Inelastic Confinement-Induced Resonances in Quantum Dots

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Recently, it was shown that the coupling of center-of-mass and relative motion in atomic systems leads to inelastic confinement-induced resonances (ICIRs) [Phys. Rev. Lett. 109, 073201 (2012)]. In the present work, the possible occurrence of ICIRs in quantum dots is investigated. Particularly, electron-hole and electron-electron two-body systems with long-range Coulomb interaction are considered using the material parameters of GaAs. ICIRs are identified for the electron-hole system verifying the universal nature of the ICIR and, additionally, resonances due to the coupling of center-of-mass and relative motion are found also for the electron-electron system. In analogy to the coherent molecule formation appearing at ICIR in atomic systems a significant change in the mean distance between electrons and holes at the resonance is observed. By using the redistribution of the particle densities at the resonance position in modern quantum-dot experiments, the ICIR can provide a new technique for the control of the electron distribution in quantum dots and for the generation of single photons on demand.

I. INTRODUCTION

Artificial atoms and quantum dots (QDs) have attracted a great deal of attention during recent years [1]. Their modifiable physical properties offer a variety of new technologies in electronics and optoelectronics, such as single-photon sources [2, 3] or single-electron transistors [4, 5]. In QDs, the charge carriers, electrons and holes, are strongly confined in each spatial direction by an external potential leading to a discretization of the energy spectrum. The external confinement can be realized by modern fabrication techniques like lithography and epitaxy or electrostatically.

While in theoretical treatments a simplified external potential such as a box potential [6, 7] or a harmonic potential [8–10] is often adopted, the exact shape of the confinement of a quantum dot is in general not known. Yet, the confinement is definitely finite and hence never purely harmonic. Such an anharmonicity leads to a coupling of the center-of-mass (c.m.) and relative (rel.) motion. It was demonstrated recently for ultracold atoms [11, 12] that the c.m.-rel. coupling allows for a controlled transfer of two atoms into a bound molecular state. This phenomenon is denoted as inelastic confinement-induced resonance (ICIR) [13].

In the present work the appearance of resonances due to c.m.-rel. coupling and thus ICIRs for a two-body system of Coulomb-interacting particles is investigated. The occurrence of ICIR is demonstrated, thus further demonstrating their universality. It is also shown that the absence of a well-defined last bound state as is the case for ultracold atoms leads to modifications reflecting the influence of the long-range Coulomb interaction.

In fact, ICIRs occur both for attractive interactions (excitons) and for repulsive interactions (electron pairs). For electron pairs it is demonstrated that the com.-rel. coupling does not cause a significant change in the mean interparticle distance but nevertheless such a coupling can result in instabilities and modifications of the charge distribution. In the case of excitons, a variation of the QD geometry allows, however, for a substantial modification of the mean distance between the electron and the hole. It is demonstrated that an adiabatic transition from an unbound electron-hole pair to a more tightly bound state seems experimentally feasible in an exciton system. Since a reduced mean distance changes the recombination rate [14], ICIR are expected to deliver a novel kind of deterministic single-photon sources. Excitons in electrostatic traps might be especially suitable for this purpose, since they can be manipulated in situ.

The paper is organized in the following way. In Sec. II, the mechanism of ICIR is introduced briefly for ultracold atoms. In Sec. III the full two-body energy spectrum of a confined Coulomb system and the computational approach are introduced. Sec. IV describes the model for the QD confinement. The results are presented in Sec. V. This includes the discussion of the energy spectra in Sec. VA, the analysis of the coupling strength in Sec. VB and the consequences of a variation of the confinement in Sec. VC. Finally, the paper closes with a conclusion and outlook (Sec. VI).

II. INELASTIC CONFINEMENT-INDUCED RESONANCES

Recently, ICIR were discovered in the context of trapped ultracold atoms. Large losses of the trapped atoms for a given interatomic interaction strength (tuned with the aid of magnetic Feshbach resonances) were observed in [15] and explained by the occurrence of an ICIR in [11]. In a dedicated experiment [12] the occurrence of the ICIR was then more directly confirmed.

The interatomic interaction in the ultracold regime is well described by the Fermi-Huang δ pseudopotential

\[ U_\delta(r) = \frac{4\pi\hbar^2a}{m} \delta(r) \frac{\partial}{\partial r} r \]  

(1)

where \( m \) is the atomic mass and \( a \) the s-wave scattering length describing the collision in the limit of vanish-
ing collision energy (temperature). Thus the interparticle interaction strength is fully characterized by the single parameter $a$. Experimentally, it is possible to vary this parameter to almost arbitrary values using magnetic Feshbach resonances [16]. The spectrum of two ultracold atoms confined in a harmonic trapping potential that interact via the $\delta$ pseudopotential is analytically solvable [17, 18] and is shown in Fig. 1 for the example of an isotropic harmonic potential and for a variation of the inverse scattering length $d_{ho}/a$ where $d_{ho} = \sqrt{\hbar/(\mu \omega)}$ is the harmonic-oscillator length with the harmonic-oscillator frequency $\omega$ and the reduced mass $\mu = m_1 m_2/(m_1 + m_2)$ of the two particles with masses $m_1$ and $m_2$ respectively. The reduced mass is equal to $m/2$ for the here considered case of atoms with equal masses.

