

Density Profiles, Energy, and Oscillation Strength of a Quantum Dot in Two Dimensions with a Harmonic Oscillator External Potential using an Orbital-free Energy Functional Based on Thomas–Fermi Theory

Suhufa Alfariisa^{2,3}, Wipsar Sunu Brams Dwandaru^{1*}, and Denny Darmawan¹

1. Department of Physics, Universitas Negeri Yogyakarta, Yogyakarta 55281, Indonesia
2. Department of Physics, Universiti Pendidikan Sultan Idris, Tanjung Malim, Perak 35900, Malaysia
3. Department of Physics, Universitas PGRI, Palembang 30263, Indonesia

*E-mail: wipsarian@uny.ac.id

Received March 4, 2015 | Accepted January 6, 2016

Abstract

This research aims i) to determine the density profile and calculate the ground state energy of a quantum dot in two dimensions (2D) with a harmonic oscillator potential using orbital-free density functional theory, and ii) to understand the effect of the harmonic oscillator potential strength on the electron density profiles in the quantum dot. This study determines the total energy functional of the quantum dot that is a functional of the density that depends only on spatial variables. The total energy functional consists of three terms. The first term is the kinetic energy functional, which is the Thomas–Fermi approximation in this case. The second term is the external potential. The harmonic oscillator potential is used in this study. The last term is the electron–electron interactions described by the Coulomb interaction. The functional is formally solved to obtain the electron density as a function of spatial variables. This equation cannot be solved analytically, and thus a numerical method is used to determine the profile of the electron density. Using the electron density profiles, the ground state energy of the quantum dot in 2D can be calculated. The ground state energies obtained are 2.464, 22.26, 90.1957, 252.437, and 496.658 au for 2, 6, 12, 20, and 56 electrons, respectively. The highest electron density is localized close to the middle of the quantum dot. The density profiles decrease with the increasing distance, and the lowest density is at the edge of the quantum dot. Generally, increasing the harmonic oscillator potential strength reduces the density profiles around the center of the quantum dot.

Abstrak

Profil Kerapatan, Energi, dan Kuat Osilasi sebuah Kuantum Dot dalam Dua Dimensi dengan sebuah Potensial Eksternal Osilator Harmonik menggunakan Fungsional Energi Bebas-orbital berdasarkan Teori Thomas–Fermi. Tujuan dari penelitian ini adalah: i) menentukan profil kerapatan dan menghitung energi keadaan dasar sebuah kuantum dot dalam dua dimensi (2D) dengan sebuah potensial osilator harmonik menggunakan teori fungsional kerapatan bebas-orbital, dan ii) memahami efek dari kekuatan potensial osilator harmonik terhadap kerapatan elektron dalam kuantum dot. Penelitian ini menentukan fungsional energi total kuantum dot yang merupakan fungsional dari kerapatan dan hanya bergantung pada variabel posisi. Fungsional energi total terdiri dari tiga suku. Suku pertama adalah fungsional energi kinetik yang dalam hal ini digunakan pendekatan Thomas–Fermi. Suku kedua adalah potensial eksternal. Dalam penelitian ini, potensial osilator harmonik yang digunakan. Suku terakhir adalah interaksi elektron–elektron yang dideskripsikan oleh interaksi Coulomb. Fungsional ini secara formal ditentukan solusinya untuk memperoleh kerapatan elektron sebagai fungsi posisi. Persamaan ini tidak dapat diselesaikan secara analitik, oleh karenanya, sebuah metode numerik digunakan untuk menentukan profil kerapatan elektron. Menggunakan profil kerapatan elektron yang diperoleh, energi keadaan dasar kuantum dot dalam 2D dapat dihitung. Nilai-nilai energi keadaan dasar yang diperoleh adalah 2,464; 22,26; 90,1957; 252,437; dan 496,658 au untuk masing-masing jumlah elektron 2, 6, 12, 20, dan 56. Kerapatan elektron tertinggi terlokalisasi pada bagian tengah kuantum dot. Profil kerapatan berkurang dengan bertambahnya jarak, dan kerapatan terendah berada pada ujung kuantum dot. Secara umum, meningkatkan kuat osilasi akan menurunkan profil kerapatan elektron di sekitar bagian tengah kuantum dot.

Keywords: harmonic oscillator potential, orbital-free density functional theory, quantum dot, Thomas–Fermi theory

Introduction

The recent progress in semiconductor fabrication technology enables us to produce very small systems on a nanometer scale that can contain one electron only [1]. The motion of the electron in this system is restricted to a zero dimension, *i.e.*, the electron is confined and not free to move in any direction. This system is called a quantum dot, and it is in the mesoscopic regime because its size ranges from nanometers to a few microns.

