Congreso Investigación

Effect of electric field and of disorder on the transmission coefficient in one-dimensional systems

J. Flores and G. Monsiváis

Instituto de Física, Universidad Nacional Autónoma de México, Apdo. Postal 20-364, 01000 México, D.F., México

(recibido el 16 de junio de 1987; aceptado el 16 de junio de 1987)

Abstract. We present in graphical form the effect of an external electric field and of disorder on the transmission coefficient of an electron wave in a one-dimensional chain of delta function potentials. For certain values of the electric field, the resonances forming the Stark ladders are apparent, even for small disorder.

Resumen. Se presentan en forma gráfica los efectos de un campo eléctrico externo y del desorden sobre el coeficiente de transmisión de una función de onda electrónica en una cadena unidimensional de potenciales delta. Para ciertos valores del campo eléctrico, aun cuando haya un pequeño desorden, aparecen claramente las resonancias que forman las escaleras de Stark.

PACS: 71.55.Jv; 71.10.+x; 71.50.+t

The properties of electrons in disordered potentials subjected to a constant electric field have received attention in a number of recent papers [1–9]. This problem is, among other things, interesting since such systems show a set of resonances, the Stark ladder resonances, (SLR's) first predicted for periodic systems by Wannier [10]. Although their existence was controversial for some time, there is now theoretical evidence which shows that the SLR's indeed exist. The experimental conditions to see them are very stringent and, although several experiments have claimed to see the SLR's [11], there is no convincing evidence supporting these claims. In what follows

we shall present in graphical form some further theoretical evidence regarding the SLR's.

The theoretical model we shall use for the one-dimensional system is defined by the Schrödinger equation

$$-rac{\hbar^2}{2m}rac{d^2\psi(x)}{dx^2}+[V(x)-Fx]\psi(x)=E\psi(x),$$
 (1)

where $\psi(x)$ is the electron wave function, F > 0 is the electric field intensity times the electronic charge, and V(x) is a random potential, which in the following will always be a sum of N equally spaced delta functions, *i.e.*

$$V(x) = \sum_{i=0}^{N-1} \beta_i \delta(x-ia), \qquad (2)$$

where β_i is a uniformly distributed random number, with distribution

$$P(\beta_i) = \begin{cases} \frac{1}{Q} & -\frac{Q}{2} + \langle \beta \rangle < \beta_i < \frac{Q}{2} + \langle \beta \rangle \\ 0 & \text{otherwise} \end{cases}$$
(3)

Here $\langle \beta \rangle$ is the average value of β_i over the ensemble of one-dimensional chains defined by distribution (3); we shall call the fixed number Q, the disorder. In all our calculations we use units such that $\hbar^2/2m = 1$ and the lattice spacing a = 1; the length L of the system is then L = N-1. We assume that the electric field is present only in the interval $0 \leq x \leq L$.

We approach the problem by calculating the transmission coefficient T as a function of the electron energy $E = k^2$. We assume that a plane wave e^{ikx} is incident from the left, so a reflected wave re^{-ikx} and a transmitted one $te^{ik'x}$ exist, as shown schematically in Fig. 1; here $k'^2 = k^2 + FL$. The connection with the dimensionless resistance ρ is provided by Landauer's formula [12]

$$\rho = \frac{R}{T} \,, \tag{4}$$



FIGURE 1. Finite one-dimensional chain of N equally spaced delta function potentials of intensity β_i under the effect of an external electric field F.

where R and T are respectively the reflexion and transmission coefficients defined as $R = |r|^2$ and $T = |t|^2$. These coefficients are computed using the Poincaré map as explained in Ref. [4].

For F = 0, that is, when no external electric field is present, and random V(x), it has been established rigorously that all states are localized [13] with an envelope that decays exponentially with distance. For $F \neq 0$ and FL < E essentially the same remains true; but for FL > E, that is when the electric field is strong, T has a power-law decay with L instead of an exponential one and there is a critical field F_c above which the states are extended [4]. The transmission coefficient T can then be large enough, and resonant states could show up as maxima of T when plotted as function of E; when the states are localized, on the other hand, T will decrease and be even close to zero.



FIGURE 2. The transmission coefficient T as a function of the incident electron energy E for different values of L. When L is large enough, Q = 0 and F = 0 the allowed and forbidden bands are apparent, and coincide with those of the infinite Kronig-Penney model.

We shall start by analyzing T(E) for different values of L without external electric field and no disorder. In Fig. 2 we show the transmission coefficient for 0 < E < 40 and L = 10,100 and 1000. In this case, Eq. 1 describes a finite-length Kronig-Penney model; the first two bands of conducting states, for which $T \neq 0$, are apparent. For L > 100 the energy limits of these bands coincide with those obtained in the text-book treatment of this model with $L \rightarrow \infty$. Notice that for L = 10 one can still count the number of values of E for which T(E) shows a local maximum; this number is equal to L



FIGURE 3. Influence on the tramission coefficient T(E) of the disorder Q, with L = 100 and F = 0. As the disorder increases, the allowed bands are destroyed.

and the corresponding states are extended states even in the limit of infinite L.

We now analyze the effect of disorder on the bands of Fig. 2, starting with the case F = 0. The function T(E), for the same range of E as in Fig. 2, is shown for one particular member of the ensemble of one-dimensional chains and several values of the disorder Q in Fig. 3 for L = 100. We see that the disorder destroys the bands, which is consistent with the fact that the electronic states become localized. Notice that for our model in which V is a set of delta functions, T remains different from zero near values of E which coincide with the upper bounds of each band. This has to do with a special feature of our model, since the highest-lying stationary states of each band have nodes at x = i [14], and therefore are not affected by the random potential V(x) given in Eq. 2; there always exists a set of states which remain extended, one for each band of the corresponding periodic system, no matter what the disorder is. When $L \to \infty$, however, this set is of zero measure.



