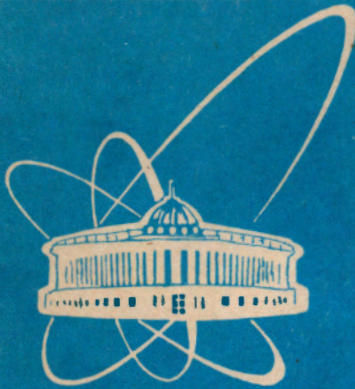


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PAIRING EFFECTS IN SODIUM CLUSTERS

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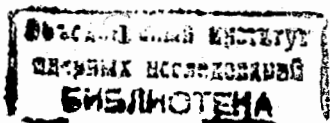
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1 Introduction

The odd-even staggering (OES) of separation energies and ionization potentials (IP) observed in metal clusters (see, for example, [1-9]) is an unexplained experimental fact that can reveal new information about the electron correlations in metal clusters not obtainable from experiments on bulk metals. The most complete experimental data for IP in sodium clusters [9] show that the strong OES takes place for the distinct regions $N = 21 - 38, 43 - 51, 59 - 68$ and $95-108$, where N is the number of atoms in a cluster (for sodium clusters $N = N_e$ where N_e is the number of valence electrons). The value of OES is about 0.2 eV for small clusters and 0.1 eV for larger clusters ($N = 59 - 68$ and $95-108$). On the other hand, there are regions (for example, $N = 51 - 58$ and $71-92$) where the OES is practically absent. The OES is also observed in small lithium [8], potassium [2,10], silver [11] and aluminum [12] clusters.

Possible ways of explanation of the OES are now intensively discussed [13-21]. It has been shown [14,15] that the quadrupole deformation of metal clusters with open shells leads to strong fluctuations in the IP and can explain, to a large extent, the behavior of the IP in size regions with $N = 4 - 20, 34 - 40$ and $59-68$. Deformation effects seem to be most important for the description of the IP. However, a very regular character of the OES in some size regions initiates consideration of additional physical effects which could be responsible for the OES. In this sense, the pairing between valence electrons (creation of Cooper pairs of valence electrons with moment $L = 0$) as a possible origin of a regular OES seems to be rather attractive. This point is based on the analogy with atomic nuclei where just pairing of nucleons (which can be considered as counterparts of valence electrons in metal clusters) is responsible for the regular OES in binding energies of nuclei [22]. The pairing and some other effects with similar consequences have been investigated for metal clusters in papers [13,16-19]. In [16] the "pairing" OES term $(-1)^N f(N)$ in the IP of sodium clusters, caused by spin degrees of freedom, was considered in the framework of the simple electron gas model and the electron spin-density functional model in the spherical jellium approxi-



mation. The comparison with experimental data [9] shows that this term underestimates considerably the OES effects and does not explain the absence of the OES in $N = 51 - 58$ and $N = 71 - 92$ size regions. In [17] the pairing in aluminum and sodium clusters was considered within the BCS method. For sodium clusters, the typical value 0.2 eV of the OES was proposed. However, as is shown in the present paper below, only a weak pairing is reasonable for sodium clusters and, as a result, the use of the BCS is not correct. A pairing origin of the OES in potassium clusters was studied in the framework of the seniority scheme in [18]. The calculations are in agreement with experimental data but in this paper only a group of small clusters was considered where the OES is rather strong. Other cluster regions, where the OES is small or absent were not studied. The OES was also discussed in [13] (schematic model, influence of temperature) and in [19] (shell-model calculations for small sodium clusters). It should be noted that in [13,16-19] an important influence of quadrupole deformation on the OES was not taken into account while, vice versa, in [14,15] the pairing effects were omitted.

The studies mentioned above provide a valuable information about features of the OES in metal clusters. However, as has been shown above, these studies are not sufficient to be sure that we really need the pairing for the description of the IP. A comprehensive study of this problem for sodium clusters is the aim of the present paper. As compared to the previous investigations [13-19] our study has three important features:

- 1) Both deformation and pairing effects are taken into account simultaneously. Particularly, competition between deformation and pairing (well known in atomic nuclei [22]) is taken into account. Calculations of cluster deformation are performed within the shell correction method [23,24] firstly developed in nuclear physics and adapted recently to alkali clusters [21,25].

