Electronic properties of anisotropic quantum dots in a magnetic field

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We have studied the electronic properties of anisotropic quantum dots in a magnetic field. The evolution of single-electron energy levels as a function of magnetic field and the corresponding chemical potentials are investigated for various cases of anisotropy. We have also analyzed the effect of interelectron interaction on the isotropic as well as anisotropic quantum dots by calculating the energy spectra and the pair-correlation function of a two-electron system.

I. INTRODUCTION

Artificial atoms[1,2] created in semiconductor heterostructures are mesoscopic systems whose electronic properties are very much of current interest.[3–5] These few-electron nanostructures have been probed recently by a variety of techniques, viz., optical spectroscopy on dot arrays,[6] capacitance spectroscopy on a single dot,[7] and magnetotransport measurements.[8] The most unique feature of these experiments is that they all provide information about the energy spectra (and other related quantities) for which reliable theories can be formulated.[1,2] One such case is the spin transitions studied in Refs. 2 and 9, and its possible detection as reported in Ref. 7. Although most of the work on these systems is for circular dots, there have been some recent experimental studies on elliptical dots.[10] Also, the confinement potential of the dots studied by McEuen *et al.*[8] was found to be anisotropic. In this paper, we have reported results for the electron states of anisotropic quantum dots. We have studied the evolution of the energy levels (single- as well as two-electron systems) with increasing magnetic field and anisotropy. The selection rules for the dipole transitions are also calculated. We then calculate the chemical potential based on a simple approximation. This quantity has been measured recently in a single quantum dot.[7] Anisotropy in a quantum dot has been treated earlier as a perturbation[11] to the isotropic parabolic quantum dot, which is not expected to be correct for large anisotropy. However, one can derive, as demonstrated below, analytical results for the single-electron system. Finally, we have included a model interelectron interaction, which results in a considerable simplification of the problem. The numerical results are found to be qualitatively reliable when compared with the Coulomb interaction results.

The paper is organized as follows: In Sec. II, the analytical results for a single electron in an anisotropic quantum dot are derived. The method of calculating the chemical potential is also discussed there. The analysis of the two-electron system is presented in Sec. III. A summary of the work is available in Sec. IV.

II. SINGLE-ELECTRON SYSTEM

Let us consider a lone electron in a lateral anisotropic parabolic confinement potential in the presence of a quantizing perpendicular magnetic field. The Hamiltonian is

$$\mathcal{H}=\frac{1}{2m_e}\left[\mathbf{p}-\frac{e}{c}\mathbf{A}\right]^2+V_{\rm conf}(x,y)\ , \tag{1}$$

where the confinement potential is

$$V_{\rm conf}(x,y)=\tfrac{1}{2}m_e(\omega_x^2x^2+\omega_y^2y^2)\ . \tag{2}$$

We choose the symmetric gauge vector potential $\mathbf{A}=\frac{1}{2}B(-y,x,0)$ and make the following transformations:

$$\begin{aligned} x&=q_1\cos\chi-\frac{\chi_2}{\chi}p_2\sin\chi\ ,\\ y&=q_2\cos\chi-\frac{\chi_2}{\chi}p_1\sin\chi\ ,\\ p_x&=p_1\cos\chi+\frac{\chi_1}{\chi}q_2\sin\chi\ ,\\ p_y&=p_2\cos\chi+\frac{\chi_1}{\chi}q_1\sin\chi\ . \end{aligned} \tag{3}$$

