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Estimation of the Minimizer of the Thomas-Fermi-Dirac-von Weizsäcker Functional of NaCl Crystal Lattice

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Abstract. Estimation of the minimizer of the Thomas-Fermi-Dirac-von Weizsäcker functional of NaCl crystal lattice is calculated by making use of a direct method we have developed recently. The method is referred to as direct method for the reason that in the course of the calculation of the estimation, we do not derive the Euler-Lagrange equation at all. By using the graph of the umbrella functions, the estimation of the minimizer function is represented. The minimizer is bounded from above by the umbrella functions.

1. Introduction

The Thomas-Fermi (TF) theory was proposed by Thomas and Fermi independently in 1927. Dirac introduced the exchange correction to the theory in 1930, so that the corrected model is called the Thomas-Fermi-Dirac (TFD). Then the gradient correction of the kinetic energy was added by von Weizsäcker in 1935, so that it is called the Thomas-Fermi-von Weizsäcker (TFW) model. Those theories were placed on a firm mathematical footing by Lieb [1]. Although the Thomas-Fermi-Dirac-von Weizsäcker (TFDW) theory has not been studied as extensively as other theories, some authors studied it, such as Engel and Dreizler [2], who presented an accurate numerical solution of the variational equation resulting from the standard TFDW energy functional plus fourth-order gradient terms of the kinetic energy.

Chan et.al. [3] perform a numerical study of the TFDW theory in finite systems to gain an understanding of the variational behavior of kinetic energy functionals. Their findings indicate that the TFDW theory can give an approximate description of matter, with atomic energies, binding energies, and bond lengths of the correct order of magnitude, though not to the accuracy required of a qualitative chemical theory.

Zhuravlev *et.al.* [4] calculate valence electron densities in series of crystal substances MA (M = Li, Na, K, Rb, Ag, Mg, Ca; A = F, Cl, Br, O, S) with a NaCl lattice using the ab initio local DFT method combined with the ab initio pseudopotential technique. They found that systematic variations of valence electron density are depending on the atomic number of anion and cation.

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The existence of a minimizer is an interesting theme to be investigated [5]. The existence of the minimizer for TFW model was proved by Benguria, Brezis and Lieb in 1981 [6]. The nonexistence of a minimizer for TFDW model for electrons with no external potential has been investigated by Lu and Otto [7]. They showed that the TFDW functional energy without external potential has no minimizer when the number of electrons exceeds a certain positive integer. They also gave an estimation that the value of the functional is in the interval $[0,(4/5)^3]$. Wahyuni *et.al.* [8] have found the estimate of the minimizer for TFDW model of electrons in the influence of an external potential, without "touching" the associate Euler-Lagrange equation, the so-called direct method.

The TFDW energy functional for electrons with external potential V is given as

$$E(\phi) := \int_{\mathbb{R}^3} \left[|\nabla\phi|^2 + F(\phi^2)\right] dx + D(\phi^2,\phi^2) + \int_{\mathbb{R}^3} V\phi^2 \, dx, \tag{1}$$

where $F(t) = t^{5/3} - t^{4/3}$ and $D(\cdot,\cdot)$ is the Coulomb interaction in $\mathbb{R}^3$, i.e.:

$$D(f,g) = \int\int_{\mathbf{R}^3\times\mathbf{R}^3} \frac{f(x)g(y)}{|x-y|} dx \, dy. \tag{2}$$

The above functional can be rewritten as

$$E(\phi) := \int_{\mathbb{R}^3} \left[|\nabla\phi|^2 + \bar{F}(\phi^2)\right] dx + D(\phi^2,\phi^2), \tag{3}$$

where $\bar{F}(t) = t^{5/3} - t^{4/3} + Vt$.

The variational principle related to TFDW model is to find the minimizer of the TFDW functional energy, i.e. a function φ that minimizes $E(\phi)$ in the sense

$$E(\varphi) = \inf_{\phi\in X,\ \int\phi^2 = m} E(\phi), \tag{4}$$

for suitable function space X.

Wahyuni *et.al.* [8] have shown that this minimizer function is bounded from above by the "umbrella" function $b(x)$ which depends on the external potential $V(x)$. This function is given by

$$b(x) = \left(\frac{4+\sqrt{16-60V(x)}}{10}\right)^{3/2}. \tag{5}$$

This current work is a part of our continued work as in [8]. We want to find out the application of this direct methods to crystal physics by making use of the umbrella function to estimate the minimizer of the TFDW functional of NaCl crystal lattice.

