Magnetoexcitons in quantum wires with an anisotropic parabolic potential

Takuji Tanaka and Yasuhiko Arakawa
Institute of Industrial Science, University of Tokyo, 7-22-1 Roppongi, Minato-ku, Tokyo 106, Japan

Gerrit W. E. Bauer
Faculty of Applied Physics, Delft University of Technology, Lorentzweg 1, 2628 CJ Delft, The Netherlands
(Received 16 February 1994; revised manuscript received 20 May 1994)

We study theoretically exciton properties of quantum wires (QWR's) with an anisotropic two-dimensional parabolic potential in a magnetic field. First, the analytical solution for the single-particle states of the QWR's in the magnetic field is obtained. Then, the energy states are analyzed numerically including the Coulomb interaction between an electron-hole pair. The results show that the experimental results on magnetophotoluminescence (magneto-PL) of GaAs QWR's [Y. Nagamune, Y. Arakawa, S. Tsukamoto, M. Nishioka, S. Sasaki, and N. Miura, Phys. Rev. Lett. **69**, 2963 (1992)] can be well explained by this model, demonstrating the importance of the exciton effect to understand the magneto-PL properties of QWR's. On the other hand, the diamagnetic energy shift can be understood even without considering the Coulomb interaction, because the change of the exciton binding energy due to the magnetic field is relatively small compared to the total energy shift.

I. INTRODUCTION

Two-dimensional (2D) confinement of carriers in quantum wires (QWR's) is an important phenomenon in physics, and is expected to significantly improve performance of lasers and electronic devices.[1,2] Recently, several types of quantum wires of high quality have been realized by metal organic chemical vapor deposition (MOCVD).[3,4] In Ref. 4 clear blueshifts of the photoluminescence (PL) peak with decreasing lateral width of the QWR's have been reported. In addition, an anisotropic magneto-PL effect[5] confirms the quantum confinement effect, where the experimental data of the magneto-PL were compared to a simple model which neglected the exciton binding energy. Measurement of the polarization dependence of PL (Ref. 6) and of magneto-PL (Ref. 7) in multiple-quantum-well wire structures with lateral widths of 70–200 nm has also been reported. Previously, the analytical solution of magneto-PL energy in quantum structures [i.e., quantum wells (QW's), QWR's, and quantum dots (QD's)] has also been obtained only for noninteracting particles in parabolic potentials.[8–11] Recently, exciton properties of quantum dots in a magnetic field were analyzed for the special case of an isotropic parabolic confinement.[12] Quantum confinement, magnetic field, and electron-hole interactions are all expected to affect the optical properties of QWR's significantly. Therefore it is important to include all of these mechanisms in the analysis of the spectra.

In this paper, we first derive the analytical solution of the energy levels of a 1D carrier gas confined by an anisotropic 2D parabolic potential in the presence of a magnetic field without considering the Coulomb effect. Then we numerically calculate the magnetoexcitons in the QWR's, i.e., the effect of Coulomb interaction in the presence of a magnetic field and a QWR potential, by a variational method. The mutual relations among quantum confinement, magnetic field, and the exciton effect are discussed. Furthermore, the numerical results for magneto-PL are compared to the experimental results for the QWR's in Ref. 5.

II. THEORY

The Hamiltonian of an electron-hole pair with Coulomb interaction is

$$\hat{H}_{e,h,C} = \hat{H}_e + \hat{H}_h + \hat{H}_C, \tag{2.1}$$

where $\hat{H}_C = -e/4\pi\varepsilon r$,

$$r = \sqrt{(x_e - x_h)^2 + (y_e - y_h)^2 + (z_e - z_h)^2},$$

ε is the permittivity, and $\hat{H}_j$ is the Hamiltonian of a single particle (an electron or a hole denoted by $j = e, h$, respectively). Quantum structures (QD's, QWR's, and QW's) are assumed to be defined by a parabolic confinement potential. The single-particle Hamiltonian $\hat{H}_j$ of the structure in a magnetic field is then

$$\hat{H}_j = \frac{(\mathbf{P}_j + q\mathbf{A}_j)^2}{2m_j^*} + \sum_{\zeta=x,y,z} \tfrac{1}{2} m_j^* \omega_{\zeta,j}^2 \zeta_j^2, \tag{2.2}$$

where $\omega_{\zeta,j}$ ($\zeta = x, y, z$) is the oscillator frequency of the parabolic potential along the ζ_j direction, m_j^* is the isotropic effective mass, and q is the electron charge. If two (one, none) of $\omega_{x,j}$, $\omega_{y,j}$, and $\omega_{z,j}$ are (is) equal to zero, the structure is a QW (QWR, QD), respectively.

