Electronic spectrum of quantum-δ-wells superlattices in an electric field

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We study one-dimensional periodic chains of quantum δ wells, centering our attention on the properties of the electronic spectrum in the presence of an electric field. We study the field dependence of the quasibound and resonant states of the system, which we define clearly. The spectrum, whose absolute behavior depends on the symmetry of the potential, is universal if an appropriate origin of energy is chosen. The field finally transforms the spectrum into a continuous one. We study also the formation of Wannier-Stark ladders. Finally, we show that in superlattices, the quasibound levels are never degenerate. [S0163-1829(97)04640-7]

I. INTRODUCTION

Since the first days of quantum mechanics, electric-field effects in solids have been a controversial matter until recently. The pioneering works by Bloch, Wannier, and Zener[1] about periodic lattices in an homogeneous electric field introduced theoretically the concepts of the Wannier-Stark ladder, Stark localization, and related phenomena, but it was experimentally difficult to observe these effects. The reason was that in ordinary solids the bandwidths Δ are so large that the dimensionless parameter $f=\Delta/Fa$ ($F=e\mathcal{E}$ is the electrical force; a is the lattice spacing) is enormous and the effects above referred were unobservable for accessible fields ($\mathcal{E} \leqslant 10^5$ V/cm). This problem was eliminated with superlattices, for which $f=1$ is easily reachable. There is clear experimental evidence[2] of field-induced localization, Wannier-Stark ladders, and Bloch oscillations in superlattices. This fact has produced a great amount of theoretical work during the past few years.[3]

The aim of this paper concerns the existence of sharp Stark-shifted electron and hole states in semiconductor quantum wells and sharp resonant field-dependent states that have been found lying above the potential barriers enclosing quantum wells. This paper presents analytical and numerical calculations for a one-dimensional superlattice built with quantum δ wells. The field produces a restructuring of the ordinary ($F=0$) spectrum into field-dependent states.

The underlying question is the meaning of bound states in an electric field. Its mere existence is strange, because if a quantum well is placed in an electric field, the energy spectrum becomes continuous, from $-\infty$ to ∞. Experimental observations suggest that certain states in the continuum are ''special'' and differ from the rest by their exceptional stability.[4] The procedures used to find these states have been basically two: by identifying them with peaks in the density of states, or as transmission resonances.[5,6] In this paper, we use a different method. The ordinary bound states ($F=0$), or the quasibound states ($F\neq 0$) are calculated as the poles of the Green function of the system using the characteristic determinant method, which is briefly described in the next section.

II. METHOD OF CALCULATION

We shall consider a sequence of N δ-function potentials of the form

$$V(x)=U(x)+\sum_{n=1}^{N} V_n\delta(x-x_n), \tag{1}$$

where the potential $U(x)$ can be any external potential applied [we will concentrate on the case $U(x)=Fx$]. The Green function (GF) $G(x,x';E)$ is defined as the solution of the equation

$$\left(-\frac{d^2}{dx^2}+Fx+\sum_{n=1}^{N} V_n\delta(x-x_n)-E\right)G(x,x';E) = \delta(x-x'). \tag{2}$$

This GF satisfies Dyson's equation:

$$G(x,x')=G_0(x,x')+\int_{x_1}^{x_N} G_0(x,x'')V(x'')G(x'',x')dx'', \tag{3}$$

where $G_0(x,x')$ is the unperturbed GF of an electron in the potential Fx. We will concentrate on the retarded GF. An acceptable GF $G_0(x,x')$ for the study of the energy spectrum[7] is given by

$$G_0(x,x')=-\frac{\pi}{F^{1/3}}\mathrm{Ai}(\xi^+)\mathrm{Bi}(\xi^-), \tag{4}$$

where $\xi=(Fx-E)/F^{2/3}$, $\xi^+(\xi^-)=\max(\min)(\xi,\xi')$, and Ai and Bi are the standard Airy functions.[8] We obtain the quasibound energies of the system as the poles of the Green function of the whole system. Gasparian *et al.*[9] showed that the poles of the Green function of the potential (1) are given by the zeroes of the characteristic determinant D_N, of the matrix whose elements are defined as

$$D_{ij}=\delta_{ij}+V_j G_0(x_i,x_j), \tag{5}$$

where the indexes i and j run from 1 to N, the total number of δ wells.

It can be shown[9] that the determinant D_N can be written in tridiagonal form. Therefore, D_N, which is in general a complex function of the energy E, can be calculated using the following recurrence relation:

$$D_n=A_n D_{n-1}-B_n D_{n-2}, \tag{6}$$

where the index n goes from 1 to N. The initial conditions are $D_{-1}=0$ and $D_0=1$.

