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Intermediate-coupling exciton in a quantum well

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Abstract. The interaction expression of the surface-optical phonons with an electron (a hole) in a slab is extended to the case of a quantum well and the Hamiltonian H of the exciton-phonon system allowing for the Gabovish image potential is obtained for the first time. A double-time unitary transformation to the Hamiltonian H is carried out to obtain the Hamiltonian \mathcal{H}_{ex} of the exciton in a quantum well, and the motion of the exciton in the z direction is discussed in detail. The result obtained is suitable not only for a weak-coupling exciton system but also for an intermediate-coupling exciton system.

1. Introduction

Recently, there has been great interest in studying the behaviour of the bare exciton in a polar crystal or a quantum well [1–4]. The behaviour of the exciton-phonon system in a slab with a one-time unitary transformation to the Hamiltonian of the system was investigated in [5], but the result is only suitable for a weak-coupling exciton-phonon system. On the other hand, when we study the behaviour of the electron (the hole) near the interface in a condensed medium, it is necessary to take into account the polarisation force (image force) due to the existence of the interface [6]. With the technological development of heterostructures and superlattices, investigation of the behaviour of the exciton in a quantum well is more important. In this paper we study the behaviour of an exciton-phonon system allowing for the Gabovish image potential in a quantum well with a two-time unitary transformation to the Hamiltonian of the system and obtain some important properties of the discussed system.

2. The Hamiltonian and unitary transformation

We generalise the Hamiltonian of the exciton-phonon system in a polar slab [5] to the case of a quantum well as shown in figure 1 and obtain the Hamiltonian of the exciton-phonon system in a quantum well by replacing the vacuum dielectric constants with the dielectric constants of $\text{Al}_x\text{Ga}_{1-x}\text{As}$, i.e.

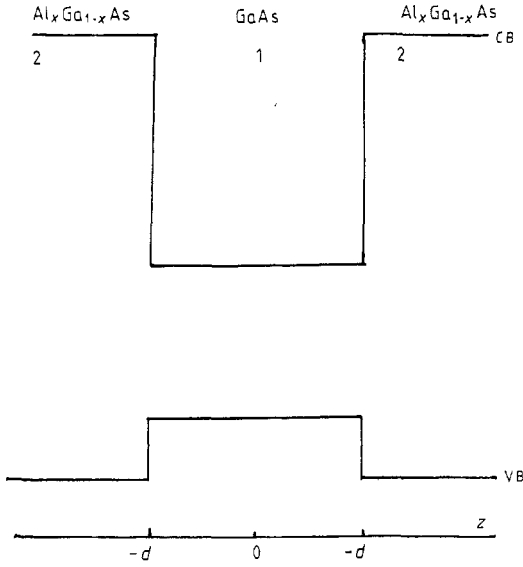


Figure 1. Quantum-well potential profile along the z axis normal to the interface of an $\text{Al}_x\text{Ga}_{1-x}\text{As}$ -GaAs- $\text{Al}_x\text{Ga}_{1-x}\text{As}$ heterostructure. The symbols CB and VB denote the conduction- and valence-band edges, respectively.

$$\begin{aligned}
 H = & \frac{P_{z_e}^2}{2m_e} + \frac{P_{z_h}^2}{2m_h} + \frac{P^2}{2M} + \frac{p^2}{2\mu} - \frac{e^2}{\epsilon_{\infty 1}[\rho^2 + (z_e - z_h)^2]^{1/2}} \\
 & + \sum_{k,m,p} a_{k,m,p}^+ a_{k,m,p} \hbar\omega_{\text{LO}} + \sum_{q,p} b_{q,p}^+ b_{q,p} \hbar\omega_{\text{sp}} \\
 & + \sum_{k,m} \{B^*[W_{k,m,+}(z_e, z_h, \rho)a_{k,m,+}^+ + W_{k,m,-}(z_e, z_h, \rho)a_{k,m,-}^+] \\
 & \times \exp(-i\mathbf{K} \cdot \mathbf{R}) + \text{HC}\} + \sum_q \left(\frac{\sinh(2qd)}{q}\right)^{1/2} \exp(-qd) \\
 & \times \{C^*[V_{q,+}(z_e, z_h, \rho)b_{q,+}^+ + V_{q,-}(z_e, z_h, \rho)b_{q,-}^+] \\
 & \times \exp(-\mathbf{q} \cdot \mathbf{R}) + \text{HC}\} + V_e(z_e) + V_h(z_h)
 \end{aligned} \tag{1}$$