- 2) It is unknown from the very beginning how strong pairing could be in clusters. Moreover, as is shown below, in sodium clusters only a weak pairing can exist. This makes the use of the BCS for the description of pairing in clusters to be very doubtful. Indeed, it is well known that the BCS gap equation has no solutions if the pairing strength constant is less

than some critical value [22]. The BCS does not conserve the particle number N , which leads to the appearance of ΔN fluctuations. The BCS accuracy is of an order of $\Delta N/N \sim \sqrt{N}$ that is not enough for small systems. So, the BCS has serious shortcomings which do not take place for a bulk but are crucial for the description of pairing in small clusters with a limited number of valence electrons. To overcome this trouble, we use here the particle-number projecting method, the so-called FBCS, which provides a good accuracy of calculations irrespective of the magnitude of pairing strength. It worth noting that this method is of quite general character and can be used for different metal clusters including the clusters that are superconductors in a bulk.

- 3) A wide region $20 \leq N \leq 80$ of sodium clusters is considered, which covers groups of clusters both with and without the OES.

Bulk sodium is not the superconductor. In this sense, the clusters of metals which are superconducting in a bulk (for example, aluminum) seem to be more promising to look for the pairing. Nevertheless, we investigate here the sodium clusters since just for these clusters there are most complete experimental data on the IP [9] and most wide calculations of the shape deformations [21,25]. Sodium clusters seem to be the best polygon to check the method proposed here for calculation of the IP.

We will not consider here a possible origin of electron pairing in sodium clusters. Since bulk sodium is not superconducting, the possible pairing in sodium clusters could have a specific origin connected, maybe, with a small size of a system (some surface effects, etc.). Residual correlations between valence electrons in clusters can include an attractive short-range component which, in turn, can lead to effects like pairing. In the present paper, the existence of electron pairing in sodium clusters is taken as some ansatz.

Temperature effects are neglected in the present calculations. The typical temperature of sodium clusters is 300-500 K which corresponds to the thermal energy 0.03-0.05 eV. This thermal energy is much smaller than the deformation energy and the pairing correlation energy (see Sec. 3) and, as a result, should not influence noticeably the results obtained.

2 Method of calculations

2.1 BCS and FBCS methods

We start from the model Hamiltonian of the form

$$H = \sum_s e_s (a_s^+ a_s + a_{\bar{s}}^+ a_{\bar{s}}) - G \sum_s a_s^+ a_{\bar{s}}^+ a_{\bar{s}} a_s. \quad (1)$$

The first term in (1) is the energy of an electron system in the independent particle model (IPM). This term is written as a sum of single-particle energies of noninteracting valence electrons moving in some mean field. The second term represents a constant pairing interaction between valence electrons. We will consider a singlet pairing which couples electrons occupied single-particle states s and \bar{s} (time reversal counterpart of state s) to the Cooper pair with zero total moment. In (1), a_s^+ and a_s are the creation and annihilation operators of the single-particle state s with the energy e_s , G is the strength constant of the pairing interaction.

It is well known that in the BCS the gap equation has solutions only in the case of sufficiently strong pairing when the strength constant G is much larger than G_{cr} , the critical value corresponding to the phase transition from the superfluid state to the normal state [22]. The closer the value G to G_{cr} , the worse the accuracy of the BCS $\sim \Delta N/N$. In this sense, the ratio G/G_{cr} can serve as a measure of the validity of the BCS. Usually, we have $G/G_{cr} \leq 1$ when a single particle spectrum is rarefied in the vicinity of the Fermi-level or single particle states contain one or several unpaired particles (the blocking effect). Both these cases take place here. Indeed, the rough estimation [13] of the pairing energy gap Δ gives $\Delta \sim 1/N$ eV that is smaller than a typical value of energy spacing between single-particle levels in the vicinity of the Fermi-level in sodium clusters with open shells. As a result, the electron pairing in sodium clusters is expected to be weak. This is especially the case for odd- N clusters where the blocking effect takes place due to the odd electron. So, for investigation of pairing in sodium clusters, one needs a more correct method than the BCS. We will use for this aim the FBCS method where the BCS wave functions are projected onto states with the

fixed particle number. In contrast with the BCS, the FBCS leads to the energy gain at any, even very small, value of G .

The FBCS was firstly suggested in [26,27] and since that time many versions of this method have appeared. In this work, we use the version which was elaborated in [28] and presented in detail in [29]. This version has the advantage that it allows one to represent quantities under computation in the form of series of small values $\beta_p = v_p/u_p < 1$ or $\beta_h^{-1} = u_h/v_h < 1$ (where p and h label single-particle states above ($p > F(N_e)$) and below ($h \leq F(N_e)$) the Fermi level $F(N_e)$) and thus to avoid time consuming calculations. The Bogoliubov coefficients u_i and v_i are determined for each state i by the variational method (variation after projection) when the total energy of a system is minimized using these coefficients as variable parameters.