A quantum dot has many applications in electrical and optical devices such as quantum dot laser [2], photo-detector [3], solar cell [4], LED [5], and sensor [6]. Research of quantum dots is rapidly growing because of their great applications. Kouwenhoven *et al.* investigated the shell structure and the magic number in a quantum dot by observing the electron transport in a quantum dot system [7].

The calculation of the ground state energy is useful to obtain information about the condition of a system, for example, in determining the entropy and the energy level. Determining the ground state energy can be conducted by various methods, and one of them is density functional theory (DFT). Generally, DFT has been applied to different physical systems such as spin polarized [8], multicomponent [9], finite temperature [10], superconducting [11], time-dependent systems [12], and self-bound systems [13]. However, research on a quantum dot system using DFT is not fully explored yet.

A quantum dot may also be called an artificial atom because of its similar properties with an atomic system. The difference between a quantum dot and an atom is related to the confinement of electrons. Electrons in a quantum dot are confined in a larger space than those in an atom. Moreover, electrons in an atom are bound to the core, whereas those in a quantum dot can be made to move freely. In an atom, the Coulomb interaction restricts the movement of electrons in a small area near the core. The potential in a quantum dot does not attract the electron to the core but looks more like a harmonic trap that is defined by an external electrode (lateral quantum dot) or by a physical dimension (vertical quantum dot) [14].

The confinement potential of electrons in a quantum dot is usually modeled simply, such as a potential well (quantum box) or a harmonic potential. The implementation of a harmonic potential in a quantum dot is effective because in this case, the electronic properties of a quantum dot can be simply predicted. This potential takes the form of [14]

$$V_{\text{ext}}(r) = \frac{1}{2} m \omega^2 r^2, \quad (1)$$

where m is the quantum dot mass, and it is $m = 1$ in this study; ω is the strength of the harmonic potential; and r is the distance of the electron in the quantum dot.

Thomas–Fermi theory describes an approximation to the electron density, $\rho(r)$, and ground state energy, $E(N)$ for many atoms or molecules with many electron numbers, N . The Thomas–Fermi functional energy is formulated as

$$E[\rho] = T[\rho] + E_{\text{ee}}[\rho] + \int V_{\text{ext}}(r)\rho(r)dr, \quad (2)$$

where the kinetic energy in 2D, $T[\rho]$, is based on the Fermi–Dirac statistics for the homogeneous electron gas, *i.e.*,

$$T[\rho] = \frac{\pi}{2} \int \rho^2(r)dr, \quad (3)$$

where $E_{\text{ee}}[\rho]$ is the energy due to the electron–electron interactions, and $V_{\text{ext}}(r)$ is an external potential, which is the spherical harmonic oscillator potential in this case.

As in orbital-free density functional theory, the electronic density and ground state energy are obtained by minimizing the functional $E[\rho]$ with respect to $\rho(r)$ for a given V_{ext} , which is called the variational principle [15]. The main principle of DFT can be expressed as [16]

$$\frac{\delta}{\delta \rho(r')} [E[\rho] - \mu(\rho(r)dr - N)] = 0. \quad (4)$$

The true density and ground state energy can be obtained using the variational principle (4) with a certain constraint. For any density profile, the canonical distribution is usually used as a constraint, and the number of electrons, N , is constant or

$$2\pi \int r\rho(r)dr = N. \quad (5)$$

Furthermore, the Lagrange multiplier of the constraint is the chemical potential, μ . Most of the DFT scheme is a modification or a development of Thomas–Fermi theory [17]. Therefore, the energy functional of the electrons in a quantum dot is given as

$$E[\rho] = \frac{\pi}{2} \int \rho^2(r)dr + \frac{1}{2} \iint \frac{\rho(r)\rho(r')}{|r-r'|} drdr' + \pi\omega^2 \int r^3 \rho(r)dr. \quad (6)$$

Applying Equation (4) to Equation (6), we can derive the equation used to determine the electron density profile and energy as follows:

$$\rho(r) = \frac{1}{\pi} \left[\mu - \frac{1}{2} \int \frac{\rho(r')}{|r-r'|} dr' - \pi\omega^2 r^3 \right]. \quad (7)$$

Equation (7) may be considered a self-consistent equation, which can be solved numerically. Therefore, by solving Equation (7), the density and energy of the quantum dot can be obtained.

