A binuclear atom — a special type of close bound state between proton and heavy atom

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It is established that a bound state of a proton with a heavy Thomas — Fermi atom should exist. On the one hand, the electrons of the atom screen the proton field. This decreases the repulsion force between the proton and the nucleus. On the other hand, the attraction force between the proton and the electrons is directed towards the gradient of the electron density, i. e. towards the nucleus. For instance, for \(Z = 80\) both forces become equal at approximately \(0.6a\) where \(a\) is the Bohr radius. The corresponding minimum of the proton potential energy is in the region of negative energies (attraction) that can be of the order of several tenths of eV. We propose to call such a system a binuclear atom.

In contrast to the molecules where a coupling with a hydrogen atom is due to an essential modification of one or several states of the outer electrons the formation of a binuclear atom is a result of collective response of the whole system of inner electrons to the screened potential of a proton that is well inside the electron system of the heavy atom. The variation of the wave function of each electron can be considered as a small perturbation. The bound state is formed as a result of joint action of a large number (of the order of \(Z\)) of perturbed inner electrons. The important problem concerning the accuracy of our calculation is discussed.

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INTRODUCTION

The purpose of the present paper is to demonstrate that a proton can be bound to a heavy atom with the charge of the nucleus \(Z \gg 1\). The principal idea of the paper can be formulated as follows: when a proton approaches the nucleus its potential is screened by the atomic electrons.

As is shown by Teller \[1\] (see also Ref. \[2\]), two Thomas — Fermi (TF) atoms cannot form a bound state. In the present paper we consider what can be looked upon as an opposite case. The principal difference of this case and the problem considered by Teller can be formulated as follows. If one considers two heavy atoms the Teller theorem states that such a system has a lower energy than the same system where the atoms are merged into a molecule. However, in the present paper we consider a situation where one of the interacting items is a heavy atom \((Z \gg 1)\) that can be described by the TF theory whereas the second item is a proton with \(Z = 1\). Our purpose is to prove that in this case (not covered by the Teller’s theory) a bound state can be formed. The screened potential of a proton can be considered as a perturbation for the electrons of the TF atom. The bound state is formed as a result of joint action on the proton of a large number of the perturbed inner electrons of the atom. The vibrational energy of the proton, i. e. the energy of its vibrations near the equilibrium position is much smaller than the binding energy. Therefore one can consider the proton in the S-state to be positioned on a sphere of a fixed radius.

There is a number of papers where bound states between a positron and an atom are considered, see for instance, Refs. \[3, 4, 5\] and the references therein. The ability of positrons to bind to a number of atoms is now well established. The attractive electron-positron interaction leads to formation of a cluster that includes a positron in the outer valence region of the atom.

In contrast to the problem of a bound state of a positron the methods and results of these papers cannot be directly applied to the situation considered here because of a great difference between the positron and proton masses. In the binuclear atom treated in the present paper the distance between the heavy nucleus and the proton is smaller than the Bohr radius \(a\). It means that in this case there is a quite different physical situation where the proton interacts practically entirely with the inner electrons of the atom.
PRELIMINARY CONSIDERATIONS

To visualize the physics of this phenomenon we start with analysis of a subsidiary problem. We will consider a Thomas — Fermi screening of a proton field by a homogeneous electron system having average density \( N \) neutralized by immobile positive charges. We have

\[
\delta N = \frac{1}{\pi^2} \frac{p_{Fm}}{\hbar^3} e \varphi, \quad \nabla_R^2 \varphi + q^2 \varphi = 0, \quad \varphi(R) = \frac{1}{R} \exp(-qR),
\]

(1)

\( p \) is the Fermi momentum, \( q \) is the reciprocal screening radius of a proton \(^\text{[6]}\), \(^\text{[40]}\). Now,

\[
q^2 = \frac{4 \cdot 3^{1/3} m e^2}{\pi^{1/3} R^2} N^{1/3} = \frac{4 \cdot 3^{1/3} 1}{\pi^{1/3} a} N^{1/3}.
\]

(2)

