# Magnetic Field Dependence of Electronic Structures in a Deformed Quantum Dot by 3D-MHFKS Calculation

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The magnetic (B) field induced transitions of the electronic states measured in a deformed single quantum dot [1] depending on the electron numbers (N) are investigated in the framework of 3-dimensional-mesh Hartree-Fock-Kohn-Sham (3D-MHFKS) method [2] and discussed to what extend the circular broken symmetry of single particle wave functions restore the circular symmetry with increasing the strength of B-field.

In the deformed dots [1], the lateral confinement potential is represented by the parabolic one $\frac{1}{2}m^*\omega^2(\delta x^2 + \frac{1}{\delta}y^2)$ using the deformation parameter $\delta$, then the wave functions are represented by the wave functions with the quantum numbers $(n_x, n_y)$ of broken circular symmetry in the limit of B=0. However it is expected that the wave functions is restored to have the characteristics with circular symmetry depending on the strength of the B-field because the field is represented by circular symmetric potential $\frac{1}{8}m^*\omega_c^2(x^2+y^2)$ and $-\frac{1}{2}\omega_c\hat{l_z}$ where $\omega_c = \frac{eB}{m^*c}$.

To investigate from the viewpoint of quantum number how far the restorations are generated, the averaged values $< l_z >$ of the angular momentum operator $\hat{l_z}$ are calculated and for the spatial viewpoint the density of the calculated wave functions are profiled.

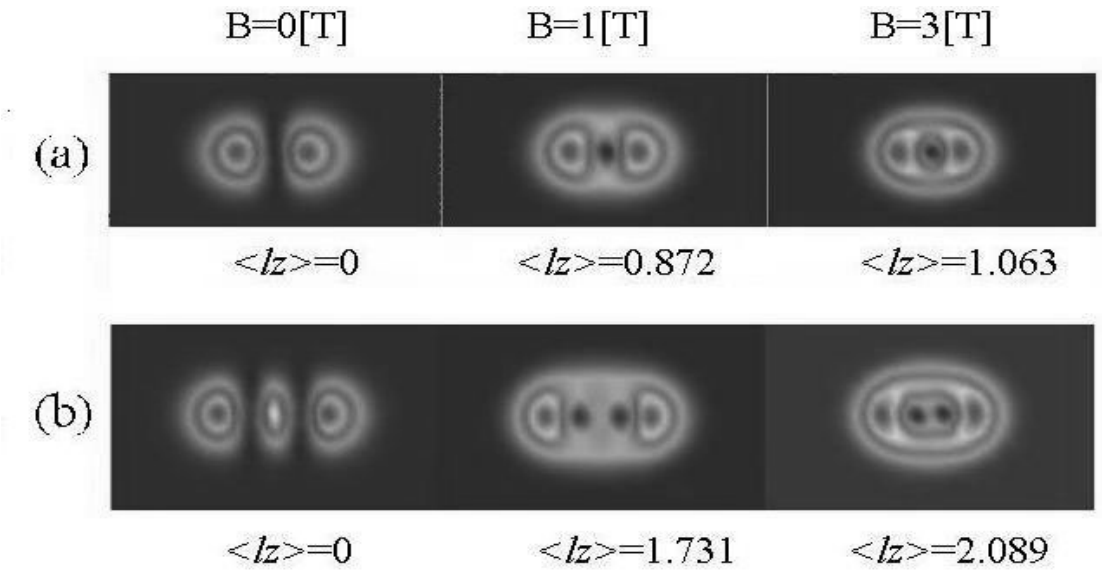


Figure 1: B-field dependence of density profile of the single particle wave function and averaged values $< l_z >$ in the case of $\delta = 1.5$ and $\hbar\omega_0 = 5$meV. (a) for $(n_x, n_y) = (0, 1)$ state and (b) $(0, 2)$ state

Firstly it is shown how the single particle wave functions depend on the strength of B-field in the case of deformation parameter $\delta = 1.5$. The $(n_x, n_y)$ states in the limit B=0T have the average values $< l_z >= 0$ because the wave functions are pure real or pure imaginary functions but the wave functions becomes complex ones in the case of B $\geq 0$ then the $< l_z >$ becomes to have the finite value. These transitions of the wave functions from pure real or imaginary functions to complex ones depending on the strength of B-field are very easily calculated in the mesh method, because the method is able properly to treat the imaginary operator $-\frac{1}{2}\omega_c\hat{l_z}$ without introducing any particular conditions.