These are consistent with the commutation relations $[p_i,q_j]=-i\hbar\delta_{ij}$ and $[q_i,q_j]=0$ if $\chi_1\chi_2=\chi^2$. Then the Hamiltonian

$$\mathcal{H}=\frac{1}{2m_e}[p_x^2+\Omega_1^2x^2+p_y^2+\Omega_2^2y^2+m_e\omega_c(yp_x-xp_y)]\ ,$$

$$\Omega_{1,2}^2=m_e^2(\omega_{x,y}^2+\tfrac{1}{4}\omega_c^2)\ ,$$

$$\omega_c=eB/m_ec\ ,$$

is diagonal if

$$\begin{aligned} \frac{\chi_1}{\chi}&=-[\tfrac{1}{2}(\Omega_1^2+\Omega_2^2)]^{1/2}\ ,\\ \frac{\chi_2}{\chi}&=\left[\frac{\chi_1}{\chi}\right]^{-1}\ ,\\ \tan2\chi&=m_e\omega_c[2(\Omega_1^2+\Omega_2^2)]^{1/2}/(\Omega_1^2-\Omega_2^2)\ . \end{aligned} \tag{4}$$

Defining

$$\Omega_3^2=[(\Omega_1^2-\Omega_2^2)^2+2m_e^2\omega_c^2(\Omega_1^2+\Omega_2^2)]^{1/2}\ ,$$

the Hamiltonian is rewritten as

$$\mathcal{H}=\frac{1}{2m_e}(\alpha_1^2 p_1^2+\alpha_2^2 p_2^2+\beta_1^2 q_1^2+\beta_2^2 q_2^2)\ , \tag{5}$$

with

$$\alpha_1^2=\frac{\Omega_1^2+3\Omega_2^2+\Omega_3^2}{2(\Omega_1^2+\Omega_2^2)}\ ,\quad \beta_1^2=\tfrac{1}{4}(3\Omega_1^2+\Omega_2^2+\Omega_3^2)\ ,$$
$$\alpha_2^2=\frac{3\Omega_1^2+\Omega_2^2-\Omega_3^2}{2(\Omega_1^2+\Omega_2^2)}\ ,\quad \beta_2^2=\tfrac{1}{4}(\Omega_1^2+3\Omega_2^2-\Omega_3^2)\ . \tag{6}$$

The energy eigenvalues are then obtained as

$$E_{n_x,n_y}=(n_x+\tfrac{1}{2})\hbar\omega_1+(n_y+\tfrac{1}{2})\hbar\omega_2\ , \tag{7}$$

where $\omega_1=\alpha_1\beta_1/m_e$ and $\omega_2=\alpha_2\beta_2/m_e$. The energy (7) has the following limiting behavior: at zero magnetic field, the system behaves like a couple of harmonic oscillators in the x and y directions. For a large magnetic field ($\omega_c \gg \omega_x,\omega_y$), we get $E_{n_x}=(n_x+\frac{1}{2})\hbar\omega_c$, i.e., Landau levels form as in the case of isotropic parabolic confinement.[1,2] When $\omega_x=\omega_y$, i.e., the confinement is isotropic parabolic, $n_x=n+\frac{1}{2}|l|-\frac{1}{2}l$ and $n_y=n+\frac{1}{2}|l|+\frac{1}{2}l$, where n and l are the principal and azimuthal quantum numbers, respectively. Also, when $\omega_x\simeq\omega_y$, the energy levels are very similar to that of the isotropic case except that the $(2n+|l|+1)$-fold degeneracies at $B=0$ are lifted[11] as a result of breaking of the circular symmetry. A similar situation also arises when the circular symmetry is broken by Coulomb coupling between two neighboring dots.[12]

The selection rules for the transition to higher energy levels can be calculated from the dipole transition matrix elements[1,2] and are as follows: polarization along the x or y axis, (i) $\Delta n_x=0$, $\Delta n_y=\pm1$, (ii) $\Delta n_x=\pm1$, $\Delta n_y=0$. There are just two modes as in the case of isotropic parabolic confinement.[1,2] The only major difference here is that at $B=0$, the two modes split, $\Delta E=\hbar(\omega_x-\omega_y)$. This mode splitting has indeed been observed experimentally.[10]