The magnitudes A_n and B_n, and then D_n can be calculated directly[10] just by fixing the values of the amplitudes V_i of the wells and their positions x_i, and using the function $G_0(x_i,x_i)$, given by Eq. (4). This method, which also can be generalized to multilayered systems,[10] has been successfully applied to study transmission properties of random[9] and quasiperiodic[11] sequences of δ barriers.

III. RESULTS

In all the calculations presented from now on, we have considered that $\hbar=2m=e=1$ ($\hbar$ is Planck's constant/2π, m is the electron mass, e is the proton charge), and then all the units are derived from this convention.

A. One δ well

If we consider one δ well of the form $-V_1\delta(x-x_1)$ (with $V_1>0$) for $F=0$, a simple calculation indicates (see, e.g., Ref. 12) that there exist always a bound state, independently of the value of V_1, with energy $E_1=-V_1^2/4$. The value of E_1 is not altered, of course, if x_1 is changed, but the corresponding wave function will have parity only if $x_1=0$. This distinction will affect the behavior of the spectrum when an electric field is considered.

To find the quasibound energy when an uniform electric field is considered, we must solve numerically the equation $D_1=0$, due to the presence of the Airy functions in G_0. In Fig. 1 it is shown the quasibound spectrum as a function of the electric field applied for three different positions x_1 of the well. The numerical values used are $V_1=1$, $x_1=0$ (circles), $x_1=1$ (crosses), and $x_1=-1$ (diamonds). As expected, the eigenenergy for a well at x_1 is equal to the energy for a well at $x=0$ shifted by the amount Fx_1. The quantitative behavior of the spectrum in the range of small fields depends clearly on x_1. By using second-order perturbation theory, we obtain, for small fields,[13]

$$E=-\frac{V_1^2}{4}+Fx_1-\frac{2\pi}{V_1^4}F^2. \tag{7}$$

The perturbative results are plotted as dotted lines in Fig. 1.

The energy of the state relative to Fx_1 allows us to distinguish between quasibound and resonant states. A pole of the GF smaller than Fx_1 corresponds to a quasibound state, while a pole of the GF bigger than Fx_1 corresponds to a resonant state. This distinction between quasibound and resonant states was not clear in previous works,[7] where the energy $E=0$ was considered to be the limit between quasibound and resonant states, independently of the position x_1 of the well. This criterium will also be applied in bigger systems.

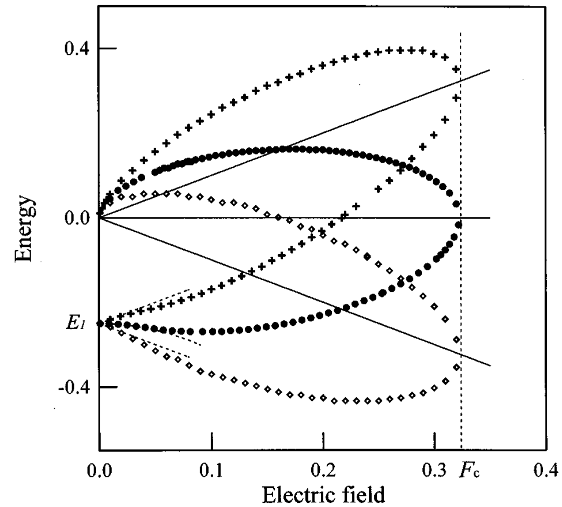

FIG. 1. Plot of the energy spectrum for one δ well, centered at different points. The values are $x_1=1$ (crosses), $x_1=0$ (circles), and $x_1=-1$ (diamonds). We also plot (solid lines) for each value of x_1 the functions $E=Fx_1$, and in dotted lines the results obtained from perturbation theory.

The results show that there exist in all cases a quasibound state inside the well, and a resonant state lying above the well (above Fx_1). This resonant state always appears at $E=0$ for very weak fields. The energy of both quasibound and resonant states is modified by the field, but as F increases, the energies of these two states approach each other. Finally, for a critical value of F (F_c in Fig. 1) the two energies coincide at a value equal to $F_c x_1$. From this value of F_c the well is unable to maintain either quasibound states or resonances, and the spectrum of the potential becomes continuous.

It is easy to show, using the standard expressions for the Ai and Bi functions for an infinitesimal argument,[8] that F_c is given by

$$F_c\cong\frac{\pi^3}{3^{5/2}[\Gamma(2/3)]^6}V_1^3. \tag{8}$$

This value, which can be very well approximated by $F_c\approx V_1^3/3$, coincides exactly with the numerical calculation.

