Thickness effect on impurity-bound polaronic energy levels in a parabolic quantum dot in magnetic fields

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Energy levels of an impurity atom and its binding energy in a quantum dot with or without electron-phonon interactions are obtained by the second-order perturbation theory. The dot is confined laterally by a parabolic potential in quantum-well structures. The energy correction is expressed as a function of the strength of lateral confinement, the applied magnetic field, and the thickness of the quantum dot in question. It is shown that the binding energy depends sensitively on the thickness if it is of the order of the polaron size or less. In the case of thicker quantum dots, the finite thickness reduces the binding energy by approximately 10%. [S0163-1829(97)03047-6]

The rapid advances of nanofabrication technology have made it possible to work with quasi-zero-dimensional quantum dots in laboratories. Such systems are of great interest in fundamental studies because of the completely discrete electronic states, as well as in practical applications for microelectronic devices because of their design flexibility. Consequently there has been a large amount of work, both experimental[1–7] and theoretical,[8–13] on quantum dots of materials such as GaAs/$Ga_xAl_{1-x}As$ compounds. One of the major concerns in such systems is the impurity states, which have attracted extensive attention in recent years.[1–3,8,9]

In theoretical studies, the quantum dot is usually assumed to be either a sphere or a dot confined laterally by a parabolic potential in a plane normal to the growth direction in a quantum well. The spherical model may be easier to solve theoretically because of its high symmetry but can be very difficult to fabricate. The description of the lateral confinement by parabolic potentials is, in this sense, more realistic. As a matter of fact, the harmonic potential confinement has been successfully applied to account for many experiments such as far infrared spectroscopy,[1–3] capacitance,[4] and transport[5,6] measurements. The influence of external magnetic fields on the impurity states has also been investigated.

There exist numerous works that have demonstrated the significant influence of electron-phonon interactions on the electronic, optical as well as transport properties of microstructures such as quantum wells,[14–21] quantum wires,[22–25] and quantum dots.[10,26] However, the thickness of laterally confined quantum dots is generally ignored and the system is approximated as a two-dimensional (2D) problem in the literature. We study in this paper the thickness dependence of the binding energy of an impurity bound polaron in a parabolic confined quantum dot of finite thickness L. An external magnetic field $\mathbf{B}_M=(0,0,B_M)$ is applied in the growing direction of the quantum well.

Consider a quantum dot confined by a square well in the z direction and a harmonic potential in the xy plane. The impurity atom is situated at the origin. The Hamiltonian of an electron in the dot takes the form

$$H=\frac{1}{2m_e}(\mathbf{p}+e\mathbf{A})^2+\frac{1}{2}m_e\omega_0^2\rho^2+V(z)-\frac{e^2}{\varepsilon_\infty r}+\sum_{\mathbf{k}}\hbar\omega_{\mathrm{LO}}a_{\mathbf{k}}^\dagger a_{\mathbf{k}}+\sum_{\mathbf{k}}(V_k^* e^{-i\mathbf{k}\cdot\mathbf{r}}a_{\mathbf{k}}^\dagger+\mathrm{H.c.}), \quad (1)$$

where m_e stands for the electron band mass, $\mathbf{p}$ and $\mathbf{r}=(\boldsymbol{\rho},z)$ are the momentum and position of the electron, and ω_0 is a parameter characterizing the confinement strength in the xy plane. The vector potential is taken as $\mathbf{A}=(-\frac{1}{2}B_M y,\frac{1}{2}B_M x,0)$. The operator $a_{\mathbf{k}}^\dagger(a_{\mathbf{k}})$ creates (annihilates) a longitudinal optical (LO) phonon of frequency ω_{LO} and wave vector $\mathbf{k}=(\boldsymbol{\kappa},k_z)$. The potential

$$V(z)=\begin{cases}0, & |z|\leqslant L/2\\ \infty, & |z|>L/2\end{cases} \quad (2)$$

and the electron-phonon coupling

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

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

Here the notation is standard.

