Asymmetric bands in solids due to interplay of topological and substitutional defects

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We have studied the combined effect of topological and substitutional impurities on the band structure of solids. An interplay of the two types of impurities can make the band asymmetric around the band center with uneven distribution of eigenenergies on either side of it. This signifies a complete breakdown of particle-hole symmetry.

In recent years, advances in microtechnology have made it possible to fabricate artificial structures as small as a few hundred angstroms, such as high-mobility metallic wires, quantum dots, point contacts, etc., grossly known as mesoscopic systems.[1,2] The transport properties across such various geometrical structures have been extensively studied. One commonly studied structure is the T-shaped structure.[3–9] It consists of a main wire that extends from $-\infty$ to $+\infty$, and there is a finite chain (or stub) attached to it. The system is often taken to be one dimensional (1D) and it represents the real situation of such quantum wires and quasi-1D systems at low temperatures when the Fermi energy is so adjusted that only the first subband propagates.[3,4,7–9] Such 2D systems have also been studied using continuum models.[5,6] The basic feature that has attracted such wide-scale attention is that these systems can produce transmission zeros (or antiresonances) and sharp changes in the transmission coefficient with changes in length of the stub, which never appears in the case of scattering by potentials. Study has been extended to a serial arrangement of stubs[4,5] and the effect of a single defect in a serial arrangement of stubs.[7] Such artificially fabricated structures are very promising as ballistic transistors and switches.

A solid in general consists of a periodic arrangement of lattices. The tight-binding model is very appropriate for describing solids, where the electron "feels" the periodicity of the underlying lattice and has a band structure due to it. However, a realistic solid consists of departures from perfect periodicity. Such departures have been studied in the form of substitutional impurities and disorder in hopping parameters in the tight-binding model.[10,11] The study of intrinsic topological defects associated with randomness in geometries has also recently attracted attention.[3] Some materials in which one encounters such defects are percolation clusters, fractals, and branched polymers. They may also explain the transport properties of dirty quantum wires. Here one intends to study a T shaped structure as a defect rather than an artificially fabricated device. Again, the fact that such defects can produce transmission zeros drastically affects the transport properties of these systems. In this paper we have focused our attention on the aspect of T-shaped structures as defects. We show that an interplay between topological and substitutional defects can produce other nontrivial changes in addition to producing transmission zeros. To this end we have considered substitutional defects located inside a topological defect (which is a T-shaped structure), and a real solid may well consist of such structures. Our study is restricted to the effect of one such defect only (the single-impurity problem). We consider the system 1D because it is sufficient to help us to draw our conclusions. Thus the system consists of a perfect periodic system with a geometrical defect made up of a few sites. There are some substitutional impurities in this finite chain. We intend to study the effect of this type of impurity on the infinite periodic system. Our study shows that such a defect can make the band of the periodic system asymmetric, with an uneven distribution of the eigenenergies on either side of the band center. This does not happen in the case of a finite amount of substitutional defects or disorder in hopping parameters or simple geometrical defects. Earlier works[8,9,12] considered potential impurities inside the stub, but, as they considered free-electron propagation as plane waves, they missed the effect that such defects can produce on the band of an infinite lattice.

When the side chain consists of a single site as in Fig. 1 the impurity can lie at either B or C or at both the sites. The perfect sites are taken to be of zero site energy according to the usual practice, and the hopping parameter V is taken as 1 everywhere. The site energies at B and C are ϵ_B and ϵ_C, respectively. We solve this problem analytically using the same procedure as in Ref. 3. That is, the effects of sites C and B can be replaced by an energy-dependent self-energy acting only on the site B, i.e., $\Sigma_B(E)$. So we have a single impurity in an infinite chain whose effective site energy is $\Sigma_B(E)$.

