# A VARIATIONAL SOLUTION OF THE SCHRÖDINGER EQUATIONS IN AN INHOMOGENEOUS COULOMB FIELD

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*Abstract: The present work is devoted to computer modeling of the emission processes from the surface of graphene. The pivotal obstacle for emission is a model of the unperturbed emission surface. The hydrogen-like atom model is one of the useful approaches describing the states of the emission surface. In [1] this model was used considering ion screening in the Brandt model [2]. To calculate the ground state of the electron, we used the variational solution of the Schrodinger equation, based on the minimization of the potential energy of an electron in the field of a homogeneous ion. However, the field of the screened singly ionized carbon atom in the Brandt model is not homogeneous. Therefore, it was shown in [3] that it is possible to obtain a binding energy error of up to 40% when using only the external screening parameter without taking into account the inhomogeneity. In this paper, we consider the effect of the ion screening parameter in the Brandt model λ and the algorithm for determining it by minimizing the total energy of the electron interaction in s state in two parameters: the effective ion charge and the ion screening parameter. The obtained solution of the Schrödinger equation is used to calculate the ground state of a hydrogen-like carbon atom in a graphene lattice at zero temperature and is compared with the results of [2, 4].*

*KEYWORDS: GRAPHENE, PSEUDOPOTENTIAL OF A HYDROGEN-LIKE ATOM, COMPUTER SIMULATION FOR GRAPHENE LATTICE*

## 1. Introduction

The present work is devoted to computer modeling of the emission processes from the surface of graphene - a perspective material for micro- and nanoelectronic devices. The pivotal obstacle for emission is a model of the unperturbed emission surface, determining the theoretical spectrum and the emission threshold current. One of the approaches to describe the states of the emission surface is the hydrogen-like atom model, which is used for light elements of the periodical table. In [1], a lattice of hydrogen-like atoms with a screened ion in the Brandt model was used to calculate the ground state of atoms of the graphene surface [2]. To calculate the ground state of an electron, the Schrödinger equation was solved by minimization of the potential energy of the electron in the ion field, which assumes homogeneity of the ion field. However, the field of the shielded singly ionized carbon atom in the Brant model is not homogeneous. Therefore, it was shown in [3] that using only the external screening parameter without taking into account the inhomogeneity, it is possible to obtain a binding energy error of up to 40%, which is unacceptable even for qualitative theory. In this paper, we consider the influence of the ion screening parameter in the Brant model λ and the algorithm for determining it by minimizing the total energy of the electron interaction in s state in terms of two parameters: the effective ion charge and the ion screening parameter. The obtained solution of the Schrodinger equation is used to calculate the ground state of a hydrogen-like carbon atom in a graphene lattice at zero temperature. The obtained solution is compared with the results of [2, 4].

## 2. Prerequisites and means for solving the problem

In [1], for the variational solution of the Schrödinger equation for an electron in a hydrogen-like atom, the method of determining the wave function in a given field was used [6]. This technique is based on minimizing the discrepancy of the difference between the total energy of an electron in a known ion field and the effective field

$$\tilde{U}_i(r) = \frac{q}{r} + A \qquad (1)$$

for which a self-similar solution of the Schrodinger equation is known, depending on the parameters of this field. For the ground state of a hydrogen-like carbon atom, this leads to a minimization of the functional

$$J_s(q,\lambda) = \int_0^\infty \psi_{2s}^2(x)\left[U_i(r,\lambda) - \frac{q}{r}\right]x^2 dx + \frac{q^2}{2n^2} + A,$$
$$\psi_{2s}^2(r) = \left(1 - \frac{x}{2}\right)^2 \exp(-x), \quad x = \frac{2q}{n} r. \qquad (2)$$

In this case, it is implicitly assumed that the field is uniform over *r*. However, the field of the screened ion in the Brandt-Kitagawa model is not uniform:

$$U_i(r) = \frac{1}{r} + \frac{Z-1}{r}\exp\left(-\frac{r}{\lambda_i}\right), \quad \frac{\partial}{\partial r}U_i(r) \neq kU_i(r). \qquad (3)$$

