mathbf{w}_3$, where n_1,n_2 are integers. If the wave function at this site is $\Psi(n_1,n_2)$, then we impose the condition on the wave function that $\Psi(n_1+3,n_2)=a\Psi(n_1,n_2)$ and $\Psi(n_1,n_2+3)=b\Psi(n_1,n_2)$, where $a=\exp(3i\mathbf{k}\cdot\mathbf{w}_1)$ and $b=\exp(-3i\mathbf{k}\cdot\mathbf{w}_3)$.

Now the Hamiltonian can be written as a 9×9 matrix for a particular representation a,b. Furthermore, since the lattice is bipartite, the only nonzero elements are between rim and hub sites, and vice versa. Thus, if we choose our basis so that the first six states are on the rim sites arranged in order, and the next three states are on the A,B,C, hub sites, then the Hamiltonian has the matrix form

$$\underline{H}=\begin{bmatrix} \underline{0}_{6\times6} & \underline{M}^\dagger \\ \underline{M} & \underline{0}_{3\times3} \end{bmatrix}.$$

The matrix $\underline{M}$ is a 3×6 matrix. $\underline{M}$ is given by

$$\underline{M}=\begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 \\ a^{-1} & b^{-1} & b^{-1} & 1 & 1 & a^{-1} \\ 1 & 1 & a & a & b & b \end{bmatrix}.$$

The three localized states about hub sites A,B,C are zero eigenvectors of $\underline{M}$, and for general a,b they will be the only zero eigenvectors, since they must be orthogonal to each of the three six-dimensional row vectors of $\underline{M}$. On the other hand, in general there will be no zero eigenvectors of the 6×3 matrix $\underline{M}^\dagger$, for they are over constrained. The remaining six nonzero eigenvectors and their eigenvalues can be found by diagonalizing the 3×3 matrix $\underline{M}\,\underline{M}^\dagger$. The eigenvalues of this matrix are E^2, and thus they each give two energy eigenvalues. The resulting cubic equation is easily solved in closed form.

Whenever $a=1$, or $b=1$, we do not have a new state. Thus all properties of the problem—and thus the energies in particular—are periodic functions of the two-dimensional vector $\mathbf{k}$. The various branches of this function, obtained by following particular eigenvalues as functions of $\mathbf{k}$, are the energy bands. The unit cell of this periodic function is the Brillouin zone. We choose the Brillouin zone as a hexagon centered at the origin, with vertices located at $\pm(4\pi/9)\mathbf{w}_j$. An idea of the band structure can be gained by following the eigenvalues from the origin O, out to a vertex V, along the perimeter to a midpoint P, and then back to the origin. These are the points of highest symmetry. The resulting band structure is shown in Fig. 2.

We see that there is no band gap at zero energy, and thus the localized states sit within the continuum. This is because when $a=b=1$, the three row vectors of $\underline{M}$ become degenerate, and therefore the dimension of the zero eigenvalue subspace is now 5. In addition, all the row vectors of $\underline{M}^\dagger$ become degenerate, and so we pick up two more zero-energy eigenstates.

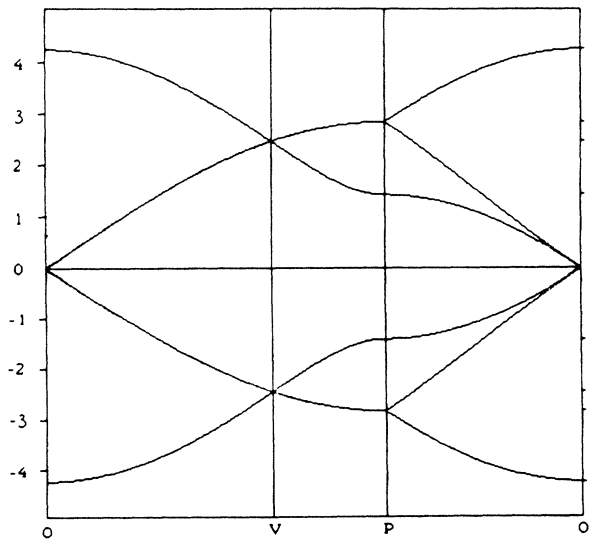

FIG. 2. Band structure of the first model, with degeneracy.

