The simulation of the spin ground states of the coulomb clusters in a broad 2D parabolic well.

B. Abdullaev, A.D. Kidisyuk and M.M. Musakhanov
Institute of Applied Physics, National University of Uzbekistan, Vuzgorodok, Tashkent, 700174, Uzbekistan

Abstract

By variational Monte-Carlo method developed Ceperley et al. for the simulation of fermi systems in macroscopic confining potential well we simulate various spin ground states of the coulomb clusters with 2, 3 and 4 particles in a broad two-dimensional (2D) parabolic well. In this method quantum state numbers determining the variational wave function are not the numbers of well quantum states but numbers of the equilibrium spatial positions of particles that give a minimum of the system potential energy. The ground states with parallel, antiparallel spins and as well, as bose state are simulated. For the cluster with three particles it is also simulated the state when two particles have one direction of spin and third opposite. The simulation shows that clusters with parallel spins have lower ground state energy than clusters with other spin configurations and bose state. That reminds a Hund’s rule in atomic physics when in not full filled atomic shells electrons prefer to have a state with parallel spins.

I. INTRODUCTION

A considerable experimental success in localization and cooling of several ions in electrostatic traps [1] and recent technological advances in the fabrication of the quantum dots in semiconductors [2,3] have induced a big theoretical interest [4–7] to these objects. A 2D parabolic potential well is a good model potential well for the confining of electrons in the quantum dots [8] in many cases. In the works [4,5] it was shown the equivalence of coulomb system in effective electrostatic potential \( U_{ext} = aR^2 \) to the Tomson model of atom. The
classic and quantum properties of coulomb clusters in traps were also investigated in work \[9\].

Here we consider the coulomb clusters that correspond to quasi two dimensional systems of ions or electrons taking place in strong anisotropic 2\(D\) traps that can be supposed as broad. By variational Monte-Carlo method developed Ceperley, Chester and Kalos \[10\] for the simulation of fermi systems in macroscopic confining potential well we simulate various spin ground states of the coulomb clusters with 2, 3 and 4 particles in a broad 2\(D\) parabolic well. In this method quantum state numbers determining the variational wave function are not the numbers of well quantum states but numbers of equilibrium spatial positions of particles that give a minimum of the system potential energy. The ground states with parallel, antiparallel spins and as well, as bose state are simulated. For the cluster with three particles it is also simulated the state when two particles have one direction of spin and third opposite. The simulation shows that clusters with parallel spins have lower ground state energy than clusters with other spin configurations and bose state. That reminds a Hund’s rule in atomic physics when in not full filled atomic shells electrons prefer to have a state with parallel spins.

II. MODEL OF SYSTEM AND THE SIMULATION METHOD

Let us consider a system - cluster having \(N\) particles in a 2\(D\) parabolic well with Hamiltonian \[1\]

\[
H = -\lambda \frac{\partial^2}{\partial R^2} + U_{\text{pot}}(R),
\]

where \(R\) corresponds to the two dimensional vectors \((\vec{r}_1, \vec{r}_2, ..., \vec{r}_N)\) and the potential energy is

\[
U_{\text{pot}}(R) = \sum_{i=1}^{N} \vec{r}_i^2 + \sum_{i>j} |\vec{r}_i - \vec{r}_j|^{-1}.
\]

Hamiltonian \[1\] contains a single quantum parameter \(\lambda = \hbar^2 a^{1/3}(2me^{8/3})^{-1}\), where \(m\) and \(e\) mass and charge of coulomb particle respectively, parameter \(a\) determines a parabolic well \(U_{\text{ext}} = aR^2\) which locates the particles. For a broad 2\(D\) parabolic well we assume \(\lambda < 1\).

We simulate the coulomb clusters by variational Monte-Carlo method proposed in \[10\] for the simulation of fermi systems in macroscopic confining potential well. It is based on the trial variational wave function

\[
\Psi(R) = \psi_J(R) D,
\]

where to take into account an interparticle electrostatic correlation and a 2\(D\) parabolic well it is introduced the Jastrow wave function:

\[
\psi_J(R) = \exp \left( -\beta \sum_{i=1}^{N} \vec{r}_i^2 - \gamma \sum_{i>j} |\vec{r}_i - \vec{r}_j|^{-1} \right).
\]
The expression for the quantity $D$ depends from the system simulating state. If it is simulating a bose state of the system then

$$D = \prod_{i=1}^{N} \exp[-\alpha(\vec{r}_i - \vec{r}_{i0})^2].$$

(5)

If there is a state of pure fermions then in according with [10]

$$D = \prod_{s=1}^{g} \det(D_{ij}^s),$$

(6)

where spin index $s$ has $g$ number of states (so for the parallel spin state $g = 1$ and for the antiparallel spin state $g = 2$) and $\det(D_{ij}^s)$ is Slater determinant, where

$$D_{ij}^s = \exp[-\alpha(\vec{r}_i - \vec{r}_j)^2]_s.$$  

(7)

In the expressions (5) and (7) the vectors $\vec{r}_{i0}$ provide a minimum of the potential energy $U_{pot}(R)$, i.e. a minimum of the potential energy for the classical system. In the expression (4) index $i$ indicates the particle’s coordinate and $j$ indicates a quantum state.

