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# Inspection of the number of electrons in the ring of a quantum dot*

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On the electronic structures of quantum dots, there is a new viewpoint saying that, in some specific states, a few electrons might behave as valence electrons moving outside surrounding a core. To clarify the validity of this viewpoint, a numerical calculation was performed in this paper. The results are against this viewpoint.

**Keywords:** quantum dots, electronic structure, symmetry consideration
**PACC:** 7115, 7320D

## 1. Introduction

In the research of condensed matter attention is specially paid to the low-dimensional (2D) systems in recent years. Among the heterostructures of semiconductors, the potential of application of the quantum dots (QD) is intriguing. In the research of QDs, when the number of electrons N is not very small, the ring-core model of electronic structure[1−4] is believed to be a reasonable model for two-dimensional QDs with axial-symmetric confinement. In the ring-core model a part of electrons ($N_{\rm ring}$) would constitute a ring outside and the remaining $N-N_{\rm ring}$ electrons would constitute a core inside. The electron densities in the ring and in the core are believed to be roughly equal; this is duo to the well known feature of incompressibility. One can imagine that each electron is associated with a circle with the diameter equal to the average electron–electron separation in the circular dot. Then these circles are put together compactly into the circular dot. In this way, the number of circles touching the outside boundary is just the number of electrons in the ring. From this simplified picture it is believed that $N_{\rm ring}$ could not be a small number unless N itself is small. However, a somewhat different point of view has been proposed recently.[5] It was argued that $N_{\rm ring}$ may be very small for some states with specific orbital angular momentum $L$. The argument is as follows:

Let $Z_k = x_k + iy_k$ denote the coordinate of the $k$-th electron. Based on the Laughlin state[6]

$$\Psi_{L_q} = \prod_{i<j}^{N}(Z_i - Z_j)^q \exp\left(-q\sum_k |Z_k|^2/4\right). \qquad (1)$$

A trial wavefunction

$$\Psi_{\rm LBP} = S\prod_{i=1}^{M}(Z_i - Z_0)\,\Psi_{L_q} \qquad (2)$$

is proposed in Ref.[5], where $q$ is an odd integer and S is the operator of symmetrization, $Z_0 = \sum Z_k/N$ denotes the coordinate of the centre of mass, and $M$ is a given integer $\leq N$ it is noted that L is a good quantum number for the Laughlin state with $L - L_q \equiv q\frac{N(N-1)}{2}$ it was proved[5] that $L$ is also a good quantum number for the $\Psi_{\rm LBP}$ with $L = L_q + M$. The charged densities given by the $\Psi_{\rm LBP}$ have been calculated, which lead to a picture with $M$ valence electrons surrounding a core with $N-M$ electrons. For example, if $N$=6, $q$=3 and $M$=2 are assumed, then we have $L_q = 15q = 45$ and the associated $\Psi_{\rm LBP}$ state has $L$=47, the density plot of this state demonstrates that there are two valence electrons surrounding a core containing four electrons.[5]

Let $\psi_{L_i}^{\rm exact}$ denote the exact eigenstate of the Hamiltonian which is the $i$-th state of an $L$-series having the given angular momentum $L$. When $i$=1, the $\psi_{L_i}^{\rm exact}$ is called the first state which is the lowest of

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the $L$-series. It is noted that both the Laughlin wavefunction and the trial wavefunction are totally antisymmetric with respect to particle permutations. The former has been proved to be very close to the exact wavefunction of the first-states with $L = L_q$ and with the total spin $S = \frac{N}{2}$ (i.e., a polarized system). Now the point is whether $\Psi_{\rm LBP}$ is close to an exact eigenstate of the polarized system. In order to see this point, exact eigenstates of a polarized $N$=6 dot have been calculated. Using the $\Psi_{\rm LBP}$ and the $\psi_{L_i}^{\rm exact}$ from a numerical calculation, the overlaps $\langle \Psi_{\rm LBP}|\psi_{L_i}^{\rm exact}\rangle$ have been evaluated.[5] It was found that, when $q$=3, the overlaps for different $M$ (or different $L$) remain within the range of 0.93 to 0.96. Based on this evaluation, it was claimed in Ref.[5] that (i) the $\Psi_{\rm LBP}$ state is a good approximation of the first-states with $L = L_q + M$ ($M \leq N$) and with $S = \frac{N}{2}$, and (ii) these first-states would have $M = L - L_q$ valence electrons surrounding a core containing $N - M$ electrons. According to this point of view, the first-states with an $L$ a little larger than $L_q$ would have a few valence electrons surrounding a core. This picture is more or less like an atom, but very different from a compact liquid.

