Hydrogenic donor states in quantum dots in the presence of a magnetic field

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We report a calculation of the binding energy of the ground state of a hydrogenic donor in a quantum dot, assumed to be in the form of a disk, in the presence of a uniform magnetic field applied parallel to the disk axis. We assume that the impurity ion is located at the center of the disk. The quantum disk is assumed to consist of a finite length cylinder of GaAs material surrounded by $Ga_{1-x}Al_xAs$. The calculations have been performed by using a suitable variational wave function for infinite confinement potential at all surfaces. The binding energy of a donor impurity located at the center of the disk depends on the radius and length of the disk. The three-dimensional confinement of the quantum disk results in a larger binding energy for the hydrogenic donor than in the corresponding quantum well and quantum wire structures. In addition for a given set of values of the radius and the length of the disk, the binding energy increases as a function of the magnetic field. We recover two- and three-dimensional limits for the binding energy for various combinations of disk radius and length.

I. INTRODUCTION

In the last few years, advances in crystal-growth techniques for the fabrication of quantum-dot (QD) structures, such as molecular-beam epitaxy (MBE) and metal-organic chemical-vapor deposition (MOCVD), have been reported.[1–12] In addition, theoretical and experimental studies on optical properties,[13–28] electronic structure,[29–37] excitonic[38–53] and impurity levels[54–60] in quantum dots have been published.

The physics of impurity states in semiconductor quantum-dot structures is an interesting subject. In the case of a spherical dot, the reduction of dimensionality can be controlled by changing the radius of the dot. An electron bound to an impurity ion located at the center of a QD never "sees" the surface of the dot for a very large dot radius, and behaves as a three-dimensional (3D) electron bound to an impurity ion in GaAs, in GaAs-$Al_xGa_{1-x}As$ structures. For very small radii, and for an infinite barrier model, the electron kinetic energy increases drastically and supercedes the attractive potential due to the impurity ion. Furthermore, it is well known that the reduction of dimensionality increases the effective strength of the Coulomb interaction, and in effect the binding energy. This can be understood by the following argument: an electron in a system of reduced dimensionality can move only in a smaller space, and spends most of its time close to the impurity ion. Therefore, the binding of the electron should be larger in lower dimensions.

Extensive theoretical work on hydrogenic impurity states in QD's has been reported. Zhu[54] and Zhu, Xiong, and Gu[55] studied the hydrogenic impurity binding energies in spherical QD's by using a series expansion for the wave function. The binding energy was calculated as a function of the disk radius, for infinite and finite confining potentials. The calculated results show stronger confinement and larger binding energies for hydrogenic impurities in QD's than in corresponding quantum wires and quantum wells. Einevoll and Chang[56] studied the same problem by applying a different method: the effective bond orbital model. The binding-energy results show the same characteristic dependence on the QD radius. Hsiao, Mei, and Chuu[57] solved the same problem analytically, for an infinite confining potential on the surface of the QD. Chuu, Hsiao, and Wei[58] have calculated the binding energy of the ground state of a hydrogenic impurity located at the center of a quantum dot by using a perturbation-variational approach. Elangovan and Navaneethakrishnan[59] have calculated the donor ionization energies and polarizabilities in a cubic quantum box. Recently Montenegro and Merchancano[60] have calculated the donor binding energies in spherical quantum dots, using a variational procedure.

Extensive experimental and theoretical investigations of the behavior of energy levels of shallow impurities in bulk semiconductors and their heterostructures, such as quantum wells, in the presence of a magnetic field have been carried out during the past 40 years. These studies have been primarily responsible for our current understanding of the nature of these impurity states. The application of the magnetic field modifies the symmetry of these states as well as the nature of the wave functions. The study of the transitions between the energy levels of these impurities leads to the determination of the binding energies, oscillator strengths, and other properties of these levels. Such studies, however, have not yet been performed in quantum dots. As in the case of bulk semiconductors and quantum wells, the study of the behavior of shallow impurity states in quantum dots in the presence of a magnetic field will lead to a better understanding of their electronic and optical properties.