with

$$V_e(z_e) = \begin{cases} V_{\text{img}}(z_e) & |z_e| \leq d \\ V_{\text{img}}(z_e) + V_0 & |z_e| > d \end{cases}$$

$$V_h(z_h) = \begin{cases} V_{\text{img}}(z_h) & |z_h| \leq d \\ V_{\text{img}}(z_h) + V'_0 & |z_h| > d \end{cases}$$

$$W_{\text{LO}}^2 = W_{\text{TO}}^2 \frac{(\epsilon_{01} + \epsilon_{02}) \mp (\epsilon_{01} - \epsilon_{02}) \exp(-2qd)}{(\epsilon_{\infty 1} + \epsilon_{\infty 2}) \mp (\epsilon_{\infty 1} - \epsilon_{\infty 2}) \exp(-2qd)}$$

$$W_{\text{LO}}^2 = W_{\text{TO}}^2 \epsilon_{01} / \epsilon_{\infty 1}$$

$$B^* = [(-4e^2 \hbar W_{\text{LO}} / V)(1/\epsilon_{\infty 1} - 1/\epsilon_{01})]^{1/2}$$

$$C^* = [-2e^2\hbar W_{LO}/A(\epsilon_{01} - \epsilon_{\infty 1})]^{1/2}$$

$$V_{q,\pm} = G_{\pm}(q, z_e) \exp(-is_2\mathbf{q} \cdot \boldsymbol{\rho}) - G_{\pm}(q, z_h) \exp(is_1\mathbf{q} \cdot \boldsymbol{\rho})$$

$$G_+(q, z) = \begin{cases} \{[\cosh(qz)/\cosh(qd)]/[(\epsilon_{\infty 1} + \epsilon_{\infty 2}) - (\epsilon_{\infty 1} - \epsilon_{\infty 2}) \exp(-2qd)]\} \\ \times \{[(\epsilon_{\infty 1} + \epsilon_{\infty 2}) - (\epsilon_{\infty 1} - \epsilon_{\infty 2}) \exp(-2qd)]/[(\epsilon_{01} + \epsilon_{02}) \\ - (\epsilon_{01} - \epsilon_{02}) \exp(-2qd)]\}^{1/4} & |z| \leq d \\ \{[\exp(-qz)/\exp(-qd)]/[(\epsilon_{\infty 1} + \epsilon_{\infty 2}) - (\epsilon_{\infty 1} - \epsilon_{\infty 2}) \exp(-2qd)]\} \\ \times \{[(\epsilon_{\infty 1} + \epsilon_{\infty 2}) - (\epsilon_{\infty 1} - \epsilon_{\infty 2}) \exp(-2qd)]/[(\epsilon_{01} + \epsilon_{02}) \\ - (\epsilon_{01} - \epsilon_{02}) \exp(-2qd)]\}^{1/4} & |z| > d \end{cases}$$

$$G_-(q, z) = \begin{cases} \{[\sinh(qz)/\sinh(qd)]/[(\epsilon_{\infty 1} + \epsilon_{\infty 2}) + (\epsilon_{\infty 1} - \epsilon_{\infty 2}) \exp(-2qd)]\} \\ \times \{[(\epsilon_{\infty 1} + \epsilon_{\infty 2}) + (\epsilon_{\infty 1} - \epsilon_{\infty 2}) \exp(-2qd)]/[(\epsilon_{01} + \epsilon_{02}) \\ + (\epsilon_{01} - \epsilon_{02}) \exp(-2qd)]\}^{1/4} & |z| \leq d \\ \{[\exp(-qz)/\exp(-qd)]/[(\epsilon_{\infty 1} + \epsilon_{\infty 2}) + (\epsilon_{\infty 1} - \epsilon_{\infty 2}) \exp(-2qd)]\} \\ \times \{[(\epsilon_{\infty 1} + \epsilon_{\infty 2}) + (\epsilon_{\infty 1} - \epsilon_{\infty 2}) \exp(-2qd)]/[(\epsilon_{01} + \epsilon_{02}) \\ + (\epsilon_{01} - \epsilon_{02}) \exp(-2qd)]\}^{1/4} & |z| > d \end{cases}$$

where $W_{k,m,+}$ and $W_{k,m,-}$ have the same expressions as those in [5], and the static image potential $V_{\text{img}}(z)$ inside the well has the following expressions [6]:

