Coexistence and coupling of zero-dimensional, two-dimensional, and continuum resonances in nanostructures

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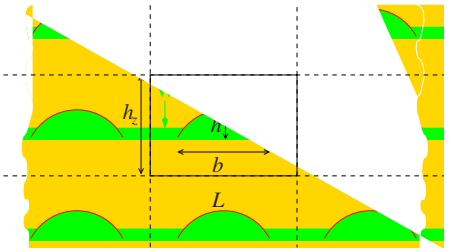
Quantum dots (QDs) embedded in a matrix exhibit a coexistence of "zero-dimensional" (0D) bound electron and hole states on the dot with "three-dimensional" (3D) continuum states of the surrounding matrix. In epitaxial QDs one encounters also "two-dimensional" (2D) states of a quantum well-like supporting structure (wetting layer). This coexistence of 0D, 2D, and 3D states leads to interesting electronic consequences explored here using multiband atomistic pseudopotential calculations. We distinguish strained dots (InAs in GaAs) and strain-free dots (InAs in GaSb) finding crucial differences: in the former case "potential wings" appear in the electron confining potential in the vicinity of the dot. This results in the appearance of localized electronic states that lie *above* the 3D continuum. Such resonances are "strain-induced localized states" (SILSs) appearing in strained systems, whereas in strain-free systems the dot resonances in the continuum are the usual "virtual bound states" (VBSs). The SILSs were found to occur regardless of the thickness of the wetting layer and even in interdiffused dots, provided that the interdiffusion length is small compared to the QD size. Thus, the SILSs are well isolated from the environment by the protective potential wings, whereas the VBSs are strongly interacting. These features are seen in our calculated intraband as well as interband absorption spectra. Furthermore, we show that the local barrier created around the dot by these potential wings suppresses the 0D-2D (dot-wetting layer) hybridization of the electron states. Consequently, in contrast to findings of simple model calculations of envelope function, 0D-to-2D "crossed transitions" (bound hole-to-wetting layer electron) are practically absent because of their spatially indirect character. On the other hand, since no such barrier exists in the hole confining potential, a strong 0D-2D hybridization is present for the hole states. We show this to be the source for the strong 2D-to-0D crossed transitions determined experimentally.

DOI: 10.1103/PhysRevB.80.045327 PACS consequences,[10] including lasing action of far infrared response,

[11,12] nonlinear upconversion,[13] or dephasing of excited carriers.[14] Quasibound states in the continuum, so-called virtual bound states (VBSs), have long been known to occur in sharply varying (e.g., square well) potentials.[15,16] We will further see that the presence of strain between the QD and the matrix within which it is embedded creates a new kind of localized resonant states at energies within the 3D continuum, which we termed strain-induced localized states (SILSs).[17]

The electronic level diagram of a QD system can be thought of at first in a simple model [Fig. 2(a)], considering dot-localized 0D states, 2D WL states, 3D matrix states, and resonant VBS. Within such a setup, one would expect to observe the following transitions:

(i) dot-localized hole (electron) to dot-localized electron (hole) states [type 1 in Fig. 2(a)];



IV. SURVEY OF EIGENSTATES IN QD SYSTEMS

A. Prototype states and their wave functions

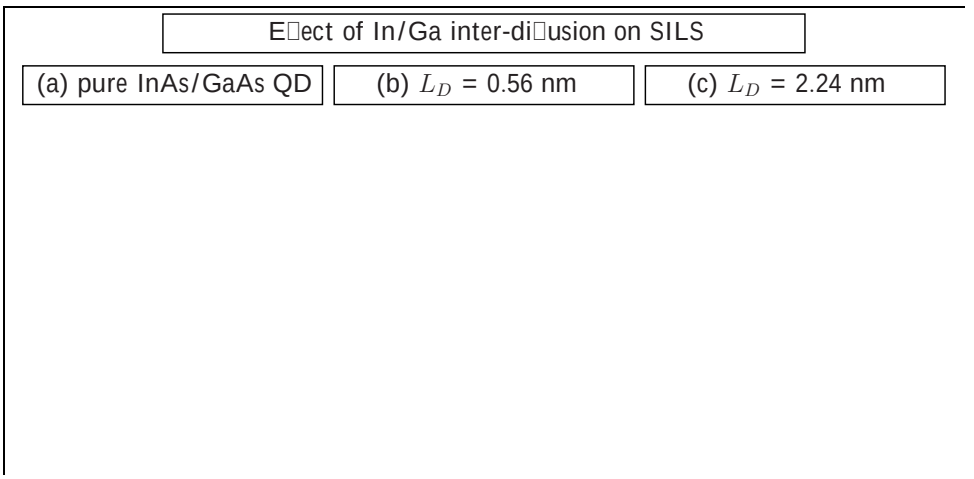
The different eigenfunctions of the single-particle problem [Eq. (2)] can be classified according to:[17] (a) their degree of localization (

the continuum by the potential wings and exist as sharp levels within an energetic resolution of $\simeq 1$ meV.

B. Stability of strain-induced localized states against interfacial

results.[48,49] This blueshift is 14 meV for QD (b) (L_D =0.56 nm) and 74 meV for QD (c) (L_D=2.24 nm). We could find the SILS level ϵ_B in the slightly interdiffused system QD (b), blueshifted by $\simeq$25 meV with respect to the reference system QD (a). As L_D increases, system QD (c), the wings are less pronounced and the confinement region is smaller, the SILS ϵ_B is no longer present. However, we could identify for QD (c), at 140 meV above the GaAs CBM, a VBS of the typical width of $\simeq$1 meV, with the same appearance as the ϵ_B SILS. Thus, in a similar manner as for (In,Ga)As/GaAs QDs,[17] SILSs appear to morph into VBSs when the strain-induced local barrier becomes weaker. We conclude that, while the QD/matrix interdiffusion certainly modifies quantitatively the electronic structure of the QD, the SILSs appear to be relatively robust, provided that the interdiffusion length is small as compared to the height of the QD.

