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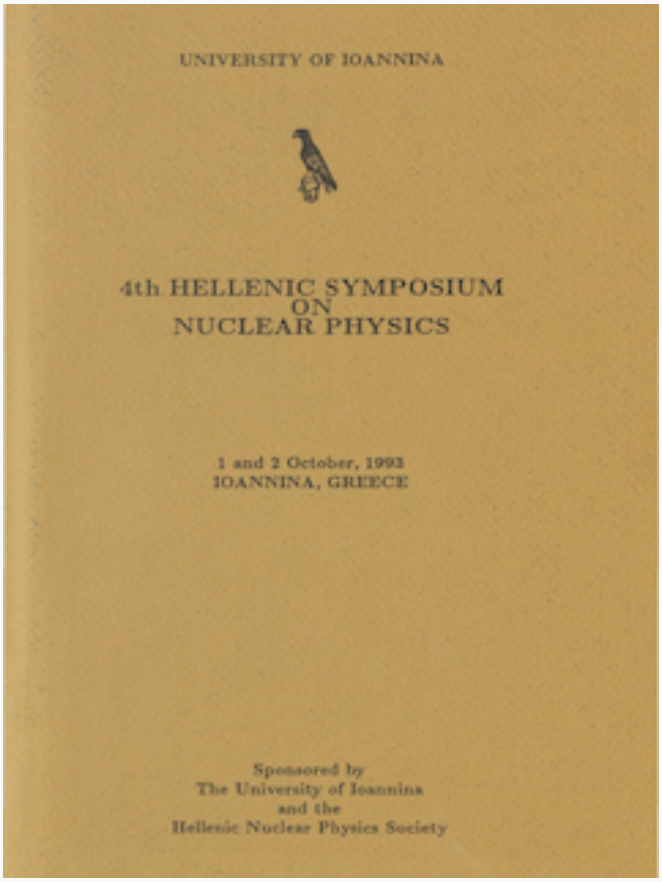

Parametrization of the effective potential in sodium clusters

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PARAMETRIZATION OF THE EFFECTIVE POTENTIAL IN SODIUM CLUSTERS

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Abstract The effective radial electronic potentials for neutral sodium clusters determined by the local density approximation and the jellium model are parametrized by means of (symmetrized) Woods-Saxon and "Wine-Bottle" symmetrized Woods-Saxon potentials. The potential parameters are determined by various least-squares fitting procedures. Particular attention is paid to the dependence of the radius parameter R on the particle number N and it is realized that for relatively smaller values of N, complex expressions of R as a function of N, are more appropriate than the standard one $R = r_0 N^{1/3}$. It is also found that improved results in these cases are obtained with an expression, of the form $R = r_0 N^{1/3} + b$, which is still very simple.

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1. Introduction

The knowledge of the mean field potentials for electrons in metal clusters is needed in various calculations, as for example, in the case of single-particle level densities, electronic binding energies etc [1,2]. In practice, it is sometimes convenient to use parametrized forms of these potentials, as in ref. [2] where the shell and supershell structure was studied for Na clusters.

+Presented by B. A. Kotsos

In this paper we investigate in some detail a parametrization procedure of the effective radial electronic potential $V_{eff}(r)$ in the spherical and homogeneous jellium model as this is determined using the local-density approximation. The density functional theory of Hohenberg, Kohn and Sham [3], has been used repeatedly in studies of metallic clusters, as for example, in refs. [4]-[8]. In our investigation, we consider the effective potentials of neutral sodium clusters determined systematically by Ekardt [7] in his spherical jellium background model (SJBM) study of work function of metal clusters, of the self-consistent determination of the charge density and self-consistent effective one-particle potential.

Ekardt's potentials have been parametrized in ref. [2] by a spherical Woods-Saxon (W-S) potential

$$V_{WS}(r) = -\frac{V_0}{1 + e^{(r-R)/a}}, \quad 0 \leq r < \infty \tag{1}$$

with $V_0 = 6eV, R = r_0 N^{1/3}, r_0 = 2.25\mathring{A}$ and $a = 0.74\mathring{A}$

Nishioka et al [2] have also considered another type of potential obtained in ref. [9] through a semiclassical approximation, aplying the Khon-Sham density functional method to a positive jellium background. The inner part of this potential is slightly shallower and the outer part is deeper than the Woods-Saxon potential. This potential of "wine-bottle" shape has also been used in ref. [2] for the study of supershells.