B. Two δ wells

Let us consider now a potential of the form $V(x)=-V_1[\delta(x-x_1)+\delta(x-x_2)]$, where $x_1<x_2$. For $F=0$, this potential presents two bound states if $V_1(x_2-x_1)>2$ is verified. When a uniform electric field F is applied, the quasibound energies have to be calculated numerically because $G_0(x,x)$ is defined in terms of the Airy functions. The numerical calculation is performed by using the characteristic determinant, which in this case is a 2×2 determinant D_2.

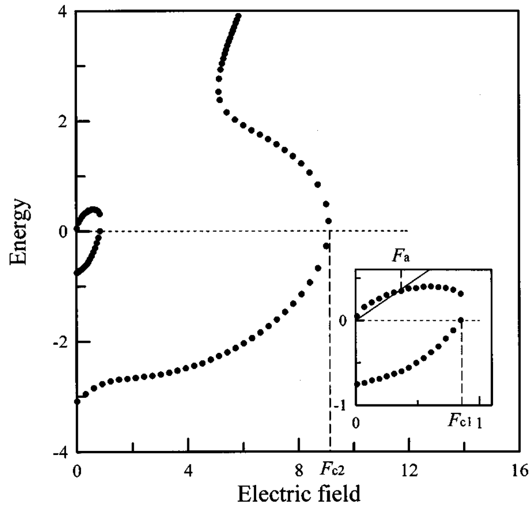

FIG. 2. Plot of the quasibound levels as a function of the electric field for a system with two δ wells. We show in squares the case $x_1=1$ and $x_2=2$, and in circles the case $x_1=1/2$ and $x_2=-1/2$.

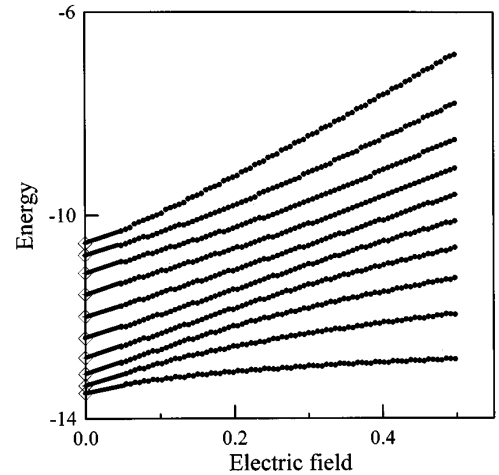

FIG. 3. Plot of the quasibound states of a system formed by 10 δ wells with $V_1=7$ and $a=1$ as a function of the electric field applied, in the weak-field regime. We show with diamonds the spectrum obtained for $F=0$.

For numerical purposes, we use the recursion relation (6), where A_2 and B_2 are defined in terms of V_1, $G_0(x,x)$, x_1 and x_2.

We have studied both the symmetrical ($x_1=-x_2$) and the asymmetrical ($x_1\neq -x_2$) cases, and the results obtained are in some way equivalent to the one found for one δ well, but with some significative differences. The absolute value of the spectrum depends on the symmetry. In the range of small fields, for the symmetric case the two quasibound energies decrease quadratically with the field; meanwhile, for the asymmetric one there is a linear behavior, as expected from perturbation theory. But the spectrum is again universal; we can obtain all the results by a proper field–dependent energy shift.

The universal spectrum is shown in Fig. 2, in which the origin of energy is taken at the top of the well placed at the point of smaller potential energy x_1. The behavior of the two quasibound states is similar. The quasibound energies are field dependent, and as the field increases, both of them approach the energy origin. Associated to each quasibound state, there is a resonant state, whose energy is also field dependent and tends to the origin of energy when F increases. For two critical values of the electric field, called F_{c1} and F_{c2} in Fig. 2, the highest and the lowest quasibound states disappear, respectively, by overlapping with their corresponding resonances, and only remains in the continuous part of the spectrum.

An interesting question is whether the states present above the origin of energy are resonant or quasibound states. The lowest quasibound state presents no problem. By Stark localization, this state must be localized in the first well, and it disappears at F_{c2} by overlapping at the energy origin with a clear resonant state, also associated to the first well. The field F_{c2} is given by Eq. (8), that is, the field needed to transform the quasibound spectrum into a continuous one. But the highest quasibound state and its associated ''resonance'' behave differently. In the inset of Fig. 2, we show as a solid line the top of this well, given by Fx_2. For very weak fields, there is a resonance above, which for a field F_a crosses Fx_2, and can be considered as a *second* quasibound state associated to the x_2 well. The two quasibound states disappear, overlapping at the natural origin of energy (dotted line in the inset).

We have also encountered very complicated patterns of resonances, above the ones plotted in Figs. 1 and 2, that disappear when the field increases. The Wannier-Stark ladder is probably only well defined for negative energies and in the weak-field regime due to the presence of these resonant states, for which evidence is presented in Ref. 14. In the following section, in which we study bigger systems, we restrict ourselves to this region to investigate the presence of the ladder.

