Energy Level Locking in Quantum Conductors

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(Received 8 November 1993)

We demonstrate theoretically that, under certain conditions, the energy levels of parallel quantum conductors lock together. This novel phenomenon is due to a charge imbalance that occurs as a transverse energy level begins to fill with electrons. The implications of our results for experiments that have been performed on semiconductor nanostructures are discussed.

PACS numbers: 73.20.Dx

In studying quantum mechanical systems it is often illuminating to view them as composed of subsystems, weakly or strongly coupled together. When a pair of energy levels belonging to two such subsystems approach each other, an energy level crossing or "anticrossing" occurs. These two possibilities are illustrated in Figs. 1(a) and 1(b), respectively. Anticrossings occur because quantum hybridization between the subsystems becomes important in near-degenerate situations. The hybridization opens an energy gap, lifting the incipient level degeneracy. Such diverse physical phenomena as the band gaps that control the electronic properties of crystalline solids [1] and the anomalously low observed flux of solar neutrinos [2] can be viewed as manifestations of anticrossings. On the other hand, simple level crossings [where a degeneracy does actually occur, as in Fig. 1(a)] happen when the matrix elements of the Hamiltonian that are responsible for the hybridization vanish, often for reasons of symmetry.

The purpose of this Letter is to demonstrate theoretically that energy level crossings and anticrossings are not the only possibilities in near-degenerate situations. For example, a third type of behavior is also possible, namely, energy level *locking*. This new phenomenon is illustrated in Fig. 1(c). Level locking may be thought of as the opposite of anticrossing; i.e., instead of nearly degenerate energy levels "repelling" each other, they lock together. We will show that energy level locking is characteristic of Coulomb-coupled quasi-one-dimensional Fermi systems. A possible physical realization is a pair of parallel narrow conductors in a semiconductor heterostructure. When the Fermi level crosses a pair of nearly degenerate transverse energy levels belonging to the different conductors, a charge imbalance occurs and, as a consequence, the energy levels show a strong tendency to lock together. Whether level locking does or does not occur depends on the relative strength of the charge imbalance and the hybridization between the energy levels involved. In addition to being interesting as a novel physical phenomenon, energy level locking may prove to be useful in the fabrication of arrays of *precisely* matched nanoscale conductors, an important and still unsolved materials science problem. Experiments suggesting that locking may be occurring between the transverse levels of closely spaced parallel conductors in semiconductor heterostructures have been reported by Smith *et al.* [3]. However, in a subsequent experimental study, Simpson *et al.* [4] reported finding no evidence of level locking. Thus the experimental situation is at present unclear, and in the absence of a theory exhibiting energy level locking in any model system, the question as to whether it should occur, even in principle, has remained open.

The theoretical study that we report here is numerical, based on the density functional formalism of Hohenberg, Kohn, and Sham [5,6]. The quantum conductors that we consider are shown schematically in Fig. 2. The electrons are confined to the x-y plane, which may represent a semiconductor heterointerface. They are, in addition, Coulomb confined laterally [7], to form a pair of parallel quasi-one-dimensional conductors, by their interaction with two uniform ribbons of positive charge. These ribbons extend infinitely in the y direction, offset from the x-y plane by a distance d. The positive charges can be

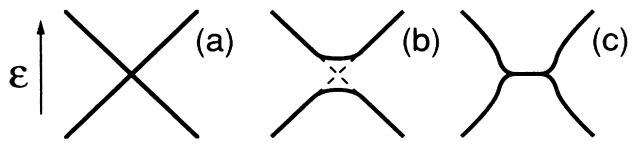

FIG. 1. The behavior of energy levels in near-degenerate situations. (a) Crossing. (b) Anticrossing. (c) Locking.

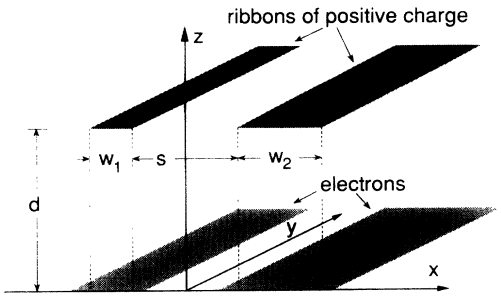

FIG. 2. Schematic drawing of a pair of parallel Coulomb-confined quantum conductors.