A characteristic feature of the rel. motion spectrum is the occurrence of a shallow molecular bound state for positive values of the $s$-wave scattering length $a$ (the state bending down to negative infinity in the rel. motion spectrum in Fig. 1). If no c.m.-rel. coupling is present, as is the case for a harmonic confinement, the energy spectrum of the full two-body system is obtained by adding the energies of the rel. and c.m. motion, respectively. As a consequence, molecular bound states with c.m. excitation cross with states of unbound atom pairs denoted as trap states, i.e. states above $1.5 \hbar \omega$ in the rel. motion plot. In case of a vanishing c.m.-rel. coupling ($W = 0$) the states cross diabatically as indicated by the black dashed lines in Fig. 2 and is visible in the inset in Fig. 1 for $W = 0$.

A coupling $W \neq 0$, e.g. induced by an anharmonic trap, leads to an avoided crossing and thus allows for an adiabatic transition (red solid line in Fig. 2) of the trap state into a molecular state. This transfer into the bound state and thus a two-body recombination is only possible, because the excess binding energy can be transferred into c.m. excitation energy due to the anharmonicity of the external confining potential. This redistribution of binding energy and kinetic energy is an inelastic process and thus these c.m.-rel. coupling resonances are denoted as \textit{inelastic confinement-induced resonances} [13]. It was demonstrated in [12] that the adiabatic transfer into the molecular bound state and the resulting reduction of the interparticle distance by one order of magnitude can be
performed fully coherently and controlled by tuning the scattering length using a magnetic Feshbach resonance.

An alternative way to reach the resonance is to vary $d_{\text{B}}$, i.e. the geometry of the external confinement which is feasible in Coulomb systems, e.g., for excitons in electrostatic traps. In contrast to atomic systems, where in the rel. motion spectrum of the $\delta$ pseudopotential only a single bound state exists, attractively interacting Coulomb systems like, e.g., excitons consisting of an electron and a hole, possess an infinite number of bound states that have the character of the ones of a hydrogen atom, i.e., they show a Rydberg series in free space approaching the continuum threshold. Inserting an exciton in a trap potential breaks the Rydberg series and leads to a smooth transition of bound to trap states. Hence the clear distinction of bound and trap states as it is present for the case of ultracold atoms is not possible. For repulsively interacting Coulomb systems, e.g., an electron-electron pair, there are no bound states present at all. A discretization is only induced by the trap potential. Thus, the different structure of the spectra of QDs provokes the natural question whether ICIR occur in a QD and if an analog to the molecule formation in the atomic system can be observed.

**III. COMPUTATIONAL APPROACH FOR THE ENERGY SPECTRUM OF THE COULOMB SYSTEM**

A system of two interacting particles with the absolute coordinates $r_1$ and $r_2$ is described by the Hamiltonian

$$H(r_1, r_2) = T_1(r_1) + T_2(r_2) + V_1(r_1) + V_2(r_2) + U(|r_1 - r_2|),$$

(2)

where $T_1$, $T_2$, $V_1$, and $V_2$ denote the kinetic and potential energies of the particles, respectively. The latter two represent the confinement of the QD. $U$ denotes the interparticle interaction. Since the Coulomb interaction

$$U_{\text{Coul}}(r) = \pm \frac{\epsilon^2}{4\pi\epsilon_0 |r_1 - r_2|},$$

(3)

with $\epsilon_\text{r}$ as the dielectric constant depends solely on the interparticle distance, the Hamiltonian is expressed in rel. and c.m. coordinates, $r = r_1 - r_2$ and $R = \frac{1}{2}(r_1 + r_2)$, respectively,

$$H(r, R) = H_{\text{rel}}(r) + H_{\text{cm}}(R) + W(r, R)$$

(4)

$$H_{\text{rel}}(r) = T_{\text{rel}}(r) + V_{\text{rel}}(r) + U_{\text{Coul}}(r)$$

(5)

$$H_{\text{cm}}(R) = T_{\text{cm}}(R) + V_{\text{cm}}(R).$$

(6)

Here, the potentials $V_{\text{rel}}(r)$ and $V_{\text{cm}}(R)$ represent the separable parts of the external potential, whereas the coupling term $W(r, R)$ includes all non-separable parts. Thus the Hamiltonians $H_{\text{rel}}$ and $H_{\text{cm}}$ correspond effectively to single-particle systems and will occasionally be denoted in the following as single-particle Hamiltonians.

