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Impurity-Bound Polarons in Double Quantum Wells in Magnetic Fields

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Energy levels of a polaron bound indirectly to impurity ions in a double quantum well system are calculated in the adiabatic approximation by means of a perturbation method, in which the unperturbed system is treated by the variational theory of Lee-Low-Pines. The polaron binding energy as well as impurity energy levels are studied for variable well width, barrier thickness and magnetic fields. It is shown that the electron-phonon interaction contributes greatly to the binding energy and must not be ignored in a system of double quantum wells in any case.

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I. Introduction

The system of a double quantum well (DQW) structure has attracted much attention in recent years for various applications in optoelectronic devices [1-12]. A particular example may be the remarkably prolonged lifetimes [11] of a spatially indirect exciton in DQW systems, which is a direct consequence of the barrier between the electron-hole pair. While the binding energy of an indirect exciton becomes much smaller than the direct exciton in a single well, it remains large enough as compared to the thermal energy [1]. The investigation of such systems may therefore shed light into interesting possibilities such as the Bose condensation [11], excitonic superconductivity [13, 14] as well as the excitonic insulator state [15-17].

While there exist calculations of indirect excitons in magnetic fields [18, 19], little work can be found on the hydrogen-like atom in a double-well structure, a polaron in one well bound to impurity ions in the other. Such systems are particularly interesting for the study of electron-phonon interactions, which can strongly modify the electronic, optical and transport properties in reduced dimensions.

In a single quantum well, theoretical investigations have been carried out in great detail on a polaron either moving freely [20-22] or bound to an impurity center [23-25], as well as on the exciton ground state [26]. The problem becomes more interesting in a double well system as the Coulomb binding is greatly reduced by the barrier. In other words, contributions of Coulomb and electron-phonon interactions to the binding energy may be of the same order of magnitude, and their relative importance depends upon the well width and barrier thickness.

We calculate in this paper energy levels of a polaron bound to the impurity in a DQW, and investigate their dependence on the magnetic field, well width and barrier thickness. It is shown that in general the contribution of electron-phonon interaction to the binding energy can be as important as and may even exceeds the Coulomb attraction because of the barrier.

II. Theory

Consider a double quantum well structure with two wells of width d separated by a barrier of thickness D. We take the center of the first well as the origin and the growth direction as the z axis, along which a uniform magnetic field $\vec{B} = (0,0,$ B) is applied. The impurity center is situated at the center of the second well, namely, at $\vec{r}_i = (0,0,\ D + $ d). With the presence of the electron-phonon interaction, the total Hamiltonian of the system is

$$H = \frac{1}{2m_c}\left(\vec{p}+\frac{e}{c}\vec{A}\right)^2 + \frac{p_z^2}{2m} - \frac{e^2}{\varepsilon\sqrt{\rho^2+(D+d-z)^2}} + \sum_{\vec{k}} \hbar\omega a_{\vec{k}}^{\dagger} a_{\vec{k}} + \sum_{\vec{k}} \left(V_k^* e^{i\vec{k}\cdot\vec{r}} a_{\vec{k}}^{\dagger} + H.c.\right) + V_e(z) + V_i(z) \tag{1}$$

where m_e stands for the electron band mass, $\vec{p} = (\vec{p}_{//}, p_z)$ and $\vec{r} = (\vec{\rho}, z)$ are the momentum and position of the electron, respectively. The vector potential takes the form $\vec{A} = \left(-\frac{1}{2}B_M y,\ \frac{1}{2}B_M x, 0\right)$. The operator $a_{\vec{k}}^{\dagger}(a_{\vec{k}})$ creates (annihilates) a longitudinal optical (LO) phonon of frequency ω and wave vector $\vec{\kappa} = (k, k_z)$. The square wells are given by

$$V_e(z) = \begin{cases} 0, & z \leq |d/2| \\ \infty, & \text{otherwise,} \end{cases} \tag{2a}$$

$$V_i(z) = \begin{cases} 0, & D \text{ t } d/2 \leq z \leq D \text{ t } 3d/2 \\ \infty, & \text{otherwise.} \end{cases} \tag{2b}$$

