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THE RADIAL DEPENDENCE OF THE SHELL MODEL POTENTIAL

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Радиальная зависимость потенциала оболочечной модели

В работе описан способ определения радиальной зависимости потенциала оболочечной модели сферического или деформированного ядра, основанный на процедуре самосогласования, в процессе которой вводится статистически усредненная плотность нуклонов. Для описания последней используется приближение, суть которого состоит в том, что пренебрегается угловой зависимостью плотности и изучается только её средняя радиальная зависимость. В работе определено понятие радиальной зависимости в деформированном ядре. В качестве примера приведены результаты расчета потенциала в ряде ядер сферической формы и в ядре ^{240}Pu при различных деформациях поверхности.

Работа выполнена в Лаборатории теоретической физики ОИЯИ.

Препринт Объединенного института ядерных исследований. Дубна 1977

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

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I. INTRODUCTION

The radial shape of the realistic shell-model potential for a spherical or deformed nucleus is usually specified in agreement with the empirical evidences that nucleon density is nearly constant inside the nucleus and decreases rapidly to zero in the thin surface layer. As an example of such a definition, one may refer to the Woods-Saxon type of the potential for the deformed nucleus (refs. [1,2]) and to the potential obtained by folding an effective two-nucleon interaction with a uniform sharp-surface pseudodensity [3] .

New experimental data such as electron scattering with large momentum transfer indicate that there exists a deviation of proton density from the Fermi distribution [4]. The theoretical calculations performed in the framework of both the shell model [5] and Hartree-Fock theory [6] also lead to the non-monotonic dependence of nucleon density on the radial variable and potential inside the nucleus. In this work we propose a method for determining the radial dependence of the shell-model potential. The shape of the nucleus is considered to be

fixed (spherical or deformed). The potential is determined by some effective nucleon-nucleon interaction, which is briefly discussed in section 2.

Following ref.[7] our aim is to define the potential in such a way that it should depend smoothly on the number of nucleons unlike the constrained Hartree-Fock potential. As a result, the newly defined potential may be used to calculate the properties of a number of nuclei of the same shape.

A smooth variation with particle number is achieved by the statistical self-consistency procedure[8]. This means that the potential should be consistent with the statistically averaged independent particle density, the exact definition of which is given in ref.[9] (see section 2).

In ref.[10] the direct numerical calculation shows that if in the Strutinsky type calculations one uses the self-consistent potential, the convergence of series in the powers of the shell corrections to the nuclear density becomes considerably better. Hence one may expect that using the statistically averaged potential in calculating nuclear masses, surface shapes and fission barriers will improve the existing theoretical predictions.

The definition of the potential and description of the effective nucleon-nucleon interaction is given in sect.2. In sect.3 a multi-parametric family of functions is introduced, which is used for an approximate description of the statistically averaged density. As illustrative examples, the potentials calculated for a number of nuclei of spherical shape and for the deformed nucleus ^{240}Pu are presented in sect.4.

2. DEFINITION OF THE STATISTICALLY AVERAGED SELF-CONSISTENT POTENTIAL

For a given proton (neutron) density $\rho_{p(n)}$ the single-particle potential is defined as a variational derivation of the nuclear potential energy $E_{pot}(\rho_p, \rho_n)$

$$U_\tau = \frac{\delta E_{pot}}{\delta \rho_\tau}, \quad \tau = p, n. \tag{1}$$

For the energy of nuclear interaction which, together with the Coulomb energy E_{Coul}, constitutes the total potential energy E_{pot} the usual[11,12] decomposition to two terms is used, i.e.,

$$E_{pot} = E_{NM} + E_{LR} + E_{Coul}. \tag{2}$$

These terms arise from the short-range (E_{NM}) and long-range (E_{LR}) components of nuclear forces.

In the local density approximation[11,12] E_{NM} has the form

$$E_{NM} = \int d\vec{r}\, w(\rho_p, \rho_n),$$

where $w(\rho_p, \rho_n)$ is assumed to be a result of the nuclear matter calculations[13-15].