$$V_{\text{img}}(z_e) = (-e^2/2\epsilon_{\infty 1}d)\{\ln[2\epsilon_{\infty 2}/(\epsilon_{\infty 2} + \epsilon_{\infty 1})] \\ + (\epsilon_{\infty 2} - \epsilon_{\infty 1})z_e^2/(\epsilon_{\infty 2} + \epsilon_{\infty 1})(d^2 - z_e^2)\} \quad |z_e| \leq d$$

$$V_{\text{img}}(z_h) = (e^2/2\epsilon_{\infty 1}d)\{\ln[2\epsilon_{\infty 2}/(\epsilon_{\infty 2} + \epsilon_{\infty 1})] \\ + (\epsilon_{\infty 2} - \epsilon_{\infty 1})z_h^2/(\epsilon_{\infty 2} + \epsilon_{\infty 1})(d^2 - z_h^2)\} \quad |z_h| \leq d.$$

$V_{\text{img}}(z)$ outside the well ($|z| > d$) has a more complex expression which is not very important to the problems that we are discussing inside the well, and so we shall not consider it here for conciseness. V_0 and V'_0 are the depths of the potential well and ϵ_{01} and ϵ_{02} are the static dielectric constants of GaAs and $\text{Al}_x\text{Ga}_{1-x}\text{As}$, respectively, and $\epsilon_{\infty 1}$ and $\epsilon_{\infty 2}$ are the optical dielectric constants. All other quantities and operators have the same meanings as in [5].

Now we introduce the following two unitary transformations [7]:

$$U_1 = \exp\left(i\mathbf{K} \cdot \mathbf{R} - i \sum_{k,m,p} a_{k,m,p}^+ a_{k,m,p} \mathbf{K} \cdot \mathbf{R} - i \sum_{q,p} b_{q,p}^+ b_{q,p} \mathbf{q} \cdot \mathbf{R}\right)$$

$$U_2 = \exp\left(\sum_{k,m,p} (a_{k,m,p}^+ f_{k,m,p} - a_{k,m,p} f_{k,m,p}^*) + \sum_{q,p} (b_{q,p}^+ g_{q,p} - b_{q,p} g_{q,p}^*)\right).$$

Then the H in equation (1) can be transformed into

$$\mathcal{H} = U_2^{-1} U_1^{-1} H U_1 U_2. \tag{2}$$

Minimising (2) by setting

$$\partial \mathcal{H} / \partial f_{k,m,p} = \partial \mathcal{H} / \partial f_{k,m,p}^* = \partial \mathcal{H} / \partial g_{q,p} = \partial \mathcal{H} / \partial g_{q,p}^* = 0$$

we obtain

$$f_{k,m,\pm} = -2MB^*W_{k,m,\pm}/\hbar^2(k^2 + u_1^2) \quad f_{k,m,\pm}^* = -2MBW_{k,m,\pm}^*/\hbar(k^2 + u_1^2)^2$$

$$g_{q,\pm} = -[2MC^*/\hbar^2(q^2 + u_{sp}^2)]\{[\sinh(2qd)]/q\}^{1/2} V_{q,\pm} \exp(-qd)$$

$$g_{q,\pm}^* = -[2MC/\hbar^2(q^2 + u_{\text{sp}}^2)]\{[\sinh(2qd)]/q\}^{1/2} V_{q,\pm}^* \exp(-qd).$$

Here, we study only the slow exciton in the low-temperature limit (at zero temperature). Assume that Φ_0 expresses the unperturbed vacuum phonon state with the following properties:

$$a_{k,m,p}|\Phi_0\rangle = 0 \quad b_{qp}|\Phi_0\rangle = 0 \quad \langle\Phi_0|\Phi_0\rangle = 1.$$

Considering the effect of the lattice vibration, we can write the Hamiltonian \mathcal{H}_{ex} of the exciton as

$$\begin{aligned} \mathcal{H}_{\text{ex}} &= \langle\Phi_0|\mathcal{H}|\Phi_0\rangle \\ &= H_{2D} - (\hbar^2/2m_e)\nabla_{z_e}^2 - (\hbar^2/2m_h)\nabla_{z_h}^2 + V_{\text{img}}(z_e) \\ &\quad + V_{\text{img}}(z_h) + V_I(z_e, z_h, \rho) \quad |z_e|, |z_h| \leq d \end{aligned} \quad (3)$$

with

$$H_{2D} = -(\hbar^2/2\mu)\nabla_\rho^2 - \lambda_e^2/\varepsilon_{\infty 1}\rho$$

where H_{2D} is the internal motion energy of the exciton on the x - y plane and its effect has been discussed clearly in [5]. The last term $V_I(z_e, z_h, \rho)$ induced by the interaction of the SO and bulk LO phonons with the exciton can be divided into three parts, i.e.