Here \( e \) is the elementary charge, \( m \) is the electron mass, \( N \) is their concentration, \( \delta N \) is its variation due to the electrostatic potential \( \varphi \). The energy of electrostatic interaction of the screened proton potential situated at \( R = 0 \) with the electron density \( N \) is

\[
E = -e^2 N \int_0^\infty d^3R \frac{1}{R} \exp(-qR) = -\frac{\pi^{4/3}}{3^{1/3} a e^2} N^{2/3}.
\]

(3)

Let us assume that \( N \) is a slow (as compared with \( 1/q \)) function of \( R: N = N(R) \). Then the electron system will act on the proton with the force \( F \) given by

\[
F = -\frac{\partial E}{\partial R} = 2 \left( \frac{\pi}{3} \right)^{4/3} a e^2 N^{-1/3}(R) \nabla_R N.
\]

(4)

Its direction is determined by \( \nabla_R N \).

CALCULATION OF THE INTERACTION POTENTIAL

Now we will treat the problem we are interested in, namely a proton in the field of electrons and a heavy nucleus. The electron system will be treated within the model of Thomas — Fermi atom (see, for instance, Ref. \(^\text{[7]}\), \(^\text{[70]}\), \(^\text{[8]}\)). This model was proposed long ago but quite recently an interest to its application was revived (for instance Refs. \(^\text{[9]}\), \(^\text{[10]}\), \(^\text{[11]}\)).

According to the model half of the electron charge of the atom is within a sphere of the radius 1.33\( aZ^{-1/3} \) where \( a \) is the Bohr radius. The electron density enhances as the distance from the nucleus becomes smaller. Let the distance between the nucleus and the proton be of the order of \( a \). Its potential should be screened by the electrons. As a result, the repulsion between the proton and nucleus becomes much smaller. As the electron density increases while \( R \) decreases the electrons should attract the proton. The force of attraction cannot be calculated using Eq. (4) as \( \nabla_R N \) now is not small. The calculations below show that for \( Z = 80 \) the force of attraction by the electrons and the force of repulsion by the nucleus are counterbalanced for \( R \approx 0.6a \). This is an indication for the possibility of a bound state formation. We will be interested in the bound state with the lowest energy, i. e. the lowest S-state.

We wish to emphasize that there is a principal difference between the unique state treated in the present paper and an ordinary molecule of a chemical compound containing a hydrogen atom. In such compounds the coupling of a hydrogen atom is due to an essential modification of one or a few outer electron states whereas here we consider a special effect that is a collective change of the whole distribution of the atom’s inner electrons by the proton potential. In ordinary molecules a coupling with a hydrogen atom is due to an essential modification of one or several states of the outer electrons. In the present paper we consider a special effect that is a collective response of the whole system of inner electrons to the screened potential of a proton. In regard to each electron the action of the potential can be considered as a small perturbation. The bound state is formed because these perturbations are summed up. Thus the perturbation theory is an adequate approach to this problem. Usually the perturbation theory cannot describe a bound state formation. However, the present case is unique as the bound state is formed as a result of united action of a large number of perturbed electrons.

Consider the screening of a proton by the electrons of a heavy atom. We assume the distance between the proton and nucleus to be \( \lesssim a \). In other words, the proton is well inside the atom. This is why we propose to call such a
system a binuclear atom. We will make estimates of the energy of such system within the TF atom model. In the first order of the perturbation theory the variation of electron density \( \delta N \) is

\[
\delta N(r) = 4 \sum_{l}^{n_{\text{max}}} \int \frac{1}{\varepsilon - \varepsilon_k} Y_{lm}(\theta, \chi) \frac{1}{\varepsilon - \varepsilon_k} Y_{n'l'm'}(\theta, \chi) \psi_{nl}(r) \psi_{n'l'}(r).
\]

Here \( i = nlm \) are the occupied states, \( k = n'l'm' \), \( n \neq n' \) and/or \( l \neq l' \); \( \theta, \chi \) are the spherical angles, \( \psi_{nl} \) is the radial quasiclassical (WKB) electron wave function in the potential \( \Phi(r) \) of the TF atom. Here and henceforth we use the atomic units \( e = \hbar = m = 1 \).