Following the recent measurements[7,8] of the electrochemical potential of a quantum dot, we have also calculated this quantity in the constant-interaction (CI) model. In this model, one estimates the total energy in a simple approximation, which is common in the studies of the Coulomb blockade.[13] In this approximation, the Coulomb interaction is taken into account via the macroscopic electrostatic energy and the total energy is written as[7,11]

$$E(N)\simeq\sum_{i=1}^{N}\mathcal{E}_i+\tfrac{1}{2}N^2U\ , \tag{8}$$

where $\mathcal{E}_i$ ($i=1,2,3,\ldots$) are the single-electron energy levels, and U is the interelectron interaction. The chemical potential is then

$$\mu_e(N)=E(N)-E(N-1)=(N-\tfrac{1}{2})U+E_N\ , \tag{9}$$

where E_N is the energy of the Nth electron. We should point out that the experiment by Ashoori *et al.*[7] indicated that the CI model is a reasonable approximation to calculate the chemical potential of the quantum dot. In what follows, we have presented the chemical potential for various values of the anisotropy of the dot and the electron number in the range $N=1-30$. In our calculations of μ_e, we have included the Zeeman energy, with the g factor to be 0.44 and the effective mass $m^*=0.067m_e$, appropriate for GaAs. For the interaction energy, we have used $U=0.6$ meV as in Ref. 7.

Figure 1(a) shows field dependence of the single-electron energy levels for a quantum dot with $\omega_x=1.0$ meV and $\omega_y=1.1$ meV. For this choice of ω_x and ω_y, the deviation from the circular dot is minimal and therefore, as expected, the energy levels are very similar to those of the circular dot[1,2] except at the origin where, as discussed above, the degeneracies are lifted. Qualitatively similar results were obtained by perturbation calculations.[11] As the number of level crossings remains unchanged, the results for the chemical potential [Fig. 1(b)] are not very different from those of the isotropic case.[7]

The energies and chemical potentials for $\omega_x=1$ meV and $\omega_y=5.0$ and 10.0 meV are plotted in Figs. 2 and 3, respectively. It is clearly seen that, as ω_y is increased, the level crossings are shifted to higher energies and the oscillations in chemical potentials are suppressed at lower energies. For example, when $\omega_y=5$, the oscillations are

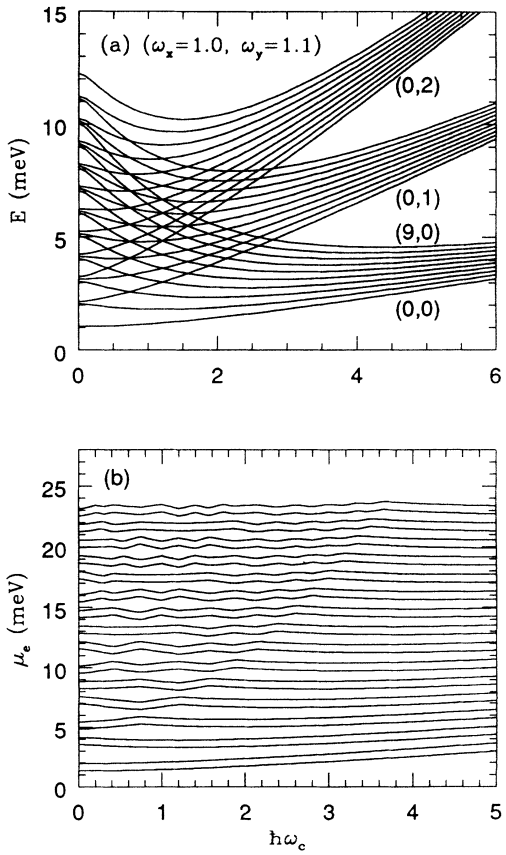

FIG. 1. (a) Energy levels of an anisotropic quantum dot as a function of the magnetic field ($\hbar\omega_c$ in meV) for $\omega_x=1.0$ meV and $\omega_y=1.1$ meV. The lines are drawn in ascending order of (n_x,n_y), as indicated. (b) The chemical potential (in the CI approximation) for the energy levels of (a).