The electron-phonon coupling strength is defined by

$$V_k = i\left(\frac{\hbar\omega_{LO}}{k}\right)\left(\frac{4\pi\alpha}{V}\right)^{1/2}\left(\frac{\hbar}{2m_e\omega_{LO}}\right)^{1/4} \tag{3a}$$

$$\alpha = \left(\frac{e^2}{2\hbar\omega_{LO} r_0}\right)\left(\frac{2m_e\omega_{LO}}{\hbar}\right)^{1/2}\left(\frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon_0}\right). \tag{3b}$$

When the magnetic field is sufficiently strong and the well width is not too large so that both the Landau level distance $eB/m_e c$ and level spacing $\pi^2\hbar^2/2m_e d^2$ due to the square-well confinement are large compared to the Coulomb attraction, the third term of the Hamiltonian can be treated as a perturbation. In the low-temperature limit, we can apply the variational theory of Lee, Low and Pine (LLP) with the adiabatic approximation and write the unperturbed wave function as [19,22]

$$|\Psi\rangle = \Phi(\vec{r})U|0\rangle = \phi(\vec{\rho})F(z)U|0\rangle. \tag{4}$$

In Eq. (4), the wave function $\phi(\vec{\rho})$ describes the electron motion in the xy-plane under the magnetic field and f(z) stands for the electron wave function in the z-direction. Their explicit forms are

$$\phi(\vec{\rho}) = \sqrt{\frac{n!}{2\pi[(n+|m|)!]}}\frac{\exp(im\varphi)}{\sqrt{\hbar c/eB}}\left(\frac{\rho}{\sqrt{2\hbar c/eB}}\right)^{|m|} L_n^{|m|}\left(\frac{\rho^2}{2\hbar c/eB}\right)\exp\left(-\frac{\rho^2}{4\hbar c/eB}\right) \tag{5a}$$

$$F(z) = \sqrt{\frac{2}{d}}\cos\left(\frac{l\pi}{d}z\right) \tag{5b}$$

where n is the quantum number labeling the Landau levels, m is the 2D angular momentum quantum number and l characterizes the z-component motion in the quantum wells. The phonon vaccum state is defined by $a_{\vec{k}}|0\rangle = 0$ and the LLP unitary transform is given by

$$U = \exp\left[\sum_{\vec{k}}\left(f_k a^\dagger_{\vec{k}} - f^*_k a_{\vec{k}}\right)\right] \tag{6a}$$

in which we have defined the variational function

$$f_k = -\frac{V^*_k}{\hbar\omega}\left\langle\Phi(\vec{r})|e^{-i\vec{k}\cdot\vec{r}}|\Phi(\vec{r})\right\rangle. \tag{6b}$$

The unperturbed energy eigenvalue of the system is therefore

$$\begin{aligned} E^0_{nml} &= \left\langle\Psi\left|H - \frac{e^2}{\varepsilon\sqrt{\rho^2+(D+d-z)^2}}\right|\Psi\right\rangle \\ &= \left(n+\frac{1}{2}\right)\hbar\omega_c + \frac{\hbar^2}{2m_e}\left(\frac{l\pi}{d}\right)^2 - \frac{4\pi\alpha\hbar\omega}{u_l d}f^{(0)}_{nml} \end{aligned} \tag{7a}$$

$$f^{(0)}_{nml} = \frac{n!}{(n+|m|)!}\int_0^\infty t^{|m|}\left[L_n^{|m|}(t)\right]^2 e^{-t}dt\int_0^{1/2}\frac{\cos^2(l\pi\xi)}{\sqrt{2\ell^2 t+\xi^2}}d\xi, \tag{7b}$$