In this paper, we report a calculation of the binding energy of the ground state of a hydrogenic impurity located at the center of a quantum circular disk of finite length, in the presence of a uniform magnetic field, applied parallel to the disk axis using a variational approach. We have calculated the binding energy for infinite confinement po-

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tentials at all surfaces as a function of the disk radius, disk length, and magnetic field. We use a variational method in which the trial wave function contains a hydrogenic part, and by taking into account the axial and radial confinement for the electron, and the appropriate axial and radial solutions[61] for an electron in a magnetic field with the appropriate boundary conditions, respectively. The axial confinement is a function of the z component only, while the radial confining potential is a function of the radial coordinate. The magnetic field is applied parallel to the disk axis and conserves the rotational symmetry of the problem.

II. THEORY

The Hamiltonian of a system consisting of an electron bound to a donor ion, inside a quantum disk of radius R and length L, with infinite potential barrier at all surfaces, in the presence of a magnetic field parallel to the disk axis, is given by

$$H=\left[\mathbf{p}+\frac{e}{c}\mathbf{A}\right]^2\Big/2m^*-\frac{e^2}{\varepsilon_0|\mathbf{r}-\mathbf{r}_0|}+V(\rho,\phi)\ , \tag{1}$$

where $|\mathbf{r}-\mathbf{r}_0|=[\rho^2+\rho_0^2-2\rho\rho_0\cos[\phi-\phi_0]+(z-z_0)^2]^{1/2}$, ε_0 is the dielectric constant of the GaAs material inside the disk, m^* is the effective electron mass, and $\mathbf{r}_0$ is the impurity ion position. $\mathbf{A}(\mathbf{r})$ is the magnetic-field potential and $V(\rho,\phi)$ is the confining potential:

$$V(\rho,\phi)=\begin{cases}0\ , & 0\le\rho\le R \text{ and } |z|\le\dfrac{L}{2}\\ \infty\ , & \rho>R \text{ and } |z|>\dfrac{L}{2}\ .\end{cases} \tag{2}$$

For an impurity ion located at the center of the quantum disk, we write $\rho_0=0$ and $z_0=0$. For a uniform magnetic field, we can write $\mathbf{A}(\mathbf{r})=(\mathbf{B}\times\mathbf{r})/2$, where $\mathbf{B}=B\hat{\mathbf{z}}$; in cylindrical coordinates, the magnetic-field potential becomes $A_\rho=A_z=0$, $A_\phi=B\rho/2$. The inclusion of the impurity potential leads to a nonseparable differential equation which cannot be solved analytically. Therefore, it is necessary to use a variational approach to calculate the eigenfunction and eigenvalue of the Hamiltonian for the ground state.

We take into account the cylindrical confining symmetry, the confinement over the z axis, the presence of the magnetic field, and the hydrogenic impurity potential, by choosing a trail wave function for the ground state which can be written as a product of a hydrogenic part, a z-dependent solution of an electron in a one-dimensional box, and a radial solution of an electron in a cylindrical disk in the presence of a magnetic field,

$$\psi(\mathbf{r})=\begin{cases}N\cos\left[\dfrac{\pi z}{L}\right]{}_1F_1(-a_{01},1;\xi)\exp\left[-\dfrac{\xi}{2}-\lambda[\rho^2+z^2]^{1/2}\right]\ , & 0\le\rho\le R \text{ and } |z|\le\dfrac{L}{2}\\ 0 \text{ otherwise}\ , & \end{cases} \tag{3}$$

where $\alpha_c=(\hbar c/eB)^{1/2}$ is the cyclotron radius, $\xi=\rho^2/2\alpha_c^2$, N is the normalization constant, and λ is a variational parameter. ${}_1F_1(a,c;\xi)$ is the confluent hypergeometric function (Kummer function) which is the radial solution of an electron in an infinite potential cylinder, in the presence of a magnetic field, applied parallel to the cylinder axis.[61] Equation (3) satisfies the boundary conditions $\psi(\rho=R,z)=\psi(\rho,z=\pm L/2)=0$, while a_{01} is in general a positive noninteger which enters in the eigenvalue for the ground state of the problem in the absence of the Coulomb term, being calculated numerically from the boundary-condition eigenvalue equation.[61] N is given by

$$N^{-2}=4\pi A \tag{4}$$

with

$$A=\int_0^R d\rho\,\rho\exp[-\rho^2/2\alpha_c^2]{}_1F_1^2(-a_{01},1;\rho^2/2\alpha_c^2)\times\int_0^{L/2}dz\cos^2\left[\frac{\pi z}{L}\right]\exp[-2\lambda r]\ . \tag{5}$$