First, we describe the analytical solution for the Hamiltonian $\hat{H} = \hat{H}_j$ (the subscript j is omitted below) of a single particle in a magnetic field B along the z axis without Coulomb interaction. A gauge with the vector potential $\mathbf{A} = B(-w^2 y, v^2 x, 0)$, where $v = \sqrt{\omega_x/(\omega_x+\omega_y)}$ and $w = \sqrt{\omega_y/(\omega_x+\omega_y)}$, is used. The eigenfunction of the Hamiltonian $\hat{H}$ can be separated into functions of (x,y) and z. The eigenenergy of the Hamiltonian is expressed as the sum of eigenenergies along the (x,y) plane (perpendicular to the magnetic field $\mathbf{B}$) $E^{(x,y)}$ and along the z axis (parallel to the magnetic field $\mathbf{B}$) $E^{(z)}$. The eigenenergy along the z axis parallel to the magnetic field is

$$E^{(z)} = \begin{cases} (l+\frac{1}{2})\hbar\omega_z & (\omega_z \neq 0), \\ \dfrac{p_z^2}{2m^*} & (\omega_z = 0), \end{cases} \tag{2.3}$$

where p_z is the momentum of a plane wave along the z axis, and l is an integer.

The problem of a carrier in the (x,y) plane perpendicular to the magnetic field along the z axis is solved as follows. In the case of $\omega_\xi = 0$ and $\omega_\eta \neq 0$ $(\xi,\eta = x,y)$, the Schrödinger equation can be solved to obtain the eigenenergy[8]

$$E^{(x,y)}_{n,p_\xi} = (n+\tfrac{1}{2})\hbar\omega_0 + \frac{p_\xi^2}{2m^*}\frac{\omega_\xi^2}{\omega_0^2}\,, \tag{2.4}$$

where $\omega_0 = \sqrt{\omega_c{}^2 + (\omega_x+\omega_y)^2}$, $\omega_c = qB/m^*$ is the cyclotron frequency, p_ξ is the momentum of the plane wave along the ξ axis, and $n = 0,1,2,\ldots$ is the order of the Hermite polynomials.

When $\omega_x\omega_y \neq 0$, we can make the ansatz $\Psi = \Phi\exp(-\frac{1}{2}X^2 - \frac{1}{2}Y^2)$, where $X = vx\sqrt{m^*\omega_0/\hbar}$ and $Y = wy\sqrt{m^*\omega_0/\hbar}$. The Schrödinger equation $\hat{H}^{(x,y)}\Psi(x,y) = E^{(x,y)}\Psi(x,y)$ is then transformed into $\hat{H}_1\Phi = (E^{(x,y)} - E_0)\Phi$, where

$$\begin{aligned}\hat{H}_1 = E_0\Bigg\{ & v^2\left(-\frac{\partial^2}{\partial X^2} + 2X\frac{\partial}{\partial X}\right) \\ & + w^2\left(-\frac{\partial^2}{\partial Y^2} + 2Y\frac{\partial}{\partial Y}\right)\Bigg\} \\ & - 2ivwE_c\left(X\frac{\partial}{\partial Y} - Y\frac{\partial}{\partial X}\right),\end{aligned} \tag{2.5}$$

$E_0 = \frac{1}{2}\hbar\omega_0$, and $E_c = \frac{1}{2}\hbar\omega_c$.

Furthermore, the wave function Φ can be expanded by basis functions

$$u_{k,m} = \frac{H_m(X)H_{k-m}(Y)}{\sqrt{m!(k-m)!}}\,, \tag{2.6}$$

where $H_n(t)$ are the Hermite polynomials

$$H_n(t) = \sum_{r=0}^{[n/2]} (-1)^r (2r-1)!! \binom{n}{2r} 2^r t^{n-2r}, \tag{2.7}$$