2. Estimation of the minimizer of the NaCl crystal lattice

NaCl has the face centered cubic (fcc) crystal lattice which results from the intersection of the Na's fcc structure and the Cl's fcc structure. In the non primitive unit cell of the Na's fcc structure there are four Na atoms, which means that there are four lattice points. So for Cl's fcc structure, there are four lattice points. Thus, in a non-primitive unit cell of NaCl, there are four Na and four Cl atoms. However, if we take primitive cells of NaCl crystal lattice, we get only one primitive cell. The NaCl crystal lattice structure is shown in Figure 1.

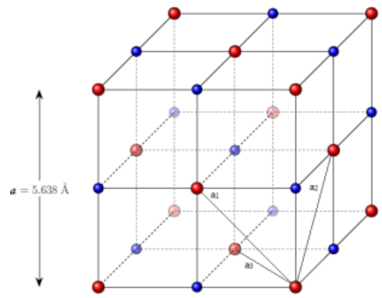


Figure 1. The primitive unit cell of NaCl

With the choice of the primitive unit cell above, the primitive unit vector is given by

$$\mathbf{a}_1 = \frac{a}{2}(\hat{y} + \hat{z}),$$
$$\mathbf{a}_2 = \frac{a}{2}(\hat{x} + \hat{z}),$$
$$\mathbf{a}_3 = \frac{a}{2}(\hat{x} + \hat{y}),$$

so that it may be written on a matrix form as

$$\mathbf{A} = \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}. \tag{6}$$

The crystal potential at any point x is obtained by summing the Coulomb terms over each charge in the crystal, i.e.:

$$V(x) = \sum_{m \in Z^3} \sum_{j=0}^{n-1} q_j |\mathbf{A}\mathbf{m} + \mathbf{d}_j - \mathbf{x}|^{-1}, \tag{7}$$

where $\mathbf{A}, \mathbf{m}$, and $\mathbf{d}_j$ are the primitive unit cell matrix, site, and position vector of the any point x to the j-th charge site q_j, respectively. Therefore, the vector from $\mathbf{x}$ to the j-th charge site (m_1, m_2, m_3) is $\mathbf{A}\mathbf{m} + \mathbf{d}_j - \mathbf{x}$ [9].

If it is applied to the NaCl crystal with the primitive unit cell, then the crystal potential is obtained as

$$\begin{aligned} V(x) \quad = \quad & \sum_{m \in Z^3} \left[\frac{1}{\sqrt{(m_2 + m_3 - x)^2 + (m_1 + m_3 - y)^2 + (m_1 + m_2 - z)^2}} \right] - \\ & \sum_{m \in Z^3} \left[\frac{1}{\sqrt{(m_2 + m_3 + 1 - x)^2 + (m_1 + m_3 + 1 - y)^2 + (m_1 + m_2 + 1 - z)^2}} \right]. \end{aligned} \tag{8}$$

The NaCl crystal potential on $z = 0$ is depicted on Figure 2. It is shown that potential forms an infinite pattern in both of the two reverse corners. It is also shown that there is an infinite potential that appail the electron to go there. The electron in this lattice tends to go to the area with narrow potential, or even to both of the cavity corners.

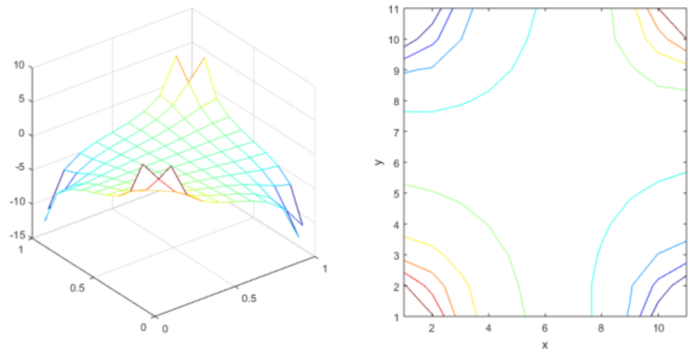


Figure 2. The 3D image of the NaCl crystal potential on $z = 0$ and its contour.