For particles with identical mass confined to a harmonic potential the coupling term $W(r, R)$ vanishes and the Hamiltonian is composed of the rel. and c.m. motion of the two decoupled single-particle Hamiltonians, respectively. While the solution of the c.m. motion is well-known for a harmonic confinement, due to the long-range behavior of the Coulomb interaction the rel. motion possesses only exact analytic solutions for certain energy levels using particular values of confinement and interaction strength [10, 19, 20].

In this work, the eigenenergies and wave functions of the stationary Schrödinger equation with the Hamiltonian $H$

$$H |\Psi_i\rangle = E_i |\Psi_i\rangle,$$

(7)

are calculated using an exact diagonalization approach [21, 22]. Herein, the solutions of c.m. and rel. motion, i.e. the decoupled parts of $H$, with their respective wave functions $\psi(R)$ and $\phi(r)$ are calculated separately. These wave functions are expanded in B splines for the radial part and spherical harmonics for the angular parts. The product states $\Psi_{\mu}(R, r) = \psi_{\mu}(R) \phi_{\kappa}(r)$ form the basis of the solution of the full Hamiltonian. Thus, the full six-dimensional wave functions of the two-particle system

$$\Psi_i(R, r) = \sum_{\kappa} C_{i,\kappa} \Phi_{\kappa}(R, r)$$

(8)

are constructed as superpositions of the $\Phi_{\kappa}$. In order treat computationally efficiently not only single wells (isolated quantum dots or ultracold atoms in a single-well potential), but also quantum-dot molecules or ultracold atoms in optical lattices, the basis functions are symmetry adapted to the eight irreducible representations of the orthorhombic point group $D_{2h}$ ($A_g, B_{1g}, B_{2g}, B_{3g}, A_u, B_{1u}, B_{2u}, B_{3u}$). This leads to a corresponding block structure of the Hamiltonian matrix.

For locating ICIRs, a distinction of the different kinds of bound states for the Coulomb system is necessary. Similarly to the atomic system the mean interparticle distance $\tau$ can be chosen as a measure of the binding strength for the attractively interacting electron-hole system. Thus, in order to characterize the Coulomb states, the mean radial distance

$$\tau = \int_0^\infty dr \ r \rho(r)$$

(9)

is considered where

$$\rho(r) = r^2 \int dV_R \ d\Omega_r |\Psi(r, R)|^2$$

(10)

is the radial pair density. The $dV_R$ denotes the c.m. volume element and $d\Omega_r$ the angular volume element of the rel. motion. A state is regarded as a bound state, if $\tau$ is of the same order of magnitude as the effective Bohr radius $a_B$, where $m_0$ is the rest mass of an electron and $a_B$ the Bohr radius. If $\tau$ is significantly larger...
than $a_{\mu}$, one can consider this state as weakly bound and its behavior is expected to be dominantly determined by the external trap potential.

As introduction into the energy spectrum of Coulomb systems, two Coulomb-interacting particles of equal mass within the harmonic potential

$$V_{i}(r_{i}) = \sum_{j=x,y,z} V_{j} k_{j}^{2} j^{2}$$

are considered. With the aid of the parameters $V_{j}$ and $k$ the potential depth and the size of the QDs are adjusted to the desired QD confinement. A characteristic length scale of the potential is given by the harmonic-oscillator length $d_{j} = \sqrt{\hbar/(\mu \omega_{j})}$ defined for each spatial direction $j = x, y, z$ with the harmonic-oscillator frequency $\omega_{j} = (V/\mu)^{1/2} k_{j}$ along direction $j$. For an isotropic harmonic confinement for which $V = V_{j}$ and $k = k_{j}$ and thus $d_{\text{ho}} = d_{j}$ and $\omega = \omega_{j}$ applies, the energy spectrum of the two-Coulomb-interacting particles is shown in Fig. 3.

Only wave functions of the total-symmetric irreducible representation $a_{g}$ of the decoupled single-particle spectra, shown in Fig. (a) and (b), are adopted when constructing the energy spectrum of the full six-dimensional two-particle system in Fig. (c). In Fig. (d) the complete two-particle energy spectrum of $A_{g}$ symmetry is constructed by using the single-particle wave functions of all symmetries. The orthorhombic $D_{2h}$ symmetry is only a subgroup of the proper symmetry group of the here considered spherical-symmetrical problem that results from the isotropic harmonic trap and isotropic interparticle interaction. The orthorhombic group is chosen since in this work mainly anisotropic systems are considered and, as discussed earlier, the code allows for the treatment of generically orthorhombic problems like atoms in optical lattices or quantum-dot arrays.

