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Bound states in continuum: Quantum dots in a quantum well

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ABSTRACT

We report on the existence of a bound state in the continuum (BIC) of quantum rods (QR). QRs are novel elongated InGaAs quantum dot nanostructures embedded in the shallower InGaAs quantum well. BIC appears as an excited confined dot state and energetically above the bottom of a well subband continuum. We prove that high height-to-diameter QR aspect ratio and the presence of a quantum well are indispensable conditions for accommodating the BIC. QRs are unique semiconductor nanostructures, exhibiting this mathematical curiosity predicted 83 years ago by Wigner and von Neumann.

1. Introduction

Semiconductor quantum dots exhibit full 3D confinement for carriers, giving a few bound integrable states with a discrete spectrum below the barrier, and free non-integrable states with continuum spectrum above the barrier. Quantum dots are often referred to as "artificial atoms" due to their discrete part of spectrum and discrete optical resonances arising from transitions between bound orbital states. Both atoms and quantum dots can be ionized, when electrons gain sufficient energy to escape the binding potential, and subsequently occupy free states – in vacuum in the case of atoms or bulk in the case of quantum dots.

However, boundedness and discreteness of an orbital state in quantum dots do not come necessarily together. We show in this Letter that novel semiconductor nanostructures, so called quantum rods, exhibit bound excited state with an energy embedded in the continuum of other free electronic states, above the ionization threshold. This is a so called bound state in continuum (BIC). There are various types of BIC reported since the foundation of quantum mechanics, but none of them were reported for atomic or condensed matter systems. In what follows, we state only a few. The first prediction originates back to 1929 when von Neumann and Wigner showed such a possibility by mathematical construction of a bounded potential accommodating a BIC [1]. This issue was revitalized by Stillinger and Herick [2] pointing out, 46 years later, that a BIC could occur in some specific molecular systems. The first artificial semiconductor nanostructure accommodating the bound state above ionization threshold, was reported in Ref. [3]. This bound state was argued to be a consequence of Bragg reflection due to the superlattice. Even though above the barrier, this state wasn't surrounded by a continuum of states and it was strictly speaking a quasi-bound state with free motion in the lateral direction. Some theoretical proposals and proofs for the BIC existence were reported for more complex quantum mechanical systems. For example, coupled system of electrons and nuclei in molecules [4] was considered. BIC, as an quantum mechanical interference effect can occur in various abstract models. Some examples of theoretical abstract systems that support BIC were reported in Refs. [5–10]. Experimentally, only photonic crystal systems with the BIC were reported [11,12]. A theoretical design of one-dimensional photonic heterostructure, supporting the BIC was provided in Ref. [13].

In what follows, we briefly describe the geometrical and compositional properties of quantum rods, and based on that we provide proof for BIC existence. The type of BIC which occurs in quantum rods is somewhat different from the majority of BICs reported in the literature. The most similar system supporting the BIC was reported by Robnik et al. [14], and one could say that the BIC reported here represents the 3D generalization of the 2D potential theoretically constructed in [14]. The rest of the Letter is dedicated to the discussion of possible interesting features arising from BIC existence, together with available experimental data and concluding remarks.

2. Quantum rods

Quantum rods are elongated InGaAs quantum dots embedded in a InGaAs quantum well sandwiched by two GaAs bulk regions. Details of the QR fabrication can be found in Refs. [15–17]. A simplified model for geometric and compositional properties of these

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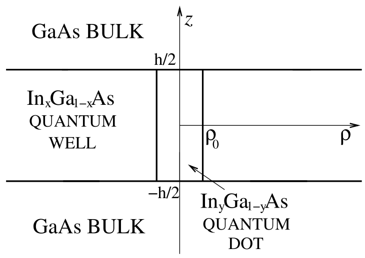

Fig. 1. Simplified geometric model of a quantum rod. Cylindrical symmetry is assumed, so the entire structure can be depicted within the z–ρ plane. Indium content of the dot region is larger than in the well region, i.e. $x < y$.

nanostructures is presented in Fig. 1. This structure consists of GaAs/InGaAs quantum well of width h over the region between $-h/2$ and $h/2$. The quantum dot is positioned within the quantum well so that the bulk region is above and below the dot in the z-direction and the quantum well is surrounding the rod in the radial direction. The entire structure is optically active giving the combined features of dot, well and the bulk as it is obvious from PL measurements [16,18]. The height of the rod and the width of the surrounding well are the same. This simplified model assumes that entire structure is cylindrically symmetric, even though such strict symmetry hasn't been reported. However, the general conclusions that follow do not depend on the exact shape of the rod basis. Therefore, we choose the circular shape of the basis in order to simplify theoretical consideration. The quantum rod has higher In content then the surrounding quantum well which makes the dot energetically deeper than the surrounding well.

3. Bound state in the continuum

One can naively expect that the quantum rod would accommodate bound states only below the quantum well barrier in the radial direction. However, due to bulk confinement in the z-direction, bound states could also appear with energies above the well barrier where also well continuum states are present giving the BIC. Such a situation resembles the one from Ref. [3] where a bound state occurs above the barrier of a superlattice, but it isn't surrounded by continuum states because the state itself is an impurity state in the superlattice, spaced from the continuum superlattice bands. Also, such a BIC is strictly speaking a quasi-bound state. We prove that in the case of a quantum rod, such state above the barrier is indeed surrounded by the continuum and is indeed bound for a wide range of parameter space.