Based on these results, our further calculations rely on the simpler construction of a sharp interface QD/matrix. We will show that: (i) in the intraband absorption SILSs exhibit similar appearance, regardless on whether the WL is included or not in the calculation;[17] (ii) neither SILS nor VBS appear to interact with the 2D WL continuum when the ECP is distorted by strain; (iii) transitions with SILS as final states can be observed also in the intraband absorption as sharp well-defined peaks.



V. CROSSED TRANSITIONS IN INTRABAND ABSORPTION

We have calculated the intraband absorption spectra for the two QD systems: the unstrained InAs/GaSb and the strained InAs/GaAs. For these systems, with confining potentials illustrated in Fig. 3, we consider both situations, with and without a WL in the structure. Initial state for all of the intraband spectra shown here is the first (S-like) electron confined level ϵ_0. Correspondingly, the intraband absorption

These features can be understood in terms of the hybridization model depicted in Fig. 13. Although one can only approximately disentangle the QD effects from those of the superlattice,[10] such a model is expected to give a fairly good prediction on the evolution of states in the full system. Let us consider an InAs/GaSb quantum well (QW) with the InAs QW thickness n ML, and having a state $E_c^{(n)}(2D)$ of symmetry compatible with the QD state ψ_C. The energetic position of $E_c^{(n)}(2D)$ will depend on n in a similar monotonic manner as shown, for example, by Piquini et al.[51] for the CBM. When forming the whole system (matrix+WL+QD), the two states $E_c^{(n)}(2D)$ and ψ_C will hybridize, giving rise to bonding-antibonding states as those shown in the middle of Fig. 13.

For this rather unusual case of no-strain InAs/GaSb system, the actual calculated intraband absorption spectra basically follow the expectations of the model and of the simple diagram depicted in Fig. 2(a). Similar theoretical results were obtained in the past using an effective-mass description[12,23,52] for [illegible] systems. Because of neglecting the strain-induced changes in the confining potential, these results are not generally valid, as it will be shown in the following.

B. Strained InAs/GaAs system: $e \rightarrow WL_e$ transitions are blocked

The intraband absorption spectrum for the InAs/GaAs QD system is shown in Fig. 14. We see, below the continuum onset E_{cont}, only S→P-like transitions ($\psi_0 \rightarrow \psi_{1,2}$). Similar to the case of no-strain InAs/GaSb, these are barely affected by the inclusion of the WL. [illegible] to InAs/GaSb, there are [illegible] transitions appearing below continuum, for any of the investigated WL thicknesses (2, 4, and 6 MLs). This indicates that, unlike the unstrained system, here, for InAs/GaAs, there is only a weak hybridization between dot e and WL$_e$ states. Thus, the predictions arising from the hybridization model (discussed above for InAs/GaSb) do not hold for real, strained systems.

The final state of transitions labeled by B_z (ψ_B) in Fig. 14 is the SILS shown in Fig. 7. As pointed out above, its energetic location and appearance are not affected much by the presence of the WL. Unlike the ψ_C state of strain-free InAs/GaSb, the SILS of InAs/GaAs shows practically no hybridization with the WL$_e$ continuum because of the "shield" provided by the potential wings, despite its position within the WL$_e$ band.

Figure 14 shows that, for the InAs/GaAs system, the number of peaks (strong transitions) above continuum is much reduced as compared to InAs/GaSb. The origin of these peaks, e.g., C_z in top panel of Fig. 14, are, like in InAs/GaSb, the VBS. We note here the disappearance of the C_z peak for the system with WL included (bottom panel of Fig. 14). This is the direct result of a change in the VBS resonance condition (a different structure) and not of a QD-WL hybridization. We therefore conclude that [illegible] eff[illegible] f[illegible] L_zL_{xy}

VI. CROSSED TRANSITIONS IN INTERBAND ABSORPTION

The calculated interband absorption spectra for the InAs/GaAs QD system, (a) without and (b) with a WL included in the structure are shown in Figs. 15 and 16, respectively. Analogously to the intraband absorption, the calculations were performed using the single-particle approximation, Eq. (4), with the delta function replaced by a Lorentzian of FWHM of 1 meV. In both figures, the continuum threshold, corresponding to the GaAs band gap $E_{\mathrm{gap}}=E_c^{\mathrm{mat}}-E_v^{\mathrm{mat}}=1.521$ eV, is marked by a vertical thick-dashed line. We will therefore find bound-to-bound ($L_zL_{xy}\rightarrow L_zL_{xy}$ or [illegible]) transitions only left of the $E_c^{\mathrm{mat}}-E_v^{\mathrm{mat}}$ line. The first of those transitions can be seen as sharp peaks in Figs. 15

electron (hole) solutions of Eq. (2) in the presence of the WL. We have marked this value in Fig. 16 by a dashed line. Consequently, [illegible] $\mathrm{WL}_h \rightarrow \mathrm{WL}_e$ transitions (of type 2 in Fig. 2) occur only right of the $E_c^{\mathrm{WL}} - E_v^{\mathrm{WL}}$ threshold. For the

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