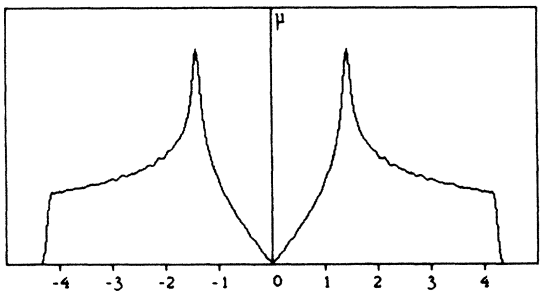

FIG. 3. Density of states for the first model, with degeneracy.

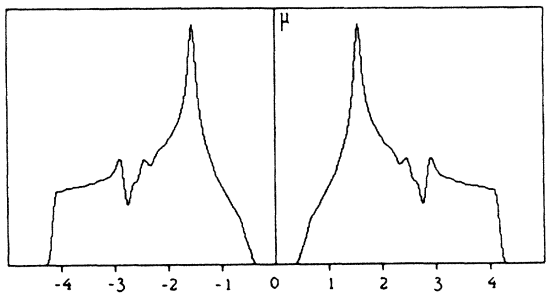

FIG. 4. Density of states for the second model, in which the degeneracy is lifted. We have taken the parameter Δ to be equal to 2. Note the band gap centered on $E=0$.

However, the localized states do exist at the energy where two band edges just touch, at the single point $\mathbf{k}=0$. This is reflected in the fact that the density of states vanishes at $E=0$. We calculate the density of states by imposing doubly periodic boundary conditions, so that $a^N=1$ and $b^N=1$. Then the vector $\mathbf{k}$ can only take values on a triangular lattice with lattice spacing $2\pi/3N$, and the Brillouin zone has exactly N^2 points corresponding to the $9N^2$ energy eigenvalues. We define the density of states $\mu(E)$ so that $9N^2\int_{-\infty}^{E}\mu(E')dE'$ is the number of states with energy less than E; it approaches the limit of a continuous function as N becomes large. We show the density of states in Fig. 3. Rather than performing a numerical integration using the analytic band structure—we are not interested in the model itself, but rather its qualitative features—we instead find the exact density of states for a finite lattice of 8100 sites. Thus the Van Hove singularities which occur at energies wherever $\nabla_{\mathbf{k}}E(\mathbf{k})=0$ are smoothed out.

IV. LIFTING THE DEGENERACY

It is qualitatively reasonable that the localized states should sit at a point with a decreased density of states, for in a sense these states have been removed from the continuum. Another way to look at it: All other states must be made orthogonal to *each* of the localized states, which places severe local constraints on the wave functions.

From the discussion of the preceding section, we understand the reason for the additional degeneracy at $\mathbf{k}=0$, which has the consequence of placing the localized states in the continuum. It might be interesting to lift this degeneracy so that the localized states actually sit in a band gap. We do this by keeping the row vectors of $\underline{M}$ nondegenerate for all a,b, by having the hopping matrix elements about each of the hub sites A,B,C different. However, we still want to preserve the localized states about each of these hubs, which constrains the possible weights.

We could investigate the general problem, but instead let us simply take an example. About each hub site of type A,B,C is a wheel of six rim sites numbered 1 to 6 as in Fig. 1. Let the hopping matrix elements be designated a_j,b_j,c_j, respectively. Impose inversion symmetry so that $a_{j+3}=a_j$, etc. For our example, we take $\mathbf{a}=(1,1,1)$, $\mathbf{b}=(1,1,\Delta)[3/(2+\Delta^2)]^{1/2}$, $\mathbf{c}=(\Delta,\Delta,1)[3/(2\Delta^2+1)]^{1/2}$. The localized state about A is now $(1,-1,\Delta,-\Delta^2,\Delta^2,-\Delta)$, with similar expressions for the others.

For the band problem, the Brillouin zone is the same hexagon, but the band structure itself no longer has this hexagonal symmetry. Instead, it only has two perpendicular reflection planes, corresponding to the symmetry of a rectangle. We present the density of states in Fig. 4, where the central band gap is apparent. As before, the infinite lattice is approximated by a finite lattice of 8100 sites. The wiggles near $E=3$ are thus smeared Van Hove singularities from extrema in the bands, as the bands in Fig. 2 separate.

V. CONCLUSION AND A THEOREM

Clearly we have demonstrated that the existence of localized states may depend only on the local topology of the hopping matrix elements. For instance, consider a wheel of six rim sites. If we fix the hopping matrix elements to each of the seven neighboring hub sites so that we have a state localized on the rim, we can do whatever we wish with the rest of the crystal—it doesn't matter—for the localized state will continue to exist. It is stable against such distortions. In particular, such a mechanism for localized states operates regardless of whether the lattice is periodic, quasiperiodic, or random. Of course, the mechanism is independent of dimensionality.