Following [28,29], the projected BCS wave function of the ground state of N_e -even cluster can be written as a superposition of particle-hole excitations:

$$|\Psi(N_e)\rangle = [T(N_e)]^{-1/2} \sum_{k=0}^n \frac{1}{(k!)^2} [\hat{P}(N_e)^+]^k [\hat{Q}(N_e)]^k |\Psi_0(N_e)\rangle \quad (2)$$

where

$$\hat{P}(N_e)^+ = \sum_{p > F(N_e)} \beta_p a_p^+ a_{\bar{p}}^+, \quad \hat{Q}(N_e) = \sum_{h \leq F(N_e)} \beta_h^{-1} a_h a_{\bar{h}},$$

a_p and a_h are the operators of creation and annihilation of the particle in the state s (in the spherical basis $|s\rangle = |nljm\rangle$); $n = \sum n_s = N/2$ is the number of pairs where n_s runs from zero up to Ω_s ; Ω_s is the pair degeneracy of the level s . In spherical clusters, $\Omega_s = 2l + 1$. In axially deformed clusters, $\Omega_s = 1$ and 2 for $\Lambda = 0$ and $\Lambda \neq 0$, respectively. $|\Psi_0(N_e)\rangle$ is the ground state of the system without pairing, i.e., in the framework of the IPM. In this approximation, electrons occupy all the levels up to $F(N_e)$. The normalization factor $T(N_e)$ in (2) has the form

$$T(N_e) = 1 + \sum_{k=1}^n P_k(N_e) Q_k(N_e); \quad (3)$$

where $P(N_e)$ and $Q(N_e)$ are symmetric polynomials:

$$P_k(N_e) = \sum_{F(N_e) < p_1 < p_2 \dots < p_k} \beta_{p_1}^2 \beta_{p_2}^2 \dots \beta_{p_k}^2, \quad (4)$$

$$Q_k(N_e) = \sum_{h_1 < h_2 \dots < h_k \leq F(N_e)} \beta_{h_1}^{-2} \beta_{h_2}^{-2} \dots \beta_{h_k}^{-2}.$$

Expression (2) corresponds to the case when the last occupied level is completely filled ($n_s = \Omega_s$). If the last level is partly filled ($n_s \leq \Omega_s$), the foregoing completely filled level should be used as $F(N_e)$. In this case, the ground state FBCS wave function is written as

$$|\Psi(N_e)\rangle = [T(N_e)]^{-1/2} \sum_{k=0}^{n-n_s} \frac{1}{k!(k+n_s)!} [\hat{P}(N_e)^+]^k [\hat{Q}(N_e)]^{k+n_s} |\Psi_0(N_e)\rangle. \quad (5)$$

States containing unpaired electrons are created by acting by appropriate a_s^+ - or a_s - operators on a ground state wave function.

Expression for the binding energy of the even- N_e system is

$$E(N_e) = 2 \sum (e_s - \frac{G}{2}) \Omega_s v_s^2 [N_e - 2]_s - G \sum_{s \neq t} \Omega_s \Omega_t u_s v_s u_t v_t [N_e - 2]_{st} \quad (6)$$

where the correcting functions

$$[N_e - 2]_s = \frac{\langle \Psi(N_e - 2)_s | \Psi(N_e - 2)_s \rangle}{T(N_e)}$$

and

$$[N_e - 2]_{st} = \frac{\langle \Psi(N_e - 2)_{st} | \Psi(N_e - 2)_{st} \rangle}{T(N_e)},$$

arise due to the particle-number projecting. $|\Psi(N_e - 2)_s\rangle$ and $|\Psi(N_e - 2)_{st}\rangle$ ($s \neq t$) are the wave functions with $N_e - 2$ paired and two unpaired electrons. The lower indices indicate energy levels occupied by unpaired electrons.

The wave function of the odd- $(N_e + 1)$ system with one unpaired electron on the single-particle level f is written as $a_f^+ |\Psi(N_e)\rangle$. The expression for the binding energy of a such system has the form

$$E_f(N_e + 1) = e_f + 2(\Omega_f - 1)e_f v_f^2 [N_e - 2]_f + 2 \sum_{s \neq f} (e_s - \frac{G}{2}) \Omega_s v_s^2 [N_e - 2]_{fs} \quad (7)$$

$$-G \sum_{s \neq t; s, t \neq f} \Omega_s \Omega_t u_s v_s u_t v_t [N_e - 2]_{fst} - 2G(\Omega_f - 1)u_f v_f \sum_{i \neq f} \Omega_i u_i v_i [N_e - 2]_{if}$$

Without the particle-number, the correcting factors in (6) and (7) are absent and these expressions have the same form as in the BCS.