In Fig.1(a), to exemplify the general characteristics, the $(n_x, n_y) = (0, 1)$ state in the B=0 limit which has $< l_z >= 0$ is shown to restore the circular symmetry as $< l_z >= 0.872$ and $< l_z >= 1.063$ in the case of B=1T and B=3T, respectively. As far as we see the averaged values $< l_z >$, it seems that the circular symmetries are completely restored in the B-field larger than B>1T. But if we see the density profile of the single particle wave functions, the restorations in space seems not complete as expected from the averaged values $< l_z >$. In Fig.1(b), the $(n_x, n_y) = (0, 2)$ state in B=0T is shown how the state develops from symmetry broken state to circular symmetry restored one from B=1T to 3T. The general tendency and characteristics of the state (0,2) is almost similar with that of the state (0,1) shown in Fig.1(a).

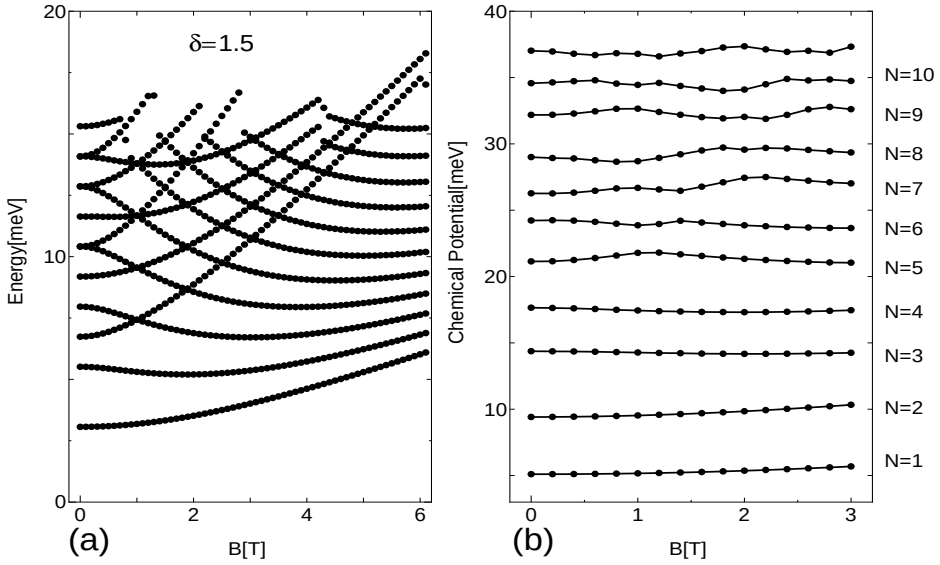


Figure 2: (a) Single particle energy levels of a deformed quantum dot as a function of B-field for the case $\delta = 1.5$. (b) The calculated chemical potential obtained by 3D-MHFKS-calculation.

Secondly, the chemical potentials $\mu_N = E_N - E_{N-1}$ obtained by the 3D-MHFKS calculations are shown in Fig.2(b) as a function of B-field from B=0T to B=3T and up to electron numbers N=11 in the case of $\delta = 1.5$, where $E_N$ is the total energy of 3D-MHFKS method. As can be expected from the B-field dependence of the single particle energy levels shown in Fig.2(a), the B-field dependences of the chemical potential are very smooth for the electron number up to N=4. For example the spin state of the N=4 correspond to spin singlet state with spin occupation $(N\downarrow, N\uparrow) = (2, 2)$. In the case of the electron numbers $N \geq 5$, the B-field dependence of the chemical potential show the wiggles which are mainly originated from the crossings of single particle energy levels shown in Fig.2(a). It should be pointed out that the B-field and electron number dependence of chemical potential obtained by 3D-MHFKS calculation almost reproduces the essential characteristics of the measured one [1].

The symmetry restoration from the broken to circular one of the single particle wave functions obtained in the 3D-MHFKS-calculation show almost similar B-field dependence shown in Fig.1. The Hartree and also exchange term in the 3D-MHFKS calculation depend rather sensitively on the symmetry of the single particle wave functions in the smallest limit of the deformation parameter $\delta \simeq 1$ too, then the electronic states of the circular dots will also be discussed from the view point of broken symmetry.


[1] S. Tarucha, et al., Appl. Phys. A **71**, 367, (2000).
[2] T. Matsuse, et al., Eur. Phys. J. D **16**, 391, (2001).