The dependence of E_{LR} on the density is as follows

$$E_{LR} = \frac{1}{2} \int d\vec{r}_1 d\vec{r}_2 \sum_{\substack{\tau,\tau' \\ p,n}} v_{\tau\tau'}(|\vec{r}_1 - \vec{r}_2|, \rho) * \\ * \rho_\tau(\vec{r}_1)[\rho_{\tau'}(\vec{r}_2) - \rho_{\tau'}(\vec{r}_1)], \tag{3}$$

which is formulated so that E_{LR} equals zero in the case of the constant density. The effective nucleon-nucleon interaction used in eq.(3) is given by

$$v_{\tau\tau'} = v_{\tau'\tau} = \sum_{i=1}^{5} (a_i^{\tau\tau'} + b_i^{\tau\tau'} k_F^{\tau\tau'}) e^{-\left(\frac{\vec{r}_1 - \vec{r}_2}{\lambda_i}\right)^2}, \qquad (4)$$

$$v_{\tau\tau} = v_{\tau'\tau'}, \tau,\tau' = p,n; \quad k_F^{\tau\tau'} = \left(\frac{\rho_\tau + \rho_{\tau'}}{2}\right)^{1/3}.$$

For the details of the definition and the meanings of the coefficients incorporated in eq.(4) the reader is referred to ref.[16].

In addition to the potential (1), the spin-orbit potential V_τ^{so} was phenomenologically taken into account but the particular choise of V_τ^{so} does not effect substantially the self-consistency procedure. It is convenient to define V_τ^{so} in terms of the derivatives of the density[9]. Here V_τ^{so} was taken proportional to the linear combinations of the derivatives of the proton and neutron densities as proposed in ref.[17]

$$V_\tau = K\left(\frac{2}{3}\vec{\nabla}\rho_\tau + \frac{1}{2}\vec{\nabla}\rho_{\bar{\tau}}\right)\cdot[\vec{s}\,\vec{p}], \qquad (5)$$

$$\tau = n,p; \quad \bar{\tau} = p,n;$$

where K is a parameter to be adjusted by comparing the experimental and theoretical positions of the single-particle levels.

The solution to the Schrödinger equation with the single-particle potential $V_\tau + V_\tau^{so}$ was found by the method described in refs.[1,2]. The eigenvalues ϵ_i^τ and eigenfunctions $\phi_i^\tau(\vec{r})$ obtained were then used in the calculations of the statistically averaged nucleon density

$$\rho_\tau(\vec{r}) = \sum_i \tilde{n}_i(\epsilon_i^\tau)|\phi_\tau^\tau(\vec{r})|^2, \quad \tau = p,n, \qquad (6)$$

where $\tilde{n}_i(\epsilon_i^\tau)$ are the occupation numbers in the Strutinsky method[9].

The newly determined density (6), in general, differs from the initial one used in the definition of the potential (1). The potential is considered to be statistically self-consistent if both densities coincide. To find such a potential one may in principle use the same iterative procedure but the complexity of the calculation remains practically the same as in the Hartree-Fock procedure. Moreover, for the deformed nucleus one has to introduce some constraints. To simplify the calculation the density is sought in a rather special family of functions. The shape of the nucleus is considered to be fixed and the variations of only the radial dependence of the density is allowed in the self-consistency process. For the specification of the shape the usual formalism is used which is developed in the theory of nuclear fission for the definition of the shell model potential[1-3,18,19]. Only axial-symmetric shapes are considered.

The "radial" variable $\ell(\vec{r})$ in the deformed nucleus is defined as a minimal distance from the given point $\vec{r}$ to an arbitrary point on the nuclear surface. The distance ℓ is considered to be negative inside the nucleus and positive outside it. This distance is found numerically. In the simplest case of

the spherical nucleus $\ell = r_{sph} - R$, where r_{sph} is a radial variable in the spherical coordinate system and R is a nuclear radius. Generally speaking, the gradient of $\ell(\vec{r})$ may have a discontinuity on the symmetry axis, but the matrix elements of the spin-orbit potential (5), which is proportional to $\vec{\nabla}\ell$, are finite. In the case of the surface shape with large curvature the function $\ell(\vec{r})$ may have a discontinuity of the derivatives not only on the symmetry axis. But we will restrict ourselves to the smooth enough shapes, which are only interesting from a physical point of view and involve no difficulties of the kind. The coordinates specifying the position of a point on the surface $\ell(\vec{r})=\text{const}$ will be referred to as "angular" variables; the exact definition of these will not be required further.

