

# LO-phonon-induced screening of electron–electron interaction in $D^-$ centres and quantum dots

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## Abstract

A problem of screening of electron–electron interaction by LO phonons is investigated for bound two-electron systems in bulk semiconductors and semiconductor quantum dots. We consider a  $D^-$  centre and a two-electron quantum dot and obtain the effective LO-phonon-induced interaction between the electrons, i.e.,  $V_{\text{eff}}(r_{12}) \sim e^2/[\epsilon_{\text{eff}}(r_{12})r_{12}]$ , where  $r_{12}$  is the interelectron distance and  $\epsilon_{\text{eff}}(r_{12})$  is the effective phonon dielectric function. The calculated phonon dielectric function rapidly increases for small  $r_{12}$  starting from the high-frequency dielectric constant,  $\epsilon_{\infty}$ , and reaches some constant value,  $\bar{\epsilon}$ , at relatively small interelectron distances. We have found that—in most cases— $\bar{\epsilon}$  is less than the static dielectric constant,  $\epsilon_s$ . Only in the weakly ionic compounds, like GaAs,  $\bar{\epsilon} \simeq \epsilon_s$ . We argue that—in the bound few-electron systems— $\bar{\epsilon}$  better approximates the average LO-phonon-induced screening than the commonly used  $\epsilon_s$ . We have also shown that the coupling with LO phonons leads to the increase of the binding energy of the two-electron system confined in the quantum dot.

## 1. Introduction

In solids, the interaction between conduction band electrons is screened by valence electrons and the crystal lattice. In compound semiconductors, the LO phonons play a dominant role in the lattice-induced screening of the electron–electron interaction. The electron–LO-phonon coupling modifies the properties of charge carriers leading to a formation of polarons [1]. In bulk ionic crystals, the two interacting, equally charged, polarons can form a bound system, called a bipolaron, if the electron–LO-phonon coupling is sufficiently strong [2–5]. The two negatively charged polarons bound on a positively charged donor impurity centre form a  $D^-$  centre [6], which exhibits a variety of properties [7] depending on material parameters of a

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semiconductor. The electron–LO-phonon coupling also modifies the properties of electrons confined in quantum dots (QDs) [8–11] and the  $D^-$  centre in the QDs [12]. The coupling of charge carriers (electrons and holes) with LO-phonons is responsible for the formation of everlasting resonant polarons, discovered in self-assembled QDs [13], ultrafast energy redistribution, observed [14] in femtosecond transmission spectra, and the long polaron lifetime measured in InAs/GaAs QDs [15].

A theory of QDs should include both the electronic and phononic components of the screening of the electron–electron interaction [16]. In electrostatic QDs [17], the electronic screening mainly results from the charges induced on the metal gates, which define the physical QD region. This effect is known as the screening of the electron–electron interaction by the gates [18]. The second effect is the phonon-induced screening. In a majority of papers, the phonon screening is taken into account in a static manner by introducing the static dielectric constant ( $\epsilon_s$ ) into the Coulomb interaction potential. When applying the static dielectric constant, we have to assume the maximal (static) crystal lattice distortion, which leads to a maximal screening of the interelectron interaction by  $\epsilon_s$ . The maximal screening results from the formation of the static lattice distortion around each electron, which requires some relaxation time. The static lattice distortion cannot entirely develop in electron transport processes, in which the electrons tunnel through the QD on a nanosecond timescale [19]. Therefore, for the description of the interaction of the tunnelling electron with the electrons confined in the QD, we have to consider the quantum dynamics of the electron–phonon system. The present paper is devoted to a study of the effective screening of the electron–electron interaction by the LO phonons. We focus on the LO phonons since they dominate in the lattice-induced screening in semiconducting compounds due to an ionic character of these materials. We will show that the LO phonons play an important role both in the strongly ionic I–VII compounds as well as in the weakly ionic III–V compounds.

The paper is organized as follows: in section 2 we present the theory, in section 3—the results, and section 4 contains the conclusions and the summary.

## 2. Theory

We consider a two-electron system localized in a solid due to a presence of a binding centre or a confining potential. Taking on the binding potential as the Coulomb potential of the positive donor centre, we deal with the  $D^-$  centre in a bulk crystal. Assuming the confining potential in a Gaussian form [20] we obtain a model of spherical QDs [21–23], i.e., nanocrystals fabricated by a colloidal chemical synthesis [21, 22]. In the present work, we are interested in an effect of the electron–LO-phonon coupling on the effective interaction between the electrons in the bound few-electron systems. We start with the Hamiltonian

$$H = H_{\text{el}} + H_{\text{ph}} + H_{\text{int}}, \quad (1)$$

where  $H_{\text{el}}$  is the Hamiltonian of the two-electron system in an absence of LO phonons,  $H_{\text{ph}}$  is the Hamiltonian of noninteracting LO phonons, and  $H_{\text{int}}$  is the electron–LO-phonon interaction Hamiltonian. In the effective mass approximation,