0031-9007/94/72(15)/2450(4)$06.00

realized physically as regions of donor ions introduced in a controlled way some distance from the heterointerface (remote doping). The system is charge neutral overall, and is embedded in a uniform dielectric. Its electronic structure must be calculated self-consistently, and the Hohenberg-Kohn-Sham theory of inhomogeneous interacting electron systems provides a suitable framework for doing this. The Kohn-Sham equations [6] that we solve [7] are

$$-\frac{\hbar^2}{2m^*}\nabla^2\Psi_{l,k}(x,y)+V_{\rm eff}[\sigma;x,y]\Psi_{l,k}(x,y) = \varepsilon_{l,k}\Psi_{l,k}(x,y),$$

where $V_{\rm eff}$ includes the Coulomb (Hartree) potential and terms arising from the exchange and correlation energy functionals of the electron density σ, which we treat in the standard local density approximation. l is the transverse energy level index and k is the longitudinal electron wave vector. The exchange-correlation energy used is that of Tanatar and Ceperly [8], suitably scaled by the dielectric constant and electron effective mass of GaAs.

The calculated electronic structure of a pair of quantum conductors is shown in Fig. 3 at $T=0$. The solid lines are the six lowest transverse energy levels $\varepsilon_{l,0}$. The dashed line is the Fermi energy. The abscissa is the (uniform) density n of the donor ions in the ribbons of positive charge shown in Fig. 2. Since the system is charge neutral overall, n can also be regarded as an electron filling parameter for the conductors. The two conductors in this case are rather similar to each other; the positively charged ribbons that define them have widths $w_1=190$ nm and $w_2=200$ nm. The energy levels in Fig. 3 are labeled N or W according to whether they belong primarily to the narrower or wider channel, respectively, as determined by inspection of the calculated eigenfunctions. Notice that when the Fermi energy rises up through the lower of a pair of adjacent energy levels with increasing n, the (algebraic) slope of the lower energy curve of the pair increases while that of the upper curve decreases. Thus the two energy levels are brought closer together. Levels 3 and 4 lock together at the Fermi energy, while the gap between levels 5 and 6 narrows by a factor of ~ 5.

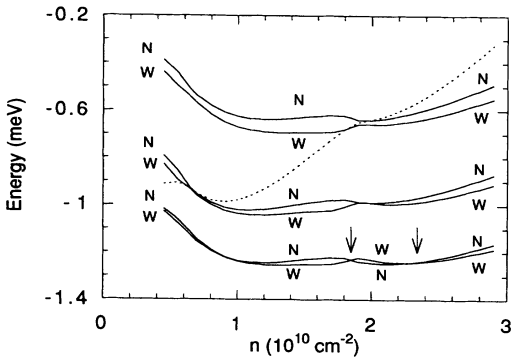

FIG. 3. The calculated transverse energy levels of a pair of quantum conductors (solid lines) and Fermi energy (dashed) vs the density n of ions in the ribbons of positive charge in Fig. 2. Energy levels are labeled N or W according to whether they belong principally to the narrower or wider channel, respectively. Arrows indicate anticrossings. Model parameters (as defined in Fig. 2) are $w_1=190$ nm, $w_2=200$ nm, $d=20$ nm, and $s=200$ nm; dielectric constant and electron effective mass are those of GaAs.

These effects can be understood qualitatively as a competition between a charge imbalance that occurs between the channels when a transverse level begins to fill and quantum hybridization. The origin of the charge imbalance is the $\varepsilon^{-1/2}$ density of states singularity, characteristic of quasi-one-dimensional systems, that crosses the Fermi energy when a transverse level begins to fill. If electrons were added to the pair of conductors without any change in the energy level structure, while maintaining equal Fermi levels in the two conductors, this singularity would result in the addition of excess electrons to the conductor in which the transverse level is beginning to fill. In this work, however, the energy level structure of the conductors is calculated *self-consistently*. Thus the potential due to the excess electrons shifts all of the transverse energy levels associated with the conductor containing them upwards. The differential charging effect is thus weakened somewhat, but it does not disappear completely. This is shown in Fig. 4, where we display the ratio r of the electron numbers in the two conductors for the range of n in which the Fermi energy crosses fifth and sixth transverse levels in Fig. 3. Because of the different widths of the ribbons of positive charge, $r=w_1/w_2=0.95$ corresponds to perfect charge balance in the two conductors. However, our calculation shows that r oscillates; its drop near $n=1.8\times10^{10}$ cm^{-2} and rise beginning at $n=2.0\times10^{10}$ cm^{-2} are due to the fifth and sixth transverse levels beginning to fill, respectively. Although the charge imbalance is small $\sim 0.5\%$, the associated electrostatic potentials shift the energy levels of the conductor

