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The strong-coupling polaron in reduced dimensionality

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Abstract. Based on the LLP-H approach, a detailed study of the electron confinement in a polar semiconductor heterostructure has been made to derive analytically the ground state energy and the effective mass of the Fröhlich polaron in quasi-two-dimensional (Q2D) and quasi-one-dimensional (Q1D) systems.

1. Introduction

A great deal of research effort is currently being devoted to the study of low-dimensional semiconductor systems because of their potential application in device technology. With the advancement in semiconductor technology, it is now possible to confine electrons (holes) in quasi-two-dimensional and quasi-one-dimensional semiconductor structures such as in hetero-junctions, quantum well or quantum-wire-like systems [1–8]. Studies on these quantum structures are important not only from the technological point of view but also for the understanding of a number of important phenomena [9, 10] concerning electrical and optical properties in these systems. In particular, the interaction of electron with longitudinal optical phonon being an important mechanism in deciding electrical and optical properties of polar semiconductor, a systematic study is crucial in achieving a detailed understanding of the polaron properties in reduced dimensionality.

Although the bulk of the literature over the years has been devoted mainly to the study of the polaronic properties in the three-dimensional (3D) system [11, 12], a considerable effort has lately gone into exploring the polaron properties in 2D systems [13–15]. Recent years have witnessed a number of experiments and theories on the polaronic effects in quantum heterostructures [16–36]. The study of the polaron effects in 2D structure [16–23] shows that the reduction of the spatial dimension greatly affects the electron–phonon interaction and it is found that polaronic properties are very much dependent on the dimensionality of the quantum structure. In most of these works the phonons are assumed to be the same as in the bulk material [18, 19]. In contrast to the bulk phonon model, the optical phonon confinement has also been considered by many authors [21–23]. Some studies on the electron–phonon interaction in Q1D systems [24–28] have also been done recently and these indicate that polaron effects are much more pronounced in Q1D structure than those in Q2D structure.

The purpose of the present paper is to report a unifying and comprehensive model yielding an explicit track of the electron–phonon interaction as a function of the effective dimensionality. Here we have made a systematic investigation of the ground state energy and the effective mass of the Q2D and Q1D polaron within the framework of the LLP-H

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method [14]. Regardless of the confined structure of the system, polar optical phonons have been treated in our approach in the spirit of bulk theory.

2. Formulation

The standard Hamiltonian for an electron or hole interacting with the optical modes in a polar crystal is given by (in Fröhlich units)

$$H_p = p^2 + \sum_{\boldsymbol{q}} b_{\boldsymbol{q}}^\dagger b_{\boldsymbol{q}} + \sum_{\boldsymbol{q}} (\xi_{\boldsymbol{qr}} b_{\boldsymbol{q}} + \mathrm{HC}) \tag{1}$$

where $\xi_{\boldsymbol{qr}} = \xi_q \exp(\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r})$, $\xi_q = -\mathrm{i}(4\pi\alpha/V)^{1/2}$, α is the usual Fröhlich constant and V is the volume of the crystal.

To address polaron formation in reduced dimensionality phonons are always considered to be 3D, although electron motions are to be localized in reduced dimensions. In a strict 2D case the electron can be assumed to be localized well around $x = 0$ and in 1D it is localized in the yz plane around the x axis.

We now consider a 3D polaron in a quantum dot potential described by the Hamiltonian

$$\tilde{H} = H_p + \lambda_1^4 x^2 + \lambda_2^4 y^2 + \lambda_3^4 z^2 \tag{2}$$

where λ_1, λ_2 and λ_3 represent the strength of the potential in the x, y and z direction respectively. Our approach is essentially directed at choosing the appropriate Hamiltonian to describe 1D and 2D polaron motion.

Now the total momentum of the system

$$\tilde{\boldsymbol{P}} = \boldsymbol{p} + \sum_{\boldsymbol{q}} \boldsymbol{q} b_{\boldsymbol{q}}^\dagger b_{\boldsymbol{q}} \tag{3}$$

commutes with the Hamiltonian $\tilde{H}([\tilde{H}, \tilde{\boldsymbol{P}}] = 0 = [\tilde{\boldsymbol{P}}, \tilde{H}])$ and is therefore a constant of motion. Following the LLP-H scheme, we now define a functional $J = \langle\tilde{\Psi}|\tilde{H} - \boldsymbol{u}\cdot\tilde{\boldsymbol{P}}|\tilde{\Psi}\rangle$ which is to be minimized with respect to the appropriate variational parameter. Here $\boldsymbol{u}$ is the Lagrange multiplier with the dimension of velocity and $\tilde{\Psi}$ is the appropriately chosen system wave function of the system.