$$H_{\text{el}} = -\frac{\hbar^2}{2m_e}(\nabla_1^2 + \nabla_2^2) + V_{\text{conf}}(r_1) + V_{\text{conf}}(r_2) + \frac{\kappa e^2}{\epsilon_\infty r_{12}}, \quad (2)$$

where  $m_e$  is the electron conduction band mass,  $r_1$  and  $r_2$  are the electron–donor centre (electron–QD centre) distances,  $r_{12}$  is the electron–electron distance,  $\epsilon_\infty$  is the high-frequency dielectric constant, and  $\kappa = 1/(4\pi\epsilon_0)$ , where  $\epsilon_0$  is the electric permittivity of vacuum. For

the  $D^-$  centre

$$V_{\text{conf}}(r) = -\frac{\kappa e^2}{\epsilon_s r}. \quad (3)$$

Form (3) results from the Platzman transformation [24] of the initial Hamiltonian, in which all the Coulomb interactions are screened by the valence electrons only, i.e., by  $\epsilon_\infty$ . The Platzman transformation [24] leads to the screening of the electron–donor interaction by the static dielectric constant  $\epsilon_s$ , which has the following physical interpretation: the interaction of electrons with the infinitely heavy positive donor centre involves the static lattice distortion, i.e., is maximally screened by the lattice and the valence electrons. We expect that the screening of the interaction between the light electrons should be different.

When applying the present approach to spherical QDs, we assume the confining potential in the Gaussian form [20], i.e.,

$$V_{\text{conf}}(r) = -V_0 \exp[-(r/R)^2], \quad (4)$$

where  $V_0$  is the depth of the confinement potential and  $R$  is its range ( $R$  can be treated as a radius of the QD). The Gaussian potential (4) accounts for the finite depth and range of the QD confinement potential. The smoothly varying form given by equation (4) is a good approximation of the confinement potential in electrostatic QDs [17], in which the confinement results from an inhomogeneous electric field. In self-assembled QDs [25] with a composition modulation [26], the confinement potential can also be approximated by the Gaussian potential [27]. In the present paper, we assume that the electron conduction band mass, dielectric constants, and LO-phonon frequency are continuous across the QD boundary. In section 4, we discuss the applicability of these assumptions.

The Hamiltonian of the LO-phonon field has a form

$$H_{\text{ph}} = \hbar\omega_{\text{LO}} \sum_{\mathbf{k}} a_{\mathbf{k}}^\dagger a_{\mathbf{k}}, \quad (5)$$

where  $a_{\mathbf{k}}^\dagger$  ( $a_{\mathbf{k}}$ ) is the creation (annihilation) operator of the LO phonon with wavevector  $\mathbf{k}$  and energy  $\hbar\omega_{\text{LO}}$ . The Hamiltonian of the electron–LO-phonon interaction can be written down as follows:

$$H_{\text{int}} = \hbar\omega_{\text{LO}} \sum_{\mathbf{k}} \{v_{\mathbf{k}} a_{\mathbf{k}} [\exp(i\mathbf{k} \cdot \mathbf{r}_1) + \exp(i\mathbf{k} \cdot \mathbf{r}_2)] + \text{H.c.}\}, \quad (6)$$

where

$$v_{\mathbf{k}} = -\frac{i}{|\mathbf{k}|} \left[ \frac{2\pi e^2}{\Omega \hbar \omega_{\text{LO}}} \left( \frac{1}{\epsilon_\infty} - \frac{1}{\epsilon_s} \right) \right]^{1/2} \quad (7)$$

is the Fröhlich interaction amplitude and  $\Omega$  is the quantization volume.

In order to determine the screening effect of the LO phonons we solve the eigenvalue problem for the two-electron Hamiltonian (1) by the variational method. For the sake of completeness, below we present the main steps of the method proposed for the  $D^-$  centre [7]. This approach is also applicable to the two-electron systems in spherical QDs. We employ the variational trial state vector in the following form [7]:

$$|\Psi\rangle = \psi(\mathbf{r}_1, \mathbf{r}_2) U(\mathbf{r}_1, \mathbf{r}_2, \{a_{\mathbf{k}}^\dagger\}, \{a_{\mathbf{k}}\}) |0\rangle, \quad (8)$$

where  $\psi(\mathbf{r}_1, \mathbf{r}_2)$  is the wavefunction of the two-electron system and  $|0\rangle$  is the LO-phonon vacuum state vector. The unitary transformation  $U$  has been taken in the form [7]

$$U(\mathbf{r}_1, \mathbf{r}_2, \{a_{\mathbf{k}}^\dagger\}, \{a_{\mathbf{k}}\}) = \exp \left\{ \sum_{\mathbf{k}} [F_{\mathbf{k}}(\mathbf{r}_1, \mathbf{r}_2) a_{\mathbf{k}} - F_{\mathbf{k}}^*(\mathbf{r}_1, \mathbf{r}_2) a_{\mathbf{k}}^\dagger] \right\}, \quad (9)$$

where

$$F_{\mathbf{k}}(\mathbf{r}_1, \mathbf{r}_2) = v_{\mathbf{k}}\{f_{\mathbf{k}}^{(1)}[\exp(i\mathbf{k} \cdot \mathbf{r}_1) + \exp(i\mathbf{k} \cdot \mathbf{r}_2)] + f_{\mathbf{k}}^{(2)}\}. \quad (10)$$