The antiparallel spin state for the cluster with two particles coincides with bose state of system.

The antiparallel spin state for the cluster with four particles has a product of two Slater determinants. We assume that in (7) $j = 1$ and $j = 4$ describe an one direction of spin and $j = 2$ and $j = 3$ the opposite direction. Therefore, in the expression (8) first determinant determines by $j = 1, 4$ and second by $j = 2, 3$.

The paralell spin state for the cluster with four particles has only one Slater determinant, where $j = 1, 2, 3, 4$.

A minimum of the ground state energy

$$E = \frac{\int dR\Psi^*(R)H\Psi(R)}{\int dR|\Psi(R)|^2}$$

(8)

is achieved by variation of parameters $\alpha, \beta$ and $\gamma$ in the expressions (4)-(7). It is assumed that variational parameters $\beta$ and $\gamma$ in the Jastrow wave function are the same for all spin and bose states of all clusters (see [10]). That means that there is no influence of the interparticle electrostatic correlation and external field on the spin part of the wave function.

The cluster ground state simulation is occured by Metropolis algorithm. In this algorithm each particle of the cluster is tested on the uniform random displacement inside square with side $\Delta$ from center of square $r_{j0}$. New spatial position of the particle is accepted by the probability

$$P = \min[1, |\psi(r_{new})/\psi(r)|^2].$$

(9)

The size of $\Delta$ is chosen by the such way that the ratio of accepted number to whole number of particle displacements has been roundly equal 1/2 for all particles. Thus, the full variation of energy (8) is taken place by the variation of four parameters $\alpha, \beta, \gamma$ and $\Delta$.

The mean values of the quantities in algorithm are calculated by the formula:
\[ < F > = \frac{\int dR \psi^*(R) F(R) \psi(R)}{\int dR |\psi(R)|^2} \approx \frac{1}{M} \sum_{i=1}^{M} F(R_i), \]  

(10)

where \( R_i \) is the \( i \)-th spatial configuration of the system whole number of which is equal \( M \).

The full energy of the system is the sum of every particle’s energy. Let’s consider the expressions for the kinetic and potential energies, for example, for the first particle.

The kinetic energy is

\[ E_{\text{KIN}} = -\frac{\hbar^2}{2m} \int \Psi^* \Psi [ (\vec{\nabla}_1 \ln \Psi)^2 + \vec{\nabla}_1^2 \ln \Psi] dR. \]  

(11)

If we introduce the determination

\[ F_1^2 = \left\langle \frac{\hbar^2}{2m} (\vec{\nabla}_1 \ln \Psi)^2 \right\rangle, \]

\[ T_1 = \left\langle -\frac{1}{4m} \vec{\nabla}_1^2 \ln \Psi \right\rangle \]  

(12)

then the expression for the full energy will have a form:

\[ E_1 = V_1 + 2T_1 - F_1^2, \]  

(13)

where

\[ V_1 = \left\langle ar_1^2 + \sum_{j=2}^{N} \epsilon_{r_{ij}}^2 \right\rangle. \]  

(14)

In the expressions (12) and (14) the angle brackets mean the mean value (10).

In the paper [11] it is shown that \( T_1 = F_1^2 \) and therefore, we are calculating the energy \( E_1 \) by the formula

\[ E_1 = V_1 + F_1^2. \]  

(15)

For the bosons containing cluster the expression for \( F_1^2 \) is

\[ F_1^2 = \frac{\hbar^2}{2m} \left\langle \left( -\sum_{j=2}^{N} \vec{\nabla}_1 u(r_{1j}) - \vec{\nabla}_1 \chi(r_1) + \vec{\nabla}_1 \Phi_1(r_1) \right)^2 \right\rangle. \]  

(16)

Here \( u(r_{1j}) = \gamma/(r_j - r_1) \), \( \chi(r_1) = \beta r_1^2 \) and \( \Phi_1(r_1) = \exp[-\alpha(\vec{r}_1^1 - \vec{r}_{101})^2]. \)

If it is simulated the fermions containing cluster then

\[ F_1^2 = \frac{\hbar^2}{2m} \left\langle \left( -\sum_{j=2}^{N} \vec{\nabla}_1 u(r_{1j}) - \vec{\nabla}_1 \chi(r_1) + \sum_{j=1}^{N} D_{ji} \vec{\nabla}_1 \Phi_j(r_1) \right)^2 \right\rangle. \]  

(17)

Here \( D_{ji}^s \) is the inverse matrix of matrix \( D_{ij}^s \).