We think that, although the above overlaps are not small, they are not large enough to draw a decisive conclusion. Therefore, further inspection is worthy. The present paper is dedicated to this purpose.

## 2. Numerical results of a six-electron polarized dot

Let us study in detail a 2D six-electron dot under a parabolic confinement; and a magnetic field $B = \nabla \times \boldsymbol{A}$ perpendicular to the plane of the dot is applied. The Hamiltonian reads

$$H = \sum_{i=1}^{N}\left[\frac{1}{2m^*}(\boldsymbol{p}_i - \frac{q}{c}\boldsymbol{A})^2 + \frac{1}{2}m^*\omega_0^2 r_i^2\right] + \frac{e^2}{4\pi\epsilon}\sum_{i<j}^{N}\frac{1}{r_{ij}} + g^*\mu_B \boldsymbol{B}\sum_{i=1}^{N}S_{zi}, \qquad (3)$$

where the effective electron mass $m*$, the dielectric constant $\epsilon$, and the strength $\omega_0$ are given as $0.067\mathrm{m_e}$, 12.4, and 3meV/$\hbar$, respectively (for the GaAs dot). $g^*$ is the effective g-factor, and $\mu_B$ the magnetic moment. $\boldsymbol{r}_i$ is the position vector, $\boldsymbol{p}_i$ the momentum, and $S_{zi}$ the $z$-component of the spin of the $i-th$ electron. The final term of the Hamiltonian will be dropped because it is very small, and because it does not affect the wavefunctions of eigenstates at all. In what follows, only the $S = N/2$ states are concerned, and therefore the orbital wavefunctions are totally antisymmetric.

For the diagonalization of the Hamiltonian, an introduction of a set of basis functions is necessary. Let us first consider the single particle harmonic oscillator state $\phi_{mk}$ satisfying

$$\left(-\frac{\hbar^2}{2m^*}\nabla^2 + \frac{1}{2}m^*\Omega^2\right)\phi_{mk} = \varepsilon_{mk}\phi_{mk}, \qquad (4)$$

with $\varepsilon_{mk} = (m + k + 1)\hbar\Omega$. This state is also called a Darwin–Fock state, where the particle has an orbital angular momentum $l_{mk} = (m - k)\hbar$. Based on the set $\phi_{mk}$, the $N$-body basis functions are defined as

$$\psi_\alpha(1,2,\cdots,N) = \frac{1}{\sqrt{N!}}\begin{vmatrix} \phi_{m_1k_1}(\boldsymbol{r}_1) & \phi_{m_1k_1}(\boldsymbol{r}_2) & \cdots & \phi_{m_1k_1}(\boldsymbol{r}_N) \\ \phi_{m_2k_2}(\boldsymbol{r}_1) & \phi_{m_2k_2}(\boldsymbol{r}_2) & \cdots & \phi_{m_2k_2}(\boldsymbol{r}_N) \\ \cdots & \cdots & \cdots & \cdots \\ \phi_{m_Nk_N}(\boldsymbol{r}_1) & \phi_{m_2k_2}(\boldsymbol{r}_2) & \cdots & \phi_{m_Nk_N}(\boldsymbol{r}_N) \end{vmatrix}, \qquad (5)$$