The parameter $\sigma = d/a_{\mu}$ can be positive or negative depending on whether the Coulomb interaction is attractive or repulsive, representing an exciton system (negative $\sigma$) or an electron pair (positive $\sigma$), respectively. The value of $\sigma$ depends on $\epsilon_{r}$ included in $a_{\mu}$. A change in $\epsilon_{r}$ can considered as a screening effect. A variation of the interaction strength is a result of the modified properties of the environment, such as a modified charge density in the QD. However, a complete screening caused by $\epsilon_{r}$, which suppresses the long-range behavior of the Coulomb potential, is usually not obtained in semiconductors.

The c.m. spectrum in Fig. 3(a) reveals the well-known simple harmonic-oscillator solution

$$E_{\text{ho}} = (2n + l + \frac{3}{2}) \hbar \omega$$

where the quantum numbers $n$ and $l$ are restricted to $0 \leq n, l$ (with only even numbers in $a_{g}$ symmetry). The energy levels are not influenced by a change of the interaction strength. The relative-motion spectrum shown in Fig. 3(b) varies with the interaction strength. At $\sigma = 0$, the Coulomb interaction is zero and the harmonic oscillator energies are revealed. For the even $a_{g}$ symmetry, the ground state with $(n, l) = (0, 0)$ appears. The next energy level at $\sigma = 0$ comprises the states with quantum number $(n, l)$ equal to $(1, 0)$ and $(0, 2)$, and thus, it is fourfold degenerate. The degeneracy comes from the quantum number $m$ of the spherical harmonics with $-l \leq m \leq l$, but only even values occur due to the considered $a_{g}$ symmetry. A ninefold degenerate state with $(n, l)$ corresponding to $(2, 0),(1, 2)$ and $(0, 4)$ follows, etc. For positive values of $\sigma$ the repulsive Coulomb interaction pushes the energy levels to higher values until they pass the continuum limit. For the attractive Coulomb interaction, i.e. $\sigma < 0$, the states bend down in energy.

Figure 3. (Color online) Eigenenergy spectra for an exciton ($\sigma < 0$) or an electron pair ($\sigma > 0$) with $m_{e,h} = 0.067 m_{0}$ confined in a harmonic potential with the dimensions $(d_{x}, d_{y}, d_{z}) = (31.6, 31.6, 31.6)$ nm. The parameter $\sigma$ is modified by a change in $\epsilon_{r}$ contained in $a_{\mu}$. In (a) and (b) the $a_{g}$ energy spectra of the rel. and c.m. motion, respectively, are shown. The $A_{g}$ energy spectrum of the full Hamiltonian (4) for $W = 0$ is shown when adapting only single-particle wave functions of $a_{g}$ symmetry (c) or single-particle wave functions of all symmetries of the $D_{2h}$ group (d).
Thereby the states with \( l = 0 \) react more sensitively than higher \( l > 0 \) states because of the presence of the centrifugal barrier for \( l > 0 \). This leads to the occurrence of unavowed (real) crossings of states with different values of \( l \). In the limit in which the trap depth approaches zero, the attractive Coulomb interaction reproduces the Rydberg series again.

The \( A_g \) energy spectrum of the full Hamiltonian \( \hat{H} \), shown in Fig. \( 3 \text{(c)} \), is only composed of \( a_g \) rel. and c.m. states. Since the c.m.-rel. coupling vanishes for this system, the spectrum is obtained by adding the two single-particle spectra of the c.m. and rel. motion. If all symmetries of \( D_{2h} \) from the rel. and c.m. motion are used for the construction of the full energy spectrum, as shown in Fig. \( 3 \text{(d)} \), some additional states appear that are (approximately) built from single-particles states of the same symmetry, e.g., \( b_{1g} \otimes b_{1g} = A_g \). The lowest energy levels still belong to the rel. and c.m. states in \( a_g \) symmetry as the comparison with the spectrum in Fig. \( 3 \text{(c)} \) shows.

The \( A_g \) symmetry is chosen, since it contains the ground state. If the coupling term \( W(\mathbf{r}, \mathbf{R}) \) does not vanish, all symmetries should be included in the full energy-spectrum calculations since they contribute to the composition of the full wave function \( \Psi_j(\mathbf{r}, \mathbf{R}) \).