Existence of the BIC in quantum rods is purely due to the interplay of the combined well and dot confinement. In order to prove this statement, consider the idealized quantum rod structure presented in Fig. 1. The quantum rod is considered isolated from the other quantum rods. We assume cylindrical symmetry of the entire structure, and the value of the embedding bulk barrier is set to infinity. The assumption of infinitely high bulk walls does not affect the general conclusion since the same conclusion follows from the full 8-band $\boldsymbol{k}\cdot\boldsymbol{p}$ model where the values for all barriers in the structure were taken with precise offsets and included strain effects. Now it becomes clear that this simplified model of realistic quantum rods presents the 3D generalization of the 2D potential constructed by Robnik et al. [14] in order to obtain the BIC, with the quantum well as escaping channel. However, it was pointed out in the same reference that existence of BIC in such potential is sensitive to perturbation, especially the one which might break the parallel geometrical shape of escaping channel. That shouldn't be a problem in this case, since the existence of quality quantum well seems very eminent, and the walls of quantum well escaping channel can be considered parallel to the infinity.

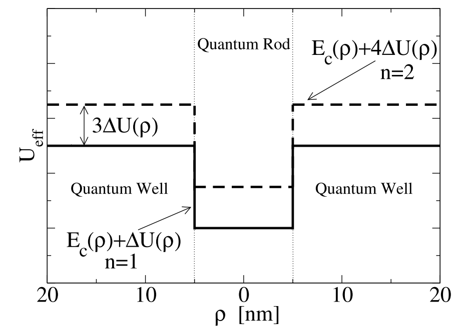

Fig. 2. Illustration of the energy span where a BIC can occur. The effective potential U_{eff} for the remaining one-dimensional radial eigenproblem is given for $l = 0$ and $n = 1, 2$. For $n = 1$ continuum states or quasi-bound well states occur for $E > U_b + \Delta U$. For $n = 2$ bound states might occur for $E < U_b + 4\Delta U$, whereas continuum states occur for $E > U_b + 4\Delta U$. Therefore the excited bound state in the well quasi-band continuum might occur for energies in the range $U_b + \hbar^2\pi^2/2m_w h^2 < E < U_b + 2\hbar^2\pi^2/m_w h^2$.

In this simple model we solve one spinless electron single-band envelope function equation in polar coordinates:

$$\left(\frac{\hbar^2}{2}\nabla\frac{1}{m_e(\boldsymbol{r})}\nabla + E_c(\rho) + E_c^z(z)\right)\Psi(\boldsymbol{r}) = E\Psi(\boldsymbol{r}) \tag{1}$$

where

$$E_c(\rho) = \begin{cases} 0 & \text{for } \rho < \rho_0 \\ U_b & \text{for } \rho > \rho_0 \end{cases}$$

and

$$E_c^z(z) = \begin{cases} 0 & \text{for } -\frac{h}{2} < z < \frac{h}{2} \\ \infty & \text{for } z < -\frac{h}{2} \text{ or } z > \frac{h}{2} \end{cases}$$

Values of the effective mass $m_e(\boldsymbol{r})$ are m_d and m_w in the dot and the well respectively. In the bulk, where the value of the potential is set to infinity, the value of the effective mass is unnecessary. The potential offset between dot and the well region is U_b. Parameters ρ_0 and h are the radius and the height of the QR. Due to infinite bulk barrier and cylindrical symmetry, one can separate the variables of the wavefunction $\Psi(\boldsymbol{r}) = \Phi(\phi)Z(z)R(\rho)$. Furthermore, the solutions for $\Phi(\phi)$ and $Z(z)$ are $\Phi_l(\phi) = \frac{1}{\sqrt{2\pi}}e^{il\phi}$ and $Z_n(z) = \sqrt{\frac{2}{h}}\sin\left(\frac{n\pi}{h}\left(z+\frac{h}{2}\right)\right)$ where we introduce good quantum numbers l and n, integer and positive integers respectively. The remaining Schrödinger-like equation in the radial direction reads:

$$-\frac{\hbar^2}{2}\frac{1}{\rho}\frac{\mathrm{d}}{\mathrm{d}\rho}\frac{\rho}{m_e(\rho)}\frac{\mathrm{d}}{\mathrm{d}\rho}R_{nl}(\rho) + \left(E_c(\rho) - E + \frac{\hbar^2}{2m_e(\rho)}\left(\frac{n^2\pi^2}{h^2} + \frac{l^2}{\rho^2}\right)\right)R_{nl}(\rho) = 0 \tag{2}$$

We provide the full solution to Eq. (2) in Appendix A. In order to maintain the simplicity, we will demonstrate the existence of the BIC by considering only the case with $l = 0$ and $n = 1, 2$.

The effective potential for the last eigenproblem in Eq. 2 is the expression given in brackets. The effective potential for $n = 1$ is $U_{\text{eff}}(\rho) = E_c(\rho) + \Delta U(\rho)$, where $\Delta U(\rho) = \hbar^2\pi^2/2m_e(\rho)h^2$ and for $n = 2$ it is $U_{\text{eff}}(\rho) = E_c(\rho) + 4\Delta U(\rho)$. The effective potential for $l = 0$ and $n = 1, 2$ is given in Fig. 2. Note that the effective mass depends only on the radial coordinate since the value of the effective mass in bulk is irrelevant due to infinite potential.

For $n = 1$ continuum states or quasi-bound well states occur for $E > U_b + \hbar^2\pi^2/2m_w h^2$. For $n = 2$ bound states might occur for $E < U_b + \hbar^2 2\pi^2/m_w h^2$, whereas continuum states occur for $E > U_b + 2\hbar^2\pi^2/m_w h^2$. Therefore, the excited bound state for $n = 2$