$(k = 1,2,\ldots;\ m = 0,1,2,\ldots,k)$. Then the Hamiltonian $\hat{H}_1$ is determined by the matrix with dimension $(k+1)\times(k+1)$ as follows:

$$\begin{aligned}\langle u_{k,n}|\hat{H}_1|u_{k,n'}\rangle = & [k - (v^2-w^2)(k-2n)]E_0\delta_{n,n'} \\ & - 2ivwE_c\sqrt{k-n+1}\sqrt{n} \\ & \times(\delta_{n,n'-1} - \delta_{n-1,n'}).\end{aligned} \tag{2.8}$$

The eigenenergy $E^{(x,y)}_{k,m}$ of the Schrödinger equation can be found by diagonalizing this matrix,

$$E^{(x,y)}_{k,m} = (1+k)E_0 + (k-2m)E_1, \tag{2.9}$$

where $E_0 = \frac{1}{2}\hbar\sqrt{\omega_c{}^2 + (\omega_x+\omega_y)^2}$, and $E_1 = \frac{1}{2}\hbar\sqrt{\omega_c{}^2 + (\omega_x-\omega_y)^2}$. This eigenenergy is equal to the value obtained in a somewhat different context.[9] In the isotropic case of $\omega_x = \omega_y$, the eigenvalue is equal to the value given by Fock[10] and Liu *et al.*[11] In this paper, we focus on the ground state with the energy $E = E_0 + \frac{1}{2}\hbar\omega_z$ and the eigenfunction along the (x,y) plane $\Psi = \exp(-\frac{1}{2}X^2 - \frac{1}{2}Y^2)$.

In the following, we discuss our numerical method for the magnetoexciton effect on an electron-hole pair in a QWR. The variational method is used for the Hamiltonian $\hat{H}_{e,h,C}$ determined by Eq. (2.1). We assume a variational function of the form $\Psi_{e,h,C} = \phi_1\phi_2$, where

$$\phi_1 = \exp\left(-\sum_{j=e,h}\left(\alpha_{x,j}x_j^2 + \alpha_{y,j}y_j^2 + \alpha_{z,j}z_j^2\right)\right), \tag{2.10}$$

$$\phi_2 = \exp(-\beta r), \tag{2.11}$$

and $\alpha_{\zeta,j}, \beta$ are variational parameters. ϕ_1 is the Gaussian function which gives the correct eigenfunction for the Hamiltonian $\hat{H}_e + \hat{H}_h$, describing the effect of the 2D parabolic confinement and of the magnetic field. ϕ_2 is the hydrogenic function which gives the correct eigenfunction for the Hamiltonian $\hat{H}_C$, describing the effect of the Coulomb force. The energy is computed as

$$E_{e,h,C} = \min\frac{\langle\Psi_{e,h,C}|\hat{H}_{e,h,C}|\Psi_{e,h,C}\rangle}{\langle\Psi_{e,h,C}|\Psi_{e,h,C}\rangle}. \tag{2.12}$$

The exciton binding energy of the system is defined as $E_C = E_e + E_h - E_{e,h,C}$. We parametrize the parabolic confinement potentials in terms of equivalent widths L_ζ, which are chosen such that the ground state single-particle energies $\frac{1}{2}\hbar\omega_{\zeta,j}$ agree with that of an infinite-barrier square well $\hbar^2\pi^2/2m_j^*L_\zeta^2$.

III. RESULTS AND DISCUSSION

Figure 1 shows calculated exciton binding energies E_C of the following quantum structures: (a) a QW with $L_z = L_W, L_x = L_y = \infty$, (b) a QWR with $L_x = L_y = L_W, L_z = \infty$, and (c) a QD with $L_x =$

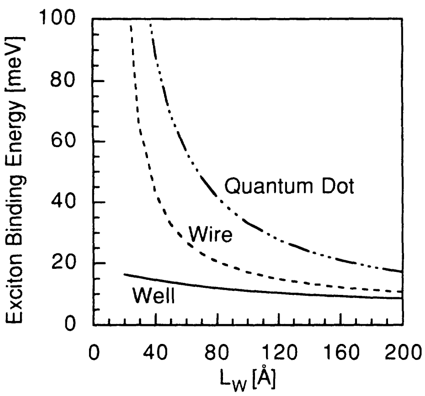

FIG. 1. Exciton binding energies of quantum structures: (a) quantum well with $L_z = L_W, L_x = L_y = \infty$, (b) quantum wire with $L_x = L_y = L_W, L_z = \infty$, (c) quantum dot with $L_x = L_y = L_z = L_W$.