The binding energy $E_b(R,B,L)$ of the hydrogenic impurity is defined as the ground-state energy of the system in the absence of the Coulomb term, minus the ground-state energy $\langle H(R,B,L)\rangle$ in the presence of the Coulomb term, i.e.,

$$E_b(R,B,L)=\hbar\omega_c(a_{01}+\tfrac{1}{2})+\frac{\hbar^2\pi^2}{2m^*L^2}-\langle H(R,B,L)\rangle\ , \tag{6}$$

where $\omega_c=\hbar/m^*\alpha_c^2$ is the cyclotron frequency, while the binding energy defined in this way is a positive quantity.

For computational purposes, we normalize the expression for the binding energy $E_b(R,B,L)$ in units of the impurity Rydberg constant: $R_B=m^*e^4/2\varepsilon_0\hbar^2=e^2/2\varepsilon_0a_B$, where $a_B=\varepsilon_0\hbar^2/m^*e^2$ is the electron Bohr radius. The expression for the binding energy is

$$E_b(R,B)=\alpha_B^2[\lambda^2-2\lambda BB-2\lambda RCC+2\pi DD]/AA+2\alpha_B(BB/AA)\ , \tag{7}$$

where

$$AA=A/R^2L\ , \tag{8}$$

$$BB=\int_0^1 dt\,tf^2(t^2\xi_R)\times\int_0^{1/2}du\exp[-2\lambda r]\cos^2[\pi u]/r\ , \tag{9}$$

$$CC=\int_0^1 dt\,t^2f(t^2\xi_R)\frac{df}{dt}(t^2\xi_R)\times\int_0^{1/2}du\,u\exp[-2\lambda r]\cos^2[\pi u]/r\ , \tag{10}$$

$$DD = \int_0^1 dt\, t f^2(t^2 \xi_R) \times \int_0^{1/2} du\, u \exp[-2\lambda r] \cos[\pi u] \sin[\pi u]/r \,, \tag{11}$$

where $\rho = Rt$, $z = Lu$, $\xi_R = R^2/2\alpha_c^2$, $f(t^2\xi_R) = \exp[-t^2\xi_R/2]\,{}_1F_1(-a_{01}, 1; t^2\xi_R)$, and $r = [t^2R^2 + u^2L^2]^{1/2}$.

We use a variational method, and search for the maximum of $E_b(R,B,L)$ with respect to λ, in order to obtain a lower bound for the binding energy. All double integrations are done numerically.

III. RESULTS AND DISCUSSION

We have calculated the values of the binding energy $E_b(R,B,L)$ of a donor where the impurity ion is located at the center of a quantum disk ($\rho_0 = 0, z_0 = 0$) in the presence of a uniform magnetic field applied along the axis of the quantum disk. The values of the physical parameters pertaining to the material GaAs in the QD's used in our calculations are $m^* = 0.067 m_0$ and $\varepsilon_0 = 12.5$.

For an infinite potential barrier, in Fig. 1 we plot the binding energy versus the disk radius for different disk lengths in the $B = 0$ case. For strong radial confinement ($R < a_B$), the binding energy diverges as $R/a_B \to 0$ in a different fashion for different disk lengths. For a strong axial confinement ($L < a_B$), the divergence is more prominent than in the weak axial confinement case ($L > a_B$), since in the former case the electron is squeezed in a smaller volume than in the latter case. The three-dimensional confinement of the quantum disk results in larger binding energies for the donor than in the corresponding quantum-well and quantum-wire structures. As the radial confinement is relaxed ($R \geq 2a_B$), the binding energy converges to the appropriate quantum-well values, depending on the length of the disk. For strong axial confinement ($L < a_B$) the binding energy tends to the value of the two-dimensional hydrogen donor, $E_b \to 4R_B$ (the quantum-well case for $L \ll R$), while for weak axial confinement ($L \gg a_B$) the binding energy tends to the three-dimensional value $E_b \to R_B$ (the quantum-wire case for $L \gg R$). Our results in the zero magnetic-field case for weak axial confinement (the infinite quantum disk) agree with those of Brown and Spector.[62]