Let us transform Eq. (5) into such a form that it gives a local relation between \( \delta N \) and \( \varphi \). \( \delta N \) being given, \( \varphi \) is determined by the Poisson equation. Inserting the relation between \( \delta N \) and \( \varphi \) we get a selfconsistent equation for \( \varphi \).

The variation of the electron energy in the first order of the perturbation theory is

\[
\delta \varepsilon_i = \langle i | \varphi | i \rangle.
\]

The perturbation for every electron is the proton potential plus the potential produced by \( \delta N \), i. e. the screened proton potential. In \[5\] and \[6\], there is a contribution of a selfacting electron. It gives a contribution to the screened potential \( \varphi \). This contribution is however negligibly small as the electron number \( Z \) is large. The total energy variation of the system \( \Delta E_1 \) is the sum of expressions \[6\] over all the particles including the nucleus

\[
\Delta E_1 = Z \varphi(0) - \int N(r) \varphi(r) d^3r.
\]

Let \( z \)-axis join the nucleus and the proton. Then \( \varphi(r) \) does not depend on the azimuthal angle and can be expanded as

\[
\varphi(r) = \sum_s \varphi_s(r) P_s(\cos \theta)
\]

where \( P_s \) is a Legendre polynomial. As \( N(r) \) has a spherical symmetry, only \( \varphi_0(r) \) contributes to Eq. (7). Now we will expand \( \delta N \) like Eq. (8) and integrate Eq. (5) over \( \theta \) using the well-known identity

\[
\sum_{m=-l}^{l} |Y_{lm}|^2 = (4\pi)^{-1}(2l+1).
\]

As a result, Eq. (5) takes the form

\[
\delta N_0(r) = \pi^{-1} \sum_{l} (2l+1) \sum_{n, n'} \frac{1}{\varepsilon_{nl} - \varepsilon_{n'l'}} \psi_{nl}(r) \psi_{n'l'}(r).
\]

The radial quasiclassical function of the state \( (n, l) \) with the energy near the Fermi level is

\[
\psi_{nl}(r) = a_n r^{1/2} e^{-1/2 p_t^{1/2}} \left( \int_{r_1}^{r} (p_t + \varepsilon_{nl} p_t^{-1}) dr' + C_l \right), \quad p_t^2 = 2 \Phi_t(r) \equiv 2 \Phi(r) - \frac{1}{r^2} \left( l + \frac{1}{2} \right)^2
\]

(\( C_l \) are constants of the order of 1). In Eq. (11) the approximation \((p_t^2 + 2 \varepsilon_{nl})^{1/2} \approx p_t + \varepsilon_{nl} p_t^{-1}\), is used. It is valid for \( \varepsilon_{nl} \ll \Phi_t \) where \( \Phi_t \) are the characteristic values of \( \Phi_t(r) \), \( a_n^2 = (2/\pi) d \varepsilon_{nl} / dr = 4 T_l^{-1}, T_l \) is the period of the classical motion at the Fermi level, \( r_1 \) (as well as \( r_2 \)) are the classical turning points.

Introducing the variable

\[
t_t(r) = \int_{r_1}^{r} |p_t(r')|^{-1} dr', \quad 2 t_t(r_2) = T_l,
\]

we expand \( \varphi_0(r) \) into Fourier series

\[
\varphi_0(r) = \sum_{n=0}^{\infty} \varphi_{0n} \cos(2\pi n T_l^{-1} t_t).
\]
Discarding the quickly oscillating part of the product of functions given by Eq. (11) one gets

\[
\delta N_0(r) = \sum_l \frac{2l+1}{2\pi^2} \sum_{\nu=0}^\infty \varphi_{0\nu} \int_{-\Phi_l(r)}^{\Phi_l(r)} \frac{dz'}{-z'} \int_0^\infty \frac{dz}{z'^2} \frac{\cos((z'-z)T_l)}{z'} \left[ \delta(z-z'+\frac{2\pi\nu}{T_l}) + \delta(z-z'-\frac{2\pi\nu}{T_l}) \right].
\] (13)