where $\sum_{i=1}^{N}(m_i - k_i)\hbar = L$ is assumed. The set $\Psi_\alpha$ spans the matrix of the Hamiltonian. After a diagonalization of the matrix, the energy eigenvalues $E_{L_1}$ and the eigenstates $\psi_{L_i}^{\rm exact}$ are thereby obtained. It is noted that there is a parameter $\Omega$ in Eq.(4) which is adjustable and is finally close at its optimal value so that the energy of the first-state $E_{L_1}$ is minimized. In order to obtain the exact solutions, infinite basis functions are necessary. In practice, only 5000 basis functions are taken into account. It was found that these basis functions are sufficient to guarantee the accuracy. In fact, very accurate solutions (in the qualitative sense) have been achieved. For example, for $L$=45 and $B$=0, we have $E_{L_1}$=176.614meV and 176.608meV, respectively, if the numbers of $N$-body basis functions are 4000 and 5000. Moreover, the density functions extracted from the wavefunctions (as we shall see) by using 4000 and 5000 basis functions, respectively, are nearly indistinguishable. Thus, the results given in the following are very accurate in the qualitative sense.

In what follows we use the simpler notation $\Psi$ to replace $\psi_{L_i}^{\rm exact}$ and use the notation $(L)_i$ to denote the $i$-th state of the $L$-series. The one-body density is defined as

$$\rho_1(\boldsymbol{r}_1) = \int {\rm d}\boldsymbol{r}_2 \cdots {\rm d}\boldsymbol{r}_N |\,\Psi|^2, \tag{6}$$

satisfying

$$1 = \int \rho_1(\boldsymbol{r}_1){\rm d}\boldsymbol{r}_1. \tag{7}$$

The two-body density is defined as

$$\rho_2(\boldsymbol{r}_1, \boldsymbol{r}_2) = \int {\rm d}\boldsymbol{r}_3 \cdots {\rm d}\boldsymbol{r}_N |\,\Psi|^2, \tag{8}$$

satisfying

$$1 = \int \rho_2(\boldsymbol{r}_1, \boldsymbol{r}_2){\rm d}\boldsymbol{r}_1{\rm d}\boldsymbol{r}_2. \tag{9}$$

The three-body density is defined as

$$\rho_3(\boldsymbol{r}_1, \boldsymbol{r}_2, \boldsymbol{r}_3) = \int {\rm d}\boldsymbol{r}_4 \cdots {\rm d}\boldsymbol{r}_N |\,\Psi|^2, \tag{10}$$

satisfying

$$1 = \int \rho_3(\boldsymbol{r}_1, \boldsymbol{r}_2, \boldsymbol{r}_2){\rm d}\boldsymbol{r}_1{\rm d}\boldsymbol{r}_2{\rm d}\boldsymbol{r}_3. \tag{11}$$

The results of the one-body densities of selected first-states ranging from $(45)_1$ to $(50)_1$ are given in Fig.1, in which the $(L)_i$ label of each state is marked in the subfigures. The $(46)_1$ has been neglected because it is simply an excited state of the $(45)_1$ with and only with the c.m. motion being excited, Furthermore, the $\rho_1$ of the $(45)_4$ has been given because it has a completely different feature. The unit of length for the abscissa is $\sqrt{\dfrac{\hbar}{m^*\omega}}$ with $\omega = \sqrt{\omega_0^2 + (\dfrac{eB}{2m^*c})^2}$. The subfigure at the left-hand side have $B$=0 while those at the right-hand side have $B$=10T. The curves at both sides are found to be one to one very similar. However, the right-hand side has a much larger $\omega$ and therefore a much smaller unit of length. It implies that the introduction of the magnetic field reduces the size of the system greatly while the feature of wavefunction remains nearly unchanged. This fact has been found before in the literature, and we confirm this finding once more via the set of one-body density plots.