In Figs. 2 and 3, we plot the binding energy versus the disk radius for different disk lengths for $B = 100$ and 200 kG, respectively. High magnetic fields confine the electron very close to the disk axis, increasing in effect the binding energy, especially in the weak radial confinement case ($R \geq 2a_B$). Our results show that in the strong radial confinement case ($R < a_B$), the binding-energy results are identical to the $B = 0$ case, an indication that the electron radial confinement prevails over the magnetic-field confinement, for values of the magnetic field considered

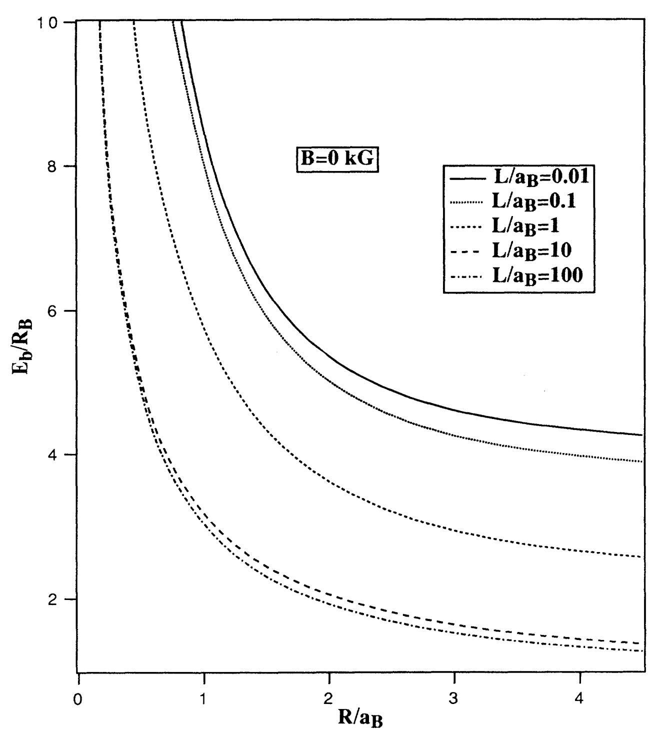

FIG. 1. Variation of the binding energy of a donor (E_b), expressed in terms of a hydrogenic rydberg (R_B) in GaAs (5.8 meV) as a function of the radius of the disk (R), expressed in terms of the Bohr radius (a_B) in GaAs ($\sim$98 Å) for several values of the disk length (L) for $B = 0$.

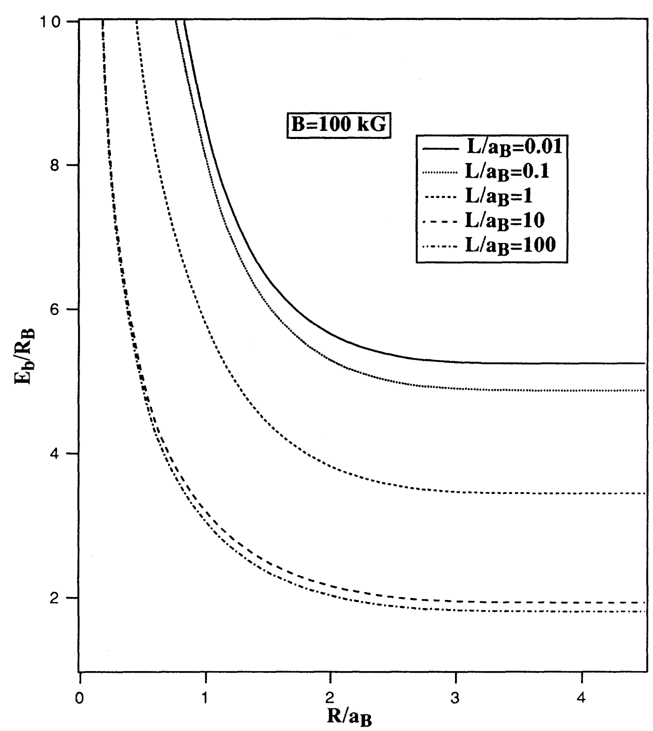

FIG. 2. Variation of the binding energy of a donor (E_b), expressed in terms of a hydrogenic rydberg (R_B) in GaAs (5.8 meV) as a function of the radius of the disk (R), expressed in terms of the Bohr radius (a_B) in GaAs ($\sim$98 Å) for several values of the disk length (L) for $B = 100$ kG.