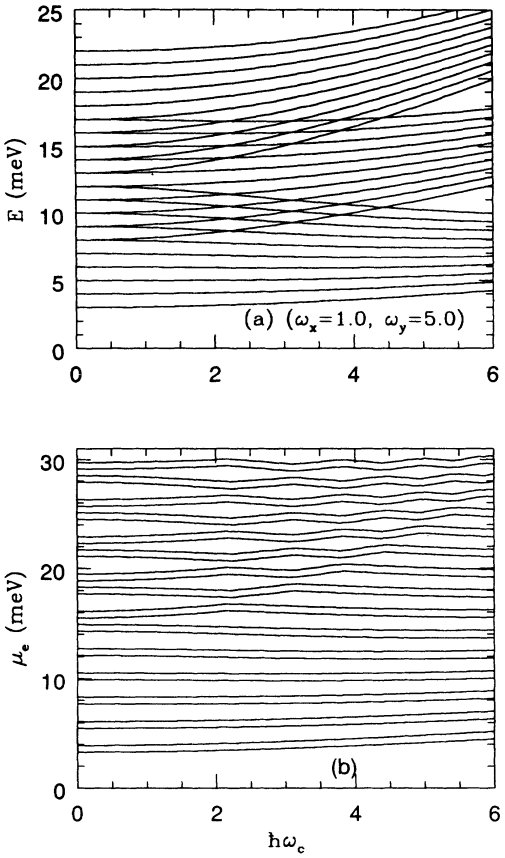

FIG. 2. Same as in Fig. 1, but for $\omega_y = 5.0$ meV.

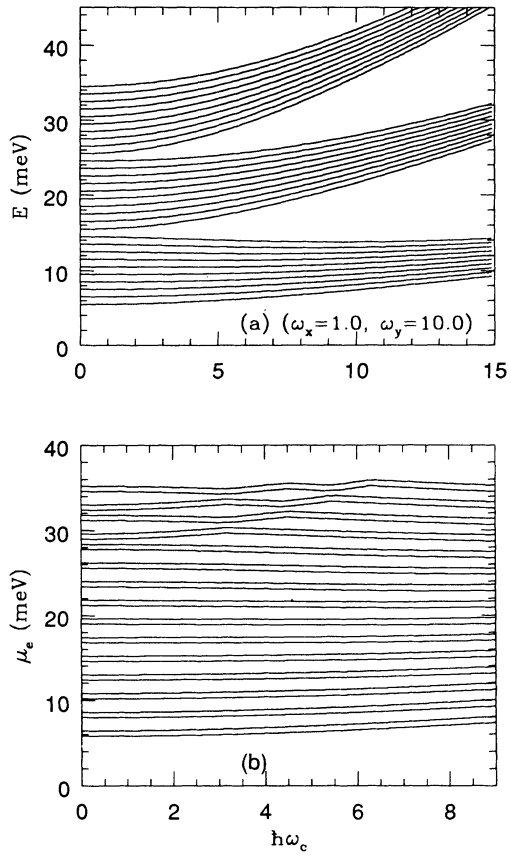

FIG. 3. Same as in Fig. 1, but for $\omega_y = 10.0$ meV.

suppressed for $N=1-12$ and $N=1-22$ when $\omega_y=10$. Furthermore, the amplitude of the oscillations decreases considerably with increasing anisotropy. On the other hand, the magnetic-field threshold beyond which the oscillations in chemical potentials cease to exist increases with increasing ω_y. With this increase of magnetic-field threshold, the oscillations also *move* to higher magnetic fields not unlike what is observed in the experimental results of Ashoori *et al.*[7] We should point out that the confinement potential for the quantum dots in the experiments of McEuen *et al.*[8] is anisotropic with $\omega_y/\omega_y \approx 4.4$, which lie in the range of $\omega_{x,y}$ considered here.