The plots in Fig.1 can be classified into three types. The $(51)_1$ belongs to the first type, in which there is a single peak, where all the six electrons prefer to stay and they form a ring outside. The probability to find an electron to be close to the centre is very small. The $(45)_4$ belong to the second type, in which there is a broad peak. A detailed observation finds that the broad peak can be divided into two with a minimum (located at $r = r_0$) lying between them. We define

$$g(r_0) = N \int_0^{r_0} \rho_1(\boldsymbol{r}){\rm d}\boldsymbol{r}, \tag{12}$$

which is the average number of electrons staying inside the circle of radius $r_0$. For the $(45)_4$, we found that $g(r_0) = 3$. It implied that this state has a double ring structure, each contains three electrons. All the rest belong to the third type, in which there are two peaks, one is located at the centre while the other is located outside with a minimum (located at $r = r_0$) lying between them. Accordingly, the circle with a radius $r_0$ can be considered as a boundary to separate the inside and outside regions. Obviously, this type is associated with the ring-core structure proposed before.[1−4] Meanwhile, the $g(r_0)$ gives the average number of electrons inside the core. The $(45)_1$ and $(50)_1$ have $g(r_0) = 1$ (refer to Table 1), thus these states have a clear centred-pentagon structure. The $(47)_1$, $(48)_1$, and $(49)_1$, have $g(r_0)$ close to but not equal to 1. Thus, mostly there is an electron in the core, but the electron might go out (or come in) occasionally. In other words, these states are not so crystal-like as the $(45)_1$ and $(50)_1$. Now, the noticeable point is that the suggested picture with a few valence electrons surrounding a core does not emerge in our numerical calculation. For example, if the $\Psi_{\rm LBP}$ with $q$=3 and $M$=2 is the main component of the $(47)_1$, then there would have two valence electrons surrounding a core of four electrons. However, instead of two, the exact solution tells us that there are mostly five, or even more, electrons in the ring outside. This numerical result does not change qualitatively if the dynamical parameters, i.e., $\omega_0, \varepsilon$, and $B$, are changed. Thus, the validity of the $\Psi_{\rm LBP}$ wavefunction is in grave doubt.

