Quasibound states in an electric field

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The Lippman-Schwinger equation in one dimension is solved for the cases of one and two δ wells in an electric field. At low field the field dependence of the quasibound levels behaves in accordance with perturbation theory, while the levels are ionized at high fields. The two-well case exhibits the onset of a Stark ladder. In both cases there is evidence for a positive-energy-resonance structure which becomes suppressed as a δ-well lattice is formed.

I. INTRODUCTION

Electric field effects have been somewhat controversial until recently,[1-5] when it became possible to engineer semiconductor heterostructures of controlled purity and dimensions. The reason is that in ordinary solids the bandwidths Δ are so large that the dimensionless parameter $f=\Delta/Fa$ ($F=e\mathcal{E}$, the electrical force; $a=$lattice spacing) is enormous and these effects are washed out in experimentally attainable fields ($\mathcal{E}\leq 10^5$ V/cm), whereas for presently standard superlattices $f=1$ is easily obtained. There is clear evidence for the existence of field-induced localization and Wannier-Stark ladders in these structures.[6-8] The matter to be addressed in this Brief Report concerns the existence of sharp Stark-shifted electron and hole states in semiconductor quantum wells and relatively sharp resonant states that have been found in calculations and seen experimentally lying above the potential barriers enclosing quantum wells.[9-11] In addition, we shall comment on the restructuring of these field-dependent states into Wannier-Stark levels as individual quantum wells are coupled to form a lattice.

The existence of bound states in an electric field is curious in itself, for if a quantum well is placed in an electric field of any strength, the energy spectrum becomes continuous and extends from $-\infty$ to ∞. Experimental observations suggest that certain states in this continuum are somewhat "special" and differ from the background continuum by their exceptional stability. These "quasibound" states cannot be located by ordinary quantum-mechanical means, since the matching equations have acceptable solutions for all energies, but have been studied by identifying them with peaks in the density of states[12] or as transmission resonances.[13] In this Brief Report we suggest a procedure for identifying them directly and apply it to the cases of one- and two-δ potential wells, where the calculations can be carried through analytically to obtain the complete field-dependent spectrum of quasibound levels.

II. CALCULATION

In ordinary ($F=0$) quantum mechanics the Schrödinger equation with potential V can be cast into the Lippman-Schwinger form

$$|\psi\rangle=g|\phi\rangle+G_0V|\psi\rangle\ , \tag{1}$$

where ϕ denotes a basis state of the underlying representation and G_0 is an appropriate Green function. In these terms, the bound states correspond to poles of the Green function G satisfying the Dyson equation

$$G=G_0+G_0VG\ . \tag{2}$$

Then, the continuum states satisfy (1) with $g=1$ and the bound states satisfy (1) with $g=0$. We propose that this same dichotomy holds for $F\neq 0$ and that the quasibound levels can be found from the integral equation

$$\psi(x)=\int_{-\infty}^{\infty}G_0(x,x')V(x')\psi(x')dx'\ , \tag{3}$$

where, for simplicity we work in one dimension, and $G_0(x,x')$ satisfies

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}-Fx-E\right]G_0(x,x';E)=\delta(x-x') \tag{4}$$

(we shall generally not express the dependence on E explicitly). As discussed in Ref. 14, an acceptable solution is

$$G_0(x,x')=-\frac{\pi}{l^2F}A_i(Z_>)B_i(Z_<)\ , \tag{5}$$

where $l=(\hbar^2/2mF)^{1/3}$, $Z=(x-E/F)l^{-1}$, $Z_>(Z_<)=\max(\min)(Z,Z')$, and A_i,B_i denote the standard Airy functions.[15]

We consider first the case of a δ well:

$$V(x)=-\lambda\delta(x)\ , \tag{6}$$

which for $F=0$ has a single bound state

$$E_0=-\varepsilon_0=-\frac{m\lambda^2}{2\hbar^2}\ ,$$
$$\psi_0(x)=Ne^{-\kappa|x|}\ ,\qquad (7)$$
$$\kappa=\frac{m\lambda}{\hbar^2}\ .$$

In this case (3) becomes

$$\psi(x)=-\lambda G_0(x,0)\psi(0)\ ,$$
$$G_0(0,0)=-\frac{1}{\lambda}\ .\qquad (8)$$

The second equation in (8) seems to have appeared first in Ref. 16 but, as discussed in Ref. 14, an inappropriate Green function was used so they did not obtain real solutions. We shall identify the quasibound levels with the solutions to the transcendental equation

$$A_i(-\xi)B_i(-\xi)=\eta \qquad (9)$$

in terms of the dimensionless variables $\xi=E/Fl$, $\eta=l^2F/\pi\lambda$. In atomic units ($\hbar=2m=1$) with $\lambda=1/\pi$, we have

$$E=\xi\eta^2,\quad F^{2/3}=4\eta^2\ . \qquad (10)$$

Equation (9) can be solved approximately for small F by using the asymptotic expansions for the Airy functions.[15] As $F\to 0$ we recover exactly the bound-state energy (7), and for small ($F>0$) the energy decreases quadratically in F, in agreement with perturbation theory.[17] For larger F the solution was found by integrating the Airy equation numerically. The resulting spectrum is shown in Fig. 1.

Next, we look at the double δ well

$$V(x)=-\lambda[\delta(x)+\delta(x-a)]\ . \qquad (11)$$

It is straightforward to show that for $y=m\lambda a/\hbar^2<1$ there is a unique bound state, for which $x_0=\kappa a(E=-\kappa^2)$ is the sole positive root to $(x_0y^{-1}-1)e^{x_0}=1$. When $y>1$, however, there are two distinct bound states corresponding to the positive roots of $(x_0y^{-1}-1)e^{x_0}=\pm 1$.