The integral over \(z'\) can be presented as a sum of integrals over the intervals \([-\Phi_l, 0]\) and \([0, \infty]\). The contribution of the first integral vanishes as the change of the variables \(z'\) changes the sign of this expression. The conditions \(z \leq 0\) and \(z' \geq 0\) are fulfilled for the first \(\delta\)-function and \(z \in [-2\pi\nu T_l^{-1}, 0]\). In the expansion Eq. (12) only the harmonics with \(2\pi\nu T_l^{-1} \ll \Phi_l\) are physically important. Integrating over \(z'\) with regard of \(\delta\)-function and over \(z\) in the interval \(2\pi\nu T_l^{-1}, 0\), and taking into account Eq. (12) one gets

\[
\delta N_0(r) = \frac{1}{2\pi^2} \sum_l \frac{2l+1}{p_l} \varphi_{0\nu}(r).
\] (14)

\(r\) is in the classical region for the quantum numbers \(l\) satisfying the condition \(\Phi_l(r) \geq 0\). Integration over \(l\) from 0 up to the maximal value, corresponding to \(\Phi_l(r) \geq 0\) gives

\[
\delta N_0(r) = \pi^{-2} p(r) \varphi_0(r), \quad p = (2\Phi)^{1/2}.
\] (15)

Eq. (15) coincides with the first equation (1). Thus the relation between \(\delta N\) and \(\varphi\) is preserved also for nonhomogeneous electron density. Eq. (15) gives the Poisson equation

\[
\frac{1}{r} \frac{d}{dr} \left( r \frac{d\varphi_0}{dr} \right) = q^2 \varphi_0, \quad q^2 = 4\pi^{-1}\sqrt{2\Phi}
\] (16)

with the boundary conditions

\[
\left. r \varphi(r) \right|_{r \to 0} = 0, \quad \left. \varphi(r) \right|_{r \to \infty} = 0, \quad \left. \frac{d}{dr} \left( r \varphi_0 \right) \right|_{r = R - 0} - \left. \frac{d}{dr} (r \varphi_0) \right|_{r = R + 0} = \frac{1}{R}.
\] (17)

The jump of the derivative is due to the presence of the proton at the distance \(R\) from the nucleus. For small values of \(r\) we solve these equations numerically. For \(r > R\) one can use the eikonal approximation that is valid at \(d\Phi/dr \ll 2p^2q\). Using the TF variable \(x = \gamma R\), \(\gamma = Z^{1/3}/0.885\) one can see that these solutions (but not the last boundary condition at \(x = \gamma R\)) are independent of \(Z\). For \(x < \gamma R\) \(x \varphi_0(x) = CP(x)\), \(P(x)\) is given in Table 1.

| \(x\)  | \(P(x)\)  | \(x\)  | \(P(x)\)  | \(x\)  | \(P(x)\)  |
|-------|---------|-------|---------|-------|---------|
| 0.2   | 0.207   | 0.4   | 0.437   | 0.6   | 0.703   |
| 0.4   | 1.4     | 1.6   | 2.79    | 1.8   | 3.40    |
| 0.8   | 1.01    | 2.0   | 4.09    | 3.2   | 10.3    |
| 1.0   | 1.37    | 2.2   | 4.87    | 3.4   | 11.7    |
| 1.2   | 1.78    | 2.4   | 5.74    | 3.6   | 13.3    |

For \(x \to 0, P = x\). For \(x > \gamma R\)

\[
x \varphi_0(x) = bq_x^{-1/2} \exp \left( -\int_{\gamma R}^x q_x dx \right), \quad q_x^2 = 1.5 \cdot x^{-1/2} X^{1/2}, \quad \Phi = ZX/r.
\] (18)

The constants \(c\) and \(b\) are determined by continuity of function \(x \varphi_0\) and the jump of derivative of function (17) at \(x = \gamma R\).