Materials and Methods

The main instruments used in this research are i) one unit of computer with an Intel (R) Core (TM) i3 CPU and 1.00 GB RAM, ii) Dev C++ language program, and iii) Microsoft Excel. The free variable is the distance from the center to one of the ends of the quantum dot; the dependent variables are the density, $\rho(r)$, and the ground state energy, E ; and the control variables are i) the number of electrons, N , ii) the external potential strength, ω , and iii) the chemical potential, μ .

To obtain the data of the electronic density inside the quantum dot, a program code is constructed using Dev C++ program (language). The number of electrons used in this research is $N = 2, 6, 12, 20$, and 56 . The reason for using the aforementioned numbers of electrons is that they are the magic numbers in the quantum dot, in which the system is stable because all the states are full. Moreover, for $N = 6$ and $N = 56$, the density profile obtained from this study may be compared with those of other methods conducted previously. The algorithm of the programming code is given as follows: i) provide a first guess for the density profile, ii) determine the chemical potential, iii) calculate the true density using Equation (7) with a constraint provided by (5), iv) calculate the ground state energy, and v) calculate the density with external potential strength variation.

Results and Discussion

First, the density profiles with the number of particle variation in the quantum dot are determined, as shown in Figure 1. The horizontal axis is the distance, r , from the center until one end of the quantum dot, *i.e.*, from 0.0 until 1.0 . The vertical axis is the value of the density profile from 0.0 until 10.0 . The numbers of particles are $N = 2, 6, 12, 20$, and 56 electrons.

Figure 1 shows that the highest electron density is located at a distance that is closest to the center of the quantum dot for all numbers of electrons. The electron density decreases as the distance increases (going further away from the center of the quantum dot). Therefore, the lowest electron density is located at the edge of the quantum dot. Furthermore, it may also be observed that as the number of particles increases the density also increases.

The density profile of the quantum dot obtained in Figure 1 is also compared with that of other methods, as shown in Figure 2, which is obtained for $N = 6$. The first approach is the local density approximation (LDA) [18], and the second

is the fast approximation [17]. Quantitatively, our result (solid line) on the electron density profile for $N = 6$ is different from that in the other two approaches. However, qualitatively, the profile is quite appropriate. The highest density is located near the center or in the middle of the quantum dot. The density profiles decrease when the electrons are far away from the center. When the electrons are close to the center of the quantum dot, our result is slightly higher than the LDA result but lower than the fast approximation. The highest value of the density for our result is 0.163 compared with 0.243 for the fast approximation located at the center of the dot. For the LDA result, the highest density is obtained when r is about 0.2 au with a value of 0.15 . For the LDA and the fast approximation methods, the density profiles go to zero at around 5 au, but this result is not obtained in this study.

Another density profile comparison is obtained for $N = 56$, as observed in Figure 3. Our result is the solid (green) line compared with the LDA (dashed-dotted line) and the fast approximation (dashed line) results.

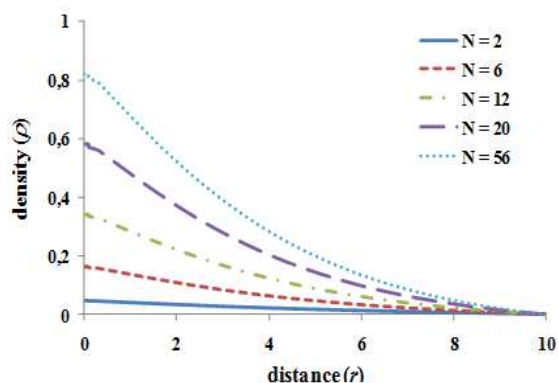


Figure 1. Density Profiles, $\rho(r)$, as a Function of the Distance, r , inside a Quantum Dot in 2D with a Number of Electron (N) Variations

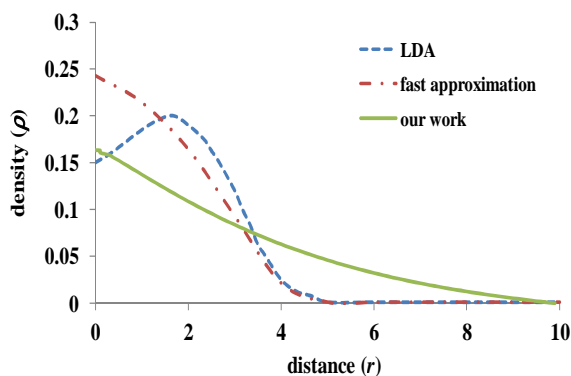


Figure 2. Comparison of the Density Profile of the Quantum Dot (solid line) with those of other Methods, *i.e.*, LDA (blue dashed line) and Fast Approximation (red dashed-dotted line) with $N = 6$