According to the virial theorem, the average total energy of the finite motion of an electron in the Coulomb field is related to the average kinetic and mean potential energy by the equation

$$\bar{E} = -\bar{T}, \quad \bar{U} = 2\bar{E}. \qquad (4)$$

Using the expression for the mean kinetic energy in a nonuniform field [5], we obtain the distribution of the total energy of the bound electron in an inhomogeneous field ion:

$$E(r) = \frac{r}{2}\frac{\partial}{\partial r}U_i(r) + U_i(r). \qquad (5)$$

Fig. 1 shows the distribution of the total energy of an electron with and without an accounting of the inhomogeneity of this field. As can be seen from the figure, the inhomogeneity of the field appears mostly near the nucleus. Therefore, taking into account the distribution of the probability density in s and p states, the influence of the field inhomogeneity on the binding energy of the electron with the ion will be larger for the electron in the s state than in the p state.

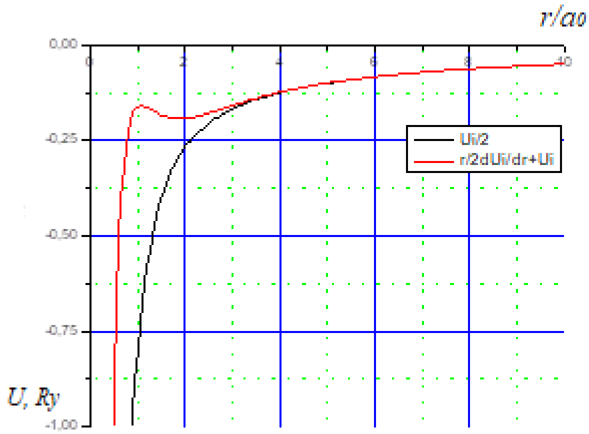


***Fig. 1.*** *Comparison of the distribution of the total energy along the radius for a finite motion of an electron*

in the field of the singly charged carbon ion in the Brandt model without and taking into account the inhomogeneity of the field.
Therefore, in an arbitrary field ion at solving the problem of variations on the characterization of the effective uniform field should be based on minimizing the total energy of the finite electron motion in a particular quantum state. The effective charge of the ion - q, and the external screening parameter - λ, are determined by the following system of nonlinear equations:

$$\frac{\partial}{\partial q}\left\{\int_0^\infty \psi_{2s}^2(x)\left[U_i(r,\lambda)-\frac{q}{r}\right]x^2dx+\frac{q^2}{2n^2}\right\}\Bigg|_{q=q_m}=0 \qquad (6)$$

$$A=-\int_0^\infty \psi_{2s}^2(x)\left[U_i(r,\lambda)-\frac{q_m}{r}\right]x^2dx-\frac{q_m^{2\,2}}{2n^2}$$

The hypothesis adopted by us was realized with the help of a numerical solution of the problem (6).

## 3. Solution of the examined problem

Figures 2a and 2b show numerical solutions of this problem for an electron in the s state with and without consideration for the inhomogeneity of the ion field for different values of the internal screening parameter λ of the ion in the Brandt model.

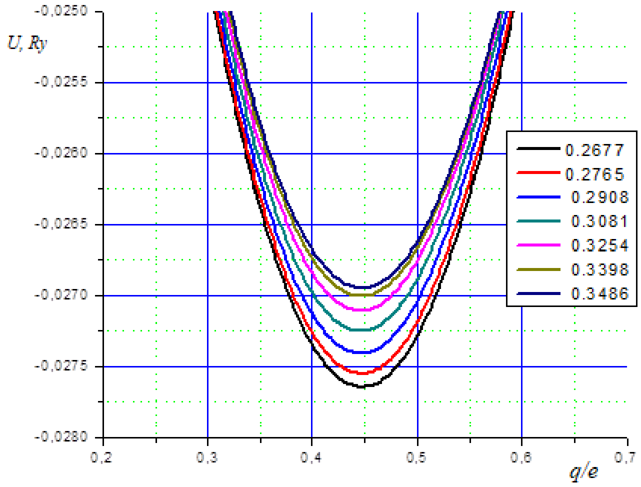


***Fig. 2a*** *Numerical solution of the variational task for an electron in the s state taking into account the inhomogeneity of the ion field.*