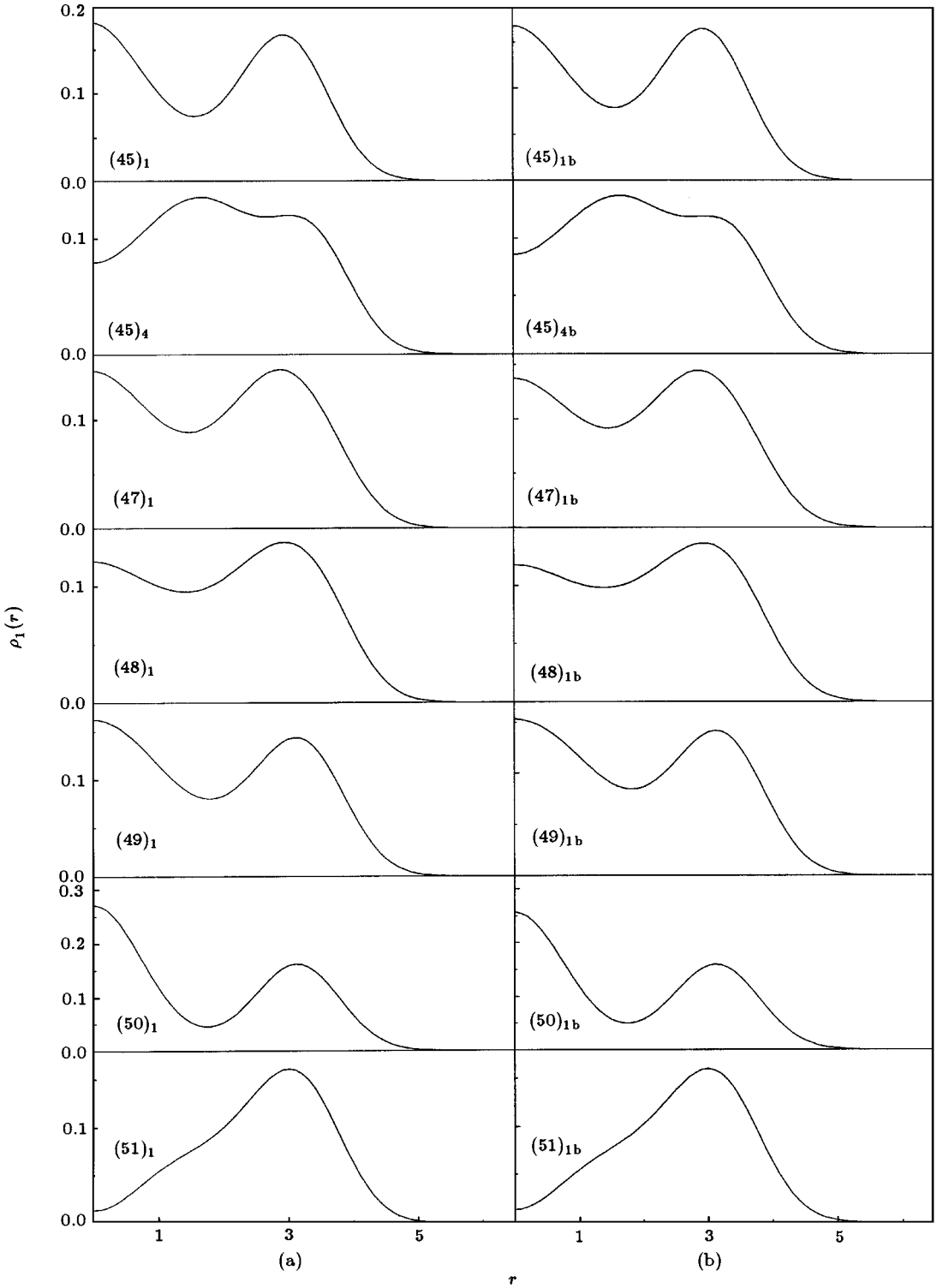



**Fig.1.** The one-body density $\rho_1$.

**Table 1.** The electronic number of difference states inside the district of $r \leq r_0$.

| types | $(45)_1$ | $(47)_1$ | $(48)_1$ | $(49)_1$ | $(50)_1$ | $(51)_1$ | $(45)_4$ |
|---|---|---|---|---|---|---|---|
| average number of electrons | 1 | 0.83 | 0.83 | 1.08 | 1 | 0 | 3 |
| $r_0$ | 1.7 | 1.5 | 1.5 | 1.8 | 1.7 | 0 | 2.7 |