We now rewrite J as

$$J = \langle\tilde{\Psi}|UU^{-1}|\tilde{H} - \boldsymbol{u}\cdot\tilde{\boldsymbol{P}}|UU^{-1}|\tilde{\Psi}\rangle = \langle\Psi|H - \boldsymbol{u}\cdot\boldsymbol{P}|\Psi\rangle \tag{4}$$

where

$$U = \exp\left\{\sum_{\boldsymbol{q}} (f_{\boldsymbol{q}} b_{\boldsymbol{q}}^\dagger - \mathrm{HC})\right\} \tag{5}$$

with $f_{\boldsymbol{q}}$ as variational functions to be determined by minimizing the functional J.

Now

$$H = U^{-1}\tilde{H}U = p^2 + \lambda_1^4 x^2 + \lambda_2^4 y^2 + \lambda_3^4 z^2 + \sum_{\boldsymbol{q}} (f_{\boldsymbol{q}} + b_{\boldsymbol{q}})^\dagger (f_{\boldsymbol{q}} + b_{\boldsymbol{q}}) + \sum_{\boldsymbol{q}} \left\{\xi_{\boldsymbol{qr}} (f_{\boldsymbol{q}} + b_{\boldsymbol{q}})^\dagger + \mathrm{HC}\right\} \tag{6}$$

$$\boldsymbol{P} = U\tilde{\boldsymbol{P}}U^{-1} = \boldsymbol{p} + \sum_{\boldsymbol{q}} \boldsymbol{q} (f_{\boldsymbol{q}} + b_{\boldsymbol{q}})^\dagger (f_{\boldsymbol{q}} + b_{\boldsymbol{q}}) \tag{7}$$

and

$$|\Psi\rangle = U^{-1}|\tilde{\Psi}\rangle. \tag{8}$$

We then choose our system wave function to be

$$|\tilde{\Psi}\rangle = \varphi(r)\exp(\mathrm{i}\boldsymbol{p}_0\cdot\boldsymbol{r})\exp\left\{\sum_{\boldsymbol{q}}(f_{\boldsymbol{q}}b^{\dagger}_{\boldsymbol{q}}) - \mathrm{HC})\right\}\kappa_0 \tag{9}$$

where $\boldsymbol{p}_0$ is an additional variational parameter, $\varphi(r)$ is the electronic wave function and κ_0 is the zero-phonon state which satisfies

$$b_{\boldsymbol{q}}\kappa_0 = 0. \tag{10}$$

Thus we obtain

$$J = \langle\varphi(r)|p^2 + \lambda_1^4x^2 + \lambda_2^4y^2 + \lambda_3^4z^2|\varphi(r)\rangle + p_0^2 + \sum_{\boldsymbol{q}}\{\langle\varphi(r)|\xi_{\boldsymbol{q}\boldsymbol{r}}|\varphi(r)\rangle f_{\boldsymbol{q}} + \mathrm{HC}\} + \sum_{\boldsymbol{q}}|f_{\boldsymbol{q}}|^2 - \boldsymbol{u}\cdot\boldsymbol{p}_0 - \sum_{\boldsymbol{q}}(\boldsymbol{u}\cdot\boldsymbol{q})|f_{\boldsymbol{q}}|^2. \tag{11}$$

Now minimizing J with respect to $\boldsymbol{p}_0$ and $f_{\boldsymbol{q}}$ we have

$$\frac{\partial J}{\partial \boldsymbol{p}_0} = 0 \rightarrow \boldsymbol{p}_0 = \boldsymbol{u}/2 \tag{12}$$

and

$$\frac{\partial J}{\partial f^*_{\boldsymbol{q}}} = 0 \rightarrow f^*_{\boldsymbol{q}} = -\frac{\langle\varphi(r)|\xi^*_{\boldsymbol{q}\boldsymbol{r}}|\varphi(r)\rangle}{(1-\boldsymbol{u}\cdot\boldsymbol{q})}. \tag{13}$$