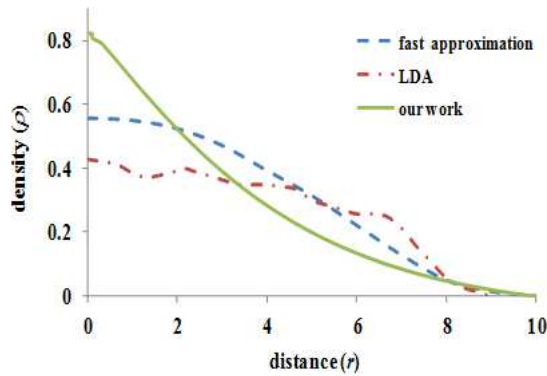


Figure 3. Comparison of the Density Profiles of the Quantum Dot (Solid Line) with those of other Methods, i.e., LDA (Red Dashed-dotted Line) and Fast Approximation (Blue Dashed Line) with $N = 56$.

Figure 3 shows that the density profile at the center of the quantum dot obtained from this work is higher than those of the other two approaches. However, away from the center of the dot, the density profile is lower than those of the LDA and fast approximation. When the density profile is further away from the center, our result is in accordance with the other two approaches. The differences in our results with those of other studies may be due to the fact that the exchange–correlation effect is not taken into account in this study. In the fast approximation approach, the electron–electron interaction is different from that used in this research, which is the Coulomb interaction in this case. For $N = 56$, the density profile generated in this study is higher than those of the two other methods. In the LDA approach, the value fluctuates but remains decreasing when the density profile is farther away from the center of the quantum dot.

Second, the results for the ground state energies are presented. The results for the ground state energy with the number of particle variations are shown in Table 1. For comparison, Räsänen *et al.* [18] reported for the value of $\omega^2 = 1$ and $N = 2$, the total energy of the ground state is 3 au. Clearly, our result of 2.2464 au is smaller than that given in [18]. Again, this result may be caused by the Thomas–Fermi approach, which does not include the exchange–correlation interaction term. Increasing the number of particles increases the energy as well, as observed in Table 1.

Finally, the results for the density profiles with oscillation strength variation are presented. In this case, we study the effect of the oscillation strength variations on the density profiles of the electrons in the quantum dot, as shown in Figure 4.

ω^2 shows the strength of the harmonic oscillator potential that traps the electron inside the quantum dot. The number of electrons used is $N = 56$ electrons.

Table 1. Ground State Energy Value of Electrons in the Quantum Dot with Various Numbers of Particles

N	E (au)
2	2.464
6	22.260
12	90.196
20	252.437
56	496.658

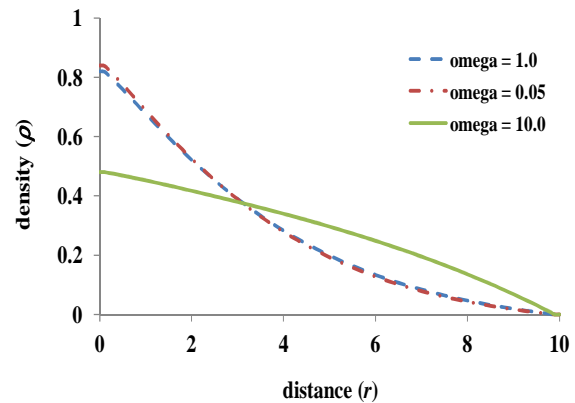


Figure 4. Density Profiles of the Electrons in the Quantum Dot with ω Variations

Figure 4 shows that increasing the oscillation strength tends to reduce the density at the center of the quantum dot. The difference in the density profiles for $\omega^2 = (0.05)^2$ and $\omega^2 = 1$ is very small. However, as the oscillation increases to $\omega^2 = 10^2$, the density decreases near the center of the quantum dot.

Conclusions

The density profiles of electrons in the quantum dot are the highest at the center or in the middle of the quantum dot. The density decreases with the increasing distance, and the lowest density is at the farthest from the center of the quantum dot. Furthermore, as the number of electrons increases, the higher the ground state energy becomes. Finally, increasing the oscillation strength reduces the density profiles of the electrons around the center of the quantum dot.

Acknowledgements

The authors would like to thank the Faculty of Mathematics and Natural Sciences at the Yogyakarta State University for funding this research.

References

- [1] Ashoori, R.C. 1996. Electrons in artificial atoms. *Nature*. 379: 413-419, doi: 10.1038/379413a0.