The main complexity of the simulation by the variational Monte-Carlo method of big number fermions containing systems is connected with technical difficulty of inversion of matrix \( D_{ij}^s \). In the paper [10] is proposed a simple algorithm for the inversion of matrix \( D_{ij}^s \) for these systems. Our clusters have a small number of particles. Therefore, we use direct method of determination of elements of inverse matrix \( D_{ji}^s \) by the elements of direct matrix \( D_{ij}^s \).
III. THE SIMULATION RESULTS

As it was said above, Hamiltonian (1) has a single quantum parameter \( \lambda = \hbar^2 a^{1/3} (2me^{8/3})^{-1} \). In accordance with this determination of parameter \( \lambda \) all length quantities are expressed in the \( e^{2/3} a^{1/3} \) units and energy quantities in the \( e^{4/3} a^{1/3} \) units.

The positions of particles \( r_0 \) that give a minimum of the potential energy \( U_{\text{pot}}(R) \) (2) for the classic systems of the clusters are determined analytically. For all spin and bose states of one cluster they are suggested identical.

For the cluster with two particles the positions of \( r_0 \) situate on the one line, on the distance \( 1/2 \) from the centre of coordinates that coincides with the centre of a parabolic well.

For the cluster with the three particles the coordinates of \( r_0 \) are the coordinates of the triangle

\[
\begin{align*}
    r_{0x1} &= -\left(\frac{3}{2}\right)^{1/3} \frac{1}{2}; & r_{0x2} &= \left(\frac{3}{2}\right)^{1/3} \frac{1}{2}; & r_{0x3} &= 0; \\
    r_{0y1} &= -\left(\frac{3}{2}\right)^{1/3} \frac{1}{2\sqrt{3}}; & r_{0y2} &= -\left(\frac{3}{2}\right)^{1/3} \frac{1}{2\sqrt{3}}; & r_{0y3} &= \left(\frac{3}{2}\right)^{1/3} \frac{1}{\sqrt{3}}.
\end{align*}
\]

For the cluster with four particles a minimum of \( U_{\text{pot}}(R) \) provides by square (with particles on the vertices of square and the centre of square on the centre of a parabolic well and coordinates). The distance between the centre coordinates and square vertex is equal

\[
r_0 = \left(\frac{(4 + \sqrt{2})/(8\sqrt{2})}{(8\sqrt{2})}\right)^{1/3}.
\]

Variational parameters \( \beta \) and \( \gamma \) that are the same for all spin and bose states of all clusters we determine by the simulation of the bose state for the two particle cluster. The numerical quantities of these are \( \beta = 0.5 \) and \( \gamma = 1.5 \).

Whole number of displacements inside \( \Delta \) for every particle we choose \( 10^4 \), so absolute exactness of the calculated mean energies is roughly equal \( 10^{-2} \) (we would like to note that for the Markov random processes, i.e. for independent random processes, absolute exactness of the calculated in simulation mean values is proportional to \( 1/\sqrt{N} \), where \( N \) is number of random simulations).

There is no a necessity for the simulation of the energies at every numerical quantity of \( \lambda \) for every spin or bose state of the one cluster. Let we have the calculated in the simulation the potential energy \( V \) and the kinetic energy \( E_{\text{KIN}} \) at any one fixed \( \lambda \). As the kinetic energy in Hamiltonian (1) is directly proportional to \( \lambda \), so for the getting of the kinetic energy for another \( \lambda_1 \) one can recalculate it by the formula \( E_{\text{KIN}}(\lambda_1) = E_{\text{KIN}}(\lambda) \cdot \lambda_1/\lambda \); the potential energy \( V \) does not depend from \( \lambda \) and one can be calculated once for this spin or bose state of cluster.

Fig. 1 shows variational parameter \( \alpha \) dependence (in the \( e^{4/3} a^{1/3} \) units) of the potential energies \( V_{\text{BS}} \), \( V_{\text{AFS}} \) and \( V_{\text{FS}} \) (bose, antiparallel spin (antiferrospin) and parallel spin (ferrospin) states respectively) for the cluster with four particles, of the full energies \( E_{\text{2BS}} \) and \( E_{\text{2FS}} \) (bose and ferrospin states respectively) for the cluster with two particles and of the kinetic energies \( E_{\text{KIN4BS}} \), \( E_{\text{KIN4AFS}} \) and \( E_{\text{KIN4FS}} \) per one particle at the fixed parameter \( \lambda = 0.01 \).