### IV. C.M.-REL. COUPLING

In order to simulate a more realistic single-well confinement of a QD, the sextic potential \( 21 \)

\[
V(\mathbf{r}) = \sum_{j=x,y,z} V_j \left( k_j^2 J_j^2 \frac{1}{3} k_j^4 J_j^4 + \frac{2}{45} k_j^6 J_j^6 \right)
\]

is chosen. This single-well potential introduces the required anharmonicity for c.m.-rel. coupling. In fact, the anharmonicity of this sextic potential is relatively weak and thus the results discussed in this work are expected to be a rather conservative estimate for the strength of the coupling between c.m. and rel. motion as occurring in many real quantum dots, especially those that are more appropriately modeled by a square-well potential. Since in the numerical approach the sextic potential is obtained by an expansion of a \( \sin^2 \) potential up to the sixth order, a parameter for the strength of the anharmonicity is the ratio \( V_j/(\hbar \omega_{ij}) \). The deeper the potential, i.e. the larger \( V_j/(\hbar \omega_{ij}) \gg 1 \), the smaller the c.m.-rel. coupling (for fixed masses of the particles).

Due to the anharmonicity of the confinement, the coupling term \( W(\mathbf{r}, \mathbf{R}) \) in \( 21 \) does not vanish and is composed of non-separable parts of the form \( r_{ij}^n R_{ij}^m \) with \( n, m \in \mathbb{N}_0 \). If the two particles have equal effective masses, such as the electron pair, the non-separable part consists of a polynomial with even values of \( n \) and \( m \), i.e. \( r_j^2 R_j^2, r_j^2 R_j^4 \) and \( r_j^4 R_j^2 \). In the case of an exciton, where usually the electron and the hole have different effective masses, odd values of \( n \) and \( m \) also appear in \( W(\mathbf{r}, \mathbf{R}) \), i.e. \( r_j R_j, r_j R_j^3, r_j^3 R_j, r_j R_j^3, r_j R_j^3, r_j R_j^3, r_j^3 R_j, \) and \( r_j^3 R_j \).

The matrix element

\[
W_{\alpha,\beta} = \langle \Psi^{(\alpha)}(\mathbf{r}, \mathbf{R}) | W(\mathbf{r}, \mathbf{R}) | \Psi^{(\beta)}(\mathbf{r}, \mathbf{R}) \rangle
\]

defines the coupling strength between the states \( \Psi^{(\alpha)} \) and \( \Psi^{(\beta)} \). In order to examine the states involved in a coupling at the resonance position, their wave function densities are explored.

### V. RESULTS

In order to obtain ICIRs comparable with those in atomic systems \( 11 \ 12 \), a strong anisotropic QD confinement is favored. In this work, inspired by the work on atomic systems, a cigar-shaped potential is chosen. In this case the longitudinal and transversal excitations experience different trap strengths and thus have distinct extensions in the spatial directions providing a significant difference in the mean distance for a transition between different excitations of them. Since a very large anisotropy is numerically challenging for the adopted computational approach, the longitudinal size, i.e., the size in \( z \) direction, is only chosen up to \( \sqrt{10} \)-times larger than the transversal sizes. Such cigar-shaped potentials are encountered in quantum dashes \( 24 \), nanorods \( 25 \), and in the quasi 1D regime also known as quantum wires \( 26 \).

All energy spectra are calculated for the \( A_g \) symmetry and taken into account single-particle wave functions of all symmetries. In the case of excitons the particles usually possess different masses and are anyhow distinguishable. In the case of an electron pair the particles are indistinguishable Fermions. Therefore, states with \( A_g \) symmetry in the spatial part correspond to spin-singlet states in the case of electron pairs.

#### A. Variation of the interaction strength

In most cases, the effective mass of an electron is much smaller than the effective mass of the hole. However, first an electron and a hole in a sextic potential are considered where the hole mass is assumed to be equal to the effective electron mass, \( m_h = m_e = 0.067 m_0 \). Here, the c.m.-rel. coupling effects can only be caused by the anharmonicity of the confinement, and thus, a clear distinction from other effects is possible.

The fully coupled energy spectrum with variation of the Coulomb interaction strength is shown in Fig. \( 4 \text{(a)} \). An avoided crossing can be identified in the framed box and is shown magnified in Fig. \( 4 \text{(b)} \). This avoided crossing, here labeled with \( \vartheta \), with a full width at half maximum (FWHM) \( \approx 0.018 \) has the position \( \vartheta_\perp/a_\mu \approx -1.78 \) with \( a_\mu \approx 17.5 \) nm.