For convenience, we adopt the operator algebra introduced by Larsen[27] to describe electron motion in the xy plane. Thus,

$$A=\frac{1}{\sqrt{\hbar}\beta}\left[\left(p_x-\frac{\beta^2}{4}y\right)-i\left(p_y+\frac{\beta^2}{4}x\right)\right], \tag{4a}$$

$$B=A^{\dagger}-\frac{i\beta}{2\sqrt{\hbar}}(x+iy), \tag{4b}$$

where $\beta^2=2eB_M/c$, with the velocity of light c. Using the Fourier expansion

$$\frac{1}{r}=\sum_{\mathbf{k}}\frac{4\pi}{VQ^2}e^{-i\mathbf{Q}\cdot\mathbf{r}}, \tag{5}$$

we can rewrite the Hamiltonian as

$$\begin{aligned}H=&\left(A^{\dagger}A+\frac{1}{2}\right)\hbar\omega_c+(A^{\dagger}A+B^{\dagger}B+1-A^{\dagger}B^{\dagger}-AB)\hbar\omega_0\tau\\&+\frac{p_z^2}{2m_e}+\sum_{\mathbf{k}}\hbar\omega_{\mathrm{LO}}a_k^{\dagger}a_{\mathbf{k}}-\frac{e^2}{\varepsilon_\infty}\sum_{\mathbf{Q}}\frac{4\pi}{VQ^2}L_QM_Qe^{-iQ_zz}\\&+\sum_{\mathbf{k}}[V_{\mathbf{k}}^*L_kM_ke^{-ik_zz}a_{\mathbf{k}}^{\dagger}+\mathrm{H.c.}],\end{aligned} \tag{6}$$

where we have defined the operators

$$L_j=\exp\left\{\frac{\sqrt{\hbar}}{\beta}[(j_x+ij_y)A-(j_x-ij_y)A^{\dagger}]\right\},\quad j=k,Q, \tag{7a}$$

$$M_j=\exp\left\{\frac{\sqrt{\hbar}}{\beta}[(j_x-ij_y)B-(j_x+ij_y)B^{\dagger}]\right\},\quad j=k,Q \tag{7b}$$

with the cyclotron frequency $\omega_c=\beta^2/2m_e$ and $\tau=\omega_0/\omega_c$.

For weak electron-phonon coupling materials such as III-V compounds, the last term in Eq. (6) can be treated as a perturbation. In the low-temperature limit, no phonon is excited and we may write the unperturbed state as

$$|\Psi\rangle=f(z)(n!m!)^{-1/2}(A^{\dagger})^n|0\rangle_A(B^{\dagger})^m|0\rangle_B|0_{\mathbf{k}}\rangle, \tag{8a}$$

$$f(z)=\sqrt{2/L}\cos(l\pi z/2),\quad l=1,3,5,\ldots. \tag{8b}$$

It is not difficult to find that the unperturbed energy levels are

$$\begin{aligned}E_{l,n,m}^{(0)}=&(n+1/2)\hbar\omega_c+\hbar^2(l\pi)^2/2m_eL^2+(n+m+1)\hbar\omega_0\tau\\&-(e^2/\varepsilon_\infty L)F_1,\end{aligned} \tag{9a}$$

$$F_1=\int_0^\infty\frac{2\sinh(lr_0x/2)}{x}\exp(-r_0^2x^2/2\lambda^2)dx, \tag{9b}$$

where the quantum number n is for the Landau levels, m for the z component of the angular momentum, and l for the subband in the z direction. The polaron radius is $r_0=\sqrt{\hbar/2m_e\omega_{\mathrm{LO}}}$, $\ell=L/r_0$ and $\lambda^2=\omega_c/\omega_{\mathrm{LO}}$. The energy correction due to LO-phonon interactions can be found by second-order perturbation theory. The calculation is tedious but straightforward and we only present the result here, namely,