Using standard Green's-function technique, we find

$$\Sigma_B(E)=\frac{V^2}{(E-\epsilon_C)}+\epsilon_B \ . \tag{1}$$

If we set $\epsilon_B=0$ ($\epsilon_C=0$), then we obtain the results for the impurity being at site C (B). Setting both at zero we obtain the same result as that of Ref. 3. We know the

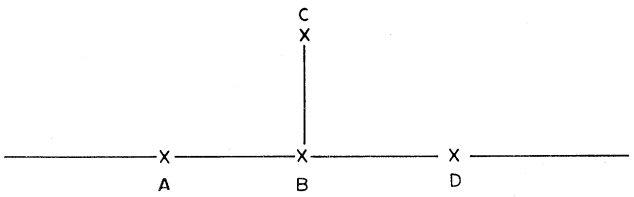

FIG. 1. A finite side chain attached to an infinite wire.

tight-binding Hamiltonian has particle-hole symmetry, and as a result the distribution of its eigenenergies, transmission coefficient, etc. are all symmetric around $E=0$. Because of the particle-hole symmetry of the Hamiltonian, the particle and hole bands (the dispersion curves) differ only by an overall sign apart from some unimportant additive constants, that can always be set to zero. The negative sign in front of the hole band can be removed by a transformation $k \rightarrow k+\pi/a$, where a is a lattice constant. So with the help of this (half a band) translation (which is just a shift of origin) the hole band can be made to coincide with the particle band completely. Even if a finite number of defect sites (substitutional impurities) are present in the chain, the band remains unchanged except at some isolated points. Hence the symmetry of the band is still maintained, and the particle and hole bands are identical.[13] Any amount of disorder in the hopping parameter or topological defects alone also cannot destroy the symmetry of the band. However, in our case, the band becomes completely asymmetric even due to a single impurity. It happens because of the special form of the effective self-energy $\Sigma_B(E)[\neq\Sigma_B(-E)]$ which arises solely due to an interplay of geometrical and substitutional impurities. As the effective site energy is asymmetric about $E=0$, it will make the band of the solid asymmetric as well. If one sets $\epsilon_B=\epsilon_C=0$, then this asymmetry disappears. This band asymmetry immediately manifests itself on the conductance of the system, as our subsequent calculations will show. They will also show the extent of the asymmetry of the band. There are also a variety of other phenomenon that depend explicitly on the symmetry of the band. Important among them are the nesting of the Fermi surface, charge-density and spin-density wave formations, Bloch oscillations and Wannier Stark localization, etc. In 1D, as the Fermi surface consists of two points, nesting is not destroyed but the band asymmetry can effect the commensurateness of the density waves. However, the form of the effective self-energy given in Eq. (1) suggests that a few such defects can also make the band of an infinite 2D periodic system (infinite or very large on all sides) asymmetric, and there the effects on charge- and spin-density waves may be more drastic. Simple substitutional defects cannot destroy the symmetry of the band, and they just result in a pinning of the charge-density waves.

The conductance of a two-port sample is directly related to the quantum-mechanical transmission by Landauer's two-probe conduction formula.[14] Using standard tight-binding techniques, one can analytically calculate the transmission coefficient across a single defect

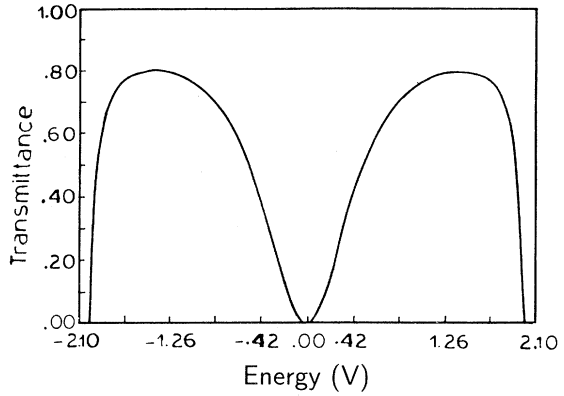

FIG. 2. Transmittance vs energy when all sites are perfect.

whose effective site energy is given in Eq. (1). In Fig. 2 we have plotted the transmission coefficient versus energy for a case $\epsilon_B=\epsilon_C=0$. This case exhibits a symmetric band. We have calculated the transmission (or the dimensionless conductance of a two-port sample) across the sample for two cases ($\epsilon_B\neq0, \epsilon_C=0$; $\epsilon_B=0, \epsilon_C\neq0$). They are shown in Figs. 3 and 4. We observe a strong energy dependence of the transport properties with the conductance vanishing at certain energies, as in Ref. 3. We observe that the conduction band becomes completely asymmetric, with a definite line shape in Figs. 3 and 4. The conduction band directly reflects the distribution of eigenenergies in the band, and the asymmetry results solely due to the asymmetry of this distribution of the eigenenergies of the infinite periodic system with a single defect. For any other type of defect the conduction band is symmetric about the center of the band, because in those cases the distribution of eigenenergies is also symmetric. It is also symmetric for geometric defects alone, as evident from Fig. 1.