The gain in the total energy of the system due to the pairing interaction is determined by the pairing correlation energy:

$$E_{corr} = E(N_e; G = 0) - E(N_e; G \neq 0) \quad (8)$$

where $E(N_e; G \neq 0)$ and $E(N_e; G = 0)$ are energies of the system (see exps. (6) and (7)) with and without pairing.

2.2 Equilibrium deformations and pairing

Single-particle energies were calculated with the Woods-Saxon potential with the parameters or radius, depth and diffuseness from ref. [30]. Parameters of axial deformations α , α_3 , α_4 , α_5 and α_6 were found for each sodium cluster by the shell correction method [21,25]. As our calculations show, the shapes of singly charged ($z = +1$) and neutral clusters with the same number of atoms coincide with good accuracy. This can be explained by the fact that single-particle potentials of charged ($z = +1$) and neutral clusters differ from each other mainly by their depth (the depth of the potential wall of a charged cluster is larger [31,32]). On the other hand, the shell corrections determining the shape of cluster are not very sensitive to the potential depth.

It is known that pairing tends to couple particles in pairs with the total angular momentum $I = 0$. Such a coupling proves to be more effective in spherical systems than in deformed ones. As a result, pairing forces tend to restore the spherical symmetry, thus decreasing the deformation of clusters with open shells. One can estimate the value of G under which the deformation of a cluster dies out. This effect is demonstrated in Fig.1

where the total energy of a system, calculated within the shell correction method taking into account pairing, is presented. Our calculations show that pairing destroys deformation of sodium clusters at $g_0 > 1.4$ eV but does not change the values of equilibrium deformation parameters at $g_0 = 0.8$ and 1.0 eV used in the present work. This is not surprising: as is seen from Fig.2, the pairing correlation energy (8) at $g_0 = 1.0$ eV is much smaller than the deformation energy $E_{def}(N_e) = E(N_e, \{\alpha\}) - E(N_e, \{\alpha = 0\})$ (see also discussion in Sect.3).

2.3 Ionization potential

Ionization potential is defined as

$$IP(N_e) = E(N_e - 1, R_N)^{+1} - E(N_e, R_N) \quad (9)$$

where $E(N_e, R_N)$ is the binding energy of N_e valence electrons in the cluster with N atoms; $R_N = r_S N^{1/3}$, r_S is the Wigner-Seitz radius, the upper index in (9) labels the charge of the cluster.

We calculated the binding energy of the charged cluster ($z = +1$) as a sum of binding energy of the neutral cluster with the same N_e and N and of the Coulomb term

$$E(N_e - 1, R_N)^{+1} = E(N_e - 1, R_N) + E_{coul} \quad (10)$$

where the charge $z = +1$ is assumed to be uniformly distributed over the surface of the cluster [33]:

$$E_{coul} = \frac{z^2}{2R_N} \left\{ 1 - \frac{1}{4\pi} \sum_{\lambda} \frac{(\lambda^2 + 3\lambda - 5)|\alpha_{\lambda}|^2}{(2\lambda + 1)} \right\} \quad (11)$$

Expression (10) is based on the assumption that single-particle levels of the ionized cluster differ from the single-particle levels of the corresponding neutral cluster by nearly constant energy shift. Our analysis of single-particle schemes [31] calculated within the Kohn-Sham prescription supports this assumption.

To simplify the calculations, it is convenient to rewrite exp. (9) as follows:

$$IP(N_e) = IP_{IPM}(N_e) + \delta E_{corr}(N_e) \quad (12)$$

where $IP_{IPM}(N_e)$ is calculated within the IPM (without the pairing but with the Coulomb contribution). The pairing contribution $\delta E_{corr}(N_e)$ has the form:

$$\delta E_{corr}(N_e) = E_{corr}(N_e - 1) - E_{corr}(N_e) \quad (13)$$

where $E_{corr}(N_e)$ is given by exp. (8). Due to the blocking effect $\delta E_{corr}(N_e) > 0$ or < 0 for even or odd N_e , respectively.

3 Results of calculations and discussion

The results of our calculations are presented in Figs. 1-3. In the calculations the pairing strength constant $G = g_0/N$ with $g_0 = 0.8, 1.0$ and 1.4 eV was used.