- [2] Raghunathan, R., Grillot, F., Mee, J.K., Murrell, D., Kovanis, V., Lester, F.L. 2014. Tuning the external optical feedback-sensitivity of a passively mode-locked quantum dot laser. *Appl. Phys. Lett.* 105: 041112, <http://dx.doi.org/10.1063/1.4891576>.
- [3] Konstantatos, G., Sargent, E.H. Colloidal quantum dot photodetectors. *Infrared Phys. Technol.* 54(3):278-282, <http://dx.doi.org/10.1016/j.infrared.2010.12.029>.
- [4] Nozik, A.J. 2002. Quantum dot solar cells. *Physica E: Low-dimensional Systems and Nanostructures* 14(1): 115-120, doi: 10.1016/S1386-9477(02)00374-0.
- [5] Schulz, W. –M., Eichfelder, M., Reischle, M., Kessler, C., Robbach R., Jetter, M., Michler, P. 2011. Pulsed single-photon resonant-cavity quantum dot LED. *J. Cryst. Growth.* 315: 127-130, doi: 10.1016/j.jcrysgro.2010.08.014.
- [6] Y. –X. Huang, Zheng, X. J., Kang, L. L., Chen, X. –Y., Liu, W. –J., Huang, B. –T., Wu, Z. –J. 2011. Quantum dots as a sensor for quantitative visualization of surface charges on single living cells with nano-scale resolution. *Biosens. Bioelectron.* 26(5):2114-2118, doi: 10.1016/j.bios.2010.09.016.
- [7] Kouwenhoven, L.P., Austing, D.G., Tarucha, S. 2001. Few-electron quantum dots. *Rep. Prog. Phys.* 64: 701-736.
- [8] Kvashnin, Y.O., Grånäs, O., Di Marco, I., Katsnelson, M.I., Lichtenstein, A.I., Eriksson, O. 2015. Exchange parameters of strongly correlated materials: extraction from spin-polarized density functional theory plus dynamical mean-field theory. *Phys. Rev. B.* 91: 125-133, <http://dx.doi.org/10.1103/PhysRevB.91.125133>.
- [9] Härtel, A., Kohl, M., Schmiedeberg, M. 2015. Anisotropic pair correlations in binary and multi-component hard-sphere mixtures in the vicinity of a hard wall: a combined density functional theory and simulation study. *Phys. Rev. E.* 92: 042-310, doi: 10.1103/PhysRevE.92.042310.
- [10] Dwandaru, W.S.B., Schmidt, M. 2011. Variational principle of classical density functional theory via Levy's constrained search method. *Phys. Rev. E.* 83: 061-133, <http://dx.doi.org/10.1103/PhysRevE.83.061133>.
- [11] Aliabad, H.A.R., Akbari, H., Saeed, M.A. 2015. Evaluation of magneto-optic properties of LaXPO (X = Mn, Fe, Ni) new superconductors by DFT. *Commatsci.* 106: 5-14, doi: 10.1016/j.commsci.2015.04.030.
- [12] Whitfield, J.D., Yung, M. –H., Tempel, D.G., Boixo, S., Aspuru-Guzik, A. 2014. Computational complexity of time-dependent density functional theory. *New J. Phys.* 16: 083035, <http://iopscience.iop.org/1367-2630/16/8/083035>.
- [13] Messud, J., Bender, M., Surau, E. 2009. Density functional theory and Kohn-Sham scheme for self-bound systems. *Phys. Rev. C.* 80: 054314, <http://dx.doi.org/10.1103/PhysRevC.80.054314>.
- [14] Helle, M. 2006. Few-Electron quantum dot molecules. PhD Dissertation, Helsinki University of Technology, Finland.
- [15] Hohenberg, P. Kohn, W. 1964. Inhomogeneous electron gas. *Phys. Rev.* 136(3B): B864, <http://dx.doi.org/10.1103/PhysRev.136.B864>.
- [16] Harrison, N.M. 2003. *Nato Science Series Sub Series III Computer and Systems Sciences.* 187: 45-70.
- [17] Räsänen, E., Bekcioglu, G., Pittalis, S. 2011. Fast approximation for the energy and density of electrons in two dimensions. arXiv:1111.6470v1 [cond-mat.str-el], https://www.academia.edu/1125723/Fast_approximation_for_the_energy_and_density_of_electrons_in_two_dimensions.
- [18] Pittalis, S., Räsänen, E. 2009. Orbital-free energy functional for electrons in tow dimensions. *Phys. Rev. B.* 80: 165112, <http://dx.doi.org/10.1103/PhysRevB.80.165112>.