FIGURE 4. Starting from the ordered chain with Q = 0, the transmission coefficient T(E) is shown for different values of the electric field F. The low energy bands are first destroyed.

Considering again the periodic system (*i.e.* Q = 0) we show the effect on the allowed bands of an external electric field. For L = 100, it will be seen in Fig. 4 how the bands disappear as F increases. The lowest-energy bands are destroyed first, since the states with eigenvalues $E \sim FL$ are seriously affected. If F is increased even more, a set of sharp resonances appears, as shown in Fig. 5. These resonances are equally spaced in energy, *i.e.*

$$E_n = E_0 + nFa, \tag{5}$$

as originally predicted by Wannier [10], and constitute what is called a Stark ladder. Here the electrons, which in a periodic system could move freely within a conducting band across the whole sample, are confined due to reflection by the tilted bands edges, giving rise to quantized states with energies E_n . Strictly speaking these states are resonant states because of the Zener tunneling. However, they only

418 J. Flores and G. Monsiváis



FIGURE 5. For the ordered chain (Q = 0) if F is large enough the Stark ladder resonances, appearing as sharp peaks in the curve T(E), are evident.

exist for values of F such that the probability of the Zener tunneling can be neglected [15]. For some ranges of the energy, more than one ladder could be present, as can be seen in Fig. 6, in which the energy range is enlarged; a fixed value of F = 0.8 was used and the SLR's are seen as a function of L. For L = 350, for example, three different ladders can be distinguished. Note also that for smaller values of L and large energies, the ladder does not exist, since then the field effect becomes negligible and T is different from zero for all values of E.

We shall now analyze the effect of disorder on the SLR's. We start in Fig. 7 with Q = 0 and a value of F (F = 0.8 in this case) for which a Stark ladder exists. Then, as Q is increased, the transmission coefficient decreases. However, for small enough values of the disorder, the Stark ladder persists, as can also be seen in Fig. 8, where we keep the disorder fixed and increase F until the ladder appears, as it did for the ordered system.



FIGURE 6. The transmission coefficient T(E) for different values of L with $F \neq 0$ fixed and Q = 0. Note the appearance of more than one Stark ladder. The range of E is here larger than in previous figures.

Finally, we should mention that it is possible to understand the above results from the following qualitative arguments, as discussed in reference [16]. When the periodic system is subjected to an external electric field, the electron wave function becomes localized, the localization length l_F being of the order of E/F [16]. On the other hand, disordered systems without external electric field also show

420 J. Flores and G. Monsiváis



FIGURE 7. The Stark ladder persists with a small amount of disorder, as shown here for T(E).



FIGURE 8. Keeping the disorder Q fixed, as F increases the Stark ladder can be recovered.

localized electronic wave functions; we shall call l_Q the corresponding localization length. When the disorder is small and an electric field is present $l_Q \gg l_F$, so the effects of disorder are not felt and the SLR's are not affected. As the disorder is increased, l_Q becomes comparable to l_F and the resonances disappear.

In conclusion, we have shown, through a set of graphs in which the transmission coefficient T is plotted as function of the electron energy E, how an external electric field affects the resistance of one-dimensional systems, both periodic and disordered. We believe that these graphs provide us, in a very pictorial way, with a better understanding of the behaviour of electrons in one-dimensional chains.

References

- V.N. Prigodin, Zh. Eksp. Teor. Fiz. 79, 2338 (1980) [Sov. Phys. JETP 52, 1185 (1980)].
- 2. F. Bentosela, V. Grecchi and F. Zironi, J. Phys. C 15, 7119 (1982).
- 3. J. Flores, J.V. José and G. Monsivais, J. Phys. C 16, L103 (1983).
- C.M. Soukoulis, J.V. José, E.N. Economou and P. Sheng, Phys. Rev. Lett. 50, 764 (1983).
- F. Delyon, B. Simon and B. Soulliard, Phys. Rev. Lett. 52, 2187 (1984).
- 6. J.V. José, G. Monsivais and J. Flores, Phys. Rev. B 31, 6906 (1985).
- 7. F. Bentosela, B. Grecchi and F. Zironi, Phys. Rev. B 31, 6909 (1985).
- 8. E. Cota, J.V. José and M. Ya. Azbel, Phys. Rev. B 32, 6137 (1985).
- 9. J. Flores, P.A. Mello and G. Monsivais, Phys. Rev. B 35, 2114 (1987).
- 10. G.H. Wannier, Phys. Rev. 117, 432 (1960).
- L.M. Lambert, J. Phys. Chem. Solids 26, 1409 (1965); Phys. Rev. 138, A1569 (1965); R. W. Koss and L.M. Lambert, Phys. Rev. B 5, 1479 (1972).
- 12. R. Landauer, Phil. Mag. 21, 863 (1970).
- 13. P. Erdös and R.C. Herndon, Adv. Phys. 31, 65 (1982).
- 14. E. Cota, J. Flores and G. Monsivais, in press (Am. J. Phys.).
- 15. S. Nagai and J. Kondo, J. Phys. Soc. Japan 49, 1255 (1980).
- 16. E. Cota, J.V. José and G. Monsivais, Phys. Rev. B 35 (1987).