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Study of Stark-ladder resonances in random chains in a constant electric field

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An electron in a disordered δ-function potential in the presence of a constant electric field is studied in one dimension. Using different criteria from scattering theory we find that there are Stark-ladder-like resonances in the electronic spectrum. A detailed analysis of the statistical properties of these resonances and their connection to the resistance as a function of disorder and field strength is given. The possibility of seeing these resonances in the resistance of ultranarrow wires is suggested.

Ever since Wannier[1] proposed the existence of Stark-ladder resonances (SLR) in periodic lattices subject to an electric field, the subject has been somewhat controversial. It is only recently that the actual existence and some properties of the SLR are becoming well established.[2] A physically intuitive argument to motivate the existence of the SLR arises from using Zener's tilted band picture when a field is applied. The band edges represent a natural boundary in momentum space for the motion of the electrons while accelerated by the field. These closed orbits can be quantized using the Bohr-Sommerfeld quantization condition, thus leading to a discrete energy spectrum. The above argument is not quite right since the electrons can tunnel from one band to the next, thus converting the discrete eigenvalues into resonances in the continuum. Proving that this is indeed what happens, starting from a Schrödinger equation for free electrons in the presence of a field, is a subtle mathematical problem.[2] In all the analyses that treat the SLR, the translational invariance of the potential has played an important role. This leads one to believe that Bloch's theorem is essential in having the SLR. Also, several attempts have been made to see these resonances experimentally in periodic systems but none of these attempts seem to have been successful.[3]

The purpose of this paper is to show, for the first time, that translational invariance is not necessary to have Stark-ladder-like resonances, and that they could be seen in disordered systems. We study here only a one-dimensional model. The existence of the SLR in a random system is connected to a recent finding that electrons in a disordered chain are power-law localized when acted on by a constant electric field.[4,5] Most of the studies of SLR in periodic models have been directed at calculating the electronic energy spectrum of a free electron in a field. Here we follow a different route, with the aim of obtaining results that can in principle be compared directly with experiments. We then concentrate on the calculation of the transmission and reflection coefficients as a function of energy and study the statistical properties of the location of the resonances and their widths for different values of the disorder, length of the system, and magnitude of the electric field. The connection to the measurable resistance is carried out via a Landauer-type formula,[5,6] and we obtain the density of states from the derivative of the phase shift in the reflectivity. Experimentally we have in mind the very narrow wires fabricated in Si inversion and accumulation layers where resonance spectroscopy seems to be possible at sufficiently low temperatures.[7-9]

We have studied the model with the Hamiltonian

$$H = -\frac{1}{2}\frac{d^2}{dx^2} + \sum_{n=1}^{N} \beta_n \delta(x - na) - Fx \ ,$$

where a is the lattice spacing, F the electric field strength times the electronic charge, and β_n an independent random variable with a uniform probability law of width W. The length of the system, which we call the sample, is L with N δ-function potentials in between. We consider a scattering problem in which we have an incoming wave incident into the sample. For an arbitrary nonzero field we have two possibilities which are clearly different from the scattering theory point of view. If we approach the potential from the right with energy smaller than FL the wave is completely reflected and the transmission coefficient is zero. Under this condition the S matrix is equal to the reflectivity and therefore the only change in S comes from the phase shift $\delta(E)$ experienced by the wave after it emerges from the sample. In this case the value of the momentum of the incoming and outgoing wave is the same. This is the situation considered in most SLR studies in periodic systems.[2,10] This possibility is not as close to the experimental situation as having the electron entering the sample from the right with an energy which is above FL. The difference is, however, that the S matrix cannot be defined in the usual way because the incoming and outgoing waves have different momenta.[11] For an electron entering above the ramp formed by the electric field potential, the transmission and reflection coefficients are on the other hand well defined. An appropriate way of defining the resonances is in terms of the maxima of the derivative of the phase shifts as a function of energy E, defined from the bottom of the ramp. In fact $\delta'(E)$ is equal to $2\pi n(E)$, where $n(E)$ is the density of states.[12]