$$V_I(z_e, z_h, \rho) = V_I^0(z_e) + V_I^0(z_h) + V_I'(z_e, z_h, \rho) \quad (4)$$

with

$$\begin{aligned} V_I^0(z_e) &= \frac{\hbar W_{\text{LO}} u_l}{d} \left\{ \sum_{m=1,3,\dots,\frac{1}{2}N} \left[(A_m + B_m s_2^2) \cos^2\left(\frac{m\pi}{2d} z_e\right) \right. \right. \\ &\quad \left. \left. + C_m \sin^2\left(\frac{m\pi}{2d} z_e\right) \right] + \sum_{m=2,4,\dots,\frac{1}{2}N} \left[(A_m + B_m s_2^2) \sin^2\left(\frac{m\pi}{2d} z_e\right) \right. \right. \\ &\quad \left. \left. + C_m \cos^2\left(\frac{m\pi}{2d} z_e\right) \right] \right\} - \frac{2M}{\hbar^2} \sum_q \frac{D_q}{\varepsilon_1(q) \cosh^2(qd)} \\ &\quad \times \left[\frac{q^2 + u_{\text{sp}}^2}{q^2} \cosh^2(qz_e) - \frac{M}{\mu} s_2^2 \cosh^2(qz_e) - \frac{M}{m_e} \sinh^2(qz_e) \right] \\ &\quad + \frac{2M}{\hbar^2} \sum_q \frac{D_q}{\varepsilon_2(q) \sinh^2(qd)} \left[-\frac{q^2 + u_{\text{sp}}^2}{q^2} \sinh^2(qz_e) \right. \\ &\quad \left. + \frac{M}{\mu} s_2^2 \sinh^2(qz_e) + \frac{M}{m_e} \cosh^2(qz_e) \right] \end{aligned}$$

with

$$A_m = \ln(m\pi/2du_l)/[u_l^2 - (m\pi/2d)^2]$$

$$B_m = (M/2\pi\mu)\{[u_l^2 - (m\pi/2d)^2]^{-1} + 2(m\pi/2d)^2 \ln(m\pi/2du_l)/[u_l^2 - (m\pi/2d)^2]^2\}$$

$$C_m = (M/2\pi m_e)(m\pi/2d)^2 [u_l^2 - (m\pi/2d)^2]^{-1} \{1/u_l^2 + 2 \ln(m\pi/2du_l)/[u_l^2 - (m\pi/2d)^2]\}$$

$$D_q = C^2 q \sinh(2qd) \exp(-2qd)/(q^2 + u_{\text{sp}}^2)^2$$

$$\varepsilon_1(q) = [(\varepsilon_{\infty 1} + \varepsilon_{\infty 2}) - (\varepsilon_{\infty 1} - \varepsilon_{\infty 2}) \exp(-2qd)]^{3/2} \\ \times [(\varepsilon_{01} + \varepsilon_{02}) - (\varepsilon_{01} - \varepsilon_{02}) \exp(-2qd)]^{1/2}$$

$$\varepsilon_2(q) = [(\varepsilon_{\infty 1} + \varepsilon_{\infty 2}) + (\varepsilon_{\infty 1} - \varepsilon_{\infty 2}) \exp(-2qd)]^{3/2} \\ \times [(\varepsilon_{01} + \varepsilon_{02}) + (\varepsilon_{01} - \varepsilon_{02}) \exp(-2qd)]^{1/2}.$$

$V_1^0(z_h)$ has the same expression as $V_1^0(z_e)$; the quantities corresponding to z_e , m_e and s_2 are z_h , m_h and s_1 , respectively.