III. TWO-ELECTRON DOTS

Quantum dots containing two electrons (artificial helium atoms) have been investigated earlier by several authors.[9,14,15] In these papers, Coulomb matrix elements, originally studied in Ref. 2 for many-electron systems, have been numerically evaluated for the two-electron systems. In what follows, we have used the interparticle potential of the form $V(r)=\hbar^2\lambda^2/2\mu r^2$, where $\mu=m^*/2$ is the effective mass. For the quantum-dot systems, this potential seems to be a reasonable approximation and has been used in earlier studies.[16] The major advantage of this choice is that most of the analysis can be performed analytically. As noted earlier by other authors,[16] this form of the interaction potential is expected to provide quite reliable qualitative results for the quantum dots. The radial part of the Schrödinger equation is then

$$\frac{1}{r}\frac{d}{dr}\left[r\frac{d\varphi}{dr}\right]-\left[\frac{l^2+\lambda^2}{r^2}\right]\varphi+\left[K_0^2 r^2-\frac{r^4}{a^4}\right]\varphi=0 ,$$

where

$$a^2=\frac{\hbar}{\mu\Omega_e} ,$$

$$K_0^2=\frac{2\mu}{\hbar^2}[E+\tfrac{1}{2}l\hbar\omega_c] ,$$

$$\Omega_e^2=\omega_0^2+\tfrac{1}{4}\omega_c^2 ,$$

and $\varphi_{\rm rel}=e^{il\theta}\varphi(r)$. Defining $m^2(l)=\lambda^2+l^2$, the radial function is written as

$$\varphi_{nl}=\frac{e^{il\theta}}{a}\left[\frac{n!}{\Gamma[n+m(l)+1]\pi}\right]^{1/2}\times\left[\frac{r}{a}\right]^{m(l)}e^{-r^2/2a^2}L_n^{m(l)}\left[\frac{r^2}{a^2}\right] .$$

The energy spectrum is

$$E(N_{\rm cm},L_{\rm cm},n_r,l_r)=[2N_{\rm cm}+|L_{\rm cm}|+2n_r+m(l_r)+2]\times\hbar\Omega_e-\tfrac{1}{2}(l_r+L_{\rm cm})\hbar\omega_c+E_{\rm spin} .$$

Here $N_{\rm cm}$ and $L_{\rm cm}$ refer to the center of mass (CM) motion. Antisymmetry of the wave function requires that even l states are singlets and odd l states triplets. Hence

$$E_{\text{spin}}=\begin{cases}0,\pm\dfrac{g^*m^*\hbar\omega_c}{2m} & \text{if } l_r \text{ is odd}\\ 0 & \text{if } l_r \text{ is even}\end{cases}.$$

We would like to emphasize that many results hitherto obtained only numerically can now be obtained analytically in this model. Our numerical results also show that this is a reasonable approximation to the Coulomb model.

The energies of the lowest states are plotted in Fig. 4 as a function of ω_c for $\lambda^2=3.0$ and $\omega_0=5.0$. The singlet-triplet transitions of the ground state, observed earlier[2,9] in numerical calculations using the r^{-1} potential, are also obtained here. Other features are also qualitatively similar as found for the Coulomb potential. In the absence of the Zeeman energy, ground-state angular momentum changes from $l\rightarrow l+1$ at

$$\omega_{c0}(l\rightarrow l+1)=\frac{4\omega_0(l+\frac{1}{2})}{\{[m(l+1)+m(l)]^2-(2l+1)^2\}^{1/2}}\ . \tag{10}$$

