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THOMAS—FERMI MODEL FOR CONFINED MULTI-ELECTRON SYSTEMS

The Thomas—Fermi model for the confined N-electron (where N is large) system is proposed as the approximation. It has been shown that the numerical solution of the Thomas-Fermi type equation for multi-electron system in a harmonic oscillator potential exists. It has been found that the electron density distribution in a system could be expressed in an analytical form.

With the advent of new technologies, the problems, connected to quantum dots, quantum wires and other related objects, has become an object of keen interest and their solution has become a reality [1, 2] (see also [3—7]). A large number of problems concerning the confinement of electrons, atoms, molecules and other microobjects have been studied recently [1—9]. The confined Coulomb systems, being placed in an external electric and magnetic fields, attract special interest [10—13]. Most of these studies have, however, been made, being based on numerical computation only [4—7]. A few attempts have been made to solve the problem of confining electrons, atoms, etc. in analytic form. As a rule, few-particle systems have been studied.

Hereby we present the Thomas—Fermi model for confined N-electron (where N is large) systems. Previously, the Thomas—Fermi type equation for multi-electron system was solved numerically for the case of a harmonic oscillator potential. The electron density distribution for such a system was found.

Let's consider a system of N electrons (almost ideal electron gas) placed into the potential field of harmonic oscillator such that

$$U(r) = \frac{1}{2}\kappa r^2, \tag{1}$$

where κ is the coefficient of quantum «rigidity» [3]. This sort of systems studies are strongly stimulated, above all, by their possible unique features, specifically magnetic properties. The case with $N = 1$ concerns the well-known classical problem of quantum mechanics concerning harmonic oscillator [4, 5].

A calculation of electron density distribution $n(r)$ in the considered system is intricate for large N when traditional approaches of self-consistent field are used. Thus, the use of the Thomas-Fermi universal statistical method [3] is appropriate. In this statistical approach, we propose to consider further the ground state of the many-electron system. The electron gas is considered as being at zero temperature. Electron gas is, also, discussed in semi-classical way, since most of electrons in the system are in state with relatively high quantum numbers. In such conditions, the quasi-classical approach could be applied.

Using the Thomas—Fermi method, one could derive an equation for general potential j, in which (hypothetically) control the electrons move inside the system. Using the well-known relations for j (r), we have (in atomic units), according to [8]:

$$\Delta(\varphi - \varphi_0) = \frac{8\sqrt{2}}{3\pi}(\varphi - \varphi_0)^{3/2}, \tag{2}$$

where φ_0 is the chemical potential.

For the electron density of system, we propose the following expression:

$$\begin{aligned} n(r) &= \frac{2\sqrt{2}}{3\pi^2}[\varphi(r) - \varphi_0]^{3/2}, \quad \varphi \geqslant \varphi_0, \\ n(r) &= 0, \qquad\qquad\qquad\quad \varphi < \varphi_0. \end{aligned} \tag{3}$$

Being based on the natural assumption that the electron density is distributed in a spherically symmetric way, and substituting in Eq. (3) the mentioned above formula for the potential, one could obtain the following:

$$\varphi(r) - \varphi_0 = \frac{1}{2}\kappa r^2 \chi(\alpha r), \tag{4}$$

where $\alpha = \kappa^{1/6}$, and turning to the new dimensionless variable, $x = \alpha r$, we have obtained the following Thomas—Fermi-like equation for the function $\chi(x)$:

$$6\chi(x) + 6x\chi'(x) + x^2\chi''(x) = Ax^3\chi^{3/2}(x), \tag{5}$$

where $A = \frac{8\sqrt{2}}{3\pi}$.

The boundary condition at zero temperature subject to Eq. (4) is:

$$\chi(0) = 1. \tag{6}$$

A boundary of spherically-symmetric oscillator in the proposed statistical model is determined by the condition $\varphi(r_0) = \varphi_0$. Taking into

account the proposed distribution of charge, potential $\varphi(r)$ could be expressed as:

$$\varphi(r) = \frac{1}{2}\kappa r^2 - \frac{N}{r}. \quad (7)$$

Right at the boundary, we have

$$\varphi(r_0) = \frac{1}{2}\kappa r_0^2 - \frac{N}{r_0} = \frac{1}{r_0}\left(\frac{1}{2}\kappa r_0^3 - N\right) = \\ = \frac{Q}{r_0} = \varphi_0. \quad (8)$$

Particularly, for the oscillator with $\kappa = 2N/r_0^3$, in accordance with Eq. (8), we have $\varphi_0 = 0$. To define the constants φ_0 and r_0, the following relation should be added to Eq. (8) (as the consequence of Gauss electrostatic theorem)

$$Q = -\frac{1}{4\pi}\left(\frac{\partial\varphi}{\partial r}\right)_{r=r_0} 4\pi r_0^2 = -r_0^2\left(\frac{\partial\varphi}{\partial r}\right)_{r=r_0}. \quad (9)$$

For dimensionless variable, the boundary condition looks like

$$\chi(x_0) = 0, \; x_0 = \alpha r_0. \quad (10)$$

It should be noted that the condition (6) is universal for different oscillators with various κ, N, whereas the condition (10) is, generally speaking, non-universal since the magnitude of x_0 can be varied for different oscillators.