In Ref. 5 the Poincaré map representation of the Schrödinger equation was used to calculate the wave functions for a fixed energy, while the electric field was approximated by a step potential. Since what we want to do here requires the calculation of the derivative of the phase $\delta(E)$ with respect to E, and this derivative is related to derivatives of the wave functions with respect to the energy as well, it turns out to be more accurate to study a Poincaré map for the derivative of the wave functions combined with a Poincaré map for the wave functions themselves. This is what we do in our calculations. To convince ourselves that our calculational procedure does converge to the correct answers, we first analyzed the location of the maxima of the derivative of the phase shifts with respect to energy in the periodic case for wave incidents below the ramp. We then compared our results with the highly accurate calculations of Benosela, Greechi, and Zironi that were obtained from finding the poles of the resolvent operator.[2] For the parameter values used by Bentosela *et al.* $N=13$, $a=6$, and $F=0.0125$, including the type of potential they use, we found that the maxima of $\delta'(E)$ do correspond with high precision to the values found in Ref. 2, i.e., a resonance is located at $E=1.556\,140\,828\,094\,9$,[2] whereas with our method of calculation we find $E=1.556\,140\,8$. In order to get the accuracy of the resonance reported in Ref. 2 we need to reduce the grid in the energy interval, which is time consuming. Since our goal is to make connections to experimentally measurable quantities we keep the accuracy in determining the location of the resonances up to six significant figures. From our calculations we notice that the resonance spectra above and below the ramp are qualitatively different. Below the ramp we see several SLR superimposed on each other. On the other hand, above the ramp we only see one ladder but with smaller lifetimes. Therefore, it is in fact easier to detect the individual ladders above the ramp than below. Looking at the numbers above the ramp we find indeed that the location of the maxima in $\delta'(E)$ corresponds to the location of the maxima in T with an accuracy of up to six significant figures. In order to study the length dependence of the results for energies $\tilde{E}$'s above the ramp we set the origin of energy, for a given FL, to zero at the top of the ramp. This procedure allows us to see the same resonances as we vary L. Also, because the calculation is done in a finite system the spacing between resonances is not exactly equal to sFa, with s an integer. Instead of analyzing the distance between any two resonances we introduce an average separation between resonances by taking an average over clearly defined resonances for a given energy interval. For example, when $F=0.4$, $a=1$, and $N=100$, we can distinguish clearly 30 resonances and the average separation distance between resonances is $\langle \Delta\tilde{E} \rangle - Fa = 0(10^{-4})$, where $\langle\ \rangle$ means a resonance average. The same comments go for the width Γ of the resonances as measured in terms of the transmission's coefficient half-width at half maximum. We find as well that the variations of Γ for different peaks are larger than the fluctuations in the location of the maxima of T for a given L. On the other hand, the location of the maxima of T does have a small oscillatory L dependence which is related to interband Zener tunneling whereas Γ is essentially independent of L when going from $L=85$ to $L=115$. Notice that since we have to calculate T for every value of $\tilde{E}$ for different L's and a small grid in $\tilde{E}$ the calculations are somewhat lengthy. In Fig. 1(a) we show the results for the logarithm of resistance defined in terms of a Landauer-type[5,6] formula, which has its minima exactly located at the points where $\delta'(\tilde{E})$ and T have their maxima.

We can now use the understanding of resonances gained in the *periodic* case given above to treat the *disordered* case, which is the central theme of this paper. As in the periodic case we calculate $\delta'(\tilde{E})$ to make sure that its maxima correspond to the maxima of T for a given realization of the random potential. In Fig. 1(b), we show an example of the results when $W=1.0$. The first thing we notice is that the essential structure of the Stark-ladder-like resonances is in fact stable against the addition of weak disorder. This is true mainly when $aFN > \tilde{E}$, which corresponds to the power-law localized regime found in Ref. 5. On the other hand, the resonances sometimes become smaller in height and their width increases while increasing W. The opposite can occur also, however. In order to get representative results about the properties of the resonances quantitatively, apart from the averages over resonances defined in the periodic case for a given realization of the random potential, we need to carry out an average over an ensemble of systems. The number of systems over which the ensemble averages are carried out need not be large, however, in order to get standard deviations of only a few percent. In our calculations we found than an ensemble with 20–30 systems gave good statistical averages. In order to have more reso-