Figure 2 shows the NaCl crystal potential on one primitive unit cell. If it is considered by many primitive unit cells, the potential is shown on the Figure 3. Next, NaCl crystal potential (8) is substituted to the umbrella function (5). Indeed, we also have to remember that the potential has to be taken lower than or equal to $4/15$ so that the minimizer has the real value. The visualization of the $b^2(x)$ is shown in Figure 4 and the contour of the $b^2(x)$ is shown in the Figure 5. Note that the minimizer is always less than this umbrella function.

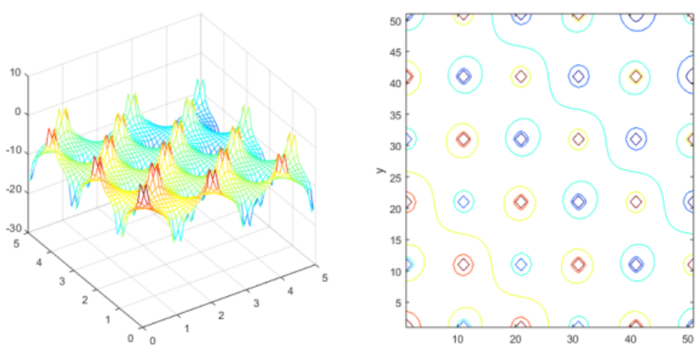


Figure 3. The 3D image of the NaCl crystal potential with five primitive unit cells and its contour.

3. Conclusion

The application of the direct method to estimate the minimizer of the TFDW functional of NaCl crystal lattice was presented. The umbrella function of NaCl crystal potential was shown in Figure 4 and the value of minimizer is bounded from above by this umbrella function.