where we have defined the phonon wave vector u_l through the relation $\hbar^2u_l^2/2m_e = \hbar\omega$ and the dimensionless quantity ℓ by the relation $\ell d = \sqrt{\hbar c/eB}$. Thus, a large ℓ means weak magnetic fields. The first term in Eq. (7a) gives the Landau level. The second term stands for the energy level of the electron motion along the z-direction, and the third term represents the electron-phonon interaction energy. Up to the first order perturbation, we find the energy levels

$$E_{nml} = E^{(0)}_{nml} + \Delta E_{nml} \tag{8a}$$

$$\Delta E_{nml} = \left\langle \Psi \left| \frac{-e^2}{\varepsilon\sqrt{\rho^2 + (D + d - z)^2}} \right| \Psi \right\rangle = -\frac{e^2}{\varepsilon d} f^{(1)}_{nml} \tag{8b}$$

$$f^{(1)}_{nml} = \frac{n!}{(n + |m|)!} \int_0^\infty t^{|m|} \left[L^{|m|}_n(t) \right]^2]e^{-t} dt \int_{-1/2}^{1/2} \frac{\cos^2(l\pi\xi)}{\sqrt{2\ell^2 t + (\delta + 1 - \xi)^2}} d\xi \tag{8c}$$

where $\delta =$ D/d. Equations (7) and (8) show clearly that only the Coulomb energy depends on the barrier thickness.

The binding energy of a polaron bound to the impurity center is defined as the difference between the bottom of conduction band and the ground state energy of the bound polaron. Thus, we have the binding energy

$$E_b = \frac{1}{2}\hbar\omega_c + \frac{\pi^2\hbar^2}{2m_e d^2} - E_{001} \tag{9a}$$

$$= \frac{4\pi\alpha\hbar\omega}{u_l d} f^{(0)}_{001} + \frac{e^2}{\varepsilon d} f^{(1)}_{001} \tag{9b}$$

in which the first term represents the contribution from the electron-phonon coupling and the second term comes from the Coulomb attraction. The two integrals in Eq. (9b) are

$$f^{(0)}_{001} = \int_0^\infty e^{-t} dt \int_0^{1/2} \frac{\cos^2(\pi\xi)}{\sqrt{2\ell^2 t + \xi^2}} d\xi \tag{10a}$$

$$f^{(1)}_{001} = \int_0^\infty e^{-t} dt \int_{-1/2}^{1/2} \frac{\cos^2(\pi\xi)}{\sqrt{2\ell^2 t + (\delta + 1 - \xi)^2}} d\xi. \tag{10b}$$

III. Results and discussion

We have obtained expressions for the energy level of impurity states in a double well system including the magnetopolaronic effects, as well as the polaron binding energy. To investigate how these energies vary with applied magnetic fields, the well width and the barrier thickness, numerical work is carried out for $GaAs/Ga_{1-x}Al_xAs$ as an example. The relevant parameters adopted in our computation are ε = 12.53, α = 0.0681, $\hbar\omega =$ 36.7 meV and $m_e =$ 0.067 mu, where mu is the electron hare mass.

We first look at the dependence of energy levels on the well width for a given barrier in a given field. The energy of the lowest three levels $(nml) = (001)$, (011) and (101) are listed in Table I for D = 20 Å and B = 10 T. It is clear that all three levels follow the same trend. The energy increases quickly with the decreasing well width. The spacing between (011) and (101) levels are roughly constant while that between (001) and (011) levels gradually increases when the well width reduces. The dependence of energy levels on the barrier thickness is calculated for d = 80 Å and ℓ^2 = 1 or $B =$ 10 T, and the results are plotted in Fig. 1. It is seen that in general the energy of all levels are insensitive to the barrier thickness, especially when $D \geq 2d$. To study the variation of energy levels with the applied magnetic field, we have calculated the energy as a function of ℓ^2 for d = 80 Å and $D =$ 10, 20 and 160 A. Only the data for D = 20 Å are plotted in Fig. 2 because the other two sets are basically the same, confirming the conclusion of Fig. 1. Recall that $\ell^2 \propto B^{-1}$ for a given well width. Our results are computed for magnetic fields within the range of 0.1 to 10 T. Figure 2 shows that as the field decreases, all energy levels drop in the high-field region but increase slightly in the low-field limit. This increase is understood as follows. The polaronic binding energy and the free electron energy carry opposite signs, and in general both of them in the well decrease in magnitude with decreasing magnetic fields. However, the latter decreases at a much faster rate as the field decreases than the former. The effect due to electron-phonon interactions is still decreasing while the free electron levels change little when the magnetic field is sufficiently low. In the weak field limit, therefore, the variation is dominated by electron-phonon interactions.