Equation (10) contains the weak-coupling,  $f_{\mathbf{k}}^{(1)}$ , and the strong-coupling,  $f_{\mathbf{k}}^{(2)}$ , phonon amplitudes that have the forms [7]

$$f_{\mathbf{k}}^{(1)} = \frac{\lambda_1}{\varrho_1^2 a_p^2 \mathbf{k}^2 + 1} \quad (11)$$

and

$$f_{\mathbf{k}}^{(2)} = \frac{\lambda_2}{(\varrho_2^2 a_p^2 \mathbf{k}^2 + 1)^2}, \quad (12)$$

where  $a_p = (\hbar/2m_e\omega_{\text{LO}})^{1/2}$  is the polaron radius. Phonon amplitudes (11) and (12) include variational parameters  $\lambda_1$ ,  $\lambda_2$ ,  $\varrho_1$ , and  $\varrho_2$ , for which the following physical interpretation can be given: parameters  $\lambda_1$  and  $\lambda_2$  determine the contributions of the weak and strong electron–LO-phonon coupling to the variational solution (equation (8)), while  $\varrho_1$  and  $\varrho_2$  are responsible for the changes of radius of the interacting polarons in the weak- and strong-coupling limits, respectively. All these variational parameters are determined from the minimization of the expectation value of Hamiltonian (1). This minimization is considerably simplified if we introduce the effective Hamiltonian

$$H_{\text{eff}} = \langle 0|U^\dagger H U|0\rangle, \quad (13)$$

which takes on the form [7]

$$H_{\text{eff}} = -\frac{\hbar^2}{2m_e}(\nabla_1^2 + \nabla_2^2) + V_{\text{conf}}(r_1) + V_{\text{conf}}(r_2) + W(r_1) + W(r_2) + V_{\text{eff}}(r_{12}) + \Sigma, \quad (14)$$

where  $W(r_1)$  and  $W(r_2)$  are the phonon-mediated electron–donor (electron–QD) interactions and  $\Sigma$  is the self-energy of the electron–phonon system. Their explicit forms are given in [7].

In the present paper, we are interested in the effective electron–electron interaction, defined in equation (14) as  $V_{\text{eff}}(r_{12})$ , i.e., the term that explicitly depends on interelectron distance  $r_{12}$ . We neglect the indirect influence of the self-energy on the screening. This effective interaction can be written down as follows:

$$V_{\text{eff}}(r_{12}) = \frac{\kappa e^2}{\varepsilon_{\text{eff}}(r_{12})r_{12}}, \quad (15)$$

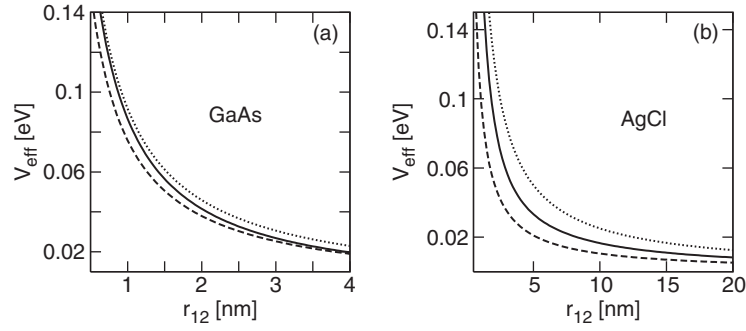
where  $\varepsilon_{\text{eff}}(r_{12})$  is the LO-phonon dielectric function of the form [7]

$$\varepsilon_{\text{eff}}^{-1}(r_{12}) = \frac{1}{\varepsilon_\infty} + \lambda_1 \left( \frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon_s} \right) \times \left\{ (\lambda_1 - 2)[1 - \exp(-r_{12}/\varrho_1 a_p)] - \frac{\lambda_1 r_{12}}{2\varrho_1 a_p} \exp(-r_{12}/\varrho_1 a_p) \right\}. \quad (16)$$

Equations (15) and (16) show that the effective electron–electron interaction also includes—besides the statically screened Coulomb interaction—the Yukawa and exponential interaction potentials.