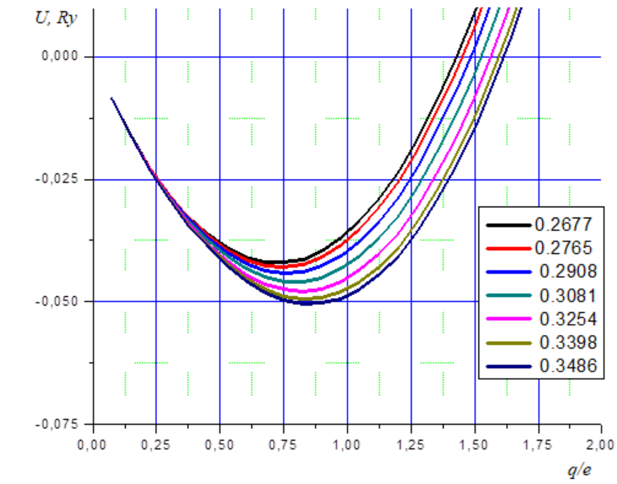


***Fig. 2b*** *Numerical solution of the variational task for an electron in the s state without taking into account the inhomogeneity of the ion field. Different lines explain different values of screening parameter λ*

Comparison of these solutions shows that the lowest value of the effective charge of the ion q and the external screening potential of the atom *A* will be when the heterogeneity of the ion field is considered.

## 4. Results and discussion

For comparison, Fig. 3 shows the solution of this task using the previously used method of the variational solution of the Schrodinger equation [1, 6].

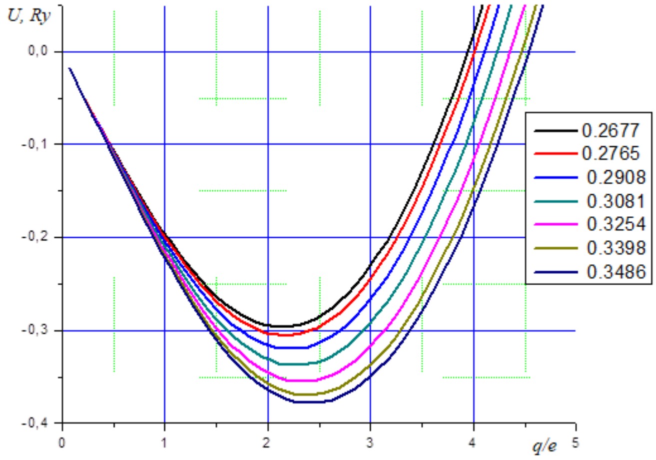


***Fig. 3*** *The variational solution of the Schrödinger equation by the method [6].*

Comparison of this solution with previous ones shows that the effective charge of the ion and the screening parameter of the atom are much higher and the binding energy exceeds the ionization potential of carbon. It can be assumed that these discrepancies go from the fact that the method of the variational solution of the Schrödinger equation [6] is more suitable for atoms with a large number of valence electrons.

An analysis of the dependence of the solution of the variational task on the parameter of the internal screening λ of an ion in the Brandt model is shown in Fig. 4.

It is interesting to note that the optimal value of λ is close to its value for a neutral atom in the Brandt model.

Figure 5 compares the obtained distribution of the field of a hydrogen-like atom along the radius with analogous distributions in [2,4].

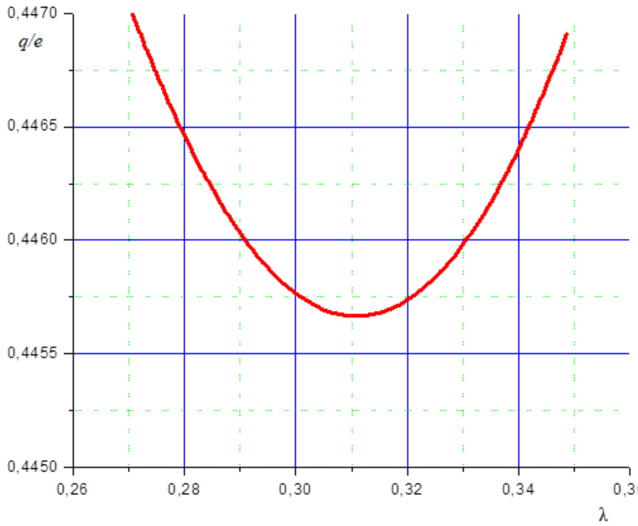


***Fig. 4*** *Dependence of the effective charge of an ion on the parameter of the internal screening of the ion λ in the Brandt model.*