The cuts through the wave-function density of the coupled states shown in Fig. \( 4 \text{(c)} \) and \( 4 \text{(d)} \) demonstrate a clear redistribution of the c.m. and rel. excitations. For
Figure 4. (Color online) The $A_\theta$ eigenenergy spectrum of the Hamiltonian (1) for an exciton with $m_b = m_e = 0.067m_0$ confined in a sextic potential with the dimensions $(d_x, d_y, d_z) = (100, 31.6, 31.6)$ nm is shown in (a), and the avoided crossing between coupled states, labeled with $\theta$, is magnified in (b). Cuts through the wave-function density $|\Psi(x_e, y_e, z_e, x_h, y_h, z_h)|^2$ of the coupled states along the $x$ direction in absolute coordinates, $x_h$ and $x_e$ ($y_e, h = z_e, h = 0$), in (c) and along the transversal $z$ direction in the absolute coordinates, $z_h$ and $z_e$ ($x_e, h = y_e, h = 0$), in (d) confirm the c.m.-rel. coupling.

Figure 5. In which two avoided crossings are marked. Here, a larger modification of the mean distance could be achieved. However, couplings between highly excited state and higher longitudinal rel. excited states occur. The interesting feature of $\theta$ corresponds thus to the ICIR found for atomic systems.

Further ICIRs between the transverse c.m. excited state and higher longitudinal rel. excited states occur. Here, a larger modification of the mean distance could be achieved. However, couplings between highly excited states are much weaker or even negligible due to the much smaller value of the integral in (14) that expresses the coupling strength.

In the following, the particle-mass values are adjusted to realistic material properties of GaAs [27]. The system of an electron and a hole with the mass $m_b = 10m_e = 0.67m_0$ is investigated. Its energy spectrum is shown in Fig. 5 in which two avoided crossings are marked.

The green dashed-framed avoided crossing presented in detail in Fig. 6 is labeled with $\lambda_0$ and has a FWHM $\approx 0.059$ at position $d_2/a_\mu = -0.90$, where $a_\mu \approx 34.5$ nm. Here, the weakly bound state with a mean distance of $\tau \approx 80$ nm couples to a bound state with $\tau \approx 24$ nm. A similar significant change in mean distance is found for the orange-framed avoided crossing labeled with $\lambda_0$ and shown in detail in Fig. 7. This crossing has a FWHM $\approx 0.006$ and is located at $d_2/a_\mu = -1.05$ with $a_\mu \approx 30$ nm. Here, the same bound state as involved in $\lambda_0$ goes over into a weak bound state with $\tau \approx 65$ nm. The interesting feature of $\lambda_0$ is the zero probability of the event that the two particles are located at the same place, i.e. the node at zero. Hence, the recombination is blocked in the weakly bound state. An adiabatic transition into this kind of states could have significant influence on photon emission. However, taking into account the coupling strength, which is discussed in more detail.
in Sec. VB the avoided crossing $\lambda_O$ is more difficult to be realized than the first avoided crossing $\lambda_G$.

In general, the coupled states at both avoided crossings of Fig. 5 are very different from the states of the system with equal-mass particles. The coupling terms that now contain also odd powers of $r$ and $R$ do not only cause avoided crossings between states, but also lead to a general change of the shape of the wave functions. Thus, a mapping of the states to comparable product states of the c.m. and rel. motion appears not to be straightforward.

Looking at unequal-mass particles in a harmonic confinement, avoided crossings can appear due to the non-vanishing coupling term $r_j R_j$. The coupling term again strongly influences the shape of the states. Here, only avoided crossings similar to $\lambda_O$ can appear.

In addition to the electron-hole system discussed above, the electron pair in a sextic potential is considered. The energy spectrum shown in Fig. 6(a) reveals avoided crossings. Due to the repulsive Coulomb interaction and the confinement the states change only slightly in the interaction strength. Hence, only coupling between states with different longitudinal excitations is observed. One of these avoided crossings is labeled with $\xi$ and magnified in Fig. 6(b). Here, no significant change in the mean interparticle distance occurs. The first transversally excited states cross only with very highly lying longitudinal excited states where due to the oscillatory behavior the coupling term becomes vanishing small. For electrons in a stronger confinement a crossing between transversally excited and low longitudinally excited states may, however, be realized. Therefore, considering a QD array a transversal coupling to another QD due to the tunnel effect is feasible. Consider the situation of a longitudinal state that is well localized in a single QD and thus tunneling to a transversally coupled QD is suppressed, since there is practically no electron density close to the tunnel barrier. If this state is adiabatically transferred to the transversally excited state, this state has a non-zero tunnel probability to the transversally coupled neighbor QD. Evidently, an in-situ transfer form one state to the other may then be used as a switch that induces a charge migration from one QD to another one.

B. Analysis of the coupling strengths

To discuss and compare the time-dependent behavior at the avoided crossings, the Landau-Zener theory [28–30] is used. The probability of an adiabatic transition at the avoided crossing can be estimated depending on the
Landau-Zener velocity, i.e., the change in parameter $\sigma$ per time $d\sigma/dt = v_{LZ}$. After calculating the linear functions for the involved diabatic states and the coupling between them, the upper bound of $v_{LZ}$ can be estimated at which the adiabatic transition is more likely than the diabatic transition.