in this work. As the disk radius becomes larger ($R \geq 2a_B$), the binding energy converges asymptotically to appropriate bulk values for different disk lengths. For strong axial confinement ($L < a_B$), the binding energy converges to the two-dimensional value in the presence of a magnetic field, while the weak axial confinement ($L \gg a_B$) corresponds to the three-dimensional value for $B \neq 0$. The nonzero magnetic-field results for weak axial and radial confinements agree with those of Aldrich and Greene.[63]

In Fig. 4, we reconfirm the previous results by plotting binding energy as a function of the disk length for different magnetic fields in the strong radial confinement case ($R = a_B$). Only very strong magnetic fields ($B \geq 400$ kG) can increase the binding energy, an indication that a small disk radius confines the electron more strongly than would the reduction of the electron cyclotron radius by the magnetic field. As the disk length increases, we recover the infinite quantum-wire results in the presence of a magnetic field applied parallel to the wire axis.[61]

In Fig. 5 we plot the binding energy versus the disk length for different magnetic fields in the weak radial confinement case ($R = 5a_B$). For small values of L/a_B, we recover the quantum-well results for different magnetic fields, while for $L \gg a_B$ the binding energy converges asymptotically to the corresponding bulk value. For example, for $B = 0$ and for small disk lengths, the binding energy reaches the two-dimensional value of $4R_B$, and for

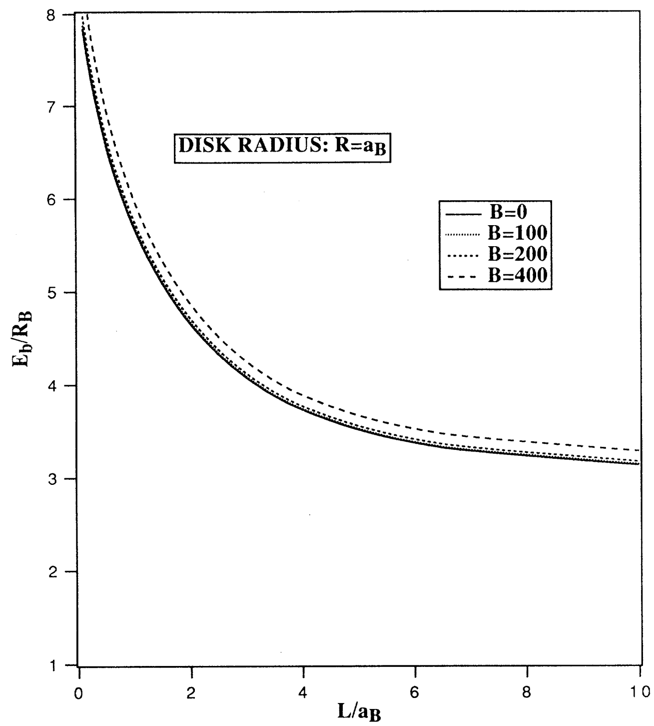

FIG. 4. Variation of the binding energy of a donor (E_b), expressed in terms of a hydrogenic rydberg (R_B) in GaAs (5.8 meV) as a function of the disk length (L), expressed in terms of the Bohr radius (a_B) in GaAs ($\sim$98 Å) for several values of magnetic field for $R = a_B$.

