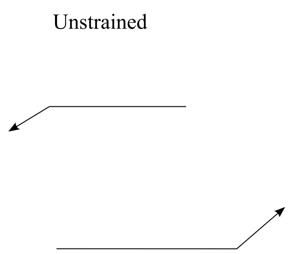
92

Supercoupling between heavy-hole and light-hole states in nanostructures

State Key Laboratory of(Received 22 July 2015; published 1 October 2015)

hole (HH) and light-hole (LH) components of the valence states in three-dimensional (3D) bulk
rs can mix quantum mechanically as the dimensionality is reduced in forming low-D nanostructures,
uantum wells, 1D quantum wires, and 0D quantum dots (QDs). This coupling controls the tuning of


Unstrained

Eq. (1), for unstrained QDs, in terms of classical perturbation theory. Figure 4(b) shows such a computed single dot V_{HL} of Gaussian-shaped GaAs QDs with varying dot height but the base size fixed to 25 nm, and all values lie around V_{HL} = 2.15 meV. This good agreement demonstrates the existence of a common coupling matrix V_{HL} for all QDs within a class of QDs. We also validate the common coupling matrix V_{HL} = 9.82 meV for strained lens-shaped InAs QDs by inserting $_{LH}$ and $_{HL}$ of a specific QD into Eq. (2) to obtain single-dot V_{HL}, as shown in Fig. 4(b).

IV. DISCUSSION OF THE SUPERCOUPLING EFFECT

The reduction of effective HH-LH splitting in Eq. (2) implies a previously unrecognized effect that will be called "supercoupling," whereby a highly dense manifold of HH-like QD states lying energetically between the HH0 and LH0 states, evidenced clearly in our directly calculated eigenvalue spectrum for strained dots (Fig. 2), mediates the HH-LH coupling and significantly enhances the mixing by reducing the energy denominator $_{HL}$ to a smaller value $_{HL}$ − . We see in Fig. 2(b)—but not in Fig. 2(a), where the LH0 state is adjacent to the HH0 state—a dense manifold of states, derived predominantly from the bulk HH band, lying between HH0 and LH0 states. We postulate that these HH-like intermediate states form a ladder of the supercoupling between HH0 and LH0. This supercoupling effect is identical for all QDs within an entire class (or ensemble), reflecting a common = 78.6 meV for all strained In(Ga)As QDs despite varying dot sizes, shape distortions, and alloy compositions, whenever the fluctuation in the number of intermediate states is small (1%).

It should be noted that for strained In(Ga)As QDs, the curve is only fitted to 11 QDs, indicated by red dots (presented elsewhere [36]), and the remaining 25 QDs, indicated by red circles, are added after fitting and thus represent (predictions) of the simple formula. Because of the large HH-LH splitting in strained QDs, the supercoupling effect (reflected in the denominator $_{HL}$) will dominate the HH-LH mixing over the direct coupling between HH0 and LH0 (reflecting in the numerator V_{HL}). Specifically, in the absence of supercoupling, i.e., = 0, the magnitude of the HH-LH mixing $^2_{LH}$, will tend to less than 1% instead of the 5–20% predicted in strained In(Ga)As QDs, even though the built-in strain significantly enhances the coupling matrix V_{HL} by a factor of 4.5 with respect to unstrained GaAs QDs.

The supercoupling is further confirmed by the presence of an abnormal point within the class of C_{2v} GaAs QDs (indicated by dot no. 1 in Fig. 3). This QD is embedded in AlAs instead of the $Al_{0.3}Ga_{0.7}As$ matrix, and it has a Gaussian shape with 25 nm base size and 3 nm height. A HH-like excited state HH1 is located between HH0 and LH0 in energy, and it has 4 meV energy separation from the LH0. For this specific QD, the coupling between HH0 and LH0 is mediated by the HH1, whereas in the remaining Gaussian-shaped QDs the state HH0 is immediately followed by LH0 without an intermediate state to mediate the interaction. Consequently, the HH-LH coupling is rather different in dots with and without intermediate states. In addition, there are dots with intermediate states but with small energy separation from the LH0, leading to a small supercoupling effect. For example, in the four lens-shaped GaAs/$Al_{0.3}Ga_{0.7}$As QDs, the HH1 state is also located between HH0 and LH0, as shown in Fig. 2(c), but this level is closer to the LH0 with a smaller energy separation of less than 2 meV. Such a small energy separation leads to a very small supercoupling effect in these lens-shaped GaAs QDs, which is consistent with their points being insignificant away from the fitted line, as shown in Fig. 3.

The origin of the supercoupling effect. We now turn to examine the supercoupling effect mediated by intermediate states in the language of classic "folded down" descriptions [1–7,11–14,16,23]. In terms of perturbation theory, the Hamiltonian of a C_{2v} QD could be divided into two parts: $H_{C_{2v}} = H_0 + V_{C_{2v}}$, where H_0 is the bare Hamiltonian with eigenstates of unperturbed HH and LH states $\{E^0_{HHn}, | ^0_{HHn}\}$ and $\{E^0_{LHn}, | ^0_{LHn}\}$ $(n = 0,1,2,\ldots)$. The perturbation potential $V_{C_{2v}}$ lowers the QD symmetry to C_{2v} and hence introduces HH-LH mixing, which modifies the ground hole state HH0 [1–7,11–14,16,18,23],

$$| _{HH0} = {}^0_{HH0} + \sum_m \frac{ {}^0_{LHm}\, V_{C_{2v}}\, {}^0_{HH0} }{E^0_{HH0} - E^0_{LHm}}\, {}^0_{LHm}. \quad (3)$$

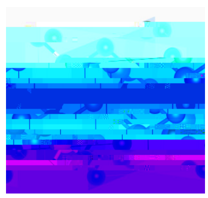
In the above equation, one usually takes LH0 into account and neglects the LH excited states [1–7,11–14,16,18,23] considering they are far from HH0 compared with LH0. Consequently,

$$_{LH} = \frac{ {}^0_{LH0}\, V_{C_{2v}}\, {}^0_{HH0} }{E^0_{HH0} - E^0_{LH0}} = \frac{V_{HL}}{_{HL}}. \quad (4)$$

In strained nanostructures, say In(Ga)As/GaAs QDs, there is a dense manifold of HH-like intermediate states lying in energy between HH0 and LH0, as observed in sophisticated calculations including multiband $k \cdot p$ approaches [19] and atomistic calculations [27–30] and shown in Fig. 2(b). These intermediate HH-like states, neglected in classical model Hamiltonian treatments [1–7,11–14,16,23], are also allowed to couple to HH0 under C_{2v} symmetry, and further modify the ground hole state,

$$| _{HH0} = | _{HH0} + \sum_{n\geq 1} \frac{ _{HHn}|\, V_{C_{2v}}\, | _{HH0} }{E_{HH0} - E_{HHn}} | _{HHn}, \quad (5)$$

where $| _{HH0}$ is given in Eq. (3) and $| _{HHn}$



92

ZZ a_z = L

and LH in self-assembled QDs is analogous to superexchange in magnetism in that it is remarkably enhanced by the presence in the QD of a dense ladder of intermediate states, which ampliÞes and propagates the coupling across a signiÞcant