Let us discuss the asymptotic properties of effective interaction (15). For  $r_{12} \rightarrow 0$ ,  $V_{\text{eff}}(r_{12}) \rightarrow \kappa e^2/(\varepsilon_\infty r_{12})$ , i.e., the LO-phonon screening becomes negligible and the electron–electron interaction is only screened by the valence electrons. In the bound systems, for  $r_{12} \gg a_p$ ,  $V_{\text{eff}}(r_{12}) \rightarrow \kappa e^2/(\bar{\varepsilon} r_{12})$ , where

$$\frac{1}{\bar{\varepsilon}} = \frac{1}{\varepsilon_\infty} - \lambda_1(2 - \lambda_1) \left( \frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon_s} \right). \quad (17)$$



**Figure 1.** Effective electron–electron interaction potential energy  $V_{\text{eff}}$  (solid line) as a function of interelectron distance  $r_{12}$  for the  $D^-$  centre in (a) GaAs and (b) AgCl. The Coulomb interaction energy screened by the static (broken line) and high-frequency (dotted line) dielectric constant is also shown for comparison.

If  $r_{12} \rightarrow \infty$ , we deal with the unbound system with the two free polarons, for which—in the weak electron–LO-phonon coupling regime—the variational parameters in equations (11) and (12) take on the following optimal values:  $\lambda_1 = \varrho_1 = 1$  and  $\lambda_2 = 0$ . In this case,  $\bar{\varepsilon} = \varepsilon_s$ , i.e., the electron–electron interaction is screened by the statically deformed lattice. For the bound systems we obtain  $\lambda_1 < 1$ , which leads to the inequality  $\bar{\varepsilon} < \varepsilon_s$ .

In order to obtain the effective LO-phonon-induced screening for the bound two-electron systems we have calculated the ground-state energy of the considered systems. This allows us to determine the optimum values of variational parameters  $\lambda_1$ ,  $\varrho_1$ ,  $\lambda_2$ , and  $\varrho_2$ , i.e., the optimized effective interaction (equations (15) and (16)). The ground-state energy has been calculated by solving the eigenproblem for the effective Hamiltonian (14) with the help of the electronic variational wavefunction [20]

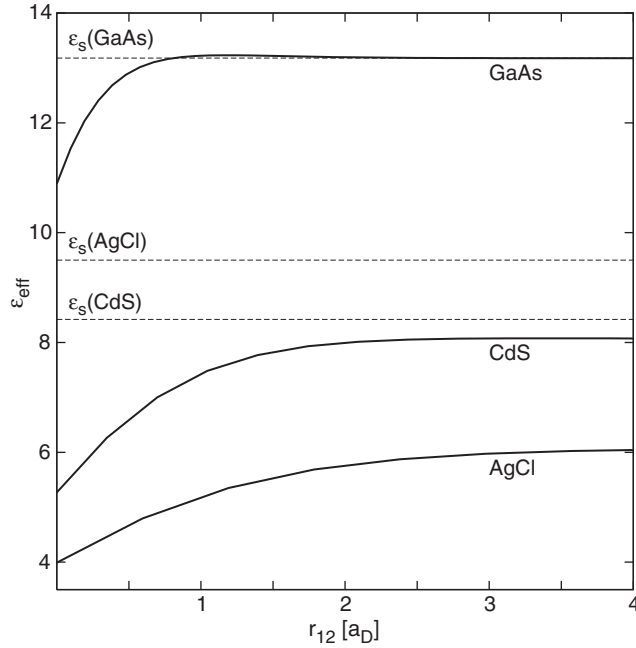
$$\psi(r_1, r_2, r_{12}) = \sum_{j=1}^N c_j (1 + P_{12}) \exp(-\alpha_j r_1^2 - \beta_j r_2^2 - \gamma_j r_{12}^2), \quad (18)$$

where  $c_j$  are the linear variational parameters and  $P_{12}$  is the permutation operator interchanging the indices 1 and 2. The nonlinear variational parameters in trial wavefunction (18) have been chosen as follows:  $\alpha_j = \alpha_1 q_\alpha^{j-1}$ ,  $\beta_j = \beta_1 q_\beta^{j-1}$ , i.e., as the geometric progressions, and  $\gamma_j = \gamma_1 + (\gamma_2 - \gamma_1) \text{frac}[\sqrt{3}j(j-1)/2]$ , i.e., as the quasi-random numbers, where  $\text{frac}(x)$  denotes the fractional part of  $x$ . Variational wavefunction (18) explicitly includes the electron–electron correlation via the  $r_{12}$ -dependent term. It contains the following independent variational parameters:  $\alpha_1$ ,  $\beta_1$ ,  $\gamma_1$ ,  $\gamma_2$ ,  $q_\alpha$ , and  $q_\beta$ . The ground-state energy has been calculated by minimizing the expectation value of  $H_{\text{eff}}$  over the variational parameters in the two-electron wavefunction (18) and phonon amplitudes (11) and (12). We have checked that the trial wavefunction (18) reproduces the results for  $D^-$  centres in bulk semiconductors, obtained previously [7] with the linear combination of correlated exponential functions.