$$V_1'(z_e, z_h, \rho) = \frac{\alpha \hbar W_{\text{LO}} u_l}{d} \left[\sum_{m=1,3,\dots,\dagger N} \cos\left(\frac{m\pi z_e}{2d}\right) \cos\left(\frac{m\pi z_h}{2d}\right) \right. \\ \left. + \sum_{m=2,4,\dots,\dagger N} \sin\frac{m\pi z_e}{2d} \sin\frac{m\pi z_h}{2d} \right] \\ \times \frac{2}{\pi} \int_0^\infty \left(1 + \frac{Ms_1 s_2 k^2}{\mu(k^2 + u_l^2)}\right) \frac{k J_0(\boldsymbol{\rho} \cdot \mathbf{k})}{(k^2 + u_l^2)[k^2 + (m\pi/2d)^2]} dk \\ + 4\alpha \hbar W_{\text{LO}} u_l \varepsilon_{\infty 1} \varepsilon_{01} \int_0^\infty \frac{\sinh(2qd) \exp(-2qd) q^2 J_0(\boldsymbol{\rho} \cdot \mathbf{q})}{\pi(q^2 + u_{\text{sp}}^2)^2} \\ \times \left(\frac{q^2 + u_{\text{sp}}^2}{q^2} + \frac{M}{\mu} s_1 s_2\right) \left(\frac{\cosh(qz_e) \cosh(qz_h)}{\varepsilon_1(q) \cosh^2(qd)} \right. \\ \left. + \frac{\sinh(qz_e) \sinh(qz_h)}{\varepsilon_2(q) \sinh^2(qd)}\right) dq.$$

3. Discussion

We rewrite \mathcal{H}_{ex} in equation (3) as

$$\mathcal{H}_{\text{ex}} = H_{2\text{D}} + H_{1\text{D}} + V_1'(z_e, z_h, \rho) \quad (5)$$

$$H_{1\text{D}} = \begin{cases} -(\hbar^2/2m_e)\nabla_{z_e}^2 - (\hbar^2/2m_h)\nabla_{z_h}^2 + V_{\text{img}}(z_e) + V_{\text{img}}(z_h) \\ \quad + V_1^0(z_e) + V_1^0(z_h) & |z_e|, |z_h| \leq d \\ -(\hbar^2/2m_h)\nabla_{z_e}^2 - (\hbar^2/2m_h)\nabla_{z_h}^2 + V_{\text{img}}(z_e) + V_{\text{img}}(z_h) \\ \quad + V_0 + V_0' & |z_e|, |z_h| > d. \end{cases}$$

The calculation shows that $V_1'(z_e, z_h, \rho)$ is smaller than $H_{2\text{D}} + H_{1\text{D}}$; so we can take $V_1'(z_e, z_h, \rho)$ as a perturbation and $H_{2\text{D}} + H_{1\text{D}}$ is unperturbed Hamiltonian of the exciton system, i.e.

$$\mathcal{H}_{\text{ex}}^0 = H_{2\text{D}} + H_{1\text{D}}$$

$$\mathcal{H}'_{\text{ex}} = V_1'(z_e, z_h, \rho).$$

For the electron, the image potential $V_{\text{img}}(z_e)$ is repulsive and, for the hole, $V_{\text{img}}(z_h)$ is attractive in the case of the GaAs–Al_xGa_{1-x}As quantum well; $V_1^0(z_e)$ and $V_1^0(z_h)$ induced by the interaction of the exciton with phonons are attractive and repulsive,

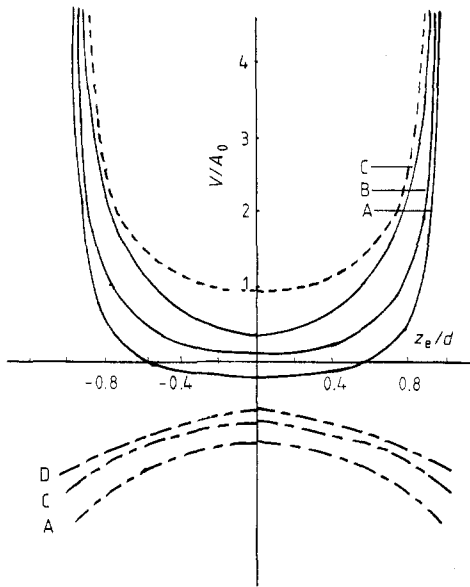


Figure 2. The potential profile of an electron in a quantum well along the z axis normal to the interface at different widths of the well. A, $N = 10$; B, $N = 20$; C, $N = 50$; D, $N = 100$. $A_0 = e^2 10^{-3} / 2\epsilon_x d$; broken curve, $V_{\text{img}}(z_e)$; chained curves, $V_1^0(z_e)$; full curves, the composition of $V_{\text{img}}(z_e)$ and $V_1^0(z_e)$.