The level crossing of the triplet (l) state and a singlet ($l+1$) state when the Zeeman energy is included is suppressed when ω_{c0} satisfies the following conditions:

$$m_l\Omega_{e0}-\frac{g^*m^*}{m}\frac{\omega_{c0}}{2}<m_{l+1}\Omega_{e0}-\frac{\omega_{c0}}{2}\ ,$$

$$m_{l+2}\Omega_{e0}-\omega_{c0}<m_l\Omega_{e0}-\tfrac{1}{2}g^*m^*\omega_{c0}\ ,$$

where $\Omega_{e0}^2=\frac{1}{4}\omega_{c0}^2+\omega_0^2$, i.e., if

$$\frac{m_{l+2}-m_l}{m_{l+1}-m_l}<1+\frac{1}{1-\dfrac{g^*m^*}{m}}\ .$$

Such a suppression of the singlet state in the presence of Zeeman energy was also noticed in Ref. 9 for a Coulomb potential. Hence, the level crossing structure of the r^{-2} potential is quite similar to that of the r^{-1} potential and reproduces all the essential features. Moreover, suitable values of λ^2 can be used to model the system appropriately. In Fig. 4(b), the energies are plotted with the Zeeman term included.

A. Pair-correlation function

This function is a measure of the probability of finding an electron at a distance r when the other is at the origin. It is defined as

$$g(r')=\pi a^2\langle\Psi_g|\delta(\mathbf{r}'-\mathbf{r})|\varphi_g\rangle\ , \tag{11}$$

where πa^2 is the normalization factor such that $\int_0^\infty xg(x)dx=1$, where $x=r/a$. The ground state always has $n_r=0$, so the pair-correlation function is

$$g(x)=\frac{x^{2m(l)}e^{-x^2}}{\Gamma[m(l)+1]}\ . \tag{12}$$

In Fig. 5, we plot the ground state $\Gamma[m(l)+1]g(x)$ vs x for $\lambda^2=2.0$ and $\lambda^2=1.0$. Clearly, $g(x)$ shows very similar behavior to that computed for the r^{-1} potential by Pfannkuche *et al.*[15] The deviations occur mostly at large

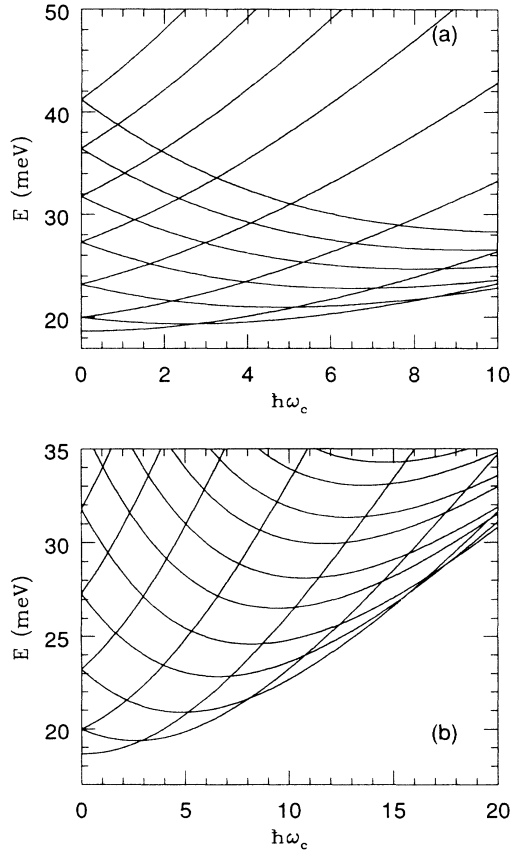

FIG. 4. Energy levels of a dot with two interacting electrons, with $\lambda^2=3.0$ and $\omega_0=5.0$ and (a) without and (b) with the Zeeman energy included.