### 3. Results

#### 3.1. $D^-$ centre

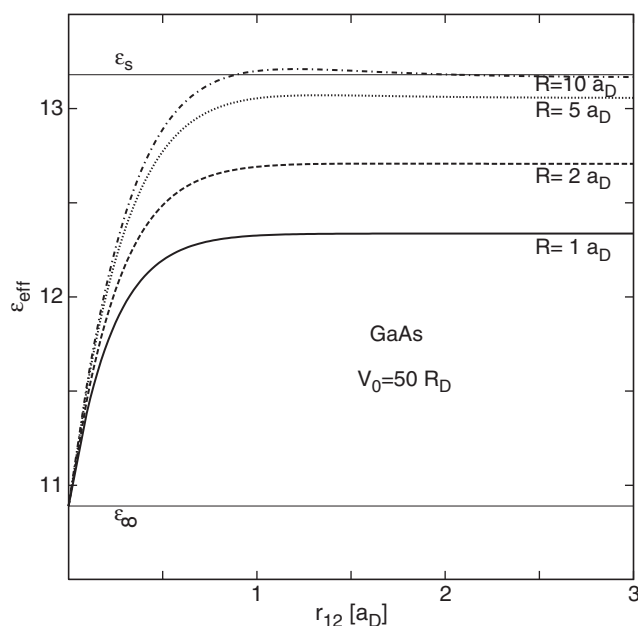
Figure 1 shows the LO-phonon screened effective interelectron interaction potential, defined by equation (15), for the  $D^-$  centre in the bulk GaAs and AgCl crystals. For all interelectron distances,  $V_{\text{eff}}(r_{12})$  is stronger than the Coulomb interaction potential, screened by the static



**Figure 2.** Effective phonon dielectric function  $\varepsilon_{\text{eff}}$  as a function of electron–electron distance  $r_{12}$  for the  $D^-$  centre in AgCl, CdS, and GaAs. Broken horizontal lines correspond to static dielectric constants  $\varepsilon_s$ .

dielectric constant  $\varepsilon_s$ , but weaker than the Coulomb interaction screened by the high-frequency dielectric constant  $\varepsilon_\infty$ . In the weakly polar GaAs as well as in the strongly polar AgCl  $V_{\text{eff}} \simeq \kappa e^2 / (\varepsilon_\infty r_{12})$  at small distances. In GaAs, the effective interaction exhibits the following asymptotic behaviour for large distances:  $V_{\text{eff}} \simeq \kappa e^2 / (\varepsilon_s r_{12})$ . In AgCl, the long-range effective interaction is always stronger than  $\kappa e^2 / (\varepsilon_s r_{12})$  (see also figure 2). In both the limits of  $r_{12}$ , the electron–electron interaction becomes purely Coulombic. At the intermediate interelectron distances the effective interaction energy considerably deviates from the Coulombic form.

The effective dielectric function for the  $D^-$  centre is plotted in figure 2 for GaAs, CdS, and AgCl, i.e., for the crystals with weak, intermediate, and strong electron–LO-phonon coupling, respectively. The energy and length are expressed in the donor units, i.e., donor Rydberg  $R_D$  and donor Bohr radius  $a_D$ , respectively. For GaAs, we take on  $R_D = 5$  meV and  $a_D = 10$  nm. Figure 2 shows that the phonon dielectric function increases monotonically with the increasing interelectron separation starting from  $\varepsilon_{\text{eff}}(0) = \varepsilon_\infty$ . In the weakly ionic material (cf the plot for GaAs in figure 2)  $\varepsilon_{\text{eff}}(r_{12})$  quickly increases with increasing  $r_{12}$  and already for  $r_{12} \leq 1a_D$  reaches the constant value  $\bar{\varepsilon}$  (equation (17)). For GaAs  $\bar{\varepsilon} \simeq \varepsilon_s$ , which means that for  $r_{12} > 1a_D$  the lattice is fully polarized and the LO-phonon-induced screening is maximal. Therefore, in GaAs we can approximate the effective dielectric function by  $\varepsilon_s$ . For the more ionic compounds (cf the plots for CdS and AgCl in figure 2), the effective phonon dielectric function is a slowly varying function of the electron–electron distance, reaching the constant value,  $\bar{\varepsilon}$ , at larger distances ( $r_{12} \simeq 3a_D$ ), and  $\bar{\varepsilon} < \varepsilon_s$ . Therefore, the increasing electron–LO-phonon coupling leads to the weakening of the screening, i.e., the electron–electron repulsion becomes stronger than in the case of the maximal screening by the lattice. At distances which correspond to the average separation between the electrons in the  $D^-$  centre, i.e.,  $2\text{--}4a_D$  [7], the