Making use of the well known relation for the Thomas — Fermi atom between \(N(r)\) and \(\Phi(r)\) and the values of \(\Phi\) given in the tables one can calculate \(\Delta E_1\) Eq. (12) for various \(R\). Note that an additional correction is needed (that,
FIG. 1: Fig. 1: 1 — the energy of the system proton — heavy atom \((Z=80)\) as a function of the distance \(R\) between the proton and the nucleus. 2 — the potential \(\Phi(R)\). For \(R > 1\) one can expect that curve 1 will tend to \(\Phi(R)\). A possible transition curve is indicated by the broken line.

however, will be small as compared with \(\Delta E_1\). We have considered the screening in a neutral atom. The total electron charge surplus near the proton due to the screening is \(-1\). Indeed, the total potential of the proton and \(\delta N\) Eq. (18) tends to zero at \(r \to \infty\) faster than \(r^{-1}\). The corresponding correction \(\Delta E_2\) should not exceed the energy of one-electron ionization of the atom. In the TF atom model this energy appears to be lower as compared to the experimental values. Such a discrepancy is due to the fact that in this model such properties are essentially related to the distances \(r \gg 1\) where the TF approximation fails. The average (over a number of different atoms) experimental value of the ionization energy is about 0.3 atomic units. The variation of the energy \(\Delta E = \Delta E_1 + \Delta E_2\) is presented in Fig. 1. Here we have assumed \(\Delta E_2 = 0\).

Let us analyze the approximations used to obtain \(\Delta E\). First, this is the one-electron approximation. The characteristic value of the kinetic energy of the electrons should be bigger than the potential energy of their Coulomb interaction, i.e. \(p^2/2 > N^{1/3}\). For the atoms where \(Z \gg 1\) this condition is satisfied. Second, this is the quasiclassical approximation. It is satisfied in the interval \(Z^{-1} < r < 1\). The solution (18) decays exponentially for \(r > R\). This is why the integral (7) is determined by the interval \(r \lesssim R\).

We have calculated the energy \(\Delta E\) for \(Z=80\) and \(R < 1\). For \(R > 1\) our theory ceases to be applicable. [When calculating the integral (7) the interval of integration has been taken from 0 to 1 where the integrand is well defined]. \(N(r)\) decreases with \(r\); \(\varphi_0(r)\) increases for \(r < R\) and decreases for \(r > R\). The integrand varies slowly for \(r < R\) and rapidly decays for \(r > R\). Thus for \(R < 0.8\) the discarded additional energy is small.

Fig. 1 shows that the energy of the system proton — heavy atom \((Z \approx 80)\) with regard of screening appears to be negative at \(R > 0.4\) a. u. and has a minimum at \(R \approx 0.6\) a. u. \((\approx 0.3\) Å\). One can expect that at the periphery of the atom \(\Delta E\) can become positive (potential barrier).

The distance between the bound proton and the nucleus \((\approx 0.3\) Å for \(Z \approx 80)\) is much smaller than the characteristic radius of the valence electron wave functions. This means that the chemical behavior of such a system after an extra electron has joined it should be similar to that of an atom of the number \(Z+1\).
CONCLUSION

The experimental search of the predicted phenomenon should be probably performed with plasmas or using a source of low-energy protons. The energy release in the course of proton trapping might be accompanied by Auger-processes and X-ray emission. The probability of a proton capture might be bigger for a heavy atom in a condensed matter (i.e. for a target) than for a vapor. The described method is applicable for estimates of the binding energy of two protons with a heavy atom. If the average distance between the protons is of the order of 0.3 Å the Coulomb energy of their repulsion is smaller that the coupling energy obtained in the present paper. Our estimates indicate that a possibility exists for trapping of α-particles and μ+ -mesons.

The TF model describes the average atomic characteristics. It cannot describe their individual properties, such as their periodicity. This point concerns also our estimates.

A few words about the accuracy of our calculation. In general the accuracy one can expect of the TF atom model is about 10 — 15 per cent. Calculating the potential curve one deals with a difference of two large quantities. This means that the difference of these quantities should be bigger than 15 per cent of each of them. Near the minimum of the potential curve these two quantities differ by 30 per cent. This means that the accuracy of our calculation is sufficient. However, it is desirable to apply in future more advanced methods to obtain a more detailed value for the potential minimum position as well as the form of potential curve near the minimum. This should facilitate the experimental search of the binuclear atoms.

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Figure caption

Fig. 1. 1 — the energy of the system proton — heavy TF atom (Z=80) as a function of the distance R between the proton and the nucleus. 2 — the potential Φ(R). For R > 1 one can expect that curve 1 will tend to Φ(R). A possible transition curve is indicated by the broken line.