Relation (9) with new variables appears in the form:

$$Q = -\frac{\sqrt{\kappa}}{2} x_0^4 [\chi'(x)]_{x=x_0} - \sqrt{\kappa} x_0^3 \chi(x_0)$$

or, taking into account Eq. (10), as follows:

$$Q = -\frac{\sqrt{\kappa}}{2} x_0^4 [\chi'(x)]_{x=x_0}. \quad (11)$$

For the oscillator with $\kappa = 2N/r_0^3$, it follows from Eq. (11) that:

$$\chi'(x_0) = 0. \quad (12)$$

It is, also, easy to verify that Eq. (5) have the exact exponential-like solution [6] in the form:

$$\chi(x) = \frac{144}{A^2 x^6}. \quad (13)$$

Please, note, that the analogous solution for Thomas—Fermi atom looks like, according to [3] the following:

$$\chi(x) = \frac{144}{x^3}.$$

One could state, that the solution $\chi(x)$, tending to zero in the same way as $1/x^6$ under $x \to \infty$ could be written down as follows, according to [8]:

$$\chi(x) = \frac{144}{A^2 x^6} \times \\ \times\left(1 - \frac{F}{x^\gamma} f_1(\gamma) + \frac{F^2}{x^{2\gamma}} f_2(\gamma) - \frac{F^3}{x^{3\gamma}} f_3(\gamma) + \ldots\right), \quad (14)$$

where

$$\gamma = \frac{\sqrt{73} - 7}{2}; \; f_1(\gamma) = 1; \; f_n(\gamma) = \frac{\sum_{m=0}^{n(n+1)} p_{nm}\gamma^m}{\sum_{m=0}^{n(n+1)} q_{nm}\gamma^m};$$

where F is the some parameter, defining the slope of curve $\chi(x)$ at the point of $x = 0$; whereas p_{nm} and q_{nm} are certain coefficients, calculated through the substitution of expansion (14) into Eq. (5). It is interesting to note that for Thomas—Fermi atom, the coefficient, similar to γ in the expansion of Eq. (14), equals, also, to $\frac{\sqrt{73} - 7}{2}$ as it follows from [3]. The substitution of (13) into formula (4), and, further, to Eq. (3), results in $\lim_{r\to\infty} n(r) \infty \frac{1}{r^6}$.

As a result, the electron density at the boundary, diminishes as $1/r^6$ in the proposed model of many-particle oscillator (it is obvious that quantum-mechanical calculations give the exponential diminishing). Naturally, this result points to the well-known incorrectness of statistical model, when defining the boundary regions for the given many-electron system, where the electron density becomes too little.

It is necessary to keep in mind that, when the local relation is being applied to the Thomas-Fermi theory results, the density of kinetic energy becomes proportional to $n^{5/3}(r)$, and this is the major shortcoming of the cited theory.

This limitation should be weakened in the proposed consistent theory. Here, the situation is again analogous to that as in the theory of Thomas—Fermi atom. The analysis shows that at the point $x = 0$, the Eq. (5) has the discontinuous solution. Following the Thomas-Fermi theory of nuclear matter [3], this fact could be explained through neglecting the exchange interaction. Equation (5), under the boundary conditions (6), gives (12), then being numerically solved by means of Adams method [8].

Figure 1 shows the graph of function $\chi(x)$.

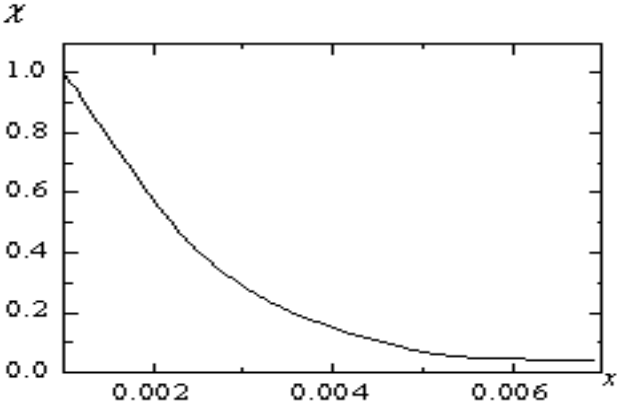

Fig. 1. Graph of function $\chi(x)$

The distribution of electron density $n(r)$ (using the condition of normality in a form $\int n(r)\mathrm{d}V = N$) subject to Eqs. (3) and (4), could be easily found in a form:

$$n(r) = \frac{\kappa^{3/2}}{3\pi^2} r^3 \chi^{3/2}(\alpha r). \qquad (15)$$

Using the constancy of the chemical potential inside the cloud of charges and taking into account the theorem of virial, one could obtain for the oscillator energy:

$$E = \frac{2I}{3\pi}\kappa^{7/6}, \quad I = \int_0^{x_0} x^7 \chi^{3/2}(x)\mathrm{d}x \approx 10^{-9}. \qquad (16)$$

For the special case of $\kappa = 2N/r_0^3$ condition, this implies that:

$$E = \frac{2^{13/6} \cdot I}{3\pi} \frac{N^{7/6}}{r_0^{7/2}}. \qquad (17)$$

It should be mentioned that the extension of the proposed model for the case of exchange, correlative, quantum, and shell effects being present, could be realized by standard method in full analogy with the Thomas-Fermi model of many-electron atom [3]. More detailed consideration and application of the model to the theory of a nucleus will be given elsewhere.