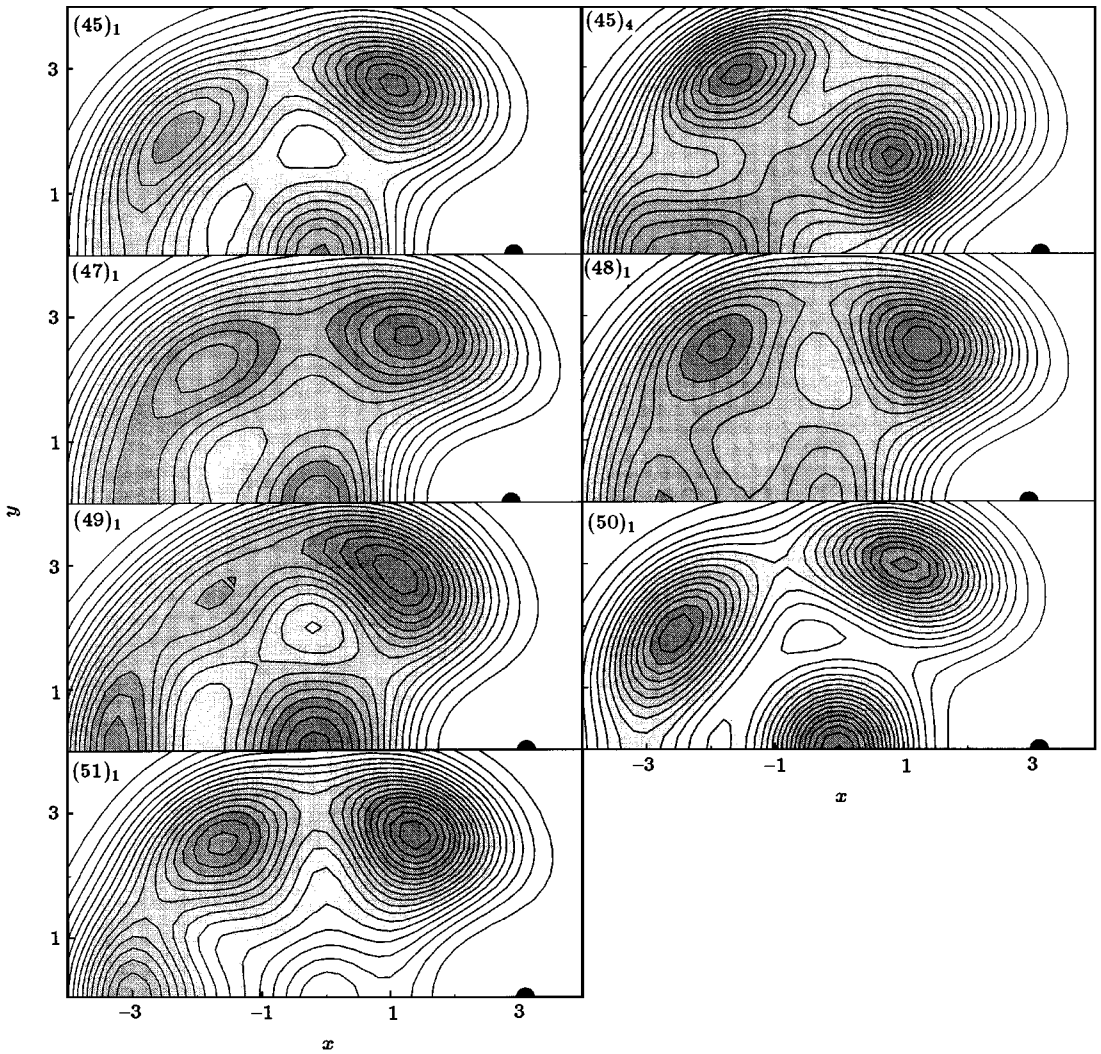



**Fig.2.** The two-body densities $\rho_2$.

For a more detailed inspection, we observe the contour plots of the two-body densities $\rho_2(\boldsymbol{r}_1, \boldsymbol{r}_2)$. In what follows only the results of $B$=0 will be given. In Fig.2 $\rho_2$ are given in the upper X-Y plane with $\boldsymbol{r}_2 = \boldsymbol{r}_{20}$ fixed at the X-axis (marked by a black spot). The darker area is associated with a larger $\rho_2$, and the peak denotes the most probable location of the first electron $e_1$ when $e_2$ is fixed, and the $\rho_2$ in the lower X-Y plane is symmetric to that in the upper plane. The centred-pentagon structure is very clear in the $(45)_1$ and $(50)_1$, the hexagon is clear in $(51)_1$, and the double ring (each containing three electrons) is clear in $(45)_4$. On the other hand, the geometric feature of the $(47)_1$, $(48)_1$ and $(49)_1$, is not so explicit. Nonetheless, most electrons stay outside in these states.

The contour plots of the three-body densities $\rho_3(\boldsymbol{r}_1, \boldsymbol{r}_2, \boldsymbol{r}_3)$ are given in Fig.3, where the locations of $e_2$ and $e_3$ are fixed and marked by black spots. Once the locations of two electrons having been fixed, the geometric features of the relevant states become more explicit, this is true even for the $(47)_1$, $(48)_1$ and $(49)_1$. It is once more confirmed that these states do not have a few valence electrons outside the core.