Now we are in a position to formulate the main approximation. We will neglect the dependence of the statistically averaged density on the angular variables. Our aim will be to study its radial dependence. In this approximation $\rho_\tau(\vec{r})$ depends on $\vec{r}$ only through $\ell(\vec{r})$. It is noteworthy that a similar approximation has actually been introduced in the theory of nuclear fission in the definition of the shell model potential [1-2, 18, 19] or generating pseudodensity [3]. In the latter case the pseudodensity is constant if $\ell < 0$ and equals zero if $\ell > 0$.

The dependence of ρ_τ on ℓ is approximated by some of the functions $\rho_\tau^{av}(\ell)$ from the multi-parametric family of functions described in the next section. The parameters that specify $\rho_\tau^{av}(\ell)$ are found using the least-square-fit method, i.e., by the minimization

of the integral of the square of the deviation $\Delta\rho_\tau = \rho_\tau^{av}(\ell) - \rho_\tau(\vec{r})$. The integral is taken over the nuclear volume with a constant weight factor. Such an approximation may be interpreted as an averaging over the angular variables. Then $\rho_\tau^{av}(\ell)$ may be called the average value of density $\rho_\tau(\vec{r})$ at a given distance ℓ from the nuclear surface. By substituting the so obtained function $\rho_\tau^{av}(\ell)$ in the formulae (1) and (5) for the definition of the new potential we will close the iterational circle. For a first approximation a function from the same family is also to be taken. The repetition of the procedure till the coincidence of the initial and final density obtained using eq.(6) results in the potential to be referred to as a statistically self-consistent one and which is proposed to be used as a shell-model potential.

The problem of finding the self-consistent solution in our approximations is reduced to the problem of finding a fixed point in a space of finite dimensionality with parameters as coordinates. For the solution of the reduced problem one may use not only the conventional methods of nuclear physics.

The approximation used may be improved by introducing the dependence of the parameters that specify the function on the angular variables, but the approach becomes rather involved in such a case.

3. RADIAL DEPENDENCE OF THE STATISTICALLY AVERAGED NUCLEON DENSITY

An approximate expression for the density of both protons and neutrons will be sought in the form (the index specifying pro-

tons or neutrons is omitted)

$$\rho^{av}(r,z) =$$

$$= \rho_0 \frac{1+T[(\ell(r,z)-d)/(R+d)]\,/(1+e^{\ell(r,z)/a})}{1+e^{\ell(r,z)/a}}, \quad (7)$$

where ρ_0 is a scale factor, R is the radius of the sphere with a volume equal to that of the region inside the nucleus, a is the diffuseness parameter, $\ell(r,z)$ is the distance from the point with cylindrical coordinated r and z to the surface of the nucleus (see the preceeding section), T(x) is the polynomial function of x equal to zero at $x=0$. The coefficients of T(x) are the parameters defining the radial dependence. The factor of T(x) is introduced to reduce the correlation of the parameters with R and a (see discussion of this point in ref. [4]).

Parametrization (7) in the case of one parameter and without the factor of T(x), i.e. $T(x)=px^2$, is known as a "wine bottle shape". In the case of two parameters, i.e., if

$$T(x)=px^2+qx^2, \quad (8)$$

it was used in refs. [20,21] for the description of the density of a spherical nucleus, x being equal to r_{sph}.

To specify the radial dependence further one should take into account higher terms in the decomposition (8).

The reduction of correlation between the polynomial coefficients is achieved by the expansion of T(x) in terms of some orthogonal polynomials

$$T(x)=\sum_{n=1}^{M} p_n Q_n(x), \quad (9)$$

where

$$Q_n(x)=-\sqrt{1+2n}\,P_{n-1}^{(0,2)}(-2x-1), \quad (10)$$

and $P_n^{(\alpha,\beta)}(t)$ is the Jacobi polynomial [22]. The polynomials $Q_n(x)$ are orthonormal on the segment $-1\le x\le 0$ that corresponds to the nuclear interior $-R\le \ell\le d$. The number of terms in the sum (9) is chosen according to the desired accuracy of the approximations of density (6). But at very large M the strong correlation of the parameters makes the least-square method ineffective. The p_1 parameter appears to be too strongly correlated with the rest of the parameters and it was taken to be identically equal to zero. The d parameter permits expansion of the region of the orthogonality of the Q_n polynomials slightly beyond the nuclear surface $\ell = 0$.