In the presence of the electric field, Eq. (9) is replaced by the determinantal equation

$$\begin{vmatrix} A_i(-\xi)B_i(-\xi)-\eta & A_i(\alpha-\xi)B_i(-\xi) \\ A_i(\alpha-\xi)B_i(-\xi) & A_i(\alpha-\xi)B_i(\alpha-\xi)-\eta \end{vmatrix}=0\ , \qquad (12)$$

where $\alpha=a/l$ and, in atomic units, the dimensionless quantities ξ,η are related to the energy and electric field as in (10). The spectrum resulting from the numerical solution to (12) for the case $a=1$, $\lambda=10/\pi$, is shown in Fig. 2.

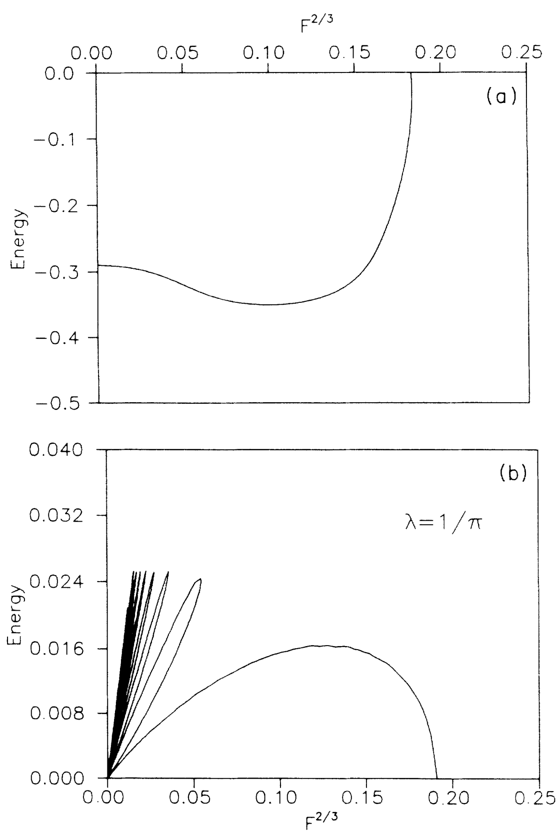

FIG. 1. Field dependence of the spectrum for the single-δ-well potential: (a) quasibound state, (b) positive-energy "resonance."

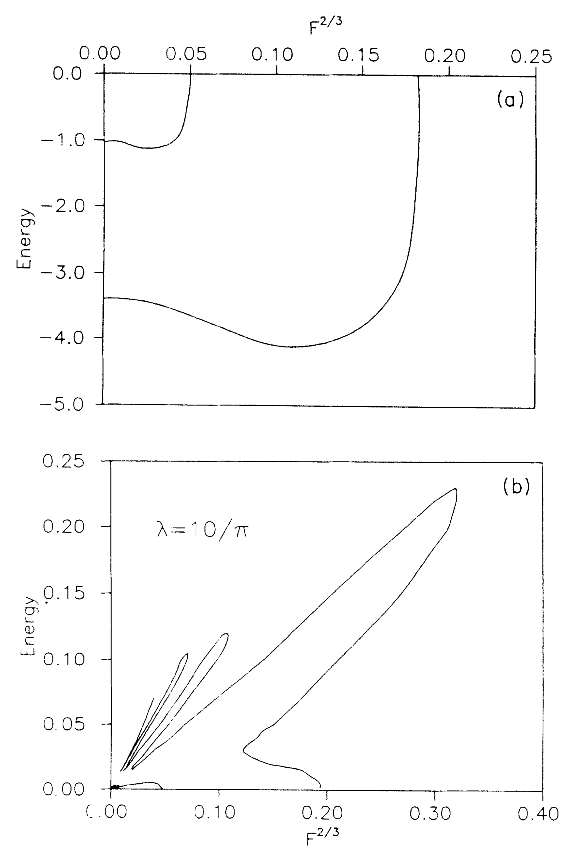

FIG. 2. Field dependence of the spectrum for the double-δ-well potential: (a) quasibound states, (b) resonances.

III. DISCUSSION

In Fig. 1(a) we show the field dependence of the quasibound state for a single well in a uniform electric field. In the absence of the field the well has a single true bound state with energy $E_0 = -\frac{1}{4}\lambda^2$. For small F, the binding energy is seen to increase quadratically, in agreement with perturbation theory.[17] As F increases, the binding energy eventually begins to decrease and vanishes abruptly at the critical value F_c. This occurs when the electric potential drop across one Bohr unit is close to $|E_0|$. At this field and above, the well is unable to maintain a quasibound state. This is in agreement with previous calculations for a square well[17] and also with physical intuition. Less intuitive, however, are the above-well quasibound levels shown in Fig. 1(b), which appear for $0 < F < F_c$ and whose number increases without limit as $F \to 0$. From Eqs. (5) and (8) one sees that the wave functions for these states are Airy functions A_i having maxima lying upfield from the well at distances $E/F^{2/3}$. Evidence for the existence of these states is discussed in Refs. 9–11.

For the two-δ-well case, we see in Fig. 2(a) the beginning of a Stark ladder. The two rungs have different critical field values, so it appears that in the case of a lattice of δ wells, the ladder is probably well defined only in the weak-field regime. In addition to the ladder states, the positive-energy "resonant" structure appears to become more complex. The upper part of the structure moves to higher energy and expands, while the lower part decreases in size and contracts toward $E = 0$. It is likely that, as more wells are introduced, this portion of the spectrum disappears, leaving only the Stark ladder states. This aspect of the problem deserves further investigation.

In conclusion, we speculate that the spectra found in the δ-well case also occur for more realistic potentials and account for phenomena observed experimentally in semiconductor heterostructures.

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