$L_y = L_z = L_W$, using the material parameters of bulk GaAs, $m_e^* = 0.067m_0$, $m_h^* = 0.45m_0$, and $\varepsilon = 12.8\varepsilon_0$. In a quantum well, the static dielectric constant ϵ under a perturbing electric field is known to be reduced by quantum confinement and to have an anisotropy along the direction of the electric field.[13] However, the reduction of ϵ is small in the parameter regime of our interest (larger than 30 Å). Therefore we used the isotropic ϵ of bulk GaAs. At $L_W = \infty$, the calculated exciton binding energy E_C of all three structures reaches the bulk exciton value of $m_r^* e^4/32\pi^2\varepsilon^2\hbar^2 \simeq 4.8$ meV, where $m_r^* = m_e^* m_h^*/(m_e^* + m_h^*)$ is the reduced effective mass. In addition, at $L_W = 0$, E_C of the QW reaches the analytical value $m_r^* e^4/8\pi^2\varepsilon^2\hbar^2 \simeq 19.4$ meV.[14] In this case, the exciton wave function is a δ function along the confined direction and a hydrogenic function along the QW plane,[14] and is asymptotically given by our variational function $\Psi_{e,h,C} = \phi_1\phi_2$ with the parameters $\alpha_{x,j}, \alpha_{y,j} \to \infty$ $(j = e, h)$. Moreover, our calculated exciton binding energies for the QWR and the QD are consistent with the results by previous workers.[12,15,16]

In order to clarify the exciton properties in our model, we calculate (a) the exciton binding energy E_C and (b) the root mean square of the relative separation $\sqrt{\langle(\zeta_e - \zeta_h)^2\rangle}$ along the ζ $(\zeta = x, y, z)$ axis for a QD with variable confinement along one axis (z) and fixed confinement along the other axes (x, y). The results are shown in Fig. 2. In Fig. 2(b), it is seen that the relative separation is not much changed along x, y, but increases strongly with L_z until it reaches a constant corresponding to the exciton radius of the QWR. A different measure of the exciton states is provided by the normalized parameter $t_\zeta = \beta/\sqrt{2\alpha_\zeta}$ $(\zeta = x, y, z)$, where $1/\alpha_\zeta = 1/\alpha_{\zeta,e} + 1/\alpha_{\zeta,h}$. t_ζ describes the character of the variational function along the ζ axis, which can be more Gaussian-like $(t_\zeta \to 0)$ or more hydrogen-like $(t_\zeta \to \infty)$. When $L_z \gg L_x, L_y$, the parameters are related as $t_z > t_x, t_y$. When $L_z \ll L_x, L_y$, $t_z < t_x, t_y$. These show that the wave function is more hydrogenlike along the direction which is less tightly confined by the parabolic potential. On the other hand, the wave function is more Gaussian-like along the direction which is more tightly confined.

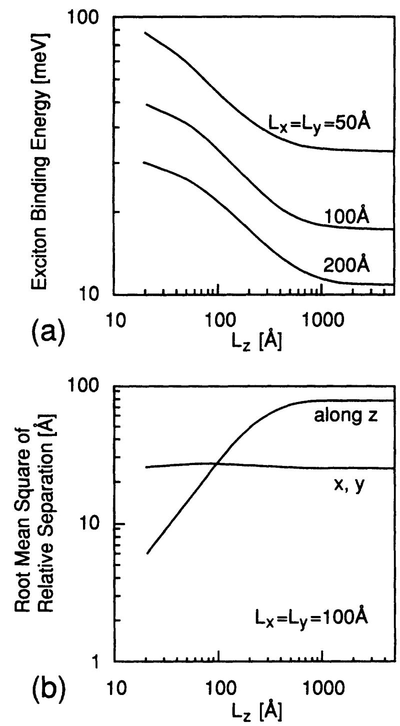

FIG. 2. (a) Exciton binding energy E_C and (b) root mean square of electron-hole separation in the ground state $\sqrt{\langle(\zeta_e - \zeta_h)^2\rangle}$ along the ζ $(\zeta = x, y, z)$ axis, for a quantum dot which has variable dimension along one axis (z) and fixed dimension along other axes (x, y).