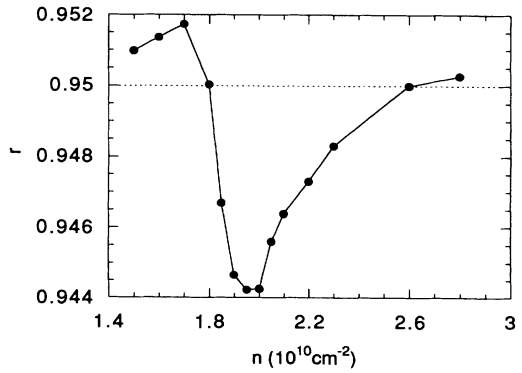

FIG. 4. Calculated charge ratio r between the two conductors. $r=w_1/w_2=0.95$ corresponds to perfect charge balance. The solid line is a guide to the eye.

with the excess (deficiency) of electrons upwards (downwards) significantly, favoring energy level locking [9]. Energy levels that lock together do not separate immediately when the Fermi energy rises above them because their density of states singularities almost coincide, which inhibits further changes of the charge differential.

As was mentioned above, quantum hybridization acts to lift degeneracies, and thus opposes energy level locking. In fact, in the presence of hybridization the energies of the locked levels cannot become *exactly* equal [10]. However, for hybridization to occur, there must be an overlap of the electron wave functions (i.e., tunneling) between the two conductors. This tunneling is *exponentially* weak when the tunnel barrier between the conductors is strong. Thus the residual energy splitting between locked levels can be made arbitrarily small by imposing a strong enough electrostatic tunnel barrier between the conductors. Notice that in Fig. 3 *all* pairs of corresponding energy levels (not just those at the Fermi energy) move closer together when the charge imbalance occurs. This is as one would expect, given the above differential charging mechanism. However, since the effect is driven by the levels *at* the Fermi energy, the other pairs of levels may anticross, or lock, or just move together slightly. All of these possibilities can be seen in Fig. 3, where anticrossings are indicated by arrows. The stronger effective tunnel barriers experienced by the electrons in the lower energy levels make it possible for the residual gaps between them (where they lock or anticross) to be much smaller than the residual gaps between levels 5 and 6; this is seen in Fig. 3.

The results presented above demonstrate energy level locking theoretically in a specific model of quantum conductors. Experimental quantum conductors are more complicated systems, with the lateral confinement usually achieved by means of gates [11] rather than the ribbons of positive charge that we have considered here. However, the physical mechanism of level locking relies on a feature of the electronic density of states that is common to all narrow fermionic conductors with multiple transverse energy levels, irrespective of the method of confinement. In gated structures [12] the lateral confinement of the electrons tends to be stronger than in Coulomb-confined systems of the type considered above, so that the hybridization that competes with level locking should be less important. However, our calculations show that locking only occurs between transverse energy levels that are close to each other to begin with. It is not clear whether the parallel conductors studied by Smith *et al.* [3] were sufficiently similar to each other for the level locking mechanism that we have described to operate. In the more recent experiments of Simpson *et al.* [4], the widths of the parallel conductors could be tuned independently. But the measurements may not have been sensitive to transverse energy level shifts such as those in Fig. 3, which, although large enough to bring adjacent energy levels together, are only $\sim 10\%$ of the subband spacings of the individual conductors.

In conclusion, we have presented the first theoretical study demonstrating that energy level locking should occur between parallel quantum conductors. This is a novel phenomenon, qualitatively different from the anticrossing behavior that is typical of nearly degenerate energy levels in quantum systems. It is driven by a charge imbalance associated with the onset of filling of transverse energy levels with electrons. Our results should stimulate further experimental and theoretical studies of this interesting phenomenon.

We wish to thank D. Loss and H. Trottier for stimulating discussions. This work was supported by the Natural Sciences and Engineering Research Council of Canada and the Center for Systems Science at Simon Fraser University.

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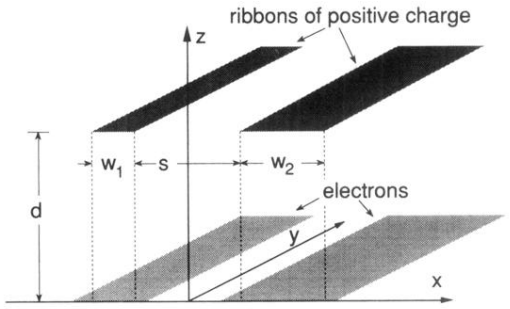

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