Fig.3 shows the IP, as measured by Persson [9], compared to the FBCS and IPM results. Both the FBCS and IPM calculations take into account the cluster axial deformations with the parameters $\alpha, \alpha_3, \alpha_4, \alpha_5$ and α_6 [21,25]. It is seen that the average value of the IP is described rather well though some underestimation of the IP takes place. The IPM results demonstrate fluctuations in the IP, caused purely by deformation effects. For most sizes regions these fluctuations do not reproduce a regular character of the experimental OES. Moreover, the IPM results exhibit the so-called quartets (the upsloping straight lines consisting of four points) which are absent in the experimental data. Until recently, these quartets were thought to be connected with fourfold degeneracy of the single-particle levels with $\Lambda \neq 0$ (see, e.g., discussion in [21]). The fourfold degeneracy should be destroyed in clusters with triaxial deformation. However, recent calculations [34,35] have shown that triaxiality does not remove quartets. So, other physical reasons should be looked for to destroy the quartets and, as is shown below, pairing could be one of them.

The FBCS results, where both pairing and deformation effects are taken into account, are presented at $g_0 = 0.8$ and 1.0 eV. The value $g_0 = 0.8$ eV seems to be most appropriate. Then, in accordance with experimental data, the FBCS provides the regular OES of the reasonable amplitude in the size regions $N = 23 - 26, 35-38, 47-50$ and $58-72$ and

destroys the quartets in large extent. On the other hand, the pairing leads to the OES in the size regions where the staggering is not observed at all ($N = 38 - 40, 51 - 58$). The results with $g_0 = 1.0$ eV, presented in the same figure, show that even rather moderate increasing of pairing leads to considerable overestimation of the OES. However, if the temperature of clusters is taken into account, the calculated OES will be smoothed and the value $g_0 = 1.0$ eV can be quite reasonable.

Let us show now that the BCS cannot be used at $g_0 = 0.8 - 1.0$ eV. Following our calculations, G/G_{cr} is about 1 for $g_0 = 1.0$ eV and considerably smaller than 1 for $g_0 = 0.8$ eV. That means that the pairing is too weak for using the BCS. Indeed, at $g_0 = 0.8 - 1.0$ eV, for the overwhelming majority of clusters we have $E_{corr}(BCS) = 0$, i.e. the BCS does not provide any energy gain. At the same time, $E_{corr}(FBCS)$ is, on the average, 0.2-0.3 eV, i.e., only the FBCS can be used for consideration of such a small pairing.

Our calculations show that the BCS becomes valid only at $g_0 \geq 1.4$ eV. But at such a strong pairing we have the drastic overestimation of the experimental OES. Moreover, the comparison of the pairing correlation energy with the deformation energy clearly demonstrates that the strong pairing ($g_0 = 1.4$ eV) destroys the deformation for the most of the clusters (see Fig.2), which is in drastic contradiction with the generally accepted picture. Vice versa, the FBCS pairing correlations obtained at $g_0 = 0.8 - 1.0$ eV do not destroy the deformation (except for the clusters where the deformation is very small). So, we again come to the conclusion that in sodium clusters only weak pairing is possible and, as a result, the use of the BCS is not correct.

4 Conclusions

For the first time, the IP in sodium clusters with $20 \leq N \leq 80$ is investigated with both deformation and pairing effects to be taken into account simultaneously. The calculations have shown that only the weak pairing is appropriate ($G = g_0/N, g_0 \leq 1.0$ eV). Then, the competition between pairing and deformation effects is negligible and pairing does not change

the equilibrium deformations. The BCS cannot be applied to such a small pairing. Only the particle-number projecting methods, like the FBSC, can be used. The strong pairing results in the drastic contradiction with the available experimental data: strong overestimation of the OES and almost total destruction of cluster's deformation. In general, including of pairing at $g_0 = 0.8$ eV leads to quite a satisfactory description of the IP. The calculations reproduce the regular behavior of the OES and result in removing the quartets. On the other hand, the pairing causes the OES even in the size regions where this effect was not observed.

The FBCS method used here for calculation of pairing in sodium clusters is of a quite general character and can be used for investigation of pairing in other metal clusters, like aluminum and etc..