$$\begin{aligned}\Delta E^{(2)}=&-\alpha\hbar\omega_{\mathrm{LO}}\frac{l^2\pi^2}{\ell}\int_0^\infty\frac{\sinh(\ell r_0k)}{k(l^2\pi^2+\ell^2r_0^2k^2)}dk\\&\times\int_0^\infty\exp\left\{-t-\frac{r_0^2k^2}{\lambda^2}[1-e^{-\lambda^2}(1+\tau)t]\right\}\\=&-\alpha\hbar\omega_{\mathrm{LO}}F_2.\end{aligned} \tag{10}$$

Combining the above results, we find the energy levels of a polaron bound to an impurity atom at the origin

$$\begin{aligned}E_{l,n,m}=E_{l,n,m}^{(0)}+\Delta E^{(2)}=&\left(n+\frac{1}{2}\right)\hbar\omega_c+\frac{\hbar^2}{2m_e}\left(\frac{l\pi}{L}\right)^2\\&+(n+m+1)\hbar\omega_0\tau-\frac{e^2}{\varepsilon_\infty L}F_1(\ell,\lambda^2)\\&-\alpha\hbar\omega_{\mathrm{LO}}F_2(\ell,\tau,\lambda^2).\end{aligned} \tag{11}$$

The first term in Eq. (11) is the Landau level. The second represents subbands in the z direction. The third term stands for the energy correction due to the parabolic confinement in magnetic fields and the fourth term is the Coulomb binding due to the impurity center. The last term represents the second-order energy correction due to LO phonon modes. If E_e denotes the electron energy level in the quantum dot without any impurity, then the binding energy is given by

$$E_b=E_e-E_{l,n,m}=\frac{e^2}{\varepsilon_\infty L}F_1(\ell,\lambda^2)+\alpha\hbar\omega_{\mathrm{LO}}F_2(\ell,\tau,\lambda^2). \tag{12}$$

Equation (12) expresses the binding energy for every state (ℓ,n,m) as a function of the magnetic field λ^2, the lateral confinement τ, and the quantum dot thickness ℓ. In the limit of strong magnetic field $\lambda^2\to\infty$ and zero thickness, the second-order energy correction reduces to

$$\Delta E_s^{(2)}=-\frac{\sqrt{\pi}}{2}\alpha\lambda\hbar\omega_{\mathrm{LO}}. \tag{13}$$

In the weak field and zero thickness limit, we have $\exp[-\lambda^2(1+\tau)t]\approx1-\lambda^2(1+\tau)t$ and find from Eq. (10) the expression

$$\Delta E_w^{(2)}=-\pi\alpha\hbar\omega_{\mathrm{LO}}/2\sqrt{1+\tau}. \tag{14}$$

As an illustration, we calculate the binding energy of an impurity atom with and without the electron-phonon interaction in a realistic sample GaAs for which $\alpha=0.068$, $\hbar\omega_{\mathrm{LO}}=36.25$ meV, and $m_e=0.067m_0$,[28] where m_0 is the electron bare mass. Generally speaking, the electron-phonon interaction increases the binding energy by about 5% in every case. In Fig. 1, the dependence of E_b on the applied magnetic field is plotted for a quantum dot of thickness $\ell=0.5$. The binding energy increases generally with increasing field. In the strong field regime, namely, when $\lambda^2\geqslant1$ for which the cyclotron frequency $\omega_c\geqslant\omega_{\mathrm{LO}}$, it is observed that the binding energy is increasing at a much higher rate than in the weak