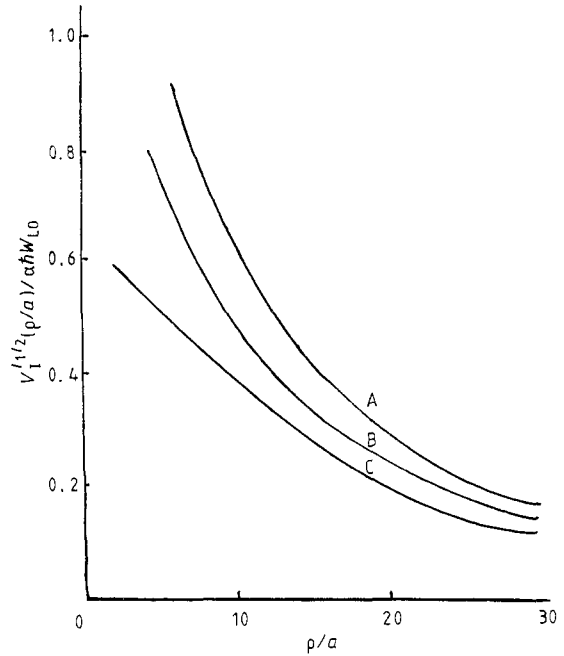


Figure 3. The induced potential as a function of the relative position between the electron and the hole ρ with lattice constant a . ($l_1 = l_2 = 1$). A, $N = 10$; B, $N = 20$; C, $N = 50$.

respectively. Figure 2 shows the composition of $V_1^0(z_e)$ and $V_{\text{img}}(z_e)$ at different widths N of the well. It is obvious that the composition of $V_1^0(z_e)$ or $V_1^0(z_h)$ and $V_{\text{img}}(z_e)$ or $V_{\text{img}}(z_h)$ can be seen approximately as a square well and, the thinner the well, the larger is $V_1^0(z_e)$ or $V_1^0(z_h)$ and the more accurate the approximation of the square well. For simplicity, supposing that (in equation (5)) $V_0, V'_0 \rightarrow \infty$, we can consider the electron (or hole) to move in a one-dimensional infinite-depth square potential well. Then the eigenfunctions and eigenenergies of H_{ID} are given by

$$|\psi_{l_1}(z_e)\psi_{l_2}(z_h)\rangle = \begin{cases} (1/d) \sin[(l_1\pi/2d)(z_e + d)] \sin[(l_2\pi/2d)(z_h + d)] & |z_e|, |z_h| \leq d \\ 0 & |z_e|, |z_h| > d \end{cases}$$

$$E_{l_1, l_2} = \pi^2 \hbar^2 l_1^2 / 8m_e d^2 + \pi^2 \hbar^2 l_2^2 / 8m_h d^2 \quad (l_1, l_2 = 1, 2, 3, 4, \dots, N).$$

Now the energy of the unperturbed exciton system is

$$E_0 = E_{2D} + E_{l_1 l_2}$$

and the first-order perturbation of $\mathcal{H}_{\text{ex}}^l$ to the exciton system energy is

$$\Delta E^{(1)} = \langle \varphi(\rho, \lambda) | V_1^{l_1 l_2}(\rho) | \varphi(\rho, \lambda) \rangle$$

with

$$V_1^{l_1 l_2}(\rho) = \langle \psi_{l_1}(z_e) \psi_{l_2}(z_h) | V_1'(z_e, z_h, \rho) | \psi_{l_2}(z_h) \psi_{l_1}(z_e) \rangle \quad (6)$$

where $|\phi(\rho, \lambda)\rangle$ is the eigenfunction of H_{2D} [5].

In equation (6), the fact that the induced potential $V_1^{l_1 l_2}(\rho)$ is relevant to the quantum numbers l_1 and l_2 shows that the magnitude of the interaction of the exciton with phonons relies on the motion state of the exciton in the z direction as well as on the width N of the well; this cannot be seen from the results in [5]. So we can see that a two-time unitary transformation to H is better than a one-time unitary transformation and the result reveals more properties of the exciton in a quantum well. Also, the calculation results are more accurate. Figure 3 shows the variation in the induced potential $V_1^{l_1 l_2}(\rho)$ with ρ (the projected distance between the electron and the hole onto the x - y plane) and N ($=d/a$, the width of the potential well) when $l_1 = 1$, $l_2 = 1$.

In our calculation, $\epsilon_{\infty 1}$ and ϵ_{01} for GaAs are 10.9 and 12.83, respectively, and $\epsilon_{\infty 2}$ and ϵ_{02} for $\text{Al}_{0.3}\text{Ga}_{0.7}\text{As}$ are 10.7 and 12.59, respectively.

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