Our results do not allow one to make final conclusions about the need for pairing for the description of the OES in sodium clusters. Pairing in these clusters remains to be rather questionable. Most probably, that the OES in sodium clusters is mainly a consequence of spin and deformation effects. To clarify this point, the calculations in the framework of the electron spin-density functional approach are very urgent. Nevertheless, we suppose that the hypothesis on pairing in metal clusters cannot be cast aside and needs additional investigation. First of all, for metals which are superconductors in a bulk. For this aim, the calculations with state dependent (not constant) pairing are very desirable. In principle, we cannot exclude the situation that this type of pairing will result in a strong dependence of the OES magnitude on the size region and thus lead to improvement of the IP description. Second, the temperature effects should be incorporated. The discovery of pairing in metal clusters would be a fundamental result with very important consequences for high temperature superconductivity and other fields of modern physics.

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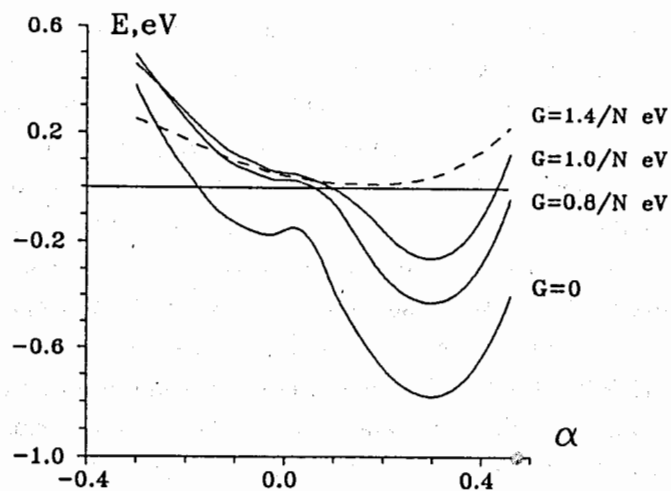


Fig.1. Total energy of Na_{22} as a function of the deformation parameter α . The calculations are performed at $g_0 = 0, 0.8, 1.0$ and 1.4 eV.

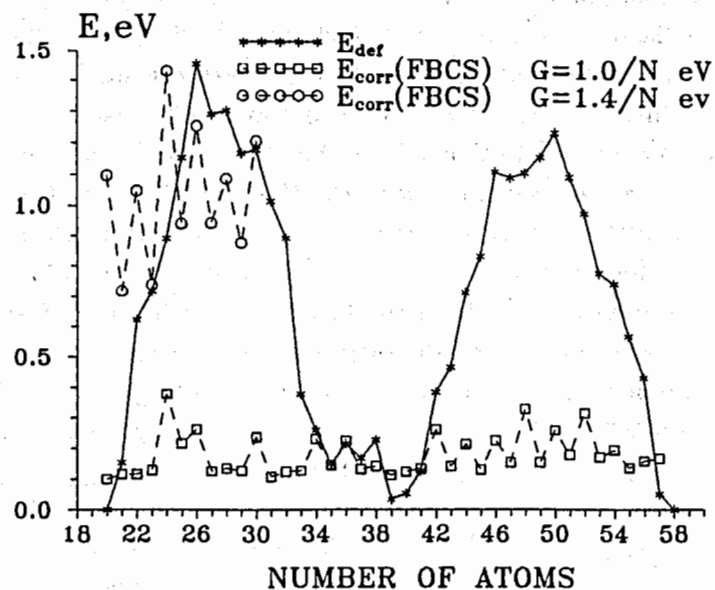


Fig.2. Deformation energies E_{def} and pairing correlation energies E_{corr} calculated within the FBCS with $g_0 = 1.0$ and 1.4 eV. All the values are given in eV.