Then the energy of the moving polaron is given by

$$E_g = \langle\Psi|H|\Psi\rangle = \langle\varphi(r)|p^2 + \lambda_1^4x^2 + \lambda_2^4y^2 + \lambda_3^4z^2|\varphi(r)\rangle + u^2/4 - 2\sum_{\boldsymbol{q}}\frac{|\langle\varphi(r)|\xi^*_{\boldsymbol{q}\boldsymbol{r}}|\varphi(r)\rangle|^2}{(1-\boldsymbol{u}\cdot\boldsymbol{q})} + \sum_{\boldsymbol{q}}\frac{|\langle\varphi(r)|\xi^*_{\boldsymbol{q}\boldsymbol{r}}|\varphi(r)\rangle|^2}{(1-\boldsymbol{u}\cdot\boldsymbol{q})^2}. \tag{14}$$

For the static polaron $\boldsymbol{u} = \mathbf{0}$ and the energy then turns out to be

$$E_p = \langle\varphi(r)|p^2 + \lambda_1^4x^2 + \lambda_2^4y^2 + \lambda_3^4z^2|\varphi(r)\rangle - \sum_{\boldsymbol{q}}|\varphi(r)|\xi^*_{\boldsymbol{q}\boldsymbol{r}}|\varphi(r)\rangle^2. \tag{15}$$

The minimum of E_p with respect to the appropriate variational parameter would give the ground state energy of the polaron in reduced dimensionality.

For the slowly moving electron, u being small, we can expand $(1-\boldsymbol{u}\cdot\boldsymbol{q})^{-1}$ and $(1-\boldsymbol{u}\cdot\boldsymbol{q})^{-2}$ in powers of u and retain only terms up to u^2 to obtain the energy of the slowly moving polaron

$$E_g = E_p + \frac{u^2}{4}\left[1 + 4\sum_{\boldsymbol{q}}q^2|\langle\varphi(r)|\xi^*_{\boldsymbol{q}\boldsymbol{r}}|\varphi(r)\rangle|^2\sin^2\vartheta\cos^2\varphi\right]. \tag{16}$$

In Fröhlich units the coefficient of $u^2/4$ can then be identified with the effective mass of the polaron.

Assuming that there is no coupling between the electron motion in the yz plane (where the electrons (holes) have the strongest confinement in the 2D case) and in the x direction (where they have the strongest confinement in the 1D case), we now define the ground state of the electron in the adiabatic approximation

$$\varphi(r) = \left(\frac{\sqrt{\pi}}{2}\right)^{-3/2}\left(\frac{1}{\lambda}\right)\left(\frac{1}{\sqrt{\beta}}\right)\exp(-\beta^2x^2/2)\exp(-\lambda^2\rho^2/2) \qquad \rho = (y,z) \tag{17}$$