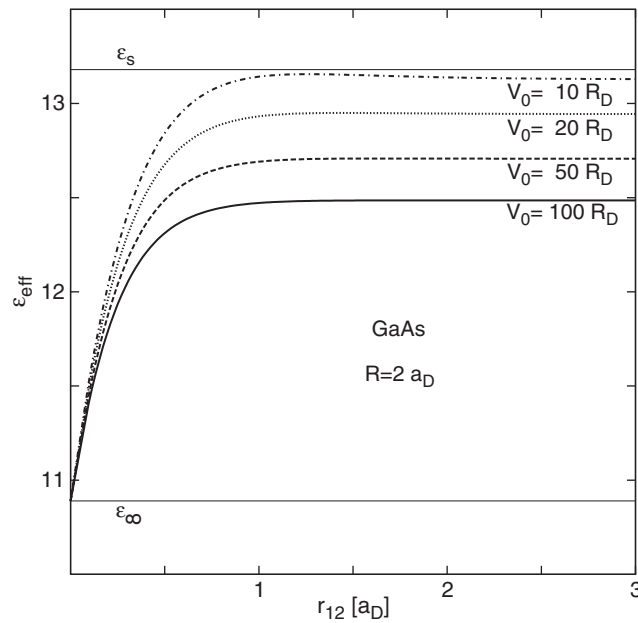
**Figure 3.** Effective phonon dielectric function  $\epsilon_{\text{eff}}$  versus interelectron distance  $r_{12}$  for the two-electron QD made of GaAs for the fixed confinement-potential depth  $V_0 = 50R_D$  and several values of the confinement-potential range  $R = 1, 2, 5,$  and  $10 a_D$ . Thin horizontal lines correspond to the high-frequency ( $\epsilon_\infty$ ) and static ( $\epsilon_s$ ) dielectric constants.

effective dielectric function can be approximated by the constant  $\bar{\epsilon}$ . We note that the stronger electron–electron repulsion is accompanied by the stronger electron–donor attraction, which is also due to the LO phonons [7].

### 3.2. Two-electron quantum dot

The results for the two-electron spherical QD with Gaussian confinement potential (4) are shown in figures 3–6. Figure 3 displays the effective phonon dielectric function for the GaAs QD with the fixed confinement-potential well depth and varying QD radius. The plots of  $\epsilon_{\text{eff}}$  versus  $r_{12}$  for the fixed radius of the QD made of GaAs and varying potential-well depth are depicted in figure 4.

Figures 3 and 4 show that the effective dielectric function rapidly increases for small interelectron distances and reaches the constant  $\bar{\epsilon}$  already at  $r_{12} \simeq 1 a_D$ . This behaviour is similar to that for the  $D^-$  centre in GaAs (cf figure 2). For fixed  $V_0$   $\bar{\epsilon}$  increases with the increasing QD radius (cf figure 3), while for the fixed QD radius  $\bar{\epsilon}$  decreases with the increasing potential-well depth (cf figure 4). For the majority of QD parameters  $\bar{\epsilon}$  is smaller than the static dielectric constant  $\epsilon_s$  and approaches  $\epsilon_s$  for the large QDs (cf the plot for  $R = 10a_D$  in figure 3) and the shallow confinement potential (cf the plot for  $V_0 = 10R_D$  in figure 4). For the large QDs and the weak confinement potential we approach the bulk crystal limit, i.e., the effective phonon dielectric function becomes similar to that for the  $D^-$  centre in the bulk GaAs (cf figure 2). For the stronger quantum confinement we observe considerable deviations from this bulk-crystal-like behaviour (cf the plots in figure 3 for small  $R$  and in figure 4 for large  $V_0$ ). Therefore, the increasing quantum confinement leads to the weakening of the LO-phonon-induced screening of the electron–electron repulsion in QDs.