The binding energy of the system is now shown in Figs. 3-5 under various conditions. In order to demonstrate the importance of polaronic effects in DQW systems, we plot in every case the binding energy with and without the electron-phonon interaction included. In Fig. 3, the binding energy is shown as a function of the well width for $D =$ 20 Å and B = 10 T. We find that within the range $1 \leq d/D \leq 10$, the electron-phonon interaction contributes ~ 27.4 to 44.3% to the binding energy of an electron bound by the impurity center in the other well. As a function of the applied field, the binding energy is plotted in Fig. 4 for d = 80 Å and two barrier thickness. The results for $D =$ 10, 20 Å are very

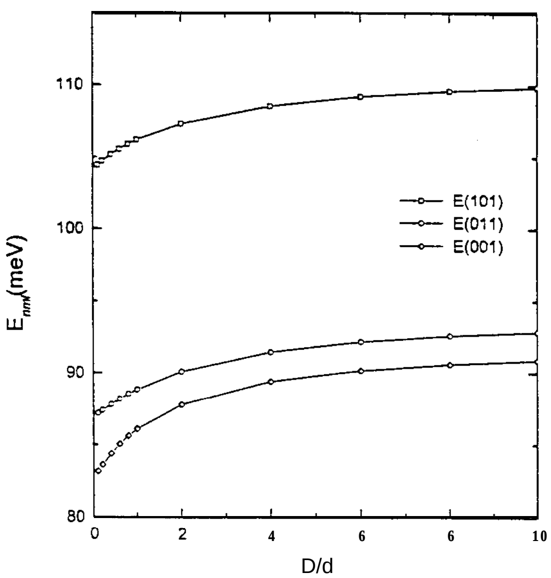

FIG. 1. Energy levels vs the barrier thickness D for a bound polaron in a double-well system of well width d = 80Å and $B =$ 10 T ($\ell^2 =$ 1).

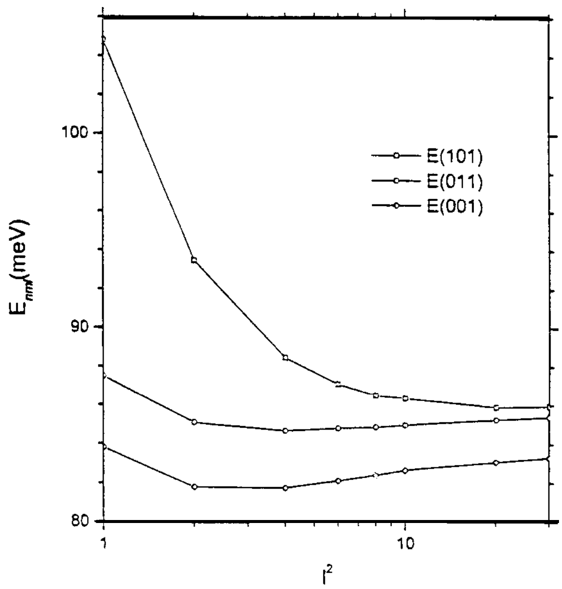

FIG. 2. Energy levels vs ℓ^2 for a bound polaron in a double-well system of well width $d = 80$Å and barrier thickness D = 20Å.