The aim of this paper is to consider Ekardt's effective potentials for neutral sodium clusters and to discuss a parametrization procedure, by means of potentials of symmentrized Woods-Saxon shape and of "wine-bottle symmetrized Woods-Saxon" shape and determine their parameters through least squares fits. Emphasis is given, in particular, to the dependence of the potential radius R on the particle number N of the cluster. These potentials are given and discussed in section 2 and 3, respectively, while in the last section numerical results are given and commented upon.

2. The symmetrized Woods-Saxon potential

The symmetrized Woods-Saxon potential we are using is the following:

$$V_{SF}(r) = -V_0 f_{SF}(r) = -V_0 \frac{sinh(R/a)}{cosh(r/a) + cosh(R/a)} =$$

$$= -V_0 \left[[1 + exp\frac{(r-R)}{a}]^{-1} + [1 + exp\frac{(-r-R)}{a}]^{-1} - 1 \right], \quad 0 \leq r < \infty \quad (2)$$

The form factor of this potential has the shape of the symmetrized Fermi distribution which has been used to describe successfully the densities of nuclei for a wide range of mass numbers [10]. The potential (2) has also been recently used in analyses of hypernuclei [11] and also as a nuclear single particle potential [12]. It is very closely related to the so-called "cosh" potential used in ref. [13] as a cluster-core potential in Nuclear Physics.

The potential (2), which unlike the Woods-Saxon potential has zero slope at the origin, resembles somehow the Gaussian one for small values of R/a, while for $R/a >> 1$ becomes very close to the Woods-Saxon one.

One feature of the potential (2) is that its volume integral is given exactly by the following simple analytic expression:

$$\left| 4\pi \int_0^\infty V_{SF}(r) r^2 dr \right| = \frac{4\pi}{3} V_0 R^3 [1 + (\frac{\pi a}{R^2})^2] \quad (3)$$

The same holds for its m.s.radius:

$$< r^2 >_{SF} = \frac{3}{5} R^2 [1 + \frac{7}{3} (\frac{\pi a}{R})^2] \quad (4)$$

More generally, the n-th moment of the potential may be given analytically [12]. In the case of the Woods-Saxon potential there are additional exponential terms, and thus its expression becomes more complex.

Since the condition $R/a >> 1$ is well satisfied, both for nuclei and atomic clusters, except for the very light ones, the symmetrized Woods-Saxon potential gives almost identical results to the Woods-Saxons one, even for small values of the mass number and particle number N, respectively. The present analysis corroborates also this fact.

3. The "Wine-bottle" symmetrized Woods-Saxon potential

Another parametrization of the effective potential, which seems to be rather interesting, is the following one which is of "wine- bottle" shape

$$V_{WB}(r) = -V_0 (1 + \frac{wr^2}{R^2}) \frac{sinh(R/a)}{cosh(r/a) + cosh(R/a)}, \quad 0 \leq r < \infty \quad (5)$$

for suitable choices of the parameter w.

The volume integral of the potential (5) may be obtained analytically though its expression is a little more complex than that of the potential (2). The result of integration leads to:

$$\left|4\pi \int_0^\infty V_{WB}(r) r^2 dr\right| = \frac{4\pi V_0}{3} R^3 \left[(1 + \frac{3w}{5}) + (1 + 2w)(\frac{\pi a}{R})^2 + \frac{7}{5} w (\frac{\pi a}{R})^4\right] \tag{6}$$

It is seen immediately that for w=0 this expression goes over to (3), as it should be the case. Analytic expressions for the various moments of the potential may be also derived.

We note that the potentials (2) or (5) should be also able to roughly reproduce the effective potential in the inhomogeneous jellium model [14] and the potential (5) of the modified jellium potential of ref. [15]. We also note that the substitution of a polynomial of a higher degree (or a suitable function of r) for $(1 + w\frac{r^2}{R^2})$ in (5), is likely to reproduce the wavy character of the local equivalent potential of ref. [16] (see fig. 2, of this reference) for individual clusters. Finally we may point out that it would be of interest to consider also the possibility of parametrizations of the form (2) or (5) of the average potential for the atom in the cluster, in the spirit of ref. [17].

4. Numerical results and discussion

In this section we give some of the results of our numerical calculations.