We now consider a situation wherein a side chain is composed of several lattice points or atoms. This will help us to understand the line shape of the transmission bands and the origin of the asymmetry more physically. Transport across such a long side chain, with substitu-

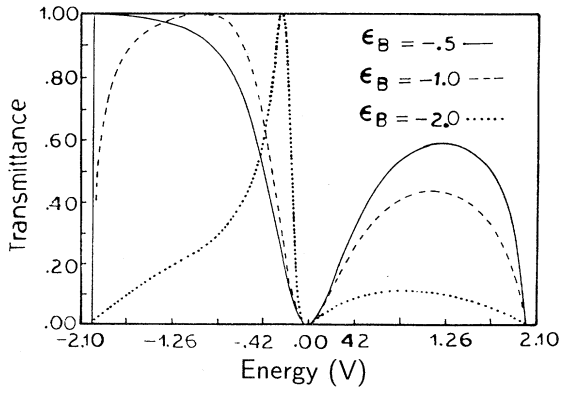

FIG. 3. Transmittance vs energy when a single substitutional impurity is at B.

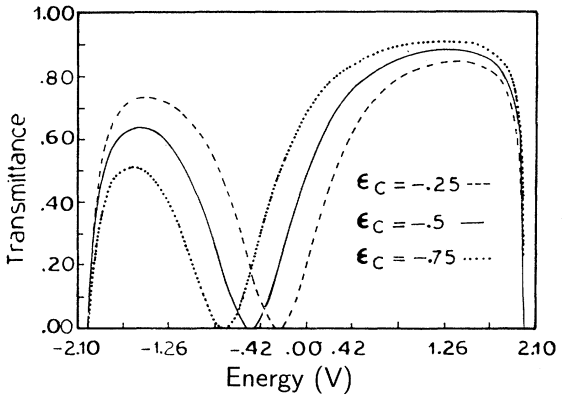

FIG. 4. Transmittance vs energy when a single substitutional impurity is at C.

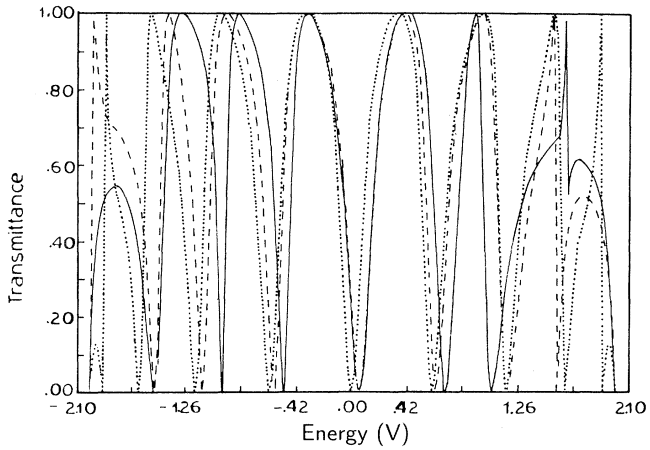

FIG. 6. Transmittance vs energy across a long finite disordered side chain.

tional impurities in it, is studied numerically using the vector recursion procedure. This formalism is discussed in detail in Ref. 15, and the procedure is well suited to tackle such geometries as this. The information about the geometry can be incorporated into the nearest-neighbor map, and then computing the transmission coefficient across the geometry is straightforward. However, we have to alter the algorithm slightly because of the 1D nature of the side chain.