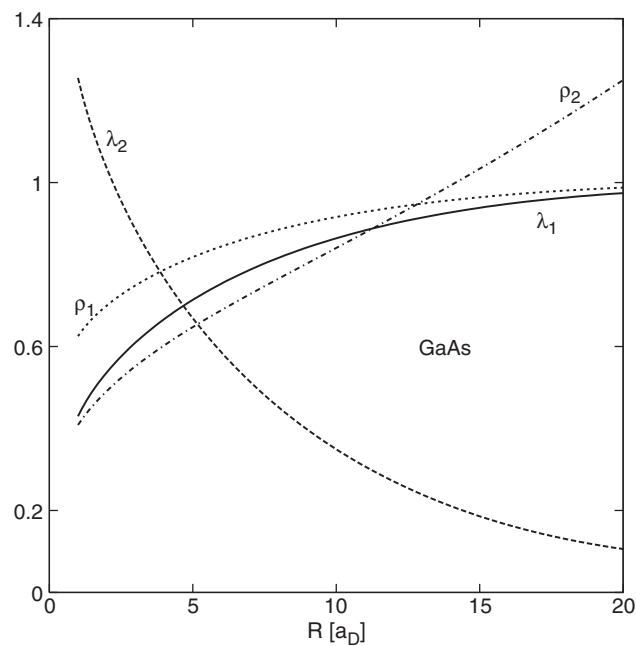


**Figure 4.** Effective phonon dielectric function  $\varepsilon_{\text{eff}}$  versus interelectron distance  $r_{12}$  for the two-electron QD made of GaAs for the fixed confinement-potential range  $R = 2a_D$  and several values of the confinement-potential depth  $V_0 = 10, 20, 50,$  and  $100 R_D$ . Thin horizontal lines correspond to the high-frequency ( $\varepsilon_\infty$ ) and static ( $\varepsilon_s$ ) dielectric constants.

The explicit formula for the effective dielectric function (equation (16)) contains the variational parameters, which modify the shape of phonon amplitudes (11) and (12). In the present paper, we have determined their values by minimizing the two-electron ground-state energy. Figure 5 shows the dependence of these variational parameters on the QD radius for the fixed confinement-potential-well depth in the QD made of GaAs. For large  $R$ , i.e., in the bulk crystal limit,  $\lambda_1 \rightarrow 1$ ,  $\varrho_1 \rightarrow 1$ , and  $\lambda_2 \rightarrow 0$ , which means that the weak-coupling phonon amplitude (11) tends to that characterizing the free polarons in the bulk crystal [28], while the strong-coupling phonon amplitude (equation (12)) vanishes. For  $\lambda_1 \leq 1$ :  $\bar{\varepsilon} < \varepsilon_s$  (cf equation (17)), i.e., the average screening of the electron–electron interaction is weaker than the screening corresponding to the static distortion of the crystal lattice.

The interaction with LO phonons modifies the energy of electron systems confined in QDs. Figure 6 displays the ground-state energy calculated for the one- and two-electron systems confined in the spherical QDs made of GaAs, CdS, and AgCl as a function of the radius. The ground-state energy of the single electron confined in the QD is denoted by  $E^{(1)}$  and the ground-state energy of the two electrons confined in the QD by  $E^{(2)}$ . The binding energy  $W$  of the two-electron system confined in the QD is defined as  $W = E^{(1)} - E^{(2)}$  [20]. Figure 6 shows that the binding energy increases with increasing radius of the QD. For small QDs the one- and two-electron systems are not bound (cf the flat parts of the curves below  $R \simeq 0.5a_D$ ). In each group of curves, corresponding to  $E^{(1)}$  and  $E^{(2)}$ , the upper (solid) curve shows the results for the elemental semiconductors, for which the electron–LO-phonon coupling vanishes. The coupling with the LO phonons lowers the ground-state energy of the electron systems confined in the QDs. The results for GaAs, CdS, and AgCl, i.e., for the materials with the weak, intermediate, and strong electron–LO-phonon coupling, show that the stronger the coupling with phonons the larger the lowering of the ground-state energy.





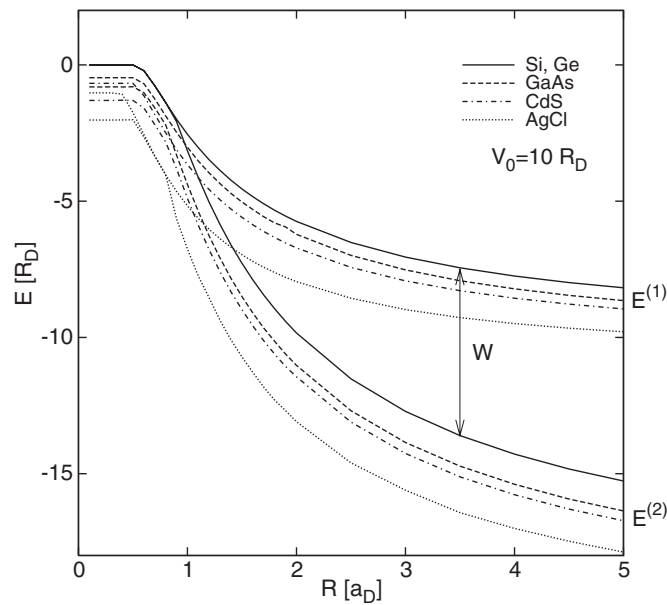
**Figure 5.** Variational parameters  $\lambda_1$  (solid line),  $\lambda_2$  (broken line),  $\rho_1$  (dotted line),  $\rho_2$  (dash-dotted line) as functions of confinement-potential range  $R$  for  $V_0 = 50R_D$  for the two-electron QD made of GaAs.

Figure 6 also shows that the binding energy increases with the increasing electron–phonon coupling.