We considered Ekardt's effective local mean field potentials for the valence electrons in neutral sodium clusters with particle numbers $N = 8, 18, 20, 34, 40, 58, 68, 90, 92, 106, 132, 138, 168, 186, 198$ and we performed "an overall least squares fit" of the symmetrized Woods-Saxon potential to the potential values of the above clusters by treating V_0, a and the parameter r_0 in $R = r_0 N^{1/3}$ as adjustable parameters. Depending on the size of each cluster, about 15-30 potential values, covering the interval where the potential differs practically from zero have been estimated from the corresponding figures of ref. [7]. The best fit values are: $V_0 = 6.05eV$, $r_0 = 2.34\mathring{A}$, $a = 0.79\mathring{A}$.

The same procedure was repeated by adopting as R a fairly complex function of N which results from the observation that, to a good approximation,

the volume integral of the potential, for each cluster varies with N as $cN+d$ where c and d are constants. In this case (in which there is an additional adjustable parameter) a marked improvement in the quality of the fitting, compared to the one in the previous case, is observed. A very similar quality in the fitting is obtained if R is taken to be of the form

$$R = r_0 N^{1/3} + b \tag{7}$$

The best fit values in the latter case are: $V_0 = 6.03eV$, $r_0 = 2.10\mathring{A}$, $b = 1.09\mathring{A}$, $a = 0.78\mathring{A}$.

Another least squares fitting procedure we attempted was to consider the average values of the potential depths and the diffuseness parameter $a(V_0 = 6.05eV, \quad a = 0.79\mathring{A})$ and determine the parameters in R by least squares fitting of the expression of $< r^2 >_{SF}$ to the corresponding values obtained by the fitting of the symmetrized W-S potential to the values of $V_{eff}(r)$ for individual clusters. The best fit values in this case are: $r_0 = 2.16\mathring{A}$, $b = 0.795\mathring{A}$.

It should be noted that the best fit values depend on the clusters considered. Thus, if among the values of N only those with $N \geq 90$ are included in the fitting, the best fit values in the first of the above mentioned fitting procedures with expression (7) for R become: $V_0 = 6.01eV$, $r_0 = 2.28\mathring{A}$, $b = 0.114\mathring{A}$ and $a = 0.87\mathring{A}$. The improvement in the quality of fitting, compared to the one in which the expression $R = r_0 N^{1/3}$ is used becomes now much smaller.

Least-squares fits analogous to the previously mentioned ones have also been carried out with the wine-bottle potential and the best fit values were obtained. For example in the case of $N \geq 90$, mentioned just previously we find $V_0 = 6.03eV$, $r_0 = 1.97\mathring{A}$, $b = 1.64\mathring{A}$, $a = 0.864\mathring{A}$, $w = 0.102$.

From our analysis we have realized that for some clusters the fitting of $V_{eff}(r)$ by a (symmetrized) Woods-Saxon potential is fairly satisfactory (see e.g. fig. 1), while for others, this is not the case (see fig.2). All these figures were obtained with the above mentioned "overall fitting" and expression (7) for R. In certain cases the fitting is improved if the "Wine-bottle" symmetrized Woods-Saxon potential is used. Different choices of w for the individual clusters may, however, be necessary in many cases.

In fig. 3 and 4 we have plotted the W-S potential and the wine-bottle potential (denoted by 1 in each figure) of ref. 10 used by Nishioka et al [2] (see

their fig. 1) together with the symmetrized Woods-Saxon and Wine-Bottle symmetrized Woods-Saxon potential respectively, obtained in this work. It is seen that there is a marked difference in the surface region. Finally in fig. 5 the variation of the radius of the (symmetrized) Woods-Saxon potential with respect to the $N^{1/3}$ is shown. The best fit values used are those of the above mentioned "overal least squares fitting" and are given after expression (7). The functional dependence of R on $N^{1/3}$ is apparent.