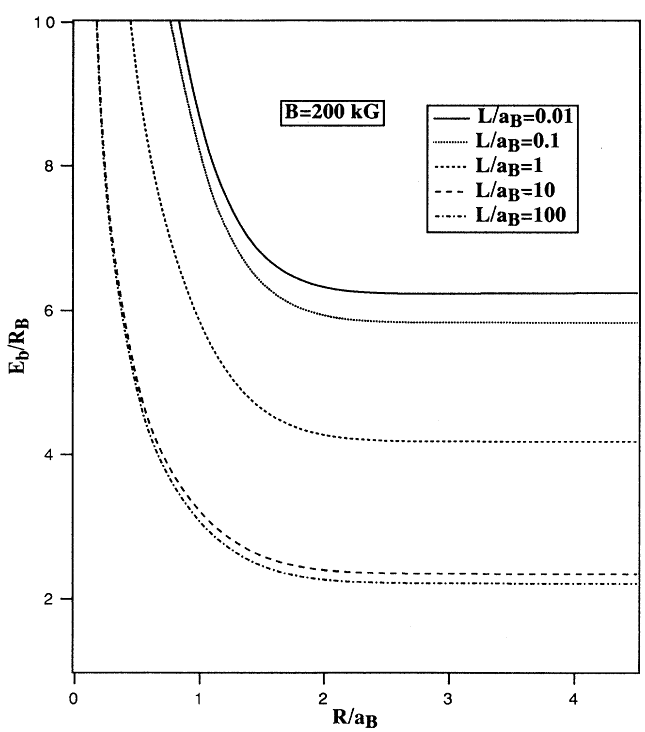

FIG. 3. Variation of the binding energy of a donor (E_b), expressed in terms of a hydrogenic rydberg (R_B) in GaAs (5.8 meV) as a function of the radius of the disk (R), expressed in terms of the Bohr radius (a_B) in GaAs ($\sim$98 Å) for several values of the disk length (L) for $B = 200$ kG.

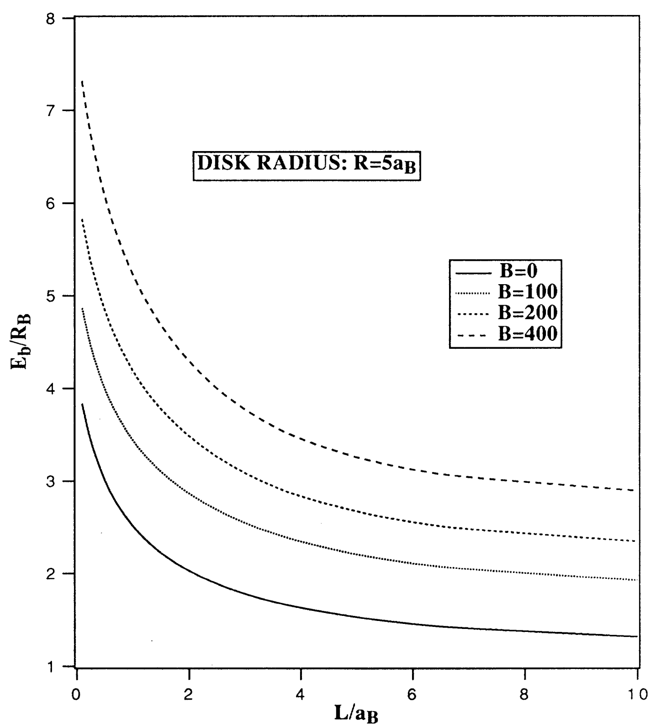

FIG. 5. Variation of the binding energy of a donor (E_b), expressed in terms of a hydrogenic rydberg (R_B) in GaAs (5.8 meV) as a function of the disk length (L), expressed in terms of the Bohr radius (a_B) in GaAs ($\sim$98 Å) for several values of magnetic field for $R = 5a_B$.

very large disk lengths the bulk value of the rydberg constant.

Finally, we would like to mention that in our calculations we have considered an infinite barrier case in which the calculations are much simpler and lead to results which, for intermediate and large values of the radius ($R/a_B > 1$) and length of the disk ($L/a_B > 1$), should agree fairly well with those in the finite barrier case, with commonly used values of Al concentration. Though the infinite barrier case, strictly speaking, does not have a physical relevance, the results thus obtained can be used as long as the values of the radius and the length of the disk are not too small.

IV. SUMMARY

We have presented a calculation of the binding energy of a hydrogenic impurity in a quantum dot, assumed to be in the form of a disk, with infinite potential barriers at all surfaces, in the presence of a uniform magnetic field applied parallel to the disk axis, for the case of an impurity located on the axis of the disk. The calculations have been performed by using a suitable variational wave function, which takes into account the confinement of the carriers in the disk (axial and radial), and the influence of the Coulomb interaction between the impurity ion and the electron. The binding energy of the impurity located at the center of the disk depends on the disk radius and length. The three-dimensional confinement of the quantum disk results in larger energies for the donor than in the corresponding quantum-well and quantum-wire structures. The binding energy continues to increase as the radius and length of the disk decrease for the infinite potential barrier case, while in the presence of magnetic field additional increases for the binding energy are reported, especially for larger disk radii. We recover two- and three-dimensional limits of the binding energy for various combinations of disk radius and length.

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