TABLE I. Variation of polaron energy levels with the well width in a DQW with $D = 20$ Å and B = 10 T.

d/D	1	2	4	6	8	10
E(OO1)	1394.32	343.96	83.64	36.77	21.05	14.15
E(011)	1400.91	349.21	87.27	39.54	23.29	16.05
E(101)	1416.43	365.46	104.11	56.54	40.34	33.12

similar as expected. The polaronic contribution to the binding energy increases with increasing magnetic field. For $1T \leq B \leq 10T$, the results in Fig. 4 indicate that 34.3 to 25.7% of the binding comes from the electron-phonon interaction. Finally, we look at the dependence of the binding on barrier thickness when d = 80 Åand B = 10 T in Fig. 5. It is observed once more that the electron-phonon interaction contributes at least 32% of the binding energy and the contribution may become exceedingly large as D increases. Hence, we conclude that the polaronic effect must be included in any discussion of impurity states in a DQW system, even though the electron-phonon interaction is in general small in single quantum wells.

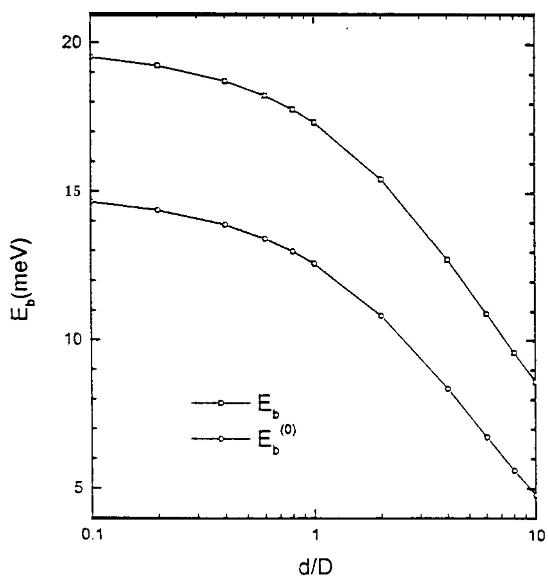

FIG. 3. Well-width dependence of the impurity binding energy with and without electron-phonon interaction for $D =$ 20Åand $B = 10$ T.

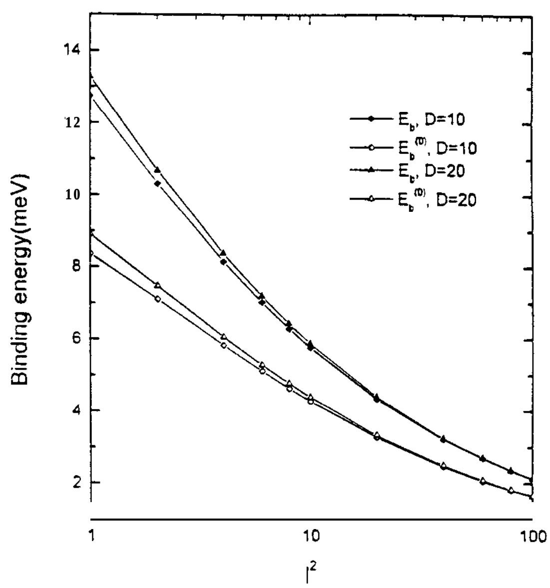

FIG. 4. Magnetic-field dependence of the impurity binding energy with and without electron-phonon interaction for d = 80Å, D = 10 and 20Å.