In fact, we can even make the following very general argument. Consider a bipartite lattice in any number of dimensions. The first sublattice consists of N_A sites of type A, the second of N_B sites of type B; the total number of sites is $N=N_A+N_B$. The electrons can only hop from A to B, or back. Assume the energy of an electron on site A is E_A, on site B is E_B. Then if we order the basis of states properly, the Hamiltonian has the form

$$\underline{H}=\begin{bmatrix} E_A\underline{I}_{N_A} & \underline{M}^\dagger \\ \underline{M} & E_B\underline{I}_{N_B} \end{bmatrix}.$$

Here, $\underline{I}_{N_A}$ is an $N_A\times N_A$ unit matrix, $\underline{I}_{N_B}$ is an $N_B\times N_B$ unit matrix, $\underline{M}$ is an $N_B\times N_A$ matrix, and $M^\dagger$ is its adjoint, an $N_A\times N_B$ matrix.

If Ψ_A^0 is a null vector of $\underline{M}$, then we may choose all components on the B sublattice to be zero, and we have an

eigenvector with eigenvalue E_A. Likewise, for a null vector of $\underline{M}^\dagger$, we have an eigenvector with eigenvalue E_B confined to the B sublattice.

Let N_A^0 be the dimension of the null space of $\underline{M}$, and N_B^0 the dimension of the null space of $M^\dagger$. However, N_B^0 is also the number of independent linear relationships between the row vectors of $\underline{M}$, and thus the dimension of the null space of $\underline{M}$ is the dimension of the row vectors of $\underline{M}$ less the number of independent row vectors of $\underline{M}$, or

$$N_A^0 = N_A - (N_B - N_B^0) \geq N_A - N_B \ .$$

Therefore, if it happens that the lattice sites are not exactly half A and half B, but instead suppose $N_A/N > N_B/N$, then we have shown that the energy level E_A is degenerate with a degeneracy proportional to the volume of the sample, or $N_A > N(N_A/N - N_B/N)$. This signals that we have a finite density of localized states in our system, entirely confined to the A sublattice. (However, the localization could conceivably be of a more general type, such as localization in momentum space.)

The eigenfunctions for values of energy other than E_A, E_B can be found by diagonalizing the non-negative $N_B \times N_B$ matrix $\underline{M}\,\underline{M}^\dagger$,

$$MM^\dagger \Psi_B = (E - E_A)(E - E_B)\Psi_B \ .$$

Let the eigenvalues of $\underline{M}\,\underline{M}^\dagger$ be ω^2. Then the energy eigenvalues are

$$E = (E_A + E_B)/2 \pm \{[(E_A - E_B)/2]^2 + \omega^2\}^{1/2} \ ,$$

so that there is an energy gap between E_A and E_B. The energy spectrum is symmetric about the point $(E_A + E_B)/2$.

Finally, we emphasize that for our general argument, we have nowhere required that our lattice be periodic or regular, either in the topology of the lattice or in the strength of the hopping matrix elements of $\underline{M}, \underline{M}^\dagger$. However, our argument does not cover the case of on-site disorder as in the Anderson model.

Note added. I would like to thank T. C. Choy for pointing out to me a reference to an earlier paper of T. Horiguchi and C. C. Chen [J. Math. Phys. 15, 659 (1974)], which calculates analytically the density of states for the diced lattice, which is our first example. The resulting expression for the density of states of Horiguchi and Chen is rather complicated, involving complete elliptic integrals whose arguments are in turn algebraic functions of the energy. In this paper, Horiguchi and Chen seem to have missed one-third of the states; these are the localized states which lie in the zero-width peak at zero energy. The analytic expressions are sufficiently complicated that we cannot check the normalization of their density of states directly.

A much more interesting example for which one can calculate exactly the fraction of localized states in the zero-width peak, even though the conditions for the theorem to apply are not met, is given in a recent paper of M. Kohmoto and this author, to be published in Phys. Rev. B.

Finally, as pointed out by Sriram Shastry, these results seem to be related to deep theorems of differential geometry, such as the Atiyah-Singer index theorem, although the exact connections are yet to be made.

ACKNOWLEDGMENT

I would like to thank Mahito Kohmoto for very helpful conversations.

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