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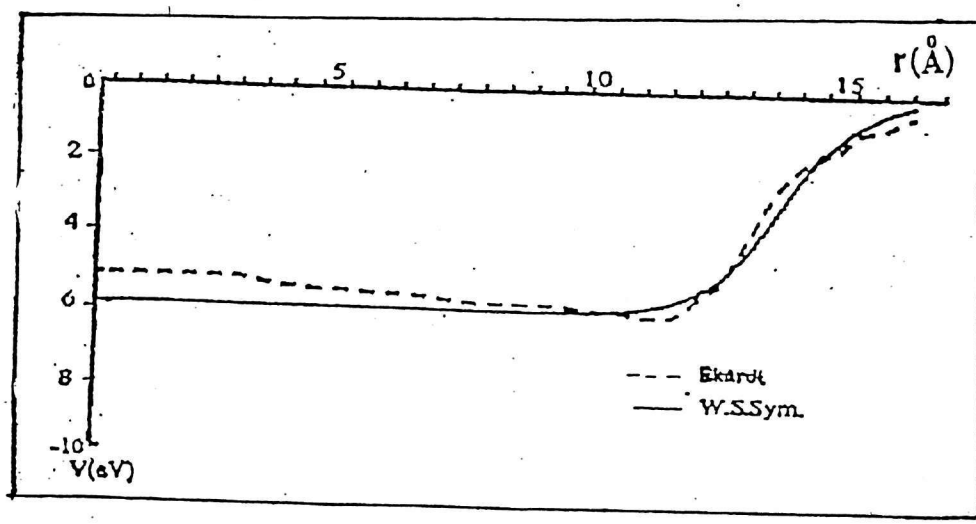

Fig. 1. The $V_{eff}(r)$ of Ekardt [7] for $N = 198$ (dotted line) and the corresponding symmetrized Woods-Saxon one (solid line) plotted with the best fit values of the "overall fitting" and $R = r_0 N^{1/3} + b$.

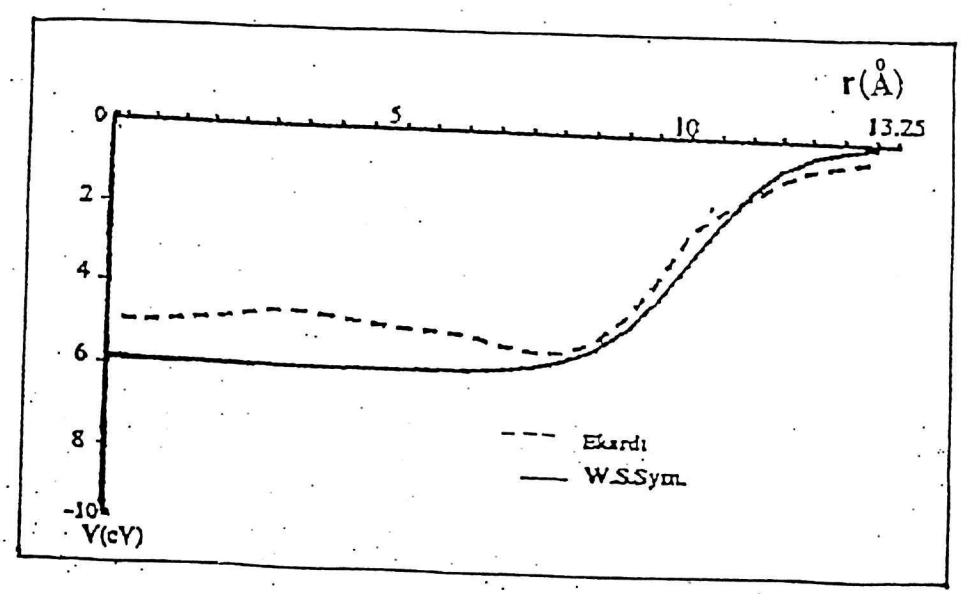

Fig. 2.The $V_{eff}(r)$ of Ekardt [7] for $N = 68$ (dotted line) and the corresponding symmetrized Woods-Saxon one (solid line) plotted with the best fit values of the "overall fitting" and $R = r_0 N^{1/3} + b$.

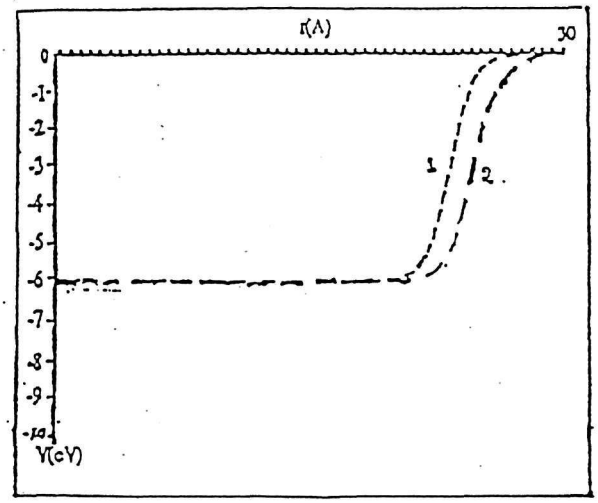

Fig. 3. The Woods Saxon potential (No 1) with the parameters of ref [2] for the cluster with N=1000 and the corresponding symmetrized Woods-Saxon potential of this work (No 2) using the expression $R = r_0 N^{1/3} + b$ and the best fit values: $V_0 = 6.014eV, r_0 = 2.28\AA$ and $b = 0.114\AA, a = 0.87\AA$.