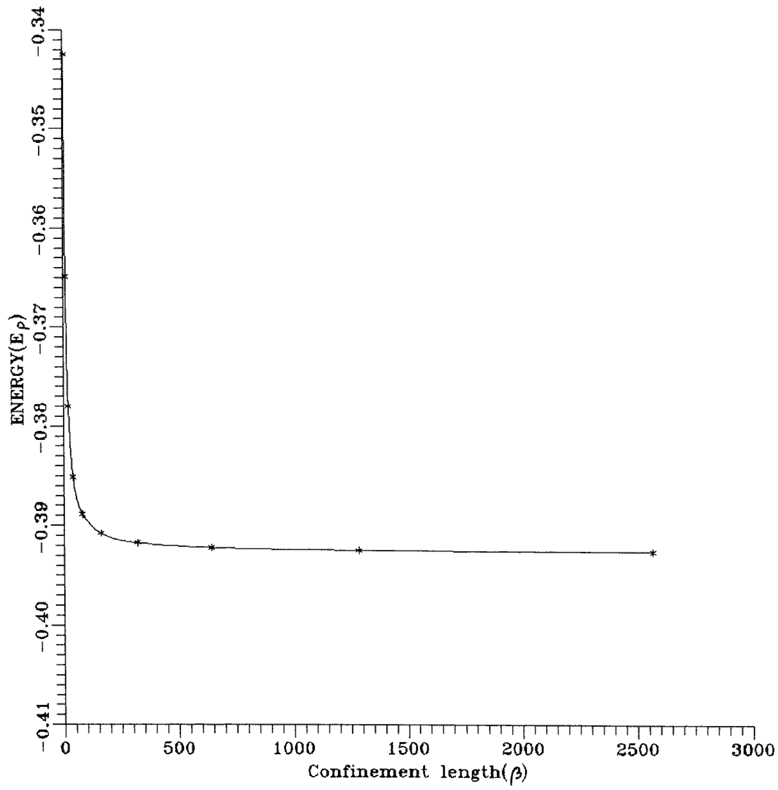

Figure 1. The ground state energy (ε_p) (in units of $\alpha h\omega$) of the Fröhlich polaron versus confinement length (β) (in Fröhlich units) in Q2D systems.

where either of λ or β is taken as a variational parameter and the other will describe the degree of confinement.

The general expression for the binding energy ($\Delta\varepsilon_p = -E_p$) and the effective mass in the quasi-2D limit becomes

$$\Delta\varepsilon_p = -\surd(1/2\pi)\alpha\lambda\{(1/b^2 - 2)\tan^{-1}(b\beta/\lambda) - (\lambda/b\beta)\}/b \tag{18}$$

$$m^*/m = 1 + 2\surd(1/2\pi)\alpha\{\sin^{-1} b - b\surd(1-b^2)\}(\lambda/\beta)^3 \tag{19}$$

where

$$b = \surd(\beta^2 - \lambda^2)/\beta \tag{20}$$

$$\lambda = \surd(1/2\pi)\alpha\{(1/b^2)\tan^{-1}(b\beta/\lambda) - (\lambda/b\beta)\}/b. \tag{21}$$

For the strict 2D case $\beta \to \infty$ and we obtain the polaron binding energy and the effective mass in the GS state [15]

$$\Delta\varepsilon_p^{2D} = \pi\alpha^2/8 \tag{22}$$

$$m^*/m = 1 + (\surd 2\pi)^4\alpha^4/64 \tag{23}$$

where

$$\lambda = (\surd 2\pi)\alpha/4. \tag{24}$$

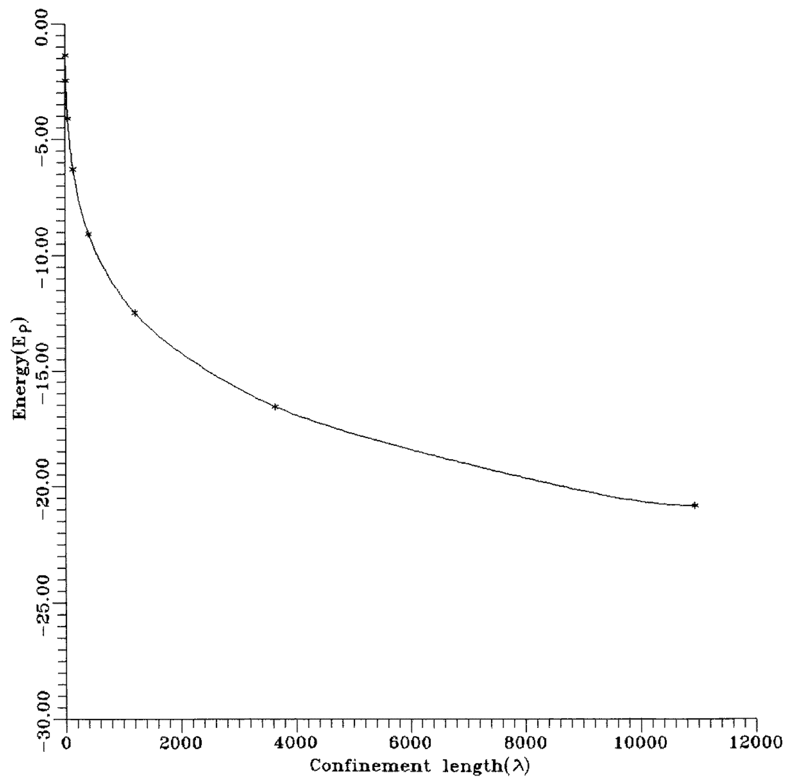

Figure 2. The ground state energy (ε_p) (in units of $\alpha h\omega$) of the Fröhlich polaron versus confinement length (λ) (in Fröhlich units) in Q1D systems.