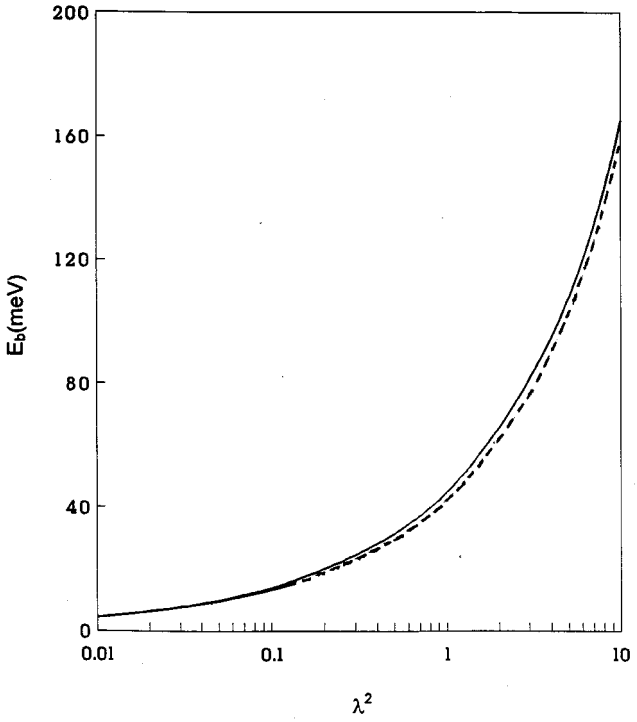

FIG. 1. Binding energy as a function of the applied magnetic field for an impurity bound electron in a quantum dot confined laterally by a parabolic potential, $l=1$, $\ell=0.5$, and $\gamma=0.5$. The solid line includes the electron-phonon interaction and the dashed line does not.

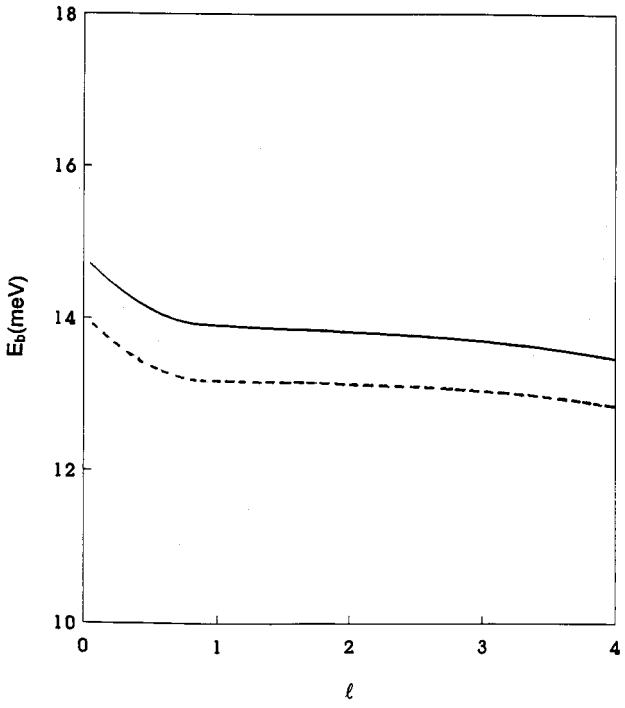

FIG. 2. Binding energy as a function of the thickness of the laterally confined quantum dot with $l=1$, $\lambda^2=0.5$, and $\gamma=0.5$. The solid line includes the electron-phonon interaction and the dashed line does not.

field region $\lambda^2<1$. This is not really surprising because the magnetic field not only adds extra binding to the orbiting electron, it also enhances the electron-phonon coupling as has been indicated in a previous study.[29] The thickness dependence of E_b is shown in Fig. 2 for a fixed field $\lambda^2=0.1$. It is clearly observed that the binding energy depends sensitively on the quantum dot thickness for $L\leqslant r_0\sim 50$ Å. In other words, when the confinement in the z direction becomes strong or when the thickness is of the order of the polaron size or smaller, measurements as well as calculations of properties involving impurity energies cannot ignore the thickness of the quantum dot.