Figure 3 shows the dependence of (a) the magneto-PL energy calculated with the Coulomb force $(E_{e,h,C} + E_g)$ and without the Coulomb force $(E_e + E_h + E_g)$, and (b) the exciton binding energy E_C of a QWR with an anisotropic 2D parabolic potential on magnetic fields along the different directions, where E_g is the band gap. In this calculation, the following parameters are used: $L_x = 102.5$ Å, $L_y = 198.8$ Å, $m_h = 0.48m_0$, $m_e = 1.42 \times 0.067m_0$, $\varepsilon = 12.8\varepsilon_0$, and $E_g = 1.519$ eV. The experimental results of magneto-PL for the QWR's in Ref. 5 are also shown in Fig. 3(a). It is seen that, assuming an electron mass 1.42 times heavier than in bulk GaAs, the magnetoexciton energy $E_{e,h,C} + E_g$ fits the experimental magneto-PL of the QWR's in Ref. 5. This heavier value of the electron mass is consistent with a theoretical calculation including nonparabolicity of the conduction band, which shows the electron mass of QWR's is heavier than that of the bulk by the factor 1.45.[17] The dimensional parameters $L_x = 102.5$ Å, $L_y = 198.8$ Å are close to the dimensions estimated in Ref. 5 (10 nm and 20 nm). However, the magneto-PL energy calculated without the exciton effect $E_e + E_h + E_g$ with the same parameters does not fit the experiments. These results show that our model including the exciton effect well explains the anisotropic magneto-PL, and supports the 2D

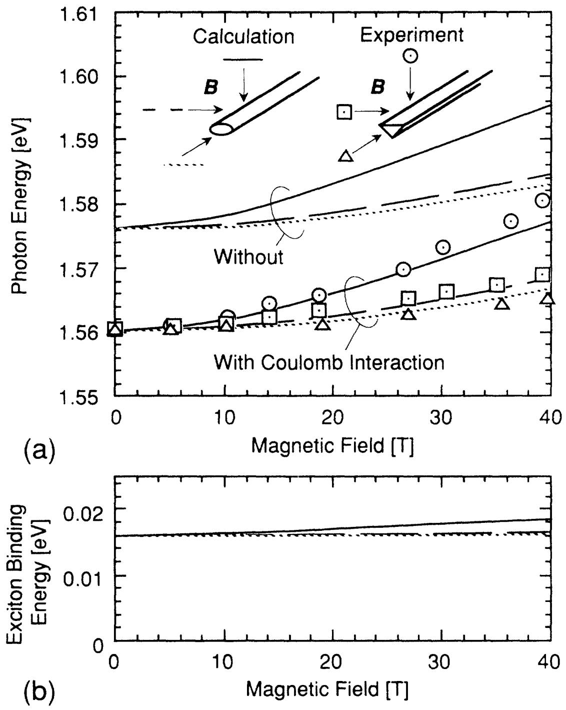

FIG. 3. (a) Photon energy $E_{e,h,C} + E_g$ (calculated with Coulomb interaction) and $E_e+E_h+E_g$ (without Coulomb interaction), (b) exciton binding energy E_C of a quantum wire with an anisotropic 2D parabolic potential (L_x = 102.5 Å, L_y = 198.8 Å, $L_z = \infty$) with different direction and magnitude of the magnetic field. Effective masses are taken as $m_h = 0.48m_0$ and $m_e = 1.42 \times 0.067m_0$. Solid, broken, and dotted lines show the magnetic field along x, y, and z, respectively. In (a), experimental magnetophotoluminescence data of the quantum wires in Ref. 5 are shown. Circles, squares, and triangles represent the data for $\mathbf{w} \perp \mathbf{B} \parallel \mathbf{k}$, $\mathbf{w} \perp \mathbf{B} \perp \mathbf{k}$, and $\mathbf{w} \parallel \mathbf{B} \perp \mathbf{k}$, respectively, where $\mathbf{w}$ and $\mathbf{k}$ are a vector parallel to the quantum wires and a vector perpendicular to the substrate, respectively. Inset: Schematic illustrations of the quantum wires and the directions of the magnetic field.

anisotropic confinement effect in QWR's. This demonstrates that the exciton effect is important to understanding magneto-PL properties.