On the other hand setting β as variational parameter and increasing λ we arrive at the quasi-1D characterization of the polaron which in the limit of $\lambda \to \infty$ will give a strict one-dimensional polaron.

Thus in the quasi-one-dimensional limit binding energy and the effective mass become

$$\Delta\varepsilon_p = \surd(1/2\pi)\alpha\beta\{{}_2F_1(1/2, 1, 3/2, \beta^2/\mu^2) + (4/3)(\beta^2/\lambda^2)\,{}_2F_1(3/2, 2, 5/2, \beta^2/\mu^2)\}. \quad (25)$$

$$m^*/m = 1 + 2\alpha\surd(2/\pi)(\beta/a')^3[a\surd(1 + a^2) - \log\{a + \surd(1 + a^2)\}] \quad (26)$$

where

$$\beta = \surd(2/\pi)\alpha\{{}_2F_1(1/2, 1, 3/2, \beta^2/\mu^2) - (2/3)(\beta^2/\lambda^2)\,{}_2F_1(3/2, 2, 5/2, \beta^2/\mu^2)\} \quad (27)$$

$$a = \surd(\lambda^2 - \beta^2)/\beta \quad (28)$$

$$a' = \surd(\lambda^2 - \beta^2)/\lambda \quad (29)$$

$$\mu = \lambda\beta/\surd(\lambda^2 - \beta^2). \quad (30)$$

Here we observe that polaron binding energy and effective mass diverge in the strict 1D limit.

For $\lambda = \beta$ we obtain the bulk value [11, 12]

$$\lambda = \beta = \surd(2/9\pi)\alpha \quad (31)$$

$$\Delta\varepsilon_p^{3D} = \alpha^2/3\pi \quad (32)$$

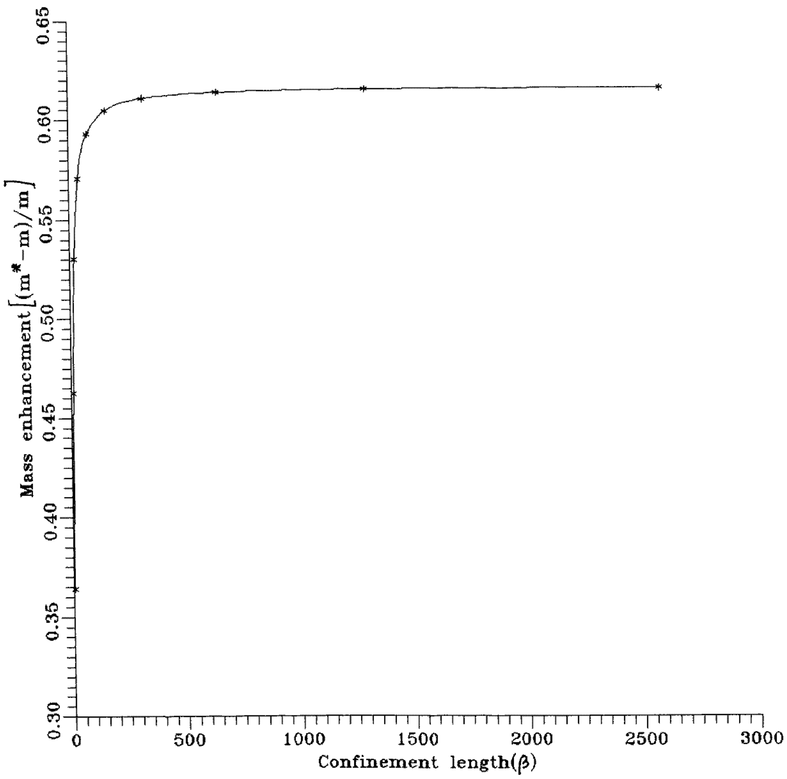

Figure 3. Relative polaronic mass enhancement $\{(m^* - m)/m\}$ (in units of α^4) versus confinement length (β) (in Fröhlich units) in Q2D systems.

and

$$m^*/m = 1 + 16\alpha^4/81\pi^2. \tag{33}$$

3. Results and discussion

According to the derivation presented in the previous section the contribution of the electron–phonon interaction to the ground state energy and the effective mass of the polaron depends on the spatial dimensions of the quantum heterostructure. It is to be noted that we have used the same Fröhlich coupling constant, α, which was derived for a three-dimensional electron gas, in reduce dimensionality also. Even though the coupling constant will not remain the same for the low-dimensional electrons and the bulk phonons, it is a reasonable approximation in our theory since we have considered the barrier part only to yield the electronic potential and thus neglect difference in masses, dielectric constants and phonon energy between the well part and barrier part [14].