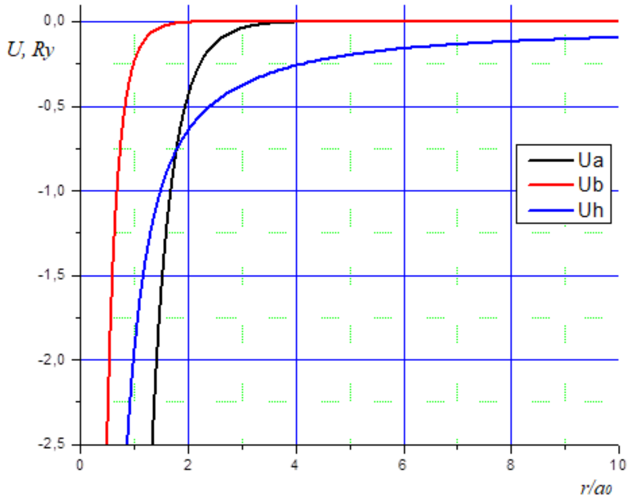


***Fig. 5*** *Comparison of the distribution of the field along the radius of a hydrogen-like atom with similar distributions in [2,4].*

It can be seen that the distribution of the field of the hydrogen-like atom is allocated between the distributions near the nucleus in other models and it decreases much more slowly in the distance.

When considering these results, it should be noted that the model Brandt atom is surrounded by an electron gas, but only the effect of neighboring atoms is taken into account in the model Abrahamson.

Because in the future we will be interested in the ground state of a hydrogen atom in the lattice of graphene, then the profiles of the potential distribution between two lattice sites in these models were calculated.

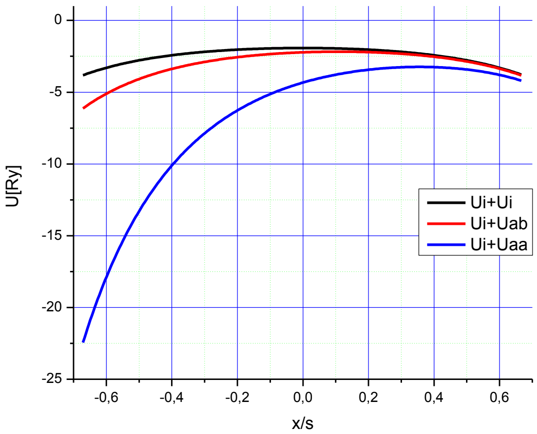


***Fig. 6*** *Potential well for a weakly bound electron accounting the field of an ion or atom at an adjacent graphene lattice site.*

Figure 6 shows that in the Abrahamson model the potential well is unnaturally deep while in the Brandt model it is close to the atom and the surrounding ion.

## *5. Conclusion*

The problems of modeling the emission processes from the graphene surface are considered. To describe the states of the emission surface at zero temperature, we used a hydrogen-like atom model, taking into account the screening of the ion in the Brandt model. To calculate the ground state of an unbound electron located in a graphene lattice site, we used the variational solution of the Schrödinger equation. It corresponds to a minimum of the total interaction energy of an unbound electron in the s state with the corresponding lattice ion. In numerical experiments, minimization was carried out in two parameters: the effective ion charge and the ion screening parameter. However, we restricted ourselves to the first iteration of the minimization of the energy functional, since it is assumed hereinafter account of the influence of the field in the immediate environment of the atoms of the electron energy with the ion in the lattice site. Our calculations showed that in the considered model it is important to take into account the inhomogeneity of the field produced by the screened lattice ion.

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