C. N δ wells

Let us consider now a potential of the form

$$V(x)=Fx-V_1\sum_{n=0}^{N-1}\delta(x-na). \qquad (9)$$

The quasibound states of the system can be obtained, as before, by solving the equation $D_N=0$, where D_N is now an $N\times N$ determinant. For numerical purposes, we use the recursion relation (6). The results obtained are presented in Fig. 3, in which we plot the energies of the quasibound states as a function of the electric field applied, F, for $N=10$, $V_1=7$, and $a=1$. When $F\to 0$, we recover exactly the spectrum obtained when F is not present, shown as diamonds in Fig. 3. The absolute value of the spectrum obtained is different if we consider symmetric or asymmetric potentials, as it happened before, with a quadratic or linear behavior, respectively. But if we shift the spectra by Fx_1, the results overlap into a universal spectrum, that is, the one plotted in Fig. 3. The energy spacing between adjacent levels is affected by the electric field, and it is approximately uniform in the central region of Fig. 3, forming a Wannier-Stark ladder.

IV. SYSTEMS WITH TWO TYPES OF WELLS

We now want to describe the properties of systems made with two different types of δ wells. In the case of no electric

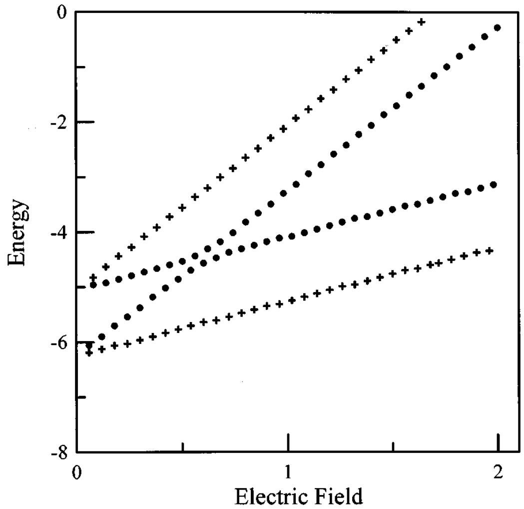

FIG. 4. Plot of the behavior of the quasibound states of a system with two different δ wells as a function of the electric field applied. In the two cases plotted, $x_1=1$ and $x_2=3$. In crosses, we show the case $V_1=5$ and $V_2=4.5$, and in circles the case $V_1=4.5$ and $V_2=5$.

field applied, it is clear that for a periodic sequence we will have two bands of bound states due to the two types of wells. But we would like to comment on a phenomenon that does not happen in systems with one type of well. Let us consider a potential formed by two different wells of the form

$$V(x)=-V_1\delta(x-x_1)-V_2\delta(x-x_2), \tag{10}$$

where $x_1<x_2$, and $V_1<V_2$. When an electric field is applied, we have an increase of the quasibound energies with the field, and the increase is faster for the quasibound state associated to the x_2 well. As $V_1<V_2$, the lowest quasibound state increases faster than the highest and they must cross at a given field. Nevertheless, we found that the two levels repel each other. This is shown in Fig. 4, where we plot the quasibound levels of a system with 2 δ wells with $x_1=1$, $x_2=3$ as a function of F; we represent in circles the case $V_1=4.5$, $V_2=5$, and in crosses the case $V_1=5$, $V_2=4.5$. In all our calculations we found that in a repulsion between two quasibound levels, these practically interchange their slopes. This means that, after the repulsion, the two levels have interchanged the wells where they are localized. The lowest quasibound state is localized in the well of smallest potential energy.

When we increase the number of wells in the system forming the sequence V_1, V_2, V_1, V_2, $\dots$, the number of repulsions increases considerably, and even we can find that there can be several repulsions between two adjacent levels due to the multiple repulsions and the corresponding interchanges of slopes between all the adjacent levels of the system. This fact produces a field-dependent and oscillatory energy spacing between adjacent levels, which can affect strongly the absorption optical spectrum of superlattices under the effect of a variable electric field.

The repulsions between adjacent levels found in all cases and, therefore, the lack of level crossing allows us to conclude that the quasibound levels are never degenerate.

V. SUMMARY

We present here a study of periodic superlattices formed by quantum δ wells when a homogeneous electric field is applied. We study the field dependence of the quasibound states, which are placed inside the wells, and also of the resonant states that lie above the well. We give a criterium to distinguish clearly between these two types of states. Although the absolute spectrum depends on the symmetry of the potential, there is in all cases a ‘‘natural’’ origin of energy, for which the spectrum is equivalent. We also study how Wannier-Stark ladders appear. If the electric field is strong enough, the lattice is unable to maintain quasibound states. Finally, we show that the quasibound levels are never degenerate.

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