On the other hand, the relative energy shift due to the magnetic field can be explained without the Coulomb interaction. As shown in Fig. 3(a), the energy shift is larger for magnetic fields normal to the direction of weaker confinement (i.e., the energy shift for $\mathbf{B} \parallel x$ is larger than that for $\mathbf{B} \parallel y$, which is again larger than that for $\mathbf{B} \parallel z \parallel$ QWR). The value of the relative energy shift due to the magnetic field is almost the same for the calculations with and without Coulomb interaction. These properties are explained as follows. The change of the exciton binding energy and the energy shift with the magnetic field is compared in Figs. 3(a) and 3(b). At $\mathbf{B} \parallel x$ and $B = 40$ T, the energy shift $E_{e,h,C}$ increases 17.0 meV compared to $B = 0$, while the exciton binding energy E_C increases only 2.2 meV. The change of the exciton binding energy is small (about 13%) compared to the energy shift due to the magnetic field. Thus, in the parameter regime of present interest[5] the ground state energy levels of QWR's in magnetic fields can be understood by the sum of electron and/or hole single-particle energies and the zero-field exciton binding energy.

IV. SUMMARY

In summary, we have described the analytical solution of energy levels of a 1D carrier gas confined by an anisotropic 2D parabolic potential in the presence of a magnetic field. The exciton properties of a QW with an anisotropic 2D parabolic potential in a magnetic field have also been calculated. The numerical calculations including Coulomb interaction agree with the experimental magneto-PL data of QWR's in Ref. 5 and the results support the 2D anisotropic confinement of the QWR's. The exciton effect turns out to be important to determine the magneto-PL in QWR's. On the other hand, the relative energy shift due to the magnetic field can be explained by noninteracting particles, because in the present structures the change of the magnetoexciton binding energy is relatively small compared to the energy shift caused by the magnetic field. Therefore the energy level of a QWR in a magnetic field can be understood as the sum of the energy level calculated without Coulomb interaction and the exciton binding energy at zero magnetic field.

ACKNOWLEDGMENTS

The authors express their thanks to Professor Y. Fujii, Professor T. Ikoma, Professor H. Sakaki, and Dr. Y. Nagamune, University of Tokyo, for their discussions and encouragement, and Dr. R. Helkey and Dr. A. B. Dzyubenko for their helpful comments. This work is supported by the University-Industry Joint Project on Mesoscopic Electronics, a Grant-in-Aid for Scientific Research on Priority Area, the TEPCO Research Foundation, and the Japan Society for the Promotion of Science.

[1] Y. Arakawa and H. Sakaki, Appl. Phys. Lett. **40**, 939 (1982).
[2] Y. Arakawa, K. Vahala, and A. Yariv, Appl. Phys. Lett. **45**, 950 (1984).
[3] E. Kapon, E. Kash, E. M. Clausen, Jr., D. M. Hwang, and E. Colas, Appl. Phys. Lett. **60**, 477 (1992).
[4] S. Tsukamoto, Y. Nagamune, M. Nishioka, and Y. Arakawa, Appl. Phys. Lett. **63**, 355 (1993).
[5] Y. Nagamune, Y. Arakawa, S. Tsukamoto, M. Nishioka, S. Sasaki, and N. Miura, Phys. Rev. Lett. **69**, 2963 (1992).
[6] M. Kohl, D. Heitmann, P. Grambow, and K. Ploog, Superlatt. Microstruct. **5**, 235 (1989).

[7] M. Kohl, D. Heitmann, P. Grambow, and K. Ploog, Phys. Rev. Lett. **63**, 2124 (1989).
[8] K.-F. Berggren, T. J. Thornton, D. J. Newson, and M. Pepper, Phys. Rev. Lett. **57**, 1769 (1986).
[9] S. K. Yip, Phys. Rev. B **43**, 1707 (1991).
[10] V. Fock, Z. Phys. **47**, 446 (1928).
[11] C. T. Liu, K. Nakamura, D. C. Tshi, K. Ismail, D. A. Antoniadis, and H. I. Smith, Appl. Phys. Lett. **55**, 168 (1989).
[12] V. Halonen, Tapash Chakraborty, and P. Pietiläinen, Phys. Rev. B **45**, 5980 (1992).
[13] Raphael Tsu and Liderio Ioriatti, Superlatt. Microstruct. **1**, 295 (1985).
[14] M. Shinada and S. Sugano, J. Phys. Soc. Jpn. **21**, 1936 (1966).
[15] W. Que, Phys. Rev. B **45**, 11 036 (1992).
[16] M. H. Degani and O. Hipólito, Phys. Rev. B **35**, 9345 (1987).
[17] T. Yamauchi, Y. Arakawa, and J. N. Schulman, Appl. Phys. Lett. **57**, 1224 (1990).