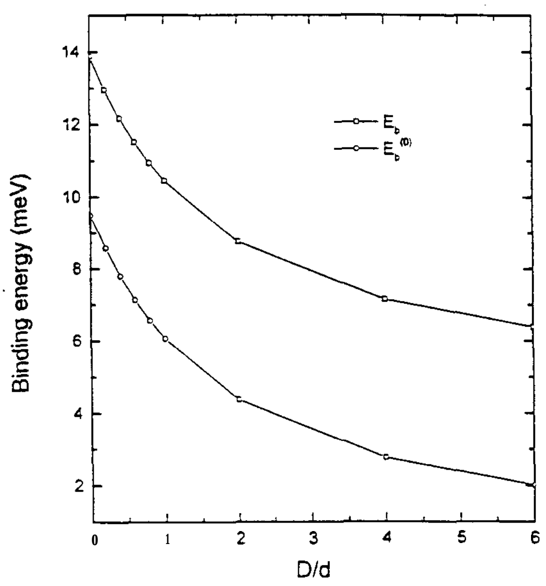

FIG. 5. Barrier-thickness dependence of the impurity binding energy with and without electron-phonon interaction for $d = 80$ Å and $B = 10$ T.

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References

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[1] Y. Kuramoto and C. Horie, Solid State Commun. 25, 713 (1978).
[2] E. J. Austin and M. Jaros, J. Phys. C19, 533 (1986).
[3] H. Kawai, J. Kaneko, and N. Watanabe, J. Appl. Phys. 58, 1263 (1985).
[4] A. Yariv, C. Lindsey and U. Siren, J. Appl. Phys. 58, 3669 (1985).
[5] Y. J. Chen, *et* al., Phys. Rev. B36, 4562 (1987).
[6] H. Q. Le, J. J. Zayhowski and W. D. Goodhue, Appl. Phys. Lett. 50, 1518 (1987).
[7] S. Charbonneau, *et* al., Phys. Rev. B38, 6287 (1988).
[8] M. Krahl, *et al.*, Appl. Phys. Lett. 52, 798 (1988).
[9] J. E. Golub, *et al.*, Appl. Phys. Lett. 53, 2584 (1988).
[10] G. Livescu, *et al.*, Phys. Rev. Lett. 63, 438 (1989).
[11] T. Fukazawa, *et* al., Surf. Sci. 228, 482 (1990).
[12] J. E. Golub, *et al.*, Phys. Rev. B41, 8564 (1990); *ibid. B45, 9477* (1992).
[13] Yu. E. Lozovik and V. I. Yudson, Zh. Eksp. Teor. Fiz. 71, 738 (1976); [Sov. Phys. JETP 44, 389 (1976)].
[14] S. I. Shevchenko, Fiz. Nizk. Temp. 2, 505 (1976); [Sov. J. Low Temp. Phys. 2, 251 (1976)].

[15] N. F. Mott, Philos. Mag. 6, 287 (1961).
[16] R. S. Knox, Theory of *Excitons, in Solid State Physics Suppl. 5,* eds. F. Seitz and D. Turnbull (Academic, New York, 1963).
[17] B. Bucher, P. Steiner and P. Wachter, Phys. Rev. Lett. 67, 2717 (1991).
[18] F. M. Peeters and J. E. Golub, Phys. Rev. B43, 5159 (1991).
[19] Yu. E. Lozovik and A. M. Ruvinsky, Phys. Lett. A227, 271 (1997).
[20] D. L. Lin, R. Chen and T. F. George, J. Phys.: Condens. Mat. 3, 4645 (1991).
[21] G. Q. Hai, F. M. Peeters and J. T. Devreese, Phys. Rev. B47, 10358 (1993).
[22] C. Y. Chen, P. W. Jin and S. Q. Zhang, J. Phys.: Condens. Mat. 4, 4483 (1992).
[23] D. L. Lin, R. Chen and T. F. George, Phys. Rev. 43, 9328 (1991); Chin. J. Phys. (Taipei) 30, 165 (1992).
[24] J. M. Shi, *et al.,* Phys. Rev. B44, 5692 (1991).
[25] R. Chen and D. L. Lin, Int. J. Mod. Phys. **B11**, 991 (1997).
[26] H. J. Xie, C. Y. Chen and S. D. Liang, Phys. Rev. B52, 1776 (1995).