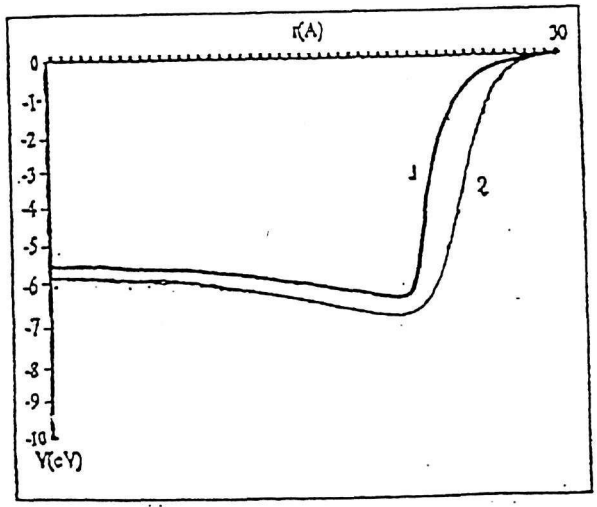

Fig. 4. The wine-bottle-potential (No 1) for $N = 1000$ obtained with the method of ref. [10] and used in ref. [2] and the "Wine-bottle" symmetrized Woods-Saxon potential (No 2) of this work using the expression $R = r_0 N^{1/3} + b$ and the best fit values: $V_0 = 6.03 eV, r_0 = 1.97\AA, b = 1.64\AA, a = 0.86\AA, w = 0.102$,.

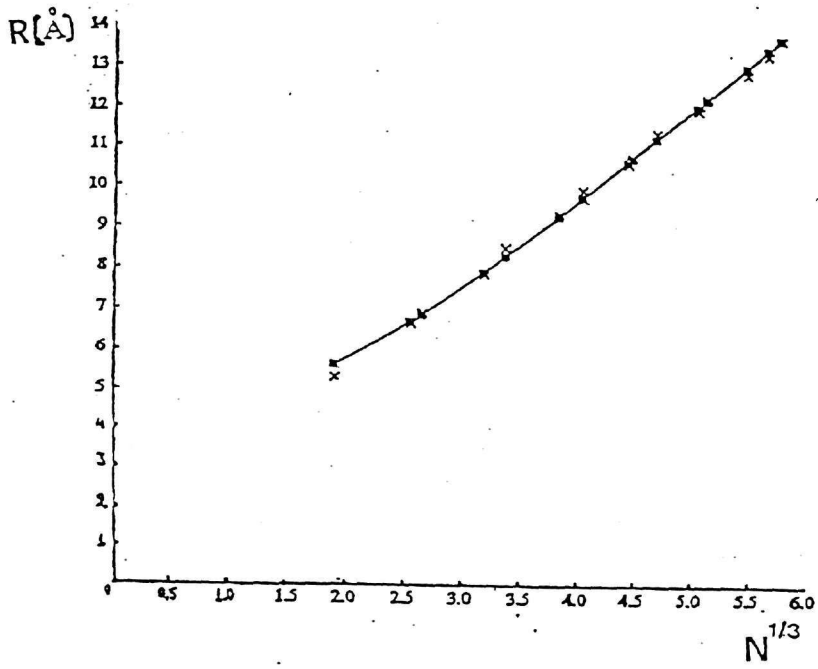

Fig. 5. The variation of the radius R of the Symmetrized Woods-Saxon potential with respect to cubic root of the particle number N. The values of R obtained by performing least squares fitting of $V_{SF}(r)$ to the $V_{eff}(r)$ of Ekardt for individual clusters are denoted by x, while those values obtained by an "overall least squares fitting" using the expression $R = r_0 N^{1/3} + b$ are denoted by ■.