#### 4. Conclusions and summary

The results for QDs presented in section 3.2 have been obtained under the assumption that the material parameters, which determine the electron–phonon system, do not change across the QD boundary. This assumption can be justified in the electrostatic QDs [29], in which the lateral confinement of electrons in the QD is caused by the external inhomogeneous electric field. In the electrostatic QDs, the QD region is made of the same material as its nearest environment in the lateral directions. However, in the vertical direction, there appear the heterojunctions, at which the material properties can change discontinuously [29]. In the self-assembled QDs [25] we deal with relatively sharp heterojunctions, which lead to a formation of the interface and confined phonons. However, in the self-assembled QDs with a compositional modulation (alloying) [26] the material parameters smoothly change across the QD boundary and the boundary region is spread over several lattice constants. For the QDs with the smoothly varying composition the present results may have a qualitative meaning. Nevertheless, in a quantitative description of the screening we have to include the interface effects and the anisotropy of the nanostructure.

The energy of the electron–LO-phonon system depends on the self-energy (cf equation (14)). This dependence enters into the expectation value of Hamiltonian (14) calculated with the wavefunction of the electronic state considered. Throughout the present paper, we study the ground state, for which the influence of the self-energy on screening



**Figure 6.** Ground-state energy of the one-electron ( $E^{(1)}$ ) and two-electron ( $E^{(2)}$ ) QDs made of the non-ionic semiconductor, e.g., Si, Ge (solid line), GaAs (broken line), CdS (dash-dotted line), and AgCl (dotted line) as a function of confinement-potential range  $R$  for fixed confinement-potential depth  $V_0 = 10R_D$ .  $W$  denotes the binding energy of the two-electron QD.

is fixed and independent of the electron–electron distance. This justifies the neglect of the influence of the self-energy on the screening. In the present work, we focus on the phonon screening; therefore, we neglect the image charges, which mainly exert the effect on the electronic screening. It was shown [30] that the image charges do not affect the electron–bulk-phonon interaction. However, the image charges can change the energy of polarons [30].

The results of the present calculations can hardly be compared with the existing experimental data, since we did not find any experimental results from which we can extract the binding energy of few-electron systems confined in QDs made of different polar materials. In the recent experiments [13–15, 31] with QDs the effect of the electron–LO-phonon coupling has been studied for the one-electron states only. The binding energy of the two-electron QD is equal to the absolute value of the chemical potential, which can be measured by the transport spectroscopy [29].

Despite some similarity of both the two-electron systems studied, i.e., the  $D^-$  centre in the bulk crystal and the two-electron system confined in the QD, there exists an essential difference between them, which results from the large difference in the binding energy. For the  $D^-$  centre in the bulk GaAs crystal  $W \simeq 0.05R_D$ , i.e., this two-electron system is very weakly bound. In contrast, the binding energy of the two-electron QD is of the order of the potential-well depth  $V_0$ , e.g.,  $W \simeq 10R_D$  for  $V_0 = 10R_D$  (cf figure 6), i.e., the two-electron QD is strongly bound. This leads to the qualitatively different behaviour of the phonon dielectric function obtained for both the two-electron systems. For example, for GaAs the average screening constant,  $\bar{\epsilon}$ , for the  $D^-$  is different from that for the two electrons in the QD (cf figures 2, 3, and 4). We have also performed calculations for the QDs with the very weak confinement potential and obtained results which are similar to that for the  $D^-$  in the bulk crystal. Let us note that for  $R \rightarrow 0$  we also approach the bulk crystal limit. However, if the QD size is too small, the

electrons do not form the bound states in the QD (cf figure 6) and the present approach to the phonon dielectric screening is not applicable.

The results of the present paper show that—in the bound two-electron systems—the LO-phonon-induced screening of the electron–electron interaction becomes weaker if the electron–LO-phonon coupling increases and/or the quantum confinement of the electrons increases. This weakening of the screening results from the enhancement of the binding, which occurs for the stronger electron–phonon coupling and the stronger confinement. In the strongly bound systems, the average interelectron separations are small [7], which leads to a partial cancellation of the virtual phonon clouds associated with each electron, which in turn causes the weaker screening of the interelectron interaction by the induced lattice polarization.

In summary, we have shown that—in the bulk crystals as well as in the QDs—the LO-phonon-induced screening of the electron–electron interaction can be described by the effective dielectric function, which is a monotonically increasing function of the interelectron distance. In the QDs, the effective dielectric function already at relatively small electron–electron separations reaches the constant value,  $\bar{\epsilon}$ , which however is usually smaller than the static dielectric constant,  $\epsilon_s$ . The average dielectric constant  $\bar{\epsilon}$  can be treated as a useful quantity that determines the LO-phonon screening of the interelectron repulsion in the bound few-electron systems. In the QDs,  $\bar{\epsilon}$  becomes equal to  $\epsilon_s$  only if the quantum confinement is weak. Moreover, the electron–LO-phonon coupling leads to the enhancement of the binding of the two-electron systems confined in the QDs made of the ionic materials.

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