First we choose all sites in the side chain to be perfect ($\epsilon=0$), and take the site at the junction to be of energy ϵ_J. This is the discrete version of the work of Tekman and Bagwell.[9] The side chain behaves as a resonant cavity that sustains standing waves. There are also continuum states in the main chain. Thus an incident electron has two alternate paths. In one, the electron does not enter the side chain; in the other, the electron enters the side chain, spends some extra time, and then comes out to mix with the continuum. The total transmission is dictated by interference between these two alternating paths. The defect site at the junction causes a weak coupling of the states in the resonant cavity with the continuum states in the main chain. In such a situation the resonances in the tight-binding model band are not the usual Breit-Wigner resonances (that are symmetric about the poles of complex transmission amplitude) (Ref. 8), but the asymmetric Fano resonances (that are asymmetric about the poles of the complex transmission amplitude). The observation in the discrete model that we have considered is that these asymmetric resonances make the entire conduction band of the tight-binding model asymmetric about $E=0$. The distribution of the poles and zeros over the entire band is asymmetric about $E=0$. In Fig. 5 we have plotted transmittance versus energy for such a system with 20 sites in the side chain. We have plotted for three values of $\epsilon_J=0$ (dotted curve), -1 (dashed curve) and -2 (solid curve). Note that when $\epsilon_J=0$ we obtain a perfect system such as that considered in Ref. 3. Note that resonances at the band edges when $\epsilon_J=0$ are asymmetric, because the states at the band edges are more localized than that at the band center. But the band is still symmetric about the band center. However, for nonzero ϵ_J all the resonances inside the band become Fano resonances, and the symmetry of the band is destroyed. Such a long chain will exhibit many zeros within a given energy range (the conduction band). As the length is gradually made shorter the zeros start moving out toward the band edges and go out of the conduction band. The shortest case is that of Fig. 1, where a single zero is left in the conduction band and the asymmetry is still maintained as in Fig. 3. Hence the line shape of the Fano resonances determine the line shape of the transmission band. This may help to engineer the line shape of the transmission band of 1D and quasi-1D solids by tuning the strength of a defect site inside an artificially built geometric structure.

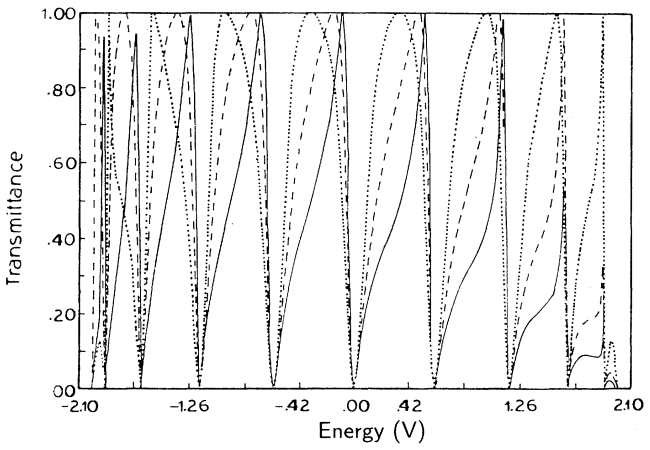

FIG. 5. Transmittance vs energy across a long finite side chain with a single impurity at the junction.

Next we choose the site energies in the side chain randomly between $-W/V$ and $+W/V$. The side chain consists of 20 sites. Again we see that the Fano resonances in the band make the band asymmetric. The origin of Fano resonances in this case is, however, slightly different from that of the case discussed in Ref. 9. Here the disor-

dered side chain causes the Anderson localization of the states inside it. Such localized states are weakly coupled to the continuum states of the main chain, and give rise to Fano-type resonances. In Fig. 6 we plot transmittance versus energy for such a chain for three values of $W/V=0$ (dotted line), 1 (dashed line), and 2 (solid line). Again $W/V=0$ is the case for perfect sites. When this chain is gradually made shorter then the zeros again move out of the band, and in the shortest situation we have the case of Fig. 1 with a substitutional impurity at C which gives the asymmetric band as in Fig. 4.

We conclude by stating the main results of this work. An interplay of substitutional impurity and geometrical defect can drastically modify the band of the host solid, making it asymmetric about the band center with an uneven distribution of eigenenergies on either side of it. This does not happen for any other type of defects or impurities. Our study of a single-impurity problem shows the robustness of the effect. This signifies a complete breakdown of particle-hole symmetry. We have explicitly shown the effect this produces on the conductance of the 1D periodic system, but this effect will manifest itself on all phenomena that depend on the symmetry of the band.

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