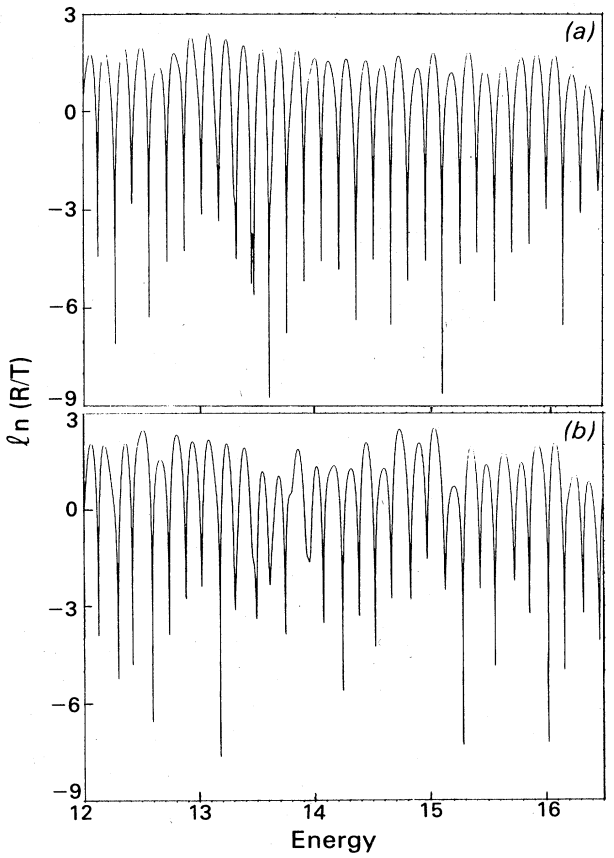

FIG. 1. Logarithm of the resistance as a function of energy for the potential treated in Ref. 2, with $N=45$, $a=6$, and $F=0.0125$. The energy grid is (10^{-3}). (a) The periodic case and (b) the disordered case with $P(\beta)=1/W$ and $-W/2-1<\beta<W/2-1$, with $W=1$.

nances over which to carry out the averages we choose a system with $N=100$, $a=1$, and $F=0.4$ with the same potential as the one studied in Ref. 5. We find that the separation distance between resonances changes *linearly* as a function of W. When we take only one system and vary W we obtain, of course, nonmonotonic results. The linear dependence of the average separation between resonances as a function of W is given in Fig. 2(b). With regard to the widths of the resonances as a function of disorder we find that they grow *quadratically* with W, as shown in Fig. 2(a). Finally we look at the behavior of the resonance widths as a function of F. We find that for a resonance and ensemble averaged analysis the width of the resonances change approximately exponentially with $-1/F$. This result is shown in Fig. 2(c) and is compared with the result for a periodic system (see Ref. 13 for a discussion of the lifetimes as a function of F).

We now give a heuristic argument to explain the existence of SLR in the model. It was found in Ref. 5 that the disordered model considered here has two qualitatively different regimes as a function of $t=aFN/\tilde{E}$. When $t<1$ the states have a transmission coefficient that decays exponentially with distance. In this case the term Fx varies slowly as a function of x for small F. We find that the ladder in this regime is not well defined. In the case when $t>1$ the electron has acquired enough energy from the field such that it "sees" less of the disordered potential and therefore the electronic wave functions decay algebraically. It is in the regime $t>1$ of quasiextended states that we distinctly observe the SLR in our calculations. Thus the existence of the SLR is directly related to the power-law nature of the electronic states.[14] An analytic analysis of the resonance spectrum of the model considered here, that would lead the results as a function of disorder quoted above, seems to be quite difficult. It is good to remember that even in the periodic case, mathematically, this is a very subtle and difficult problem in itself. We should point out the important difference between the resonance widths in the $F=0$ case as compared to the $F\neq 0$ case. In the former case the width decreases exponentially with L[8,9] whereas for $F\neq 0$ it decays as a power law. This important difference could make possible the observation of SLR in experiments like those in Ref. 7. The experiments should be carried out at sufficiently low temperatures such that the thermal broadening of the resonances is minimized. Also, an insulating material with narrow bands can be used, such that heating as well as screening effects are reduced.

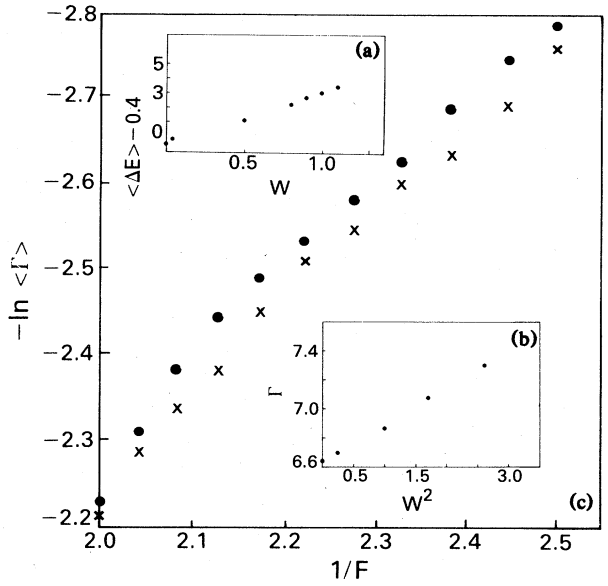

FIG. 2. The model here corresponds to $P(\beta)=1/W$ and $-W/2+1<\beta<W/2+1$, with parameter values, $N=100$, $a=1$, and $F=0.4$. In the three figures (a)–(c) we show resonance and ensemble averaged results. In (a) the vertical scale is multiplied by (10^{-4}), whereas in (b) it is multiplied by (10^{-2}). In (c) the dots correspond to $W=0$, and the X to $W=1.0$. The discussion of the results is given in the text.

Note added. After this paper was submitted for publication we learned of work by F. Bentosela, V. Grecchi, and F. Zironi [following paper, Phys. Rev. B 31, 6909 (1985)] in which the same problem is studied. Both works are complementary to each other. We thank Dr. F. Bentosela for informative correspondence.

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