A detailed study of the effect of electron confinement on the polaronic properties has been made to show that this approach may apply equally well to retrieve the bulk 2D and 3D results. In figures 1 and 2 we have plotted the GS energy of the Q2D and Q1D polaron respectively as a function of the confinement length. We notice from figure 1 that the polaron effect increases due to decrease of the layer width when β increases and as a result

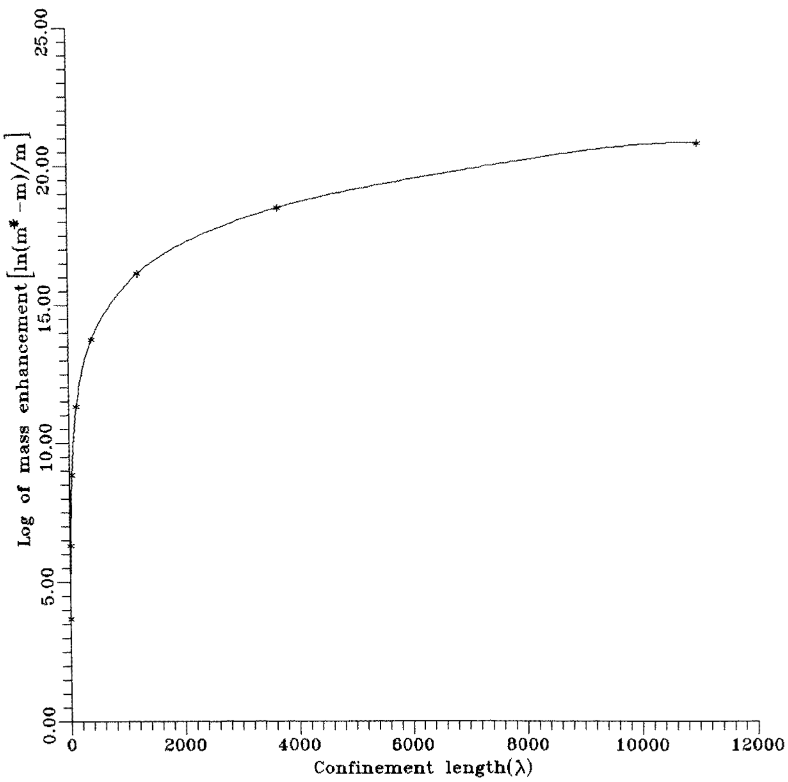

Figure 4. Relative polaronic mass enhancement $\{(m^* - m)/m\}$ (in units of α^4) versus logarithm of the confinement length (λ) (in Fröhlich units) in Q1D systems.

$|E_p|$ increases and approaches the 2D limit when $\beta \to \infty$. In figure 2 we are concerned with the effect of the dimensionality of the Q1D structure on the GS energy of the Fröhlich polaron. The GS energy of the polaron in the Q1D heterostructure increases rapidly with the increase of λ and diverges in the strict 1D case when $\lambda \to \infty$.

The behaviour of the effective mass as a function of confinement length of the quantum heterostructure is depicted in figures 3 and 4. We observe that the effective mass of the polaron in the Q2D heterostructure also increases with the decrease of the layer width and approaches the exact 2D limit. On the other hand the effective mass of the Fröhlich polaron in the Q1D structure increases more rapidly when λ increases and we notice from figure 4 that it diverges logarithmically in strictly one dimension.

Thus the high degree of localization in reduced dimensionality leads to an enhancement in the effective phonon coupling which in turn brings about the possibility that the quantum behaviour and the dynamics undergo drastic changes with respect to the bulk when carriers are artificially confined to a volume whose dimensions are well below a critical length.