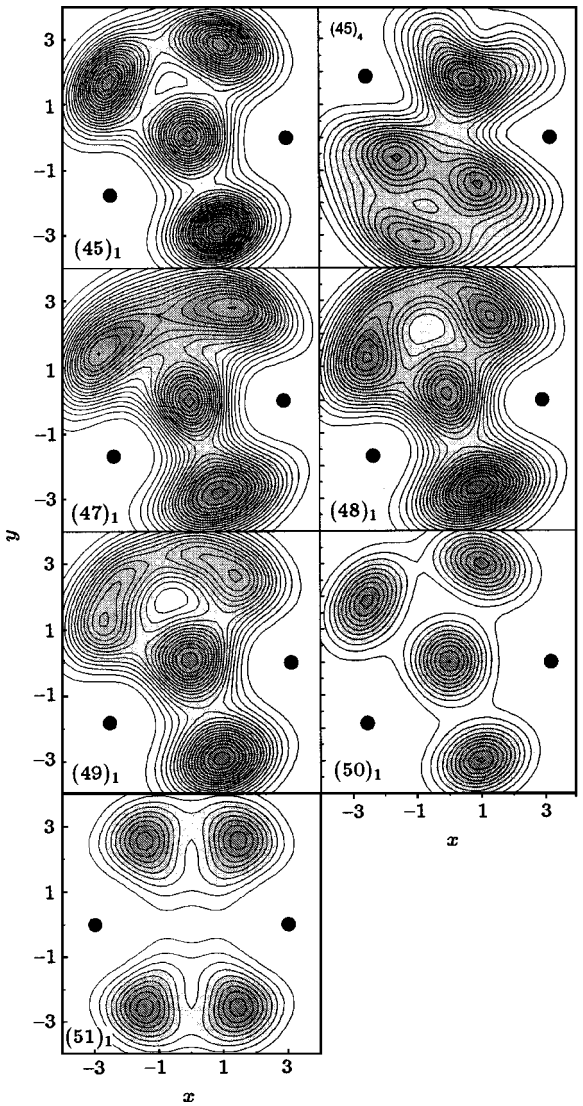



**Fig.3.** The three-body densities $\rho_3$.

## 3. An analysis based on symmetry and conclusions

The geometric structure (or the crystal-like behaviour) of quantum dots has been investigated based on symmetry consideration.[7−8] For the six-electron dot, it was found that only the states with $L = 6k + 3$ ($k$ is an integer) are allowed to possess a regular hexagon configuration, and only the states with $L = 5k$ are allowed to possess a regular centred-pentagon configuration. This is the underlying reason that six-electron ring was found in the $(51)_1$ state, and the five-electron ring was found in the $(50)_1$ state. For the $L$=45 states both the hexagon and pentagon are allowed. However, the centred-pentagon is associated with a lower total potential energy. Therefore, this shape is chosen by the $(45)_1$.

On the other hand, we found that the first-states with $L$ being neither equal to $6k + 3$ nor $5k$ have also the ring-core structure with mostly five electrons in the ring, such a structure is lower in total potential energy. However, for these states the ring-core structure is not very stable. Two points are noticeable: (i) The radial motion of the electrons might be stronger, consequently the electron in the core has a larger chance to go out (or inversely) as stated before. In other words, the electrons in the core and in the ring might exchange more frequently, this would lead to an ambiguity of the geometric feature (this point deserves a further study). (ii) The angular motion of the electrons is stronger. The second point can be directly verified by observing the wavefunction in the ring as follows.

Let us observe the $(45)_1$ and $(48)_1$ as examples, $B$=0 is assumed. Let five of the electrons be put equidistantly on a circle while one at the centre. The radius of the circle is the same as the radial distance at which the one-body density is peaked. Obviously, the five outer electrons form a regular pentagon. Now let four of them remain fixed at the vertexes of the pentagon and one is allowed to move along the circle back and forth around the vertex. Then the real and imaginary parts of the wavefunction are give in Fig.4, where the abscissa is the azimuthal angle $\theta$ apart from the vertex. In Fig.4(a) the real part of the $(45)_1$ has a peak at $\theta$=0. This means that the regular pentagon is a most probable shape. Whereas in Fig.4(b) both the real and imaginary parts of the $(48)_1$ are zero at $\theta = 0$. This means that the regular pentagon is prohibited in which a node emerges (a zero point of the wavefunction). Since the appearance of a node is a signal of a stronger oscillation. It is believed that, for the $(48)_1$, the internal motion in the ring is stronger.