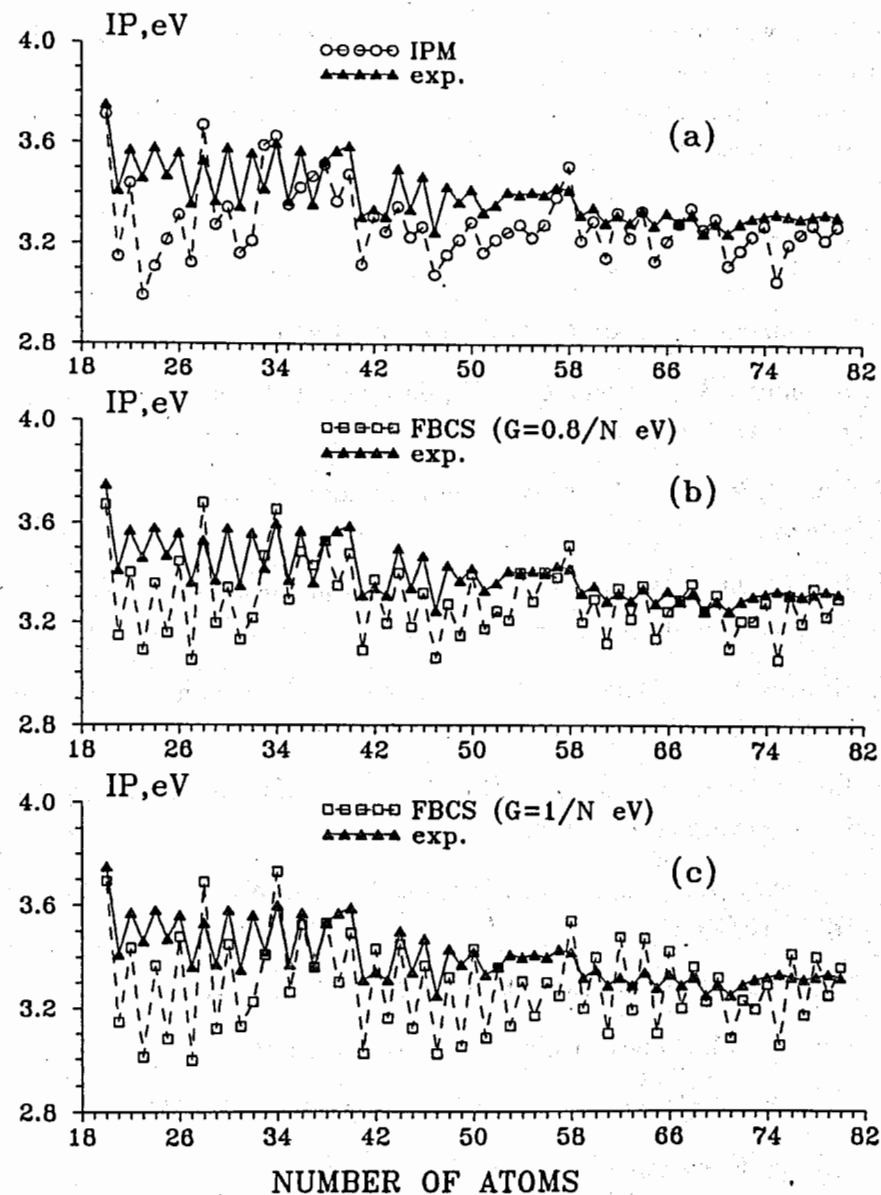


Fig. 3. Experimental [9] and calculated (within the IPM and FBCS) IP in sodium clusters with $20 \leq N \leq 80$.

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References

1. Brechignac, C. et al: Z.Phys. D12 199 (1983)
2. Saunders, W.A., Clemenger, K., de Heer, W.A. and Knight, W.D.: Phys.Rev. B32 1336 (1985)
3. Knight, W.D., de Heer, W.A. and Saunders, W.A.:Z.Phys. D3 109 (1986)
4. Kappes, M.M., Schar, M., Radi, P. and Schumacher, E.: J.Chem.Phys. 84 1863 (1986)
5. Kappes, M.M., Schar, M., Rothlisberger, U., Yerezian, C. and Schumacher, E.: Chem.Phys.Lett. 143 251 (1988)
6. Honea, E.C., Hommer, M.L., Persson, J.L. and Whetten, R.L.: Chem. Phys. Lett. 171 147 (1990).
7. Hommer, M.L., Persson, J.L., Honea, E.C. and Whetten, R.L.: Z.Phys. D22 441 (1991)
8. Dugourd, Ph. et al: J.de Physique 4 1 c7-509 (1991)
9. Persson, J.L.: Thesis Univ. of Los Angeles, 1991.
10. Brechignac, C. and Cahuzac, Ph.: Z.Phys. D3 121 (1986)
11. Laiting, K. et al: Z.Phys. D13 161 (1989)
12. Schriver, K.E. et al: Phys.Rev.Lett. 64 2539 (1990)
13. Mottelson, B.R.: Clustering Phenomena in Atoms and Nuclei, Springer Series in Nucl. and Part. Phys.:Int. Conf. on Nucl. and Atomic Clusters, Turku, Finland (1991) 571.