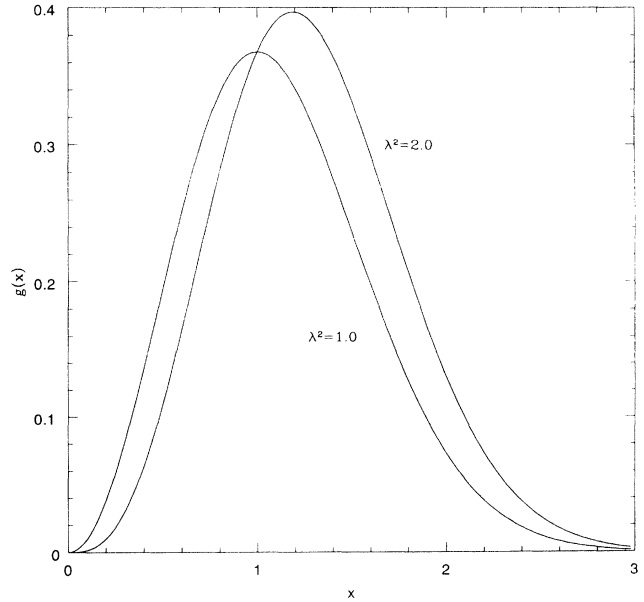

FIG. 5. The ground-state pair-correlation function for the two interacting electrons in a quantum dot.

x, but in the case of strong confinement and moderately strong field, the present results are again a good approximation.

B. Effect of anisotropy

The deviation from the circular symmetry is described by the potential

$$\mathcal{H}_1=\tfrac{1}{2}\mu(\delta\omega)^2r^2+\tfrac{1}{2}M(\delta\omega)^2R^2\ , \tag{13}$$

where R is the CM coordinate, $M=2m^*$, and $\mu=\frac{1}{2}m^*$. The CM motion may be exactly solved in Sec. II. As discussed above, the effect of anisotropy at low field is to remove the degeneracy in E at $\omega_c=0$. A perturbation correction to the energy is good for a weak anisotropy at low ω_c and is also good for much larger $\delta\omega$ at higher fields, since the first-order correction decreases as $(\delta\omega)^2/[\omega_0^2+\frac{1}{4}\omega_c^2]^{1/2}$ with ω_c. The first-order shift in energy is

$$E^{(1)}_{\mathrm{rel},nl}=[2n+|m(l)|+1]\frac{\delta\omega}{\Omega_e}\frac{\delta\omega}{4}\ .$$

Consequently, low-lying states are shifted less than the higher ones. The effect of the anisotropy is similar to that of the noninteracting case, and in this case increases the field at which the ground-state angular momentum changes.

It should be pointed out that the degeneracy at zero fields, as discussed in Sec. II, is not removed in first order. Therefore, we compute the second-order shift to the energy which lifts the degeneracy

$$E^{(2)}_{0,l}=-\sum_{n',l'=l,l\pm2}\frac{|a_{n'l'0l}|^2}{E_{n'l'}-E_{0l}}\ , \tag{14}$$

where

$$a_{n'l',0l}=K(l')\frac{\Gamma\left[\frac{m(l)+m(l')}{2}+2\right]\Gamma\left[n+\frac{m(l')-m(l)}{2}\right]}{\Gamma[n'+m(l')+1]\Gamma[m(l)+1]\Gamma\left[\frac{m(l')-m(l)}{2}-1\right]}\frac{\hbar^2}{4}(\delta\omega)^2\left[\frac{\delta\omega}{\Omega_e}\right]^2\ , \tag{15}$$

and

$$K(l')=\begin{cases}1\ , & l=l'\\ \frac{1}{4}\ , & l=l'\pm2\\ 0\ \text{ otherwise}\ .\end{cases} \tag{16}$$

For higher fields, the second-order correction is negligible and the first-order energy shift is quite accurate. Hence, the main effect of the higher-order corrections is to split the degeneracy at $\omega_c=0$. The shifting of the level crossings to higher fields is also obtained in first order.

IV. SUMMARY

We have investigated the electronic energy levels of an anisotropic quantum dot in a magnetic field. The single-electron system has been solved analytically. We have derived the selection rules for dipole transitions. We have also studied the chemical potentials in these systems, which can be measured experimentally. The level crossings are found to be shifted to higher energies and the oscillations in chemical potentials are seen to be suppressed at the low-lying energy levels. Our choice of a model interaction potential simplified the two-electron problem considerably. The results are found to be qualitatively reliable. We also analyze the anisotropic system with interacting electrons via perturbation theory.

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