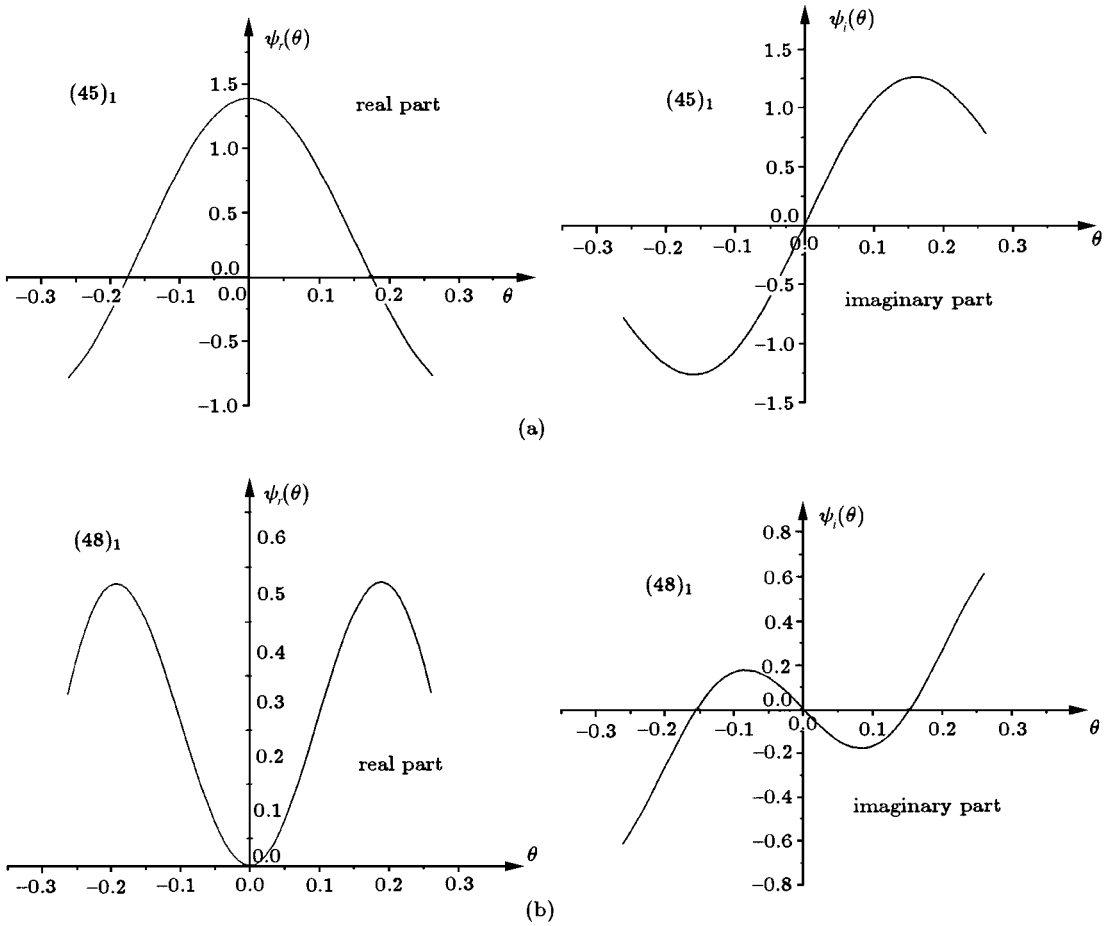



**Fig.4.** $\varphi_r(\theta)$ and $\varphi_i(\theta)$ are the real and imaginary parts of the wavefunctions of the $(45)_1$ (Fig.(a)) and $(48)_1$ (Fig.(b)) states. $\theta$ measures the angular motion of an electron around a vertex of a regular pentagon as an equilibrium point of oscillation.

In conclusion, although the trial wavefunction $\Psi_{\mathrm{LBP}}$ proposed in Ref.[5] has an elegant form and has the overlap with the exact eigenstate not small, the physical picture provided by this function deviates remarkably from the real picture. Our numerical results deny the possibility of having a few valence electrons surrounding a core, and in general support the ring-core structure.

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