14. Ekardt, W. and Penzar, Z.: Phys.Rev. B38 4273 (1988)
15. Penzar, Z. and Ekardt, W.: Z.Phys. D19 109 (1991)
16. Snider, D.R. and Sorbello, R.: Surf.Sci. 43 204 (1984)
17. Barranko, M. et al: Z.Phys. D22 659 (1992)
18. Lipparini, E.: Preprint UTF239, Trento, 1991.
19. Koskinen, M. et al: Lect. Notes in Phys., v.404 (1991) 335 (Proc Int.Conf. on Nucl. Phys. Concepts in Study of Atomic Cluster Phys., Bad Honnef FRG, Eds R.Schmidt, H.O.Lutz and R.Dreizier).
20. Nesterenko, V.O.: Part.Nucl. 23, n.6, 1665 (1992)
21. Frauendorf, S. and Pashkevich, V.V.: Preprint FZR-37, Rossendorf, 1994; subm. to Phys. Rev. B,
22. Bohr, A. and Mottelson, B.R.: Nuclear Structure, v.1, W.A.Benjamin, Inc. New York, Amsterdam, 1969.
23. Brack, M., Damgaard, J., Jensen, A.S., Pauli, H.C., Strutinsky, V.M., Wong, C.Y.: Rev.Mod.Phys. 44 320 (1972)
24. Strutinsky, V.M.: Nuc.Phys. A95 420 (1967); Nucl.Phys. A122 1 (1968)
25. Frauendorf, S. and Pashkevich, V.V.: Z.Phys. D26 S98 (1993)
26. Kerman, A.K., Lawson, R.D., Macfarlane, M.H.: Phys.Rev. 124 162 (1961)
27. Dietrich, K., Mang, H.J and Pradal, J.H.: Phys.Rev. B135 22 (1964)
28. Kuzmenko, N.K. and Mikhailov, V.M.: Bull. Acad. Nauk. USSR, ser. phys. 37 1911 (1973)
29. Kuzmenko, N.K. and Mikhailov, V.M.: Sov. J. Part.Nucl., 20 830 (1989) and references therein.

30. Nishioka, H., Hansen, K. and Mottelson, B.R.: Phys.Rev., B42 9377 (1990)
31. Ekardt, W.: Phys.Rev., B29 4273 (1984)
32. Yannouleas, C., Broglia, R.A., Brack, M. and Bortignon, P.F.: Phys. Rev. Lett., 63 255 (1989)
33. Lipparini, E. and Vitturi, A.: Z. Phys., D17 57 (1990)
34. Yannouleas, C. and Landman, Uzi: Phys.Rev B15, in press.
35. Frauendorf, S. et al: in preparation.

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Кузьменко Н.К. и др.
Эффекты спаривания в натриевых кластерах

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Рассматривается возможность объяснения нечетно-четных флуктуаций (НЧФ) в потенциале ионизации (ПИ) натриевых кластеров с $20 \leq N \leq 80$ как проявления спаривания между валентными электронами. Впервые и спаривание, и деформация кластеров учитываются в расчетах одновременно. В среднем получено достаточно неплохое описание ПИ. Показано, что в натриевых кластерах возможно только слабое спаривание. Использование метода Бардина—Купера—Шриффера (БКШ) в данном случае неправомерно. Необходимо пользоваться методами проектирования по числу частиц. Показано, что конкуренция между спариванием и деформационными эффектами мала и не приводит к изменению равновесной деформации. Спаривание вызывает регулярные отчетливые НЧФ и разрушает так называемые квартеты в ПИ. Для одних групп кластеров это приводит к заметному улучшению согласия с экспериментом, для других групп (в первую очередь, там, где НЧФ на эксперименте не обнаружено) — к ухудшению описания ПИ. В целом, существование спаривания в натриевых кластерах представляется довольно проблематичным.

Работа выполнена в Лаборатории теоретической физики им.Н.Н.Боголюбова ОИЯИ.

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Kuzmenko N.K. et al.
Pairing Effects in Sodium Clusters

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The pairing between valence electrons is considered as a possible origin of the odd-even staggering (OES) in the ionization potentials (IP) of sodium clusters with $20 \leq N \leq 80$. For the first time, both effects of pairing and shape deformation are taken into account simultaneously. On the average, quite a reasonable description of the IP is achieved. It is shown that in sodium clusters only a weak pairing can exist (if the pairing exists at all). In this case, it is not correct to use the Bardin—Cooper—Shriffier (BCS) method. Only the particle-number projecting methods can be applied. It is shown that competition between pairing and deformation effects is small and does not change the equilibrium deformations. Pairing leads to systematic and pronounced OES and destroys the so-called quartets in the IP. This improves the agreement with experimental data in some size regions. On the other hand, the pairing worsens the agreement in the size regions where the OES has not been observed at all. Finally, the existence of the pairing in sodium clusters seems to be very questionable.

The investigation has been performed at the Bogoliubov Laboratory of Theoretical Physics, JINR

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