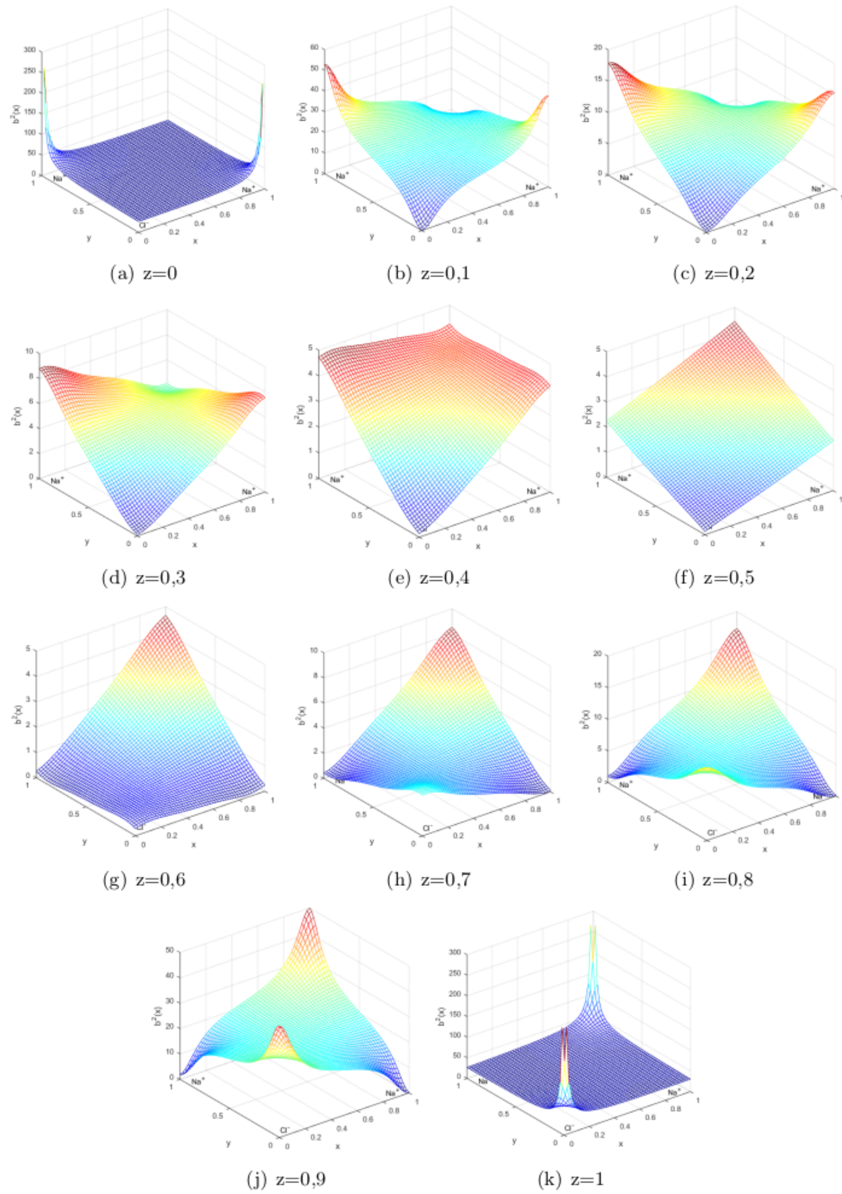
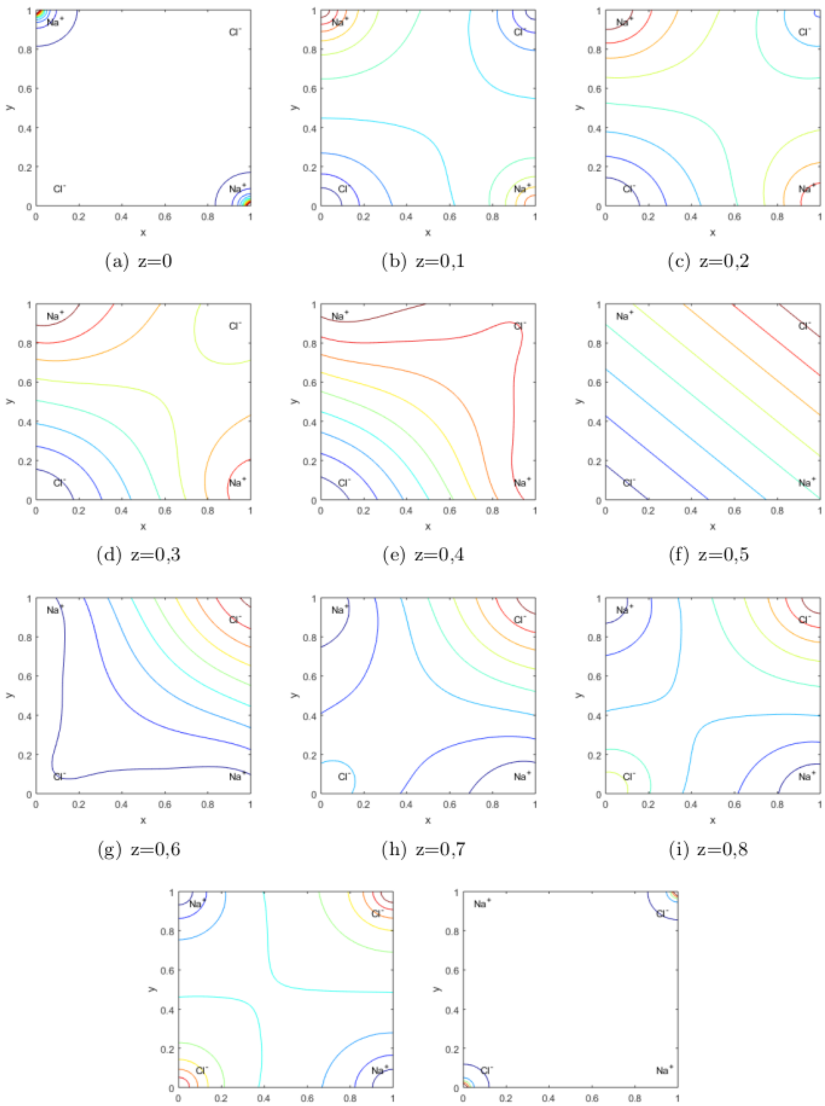


Figure 4. Picture $b^2(x)$ of the NaCl crystal potential in the many value of z



(a) z=0 (b) z=0,1 (c) z=0,2

(d) z=0,3 (e) z=0,4 (f) z=0,5

(g) z=0,6 (h) z=0,7 (i) z=0,8

(j) z=0,9 (k) z=1

Figure 5. The contour $b^2(x)$ of the NaCl crystal potential in the many value of z

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