Applying the Landau-Zener theory to the avoided crossing $\vartheta$ of the electron-hole system with equal-mass particles in Fig. 4, the velocity $v_{LZ,\vartheta} \approx 0.9$ GHz is found as upper bound for an adiabatic transition. Regarding the required change in $\sigma$ for passing this avoided crossing, $d\sigma \approx 0.1$, the transition has to be performed within $dt_{\vartheta} \gtrapprox 0.11$ ns. This transition time is in the window of the exciton lifetime which is of the order of $\tau \approx 1$ ns in GaAs [31,33]. This result indicates the potential impact of an ICIRs in QDs.

Considering the avoided crossings of the electron-hole system with $m_h = 10 m_e$ in Fig. [5] the upper bounds $v_{LZ,\lambda_0} \approx 2.9$ GHz for avoided crossing $\lambda_0$ and $v_{LZ,\lambda_0} \approx 34$ MHz for avoided crossing $\lambda_0$ are obtained. Since $v_{LZ,\lambda_0}$ is larger than $v_{LZ,\vartheta}$, different mass values of the particles enhance the coupling strength and an adiabatic transition is dominant even for shorter time scales. Here, the transition time $dt_{\lambda_0} \gtrapprox 0.01$ ns with a required change $d\sigma \approx 0.15$ is obtained. Contrary, observation of the avoided crossing of type $\lambda_0$ is expected to be difficult due to the two orders of magnitude smaller value of $v_{LZ,\lambda_0}$ in comparison to $v_{LZ,\lambda_0}$. It has only the transition time $dt_{\lambda_0} \gtrapprox 0.9$ ns with the change $d\sigma_{\lambda_0} \approx 0.3$.

For the avoided crossing $\xi$ of the electron pair from Fig. [5] the velocity $v_{LZ,\xi} = 0.15$ GHz is obtained. This velocity is considerably higher for transitions between two longitudinally excited states of the electron pair. Here, a change $d\sigma_{\lambda_0} \approx 0.02$ with the transition time $dt_{\xi} \gtrapprox 0.13$ ns has to be achieved.

In general, the observation of an ICIR in experiments strongly depends on the good resolution of the parameter $\sigma$. For this purpose, the uncertainty of the dielec-

Figure 7. (Color online) The avoided crossing $\lambda_0$ orange-framed in Fig. [3] magnified in (a). Cuts through the wave-function density $|\Psi(x_e, y_e, z_e, x_h, y_h, z_h)|^2$ of the coupled states are shown along the absolute $x$ coordinates, $x_h$ and $x_e$ ($y_e, h = z_e, h = 0$), in (b) and along the absolute $z$ coordinates, $z_h$ and $z_e$ ($x_e, y_e, h = 0$), in (c). The c.m.-rel. resonance causes a transition of a state with zero probability for $d_e, h = 0$ and a bound state.

Figure 8. (Color online) The $A_\varphi$ eigenenergy spectrum of the Hamiltonian (1) for an electron pair with $m_{e,1} = m_{e,2} = 0.067 m_0$ confined in a sextic potential with the dimensions $(d_x, d_y, d_z) = (100, 31.6, 31.6)$ nm is shown in (a), and the avoided crossing between coupled states, label with $\xi$, is magnified in (b). Even for a repulsive Coulomb interaction the c.m.-rel. coupling causes avoided crossings.
tric constant\cite{34}, of the effective mass, and of the trap confinement must be kept low. As mentioned earlier, it should on the other hand also be reminded that the sextic potential chosen in the present simulations is only weakly anharmonic. Trap potentials with higher degree of anharmonicity like square-well potentials are expected to provide stronger couplings and thus broader avoided crossings.

C. Variation of the confinement

The variation of the dielectric constant in a QD to change the Coulomb interaction strength between the particles is experimentally a complicated task. A more suitable parameter for modification is the confinement of the QD. In electrostatic QDs, a modification of the confinement is possible by a variation of the applied voltage\cite{35}. The intrinsic problem arising in connection with electrostatic traps is the exciton dissociation by applying an electric field. However, various studies report electrostatic traps for indirect excitons in coupled QDs\cite{36–39}. Also for QDs fabricated by chemical and growth processes the size can be varied in a controlled way\cite{40}. Hence, it is appropriate to investigate a confinement variation for the electron-hole system.