In this figure the potential energy for the bose state \( V_{\text{BS}} \) is increased when parameter \( \alpha \) goes to zero. This takes place due the increasing of the electrostatic interaction between
coulomb particles because the decreasing of $\alpha$ means the increasing of the mean size of the wave function per one particle. The $\alpha$ dependence of the potential energy for parallel spin state $V_{AFS}$ when $\alpha$ goes to zero has opposite character. This is occurred due the increasing of the exchange interaction between fermions.

Fig. 2 shows the $\lambda$ dependence (in the $e^{4/3}a^{1/3}$ units) of full ground state energy for every cluster per one particle. In this figure the symbol $3AFS$ corresponds to the state when two particles have one direction of spin and third opposite. The numerical quantities of the full energies in Fig. 2 are the minimums of these energies on variational parameter $\alpha$.

At last, for the demonstration of qualitative behaviour of the module of the wave function, we have simulated it for the cluster with three particles at parameters $\beta = 1.7$ and $\gamma = 1.0$ (though these parameters of $\beta$ and $\gamma$ do not give the minimum of the full energy, but they provide for the module of the wave function an obvious visual illustration). This quantity is outlined in the figures 3, 4 and 5 for the bose, parallel spin and mixed spin (i.e. $3AFS$) states respectively. From these figures one can see clearly that exchange interaction between fermions moves apart a quantum spatial distribution of the cluster particles. Bose and fermi like together behaviours of the module of the wave function are outlined in Fig. 5.

The main result of the present work is outlined in the figures 1 and 2. It turns out that for the every cluster with 2, 3 and 4 coulomb particles in a 2D parabolic well the ground states with parallel spins are energetically advantageous than other spin and bose states. That reminds a Hund’s rule in atomic physics when by taking account of exchange interaction in not full filled atomic shell it is profitable for the electrons to have a single direction of spin.

We are grateful Yu.E. Lozovik for indication on this task and helpful discussions.


REFERENCES

[1] P.E. Toschek, in Les. Houches, Session 38, New trends in atomic physics, Vol. 1, eds. G.Grynberg and R.Stora (North - Holland, Amsterdam) p.383, 1984; S. Becker et al., Rev. Sci. Instr., 66, 4902 (1995); H.J. Kluge, Nucl. Instr. Methods Phys. Res., B98, 500 (1995).

[2] M.A. Kastner, Rev. Mod. Phys., 64, 849 (1992); Phys. Today, 46, 24 (1993).

[3] R.C. Ashoori, Nature (London), 379, 413 (1996); L.P. Kouwenhoven, T.H. Oosterkamp et al., Science, 278, 1788 (1997).

[4] Yu.E. Lozovik and V.A. Mandelshtam, Phys. Lett., A145, 269 (1990).

[5] Yu.E. Lozovik, Usp.Fiz.Nauk, 153, 356 (1987);

[6] B.C. Levi, Phys. Today, 21, 17 (1988); D.H. E. Dubin and T.M. O’Neil, Phys. Today, 60, 511 (1988); J. Hoffnagle, R.G. de Voe, L. Reyna and R.G. Brewer, Phys. Today, 61, 255 (1989); R. Blumel, J.M. Chen, E. Peik, W. Quint, W. Schleich, Y.R. Shen and H. Walter, Nature (London), 334, 309 (1988).

[7] N.J. Johnson, J.Phys.: Condens. Matter, 7, 965 (1995).

[8] P. Bakshi, D.A. Broido and K. Kempa, Phys. Rev., B42, 7416 (1990); N.A. Bruce and P.A. Maksym, Phys. Rev., B61, 4718 (2000).

[9] Yu.E. Lozovik and V.A. Mandelshtam, Phys. Lett., A165, 469 (1992).

[10] D. Ceperley, G.V. Chester and M.H. Kalos, Phys. Rev., B16, 3081 (1977).

[11] H.W. Jackson and E. Feenberg, Ann. Phys. (NY), 15, 266 (1961).
FIG. 1. The $\alpha$ dependence of the potential energies $V_{4BS}$, $V_{4AFS}$, $V_{4FS}$, the full energies $E_{2BS}$, $E_{2FS}$ and the kinetic energies $E_{KINBS}$, $E_{KINAFS}$, $E_{KINFS}$ at the fixed $\lambda = 0.01$.

FIG. 2. The $\lambda$ dependence of the full energies for all clusters.
FIG. 3. The module of the wave function for the bose state for cluster with three coulomb particles in a $2D$ parabolic well.

FIG. 4. The module of the wave function for the parallel spin state for cluster with three coulomb particles in a $2D$ parabolic well.
FIG. 5. The module of the wave function for the mixed spin state for cluster with three coulomb particles in a 2D parabolic well when two particles have one direction of spin and third opposite. In the figures 3,4 and 5 the numerical quantities in the vertical axes expressed in single numerical units.