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[1] C. Sikorski and U. Merkt, Phys. Rev. Lett. **62**, 2164 (1989).
[2] T. Demel, D. Heitmann, P. Grambow, and K. Ploog, Phys. Rev. Lett. **64**, 788 (1990).
[3] A. Lorke, J. P. Kotthaus, and K. Ploog, Phys. Rev. Lett. **64**, 2559 (1990).
[4] W. Hansen, T. P. Smith III, K. Y. Lee, J. A. Brum, C. M. Knoedler, J. M. Hong, and D. P. Kern, Phys. Rev. Lett. **62**, 2168 (1989).
[5] M. A. Reed, J. N. Randall, R. J. Aggarwal, R. J. Matyi, T. M. Moore, and A. E. Wetsel, Phys. Rev. Lett. **60**, 535 (1988).
[6] L. P. Kouwenhoven, F. W. J. Hekking, B. J. van Wees, C. J. P. M. Harmans, C. E. Timmering, and C. T. Foxon, Phys. Rev. Lett. **65**, 361 (1990).
[7] C. T. Liu, K. Nakamura, D. C. Tsui, K. Ismail, D. A. Antoniads, and H. I. Smith, Appl. Phys. Lett. **55**, 168 (1989).
[8] N. Porras-Montenegro and S. T. Perez-Merchancano, Phys. Rev. B **46**, 9780 (1992).
[9] A. Kumar, S. E. Laux, and F. Stern, Phys. Rev. B **42**, 5166 (1990).
[10] M. H. Degani and G. A. Farias, Phys. Rev. B **42**, 11 950 (1990).
[11] U. Merkt, J. Huser, and M. Wagner, Phys. Rev. B **43**, 7320 (1991).
[12] S. Normura and T. Kobayashi, Phys. Rev. B **45**, 1305 (1992).
[13] S. Mukhopadhyay and A. Chatterjee, J. Phys.: Condens. Matter **8**, 4017 (1996).
[14] M. H. Degani and O. Hipolito, Phys. Rev. B **35**, 4507 (1987).
[15] R. Chen and D. L. Lin, Int. J. Mod. Phys. B **11**, 991 (1997).
[16] C. Y. Chen, S. D. Liang, and M. Li, J. Phys.: Condens. Matter **6**, 1903 (1994).
[17] C. Y. Chen, D. L. Lin, P. W. Jin, and R. Chen, Phys. Rev. B **49**, 13 680 (1994).
[18] H. J. Xie, C. Y. Chen, and S. D. Liang, Phys. Rev. B **52**, 1776 (1995).
[19] T. A. Vaughan, R. J. Nicholas, C. J. G. M. Langerak, B. N. Murdin, C. R. Pidglon, N. J. Mason, and P. J. Walker, Phys. Rev. B **53**, 16 481 (1996).
[20] L. Liu, Y. Du, H. Zhou, and T. Lin, Phys. Rev. B **54**, 1953 (1996).

[21] G. Bongicovanni, A. Mura, F. Quochi, S. Giutler, J. L. Staehli, F. Tassone, R. P. Stanley, U. Oesterle, and R. Houdre, Phys. Rev. B **55**, 7084 (1997).
[22] S. D. Liang, C. Y. Chen, S. C. Jiang, and D. L. Lin, Phys. Rev. B **53**, 15 459 (1996).
[23] A. J. Kent, A. J. Naylor, P. Hawker, M. Henini, and B. Bacher, Phys. Rev. B **55**, 9775 (1997).
[24] V. V. Paranjape, Phys. Rev. B **53**, 6908 (1996).
[25] J. A. Kenrow, Phys. Rev. B **55**, 7809 (1997).
[26] S. Mukhopadhyay and A. Chatterjee, Phys. Rev. B **55**, 5944 (1997).
[27] D. M. Larsen, Phys. Rev. B **33**, 799 (1986).
[28] S. Adachi, J. Appl. Phys. **58**, R1 (1985).
[29] R. Chen, D. L. Lin, M. Shukri, and C. Y. Chen, Phys. Rev. B **46**, 13 357 (1992).