Further, let us consider the relativistic generalization for the Thomas—Fermi model of many-electron oscillator, using the methodology similar to that of Vallarty—Rosen in relativistic theory of Thomas—Fermi for atom (see, please, [3, 8, 14, 15]).

According to the non-relativistic approach, but from the outset subtracting the rest energy, mc^2, let us write the quasi-classic equation of motion for fastest electron. If $p_F(r_i)$ is the impulse of the fastest electron at the point r_i and $\varphi(r)$ is, as usual, the self-consistent potential energy of the field, where electron moves, then, using standard relativistic expression for kinetic energy, we have (in atomic units)

$$-\varphi_0 = [c^2 p_F^2 + c]^{1/2} - c^2 - \varphi(r). \qquad (18)$$

The impulse, p_F, is assigned with the electron density, n, by standard relation

$$n(r) = p_F^3(r)/3\pi^2. \qquad (19)$$

Taking, also, into account the condition of self-consistency, contained in Poisson equation, one could put down that:

$$\Delta(\varphi_0 - \varphi) = -4\pi n(r). \qquad (20)$$

Now, applying the dimensioned transforms, as in the non-relativistic case, let us use the dimensionless values, $\varphi(x)$ and x, defined as earlier.

Taking into account a spherical symmetry of the problem and Eq. (4), one could write:

$$\frac{1}{r}\frac{\mathrm{d}^2}{\mathrm{d}r^2}[r(\varphi_0 - \varphi)] = -\frac{\kappa}{2}[6\chi(x) + 6x\chi'(x) + x^2\chi''(x)] = -4\pi n(r). \qquad (21)$$

Permuting the terms in Eq. (18) and squaring, we obtain:

$$(\varphi - \varphi_0)^2 + 2c^2(\varphi - \varphi_0) = c^2 p_F^2. \qquad (22)$$

Then, for the independent variables φ, x, and n, we have:

$$\frac{p_F^2}{2} = \frac{1}{2}(3\pi^2)^{2/3} n^{2/3} = \frac{(\varphi - \varphi_0)^2}{2c^2} + (\varphi - \varphi_0) = \frac{\kappa^{4/3}}{8c^2} x^4 \chi^2 + \frac{\kappa^{2/3}}{2} x^2 \chi. \qquad (23)$$

Using Eq. (21) for the density n, after some rearrangement of items, we have the final output in the analytical form:

$$\left(\frac{3\pi}{8\sqrt{2}}\right)^{2/3} [6\chi(x) + 6x\chi'(x) + x^2\chi''(x)]^{2/3} = x^2\chi(x)\left[1 + \frac{\kappa^{2/3}}{4c^2} x^2 \chi(x)\right]. \qquad (24)$$

CONCLUSIONS

1. The Thomas—Fermi model for the confined N-electron (where N is large) system is developed. It has been found the numerical solution of the Thomas-Fermi type equation for multi-electron system in a harmonic oscillator potential.

2. It is easy to see that Eq. (23) in non-relativistic limit (for $c \to \Gamma$; accounting the independence of left-hand member of Eq. (24) of the light speed, c), could be reduced to the proper non-relativistic equation (5).

3. The numerical solution of Eq. (3) could be realized with the use of Adams method, as well as the solution of Eq. (5) cited above. Obviously, a total energy of the system in the relativistic approach depends not only on the parameter κ and number of electrons N, but also on value $1/c^2$ (in atomic units or in usual units $(e^2/\hbar c)^2$, i. e. on fine structure constant).

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The Thomas—Fermi model for the confined N-electron (N is large) system is developed. It has been obtained and numerically solved the Thomas-Fermi type equation for multi-electron system in a harmonic oscillator potential. It has been found the expression for the electron density distribution in a system.

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МОДЕЛЬ ТОМАСА—ФЕРМИ ДЛЯ МНОГОЭЛЕКТРОННЫХ СИСТЕМ В СОСТОЯНИИ КОНФАЙМЕНТА

Развита томас—фермиевская модель N-электронной (N-велико) системы в состоянии конфаймента. Получено и численно решено томас-фермиевское уравнение для многоэлектронной системы в потенциальном поле гармонического осциллятора. Определено выражение для распределения электронной плотности в системе.

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МОДЕЛЬ ТОМАСА—ФЕРМІ ДЛЯ БАГАТОЕЛЕКТРОННИХ СИСТЕМ У СТАНІ КОНФАЙМЕНТУ

Розвинута томас—фермієвська модель N-електронної (N є великим) системи у стані конфайменту. Отримано і чисельно розв'язано томас-фермієвське рівняння для багатоелектронної системи у потенціальному полі гармонічного осцилятору. Визначений аналітичний вираз для розподілу електронної густини в системі.