In Fig. 9 the confinement is varied from an isotropic to a cigar-shaped potential with \( x \) being the longitudinal direction. The parameter \( \eta = \omega _L / \omega _x \) indicates the anisotropy. The energy levels bend down towards lower values the more anisotropic the confinement becomes. An avoided crossing labeled with \( \kappa \) can clearly be located at \( \eta \approx 2.2 \) and has a FWHM \( \approx 0.120 \). Here, a bound state with a small anisotropy of \( \eta = 1.9 \) and a mean distance \( \tau \approx 18 \text{ nm} \) couples to a weaker bound state with \( \tau \approx 45 \text{ nm} \) at \( \eta \approx 2.4 \text{ nm} \). The densities (Fig. 9(c) and (d)) of the avoided crossing \( \kappa \) reveal the redistribution of c.m. and rel. excitations, the typical characteristic of an ICIR. The change in mean distance is not as significant as in the case of the variation of the Coulomb interaction in Fig. 9 since the anisotropy at the ICIR is smaller. However, the position of the resonance may be tuned by varying the confinement strength in the transversal directions and thus leading to other changes in mean distance. Moreover, for a system of particles with different masses a resonance with zero probability for \( d_{e,h} = 0 \) similar to the ICIR \( A_0 \) can occur.

Using the Landau-Zener theory, the upper bound \( v_{L,2,e,h} \approx 0.8 \text{ GHz} \) for avoided crossing \( \kappa \) is found. This Landau-Zener velocity is similar to \( v_{L,2,e,h} \) obtained from the variation of the Coulomb interaction. With the change \( \Delta m \approx 0.5 \) in the confinement variation, the transition time \( \Delta t \approx 0.63 \text{ ns} \) is found which is still smaller than the usual exciton lifetimes\cite{31–33}. This feature makes ICIRs induced by a confinement variation accessible to an observation in experiments.

Figure 9. (Color online) The \( A_0 \) eigenenergy spectrum of the Hamiltonian\cite{4} for an exciton with \( m_h = m_e = 0.067 m_0 \) confined in a sextic potential with the transversal dimensions \( d_{y,z} = 31.6 \text{ nm} \) and dielectric constant \( \epsilon_r = 13.15 \) giving a \( d_{L} / a_m \approx -1.52 \) is shown (a), and an avoided crossing between coupled states, labeled with \( \kappa \), is magnified in (b). Cuts through the density \( |\Psi (x_e, y_e, z_e, x_h, y_h, z_h)|^2 \) of the coupled states along the \( x \) direction in absolute coordinates, \( x_h \) and \( x_e \) (\( y_{e,h} = 0 \), in (c) and along the transversal \( z \) direction in the absolute coordinates, \( z_h \) and \( z_e \) (\( x_{e,h} = 0 \), in (d) are shown.
VI. CONCLUSION AND OUTLOOK

It is demonstrated that inelastic confinement-induced resonances, first described for trapped ultracold atoms [13] [14], occur in the electron-hole Coulomb systems confined in a QD. Furthermore, the c.m.-rel. coupling leads also to other types of avoided crossings as, e.g., in electron-electron systems. In order to investigate a realistic QD, its confinement is approximated by an anharmonic and anisotropic potential. For the electron-hole system, the ICIR causes a significant change in the interparticle distance, and thus can lead to a significant influence on the recombination rate. The change in distance grows with the anisotropy of the confinement, since couplings between weakly bound longitudinally excited states and bound transversally excited states become possible. Thereby, the anharmonicity of the confinement induces the c.m.-rel. coupling. Hence, the coupling strength can be controlled by the confinement geometry. Furthermore, looking at realistic exciton lifetimes a transition between states at an ICIR appears to be in an experimentally feasible time window.

An interesting application of the ICIR in Coulomb systems studied in the present work could be a novel kind of single-photon sources on demand based on excitons. In the case of excitons in self-organized QD the in situ variation of the confinement, i.e. the change of the trap potential on a timescale shorter than the exciton lifetime, is usually impossible. However, the realization of excitons in electrostatic traps [37] [39] or laser-induced traps [11] overcomes this limitation and thus allows for real-time reduction of the relative mean distance between electron and hole at an ICIR. The enhanced recombination probability leads then to a controlled photon emission. However, in order to stabilize the exciton against dissociation an additional electric field perpendicular to the plane of electrostatic confinement is usually adopted. The influence of this alignment of the exciton for the ICIR will be subject of a future study. In the case of more than one exciton, the alignment leads to a dipole-dipole interaction between the excitons [39]. Noteworthy, the occurrence of ICIR in cold dipolar gases has recently theoretically been demonstrated in [42]. For electrons in QD arrays the ICIR may on the other hand be used as a possible switch that allows to turn-on or -off the tunnel current to a neighbor QD.

Moreover, this work confirms the universal nature of ICIR as they are now proven to appear in the two very contrary systems of quantum dots and ultracold atoms.

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