References

[1] Sakaki H 1980 *Japan. J. Appl. Phys.* **19** L735
[2] Petroof P M, Gossard A C, Lagan R A and Wiegmann W 1982 *Appl. Phys. Lett.* **41** 635
[3] Kash K, Scherer A, Worlock J M, Craighead H G and Tamargo M C 1986 *Appl. Phys. Lett.* **49** 1043

[4] Zhao X, Kosulu K and Sakka J S 1987 *J. Mater. Sci.* **22** 4103
[5] Temkin H, Dolan J G, Panish M B and Chu S N G 1987 *Appl. Phys. Lett.* **50** 413
[6] Sikorski C and Merkt U 1989 *Phys. Rev. Lett.* **62** 2164
[7] Reed M A, Randall J N, Aggarwal R G, Matyi R J, Morse T M and Wetsel A E 1989 *Phys. Rev. Lett.* **55** 168
[8] Lorke A, Kotthaus J P and Ploog K 1990 *Phys. Rev. Lett.* **64** 788
[9] Liu C T, Nakamura K and Tsui D C 1989 *Appl. Phys. Lett.* **55** 168
[10] Hansen W, Smith T P III, Lee K Y, Brun J A, Knoedler C M, Hong J M and Kern D P 1989 *Phys. Rev. Lett.* **62** 2168
[11] Kuper C G and Whitfield G D (eds) 1963 *Polarons and Excitons* (New York: Plenum)
[12] Mitra T K, Chatterjee A and Mukhopadhyay S 1987 *Phys. Rep.* **153** 91
[13] Matsura M 1976 *J. Phys. Soc. Japan* **41** 394
Matsura M 1988 *Phys. Rev.* B **37** 6977
[14] Huybrechts W J 1976 *J. Phys. C: Solid State Phys.* **9** L211
Huybrechts W J 1977 *J. Phys. C: Solid State Phys.* **10** 3761
[15] Xiaoguang W, Peeters F M and Devreese J T 1985 *Phys. Rev.* B **31** 3420
[16] Licary J J and Evrard R 1977 *Phys. Rev.* B **15** 2254
[17] Licary J J 1979 *Solid State Commun.* **29** 625
[18] Das Sarma S 1983 *Phys. Rev.* B **27** 2590
[19] Das Sarma S and Stopa M 1987 *Phys. Rev.* B **36** 9595
[20] Schmitt-Rink S, Miller D A B and Chemla D S 1987 *Phys. Rev.* B **35** 8113
[21] Liang X X, Gu S W and Lin D L 1986 *Phys. Rev.* B **34** 2807
[22] Comas F, Trallero-Giner C and Riera R 1989 *Phys. Rev.* B **39** 5907
[23] Hai G Q, Peeters F M and Devreese J T 1991 *Phys. Rev.* B **42** 11 063
Hai G Q, Peeters F M and Devreese J T 1993 *Phys. Rev.* B **48** 4666
[24] Wu X G 1989 *Phys. Rev.* B **39** 8062
[25] Degani M H 1989 *Phys. Rev.* B **40** 11 937
[26] Degani M H and Farias G A 1990 *Phys. Rev.* B **42** 11 950
[27] Cmpos V B, Degani M H and Hipolito O 1991 *Solid State Commun.* **79** 473
[28] Hai G Q, Peeters F M and Devreese J T 1993 *Phys. Rev.* B **48** 12 016
[29] Roussignol D R and Flytzanis C 1989 *Phys. Rev. Lett.* **62** 312
[30] Klein M C, Hache F, Ricard D and Flytzanis C 1990 *Phys. Rev.* B **42** 11 123
[31] Yildirim T and Ercelebi A 1991 *J. Phys. C: Solid State Phys.* **3** 1271
Yildirim T and Ercelebi A 1991 *J. Phys. C: Solid State Phys.* **3** 4357
[32] Zhu K D and Gu S W 1992 *Phys. Lett.* **163A** 435
Zhu K D and Gu S W 1993 *Phys. Rev.* B **47** 12 941
[33] Zhu K D and Kobayashi T 1994 *Solid State Commun.* **92** 353
[34] Mukhopadhyay S and Chatterjee A 1995 *Phys. Lett.* **204A** 411
[35] Sahoo S 1996 *Z. Phys.* B **101** 97
[36] Kabanov V V and Mashtakov O Y 1993 *Phys. Rev.* B **47** 6061