4. EXAMPLES OF THE CALCULATED SHELL-MODEL POTENTIAL

The shell model potential for ^{208}Pb calculated with different choices of the short-range effective interaction (SEI) is shown in fig.1. For comparison, the usual Woods-Saxon potential [23] is also shown. It is seen that the variation of SEI results in a change of the global features of the potential. The diffuseness of the nuclear surface is especially sensitive to the variation considered. The oscillations of the density inside the nucleus have a close correspondence to each other for different SEI. The results suggest

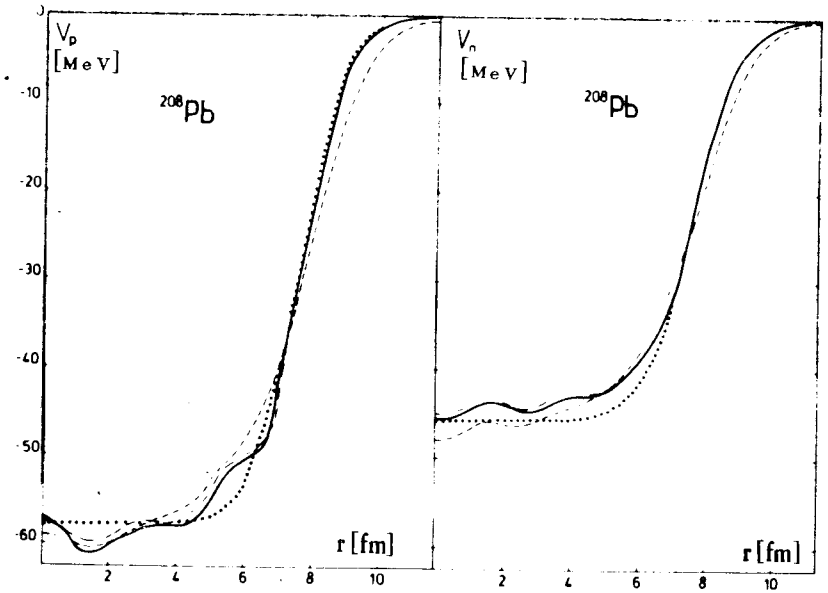

Fig.1. The statistically averaged self-consistent proton (to the left) and neutron (to the right) potentials in ^{208}Pb for different effective interactions. The solid and dash-dotted curves correspond to variants I and II of the short-range forces from ref./14/, respectively, the dashed curve is variant C from ref./15/. The long-range forces were taken from ref./16/. The dotted line represents the usual Woods-Saxon potential with parameters from ref./23/.

that after making a new fit of the SEI imposing the condition of the good reproduction of the known global features of the potential, one may study the special variations of the potential because they are not very sensitive to the details of SEI. The parameters of SEI are known to be so far chosen by fitting the results of the nuclear matter calculations to the experimental data.

The calculated spherically symmetric potentials for a number of nuclei over the whole Periodic Table are shown in fig.2. Variant II of SEI is taken from ref./14/. The long-range interaction recommended in ref./16/ was chosen (see eqs.(3,4)), which is different from that used in ref./14/. Moreover, in this paper the effective nucleon mass inside the nucleus was considered to be equal to that in vacuum. Due to this variation, the global features of the potential shown in fig.2 are slightly different from those described in ref./14/, the difference amounting to several per cent.

It is seen from fig.2 that the oscillations of the potential in all the nuclei considered are, in a good approximation, nearly the same function of the distance from the border of the nucleus. To see this easily the figure was drawn so that the borders of all nuclei coincide. To be more exact, for each potential an approximating Woods-Saxon potential was found according to the procedure described in section 2 for a particular case of $M = 0$. The radii of the approximating potentials are made to coincide in fig.2.

The differences in the functional dependence of the potential near the centre of the nuclei are not meaningful because in the

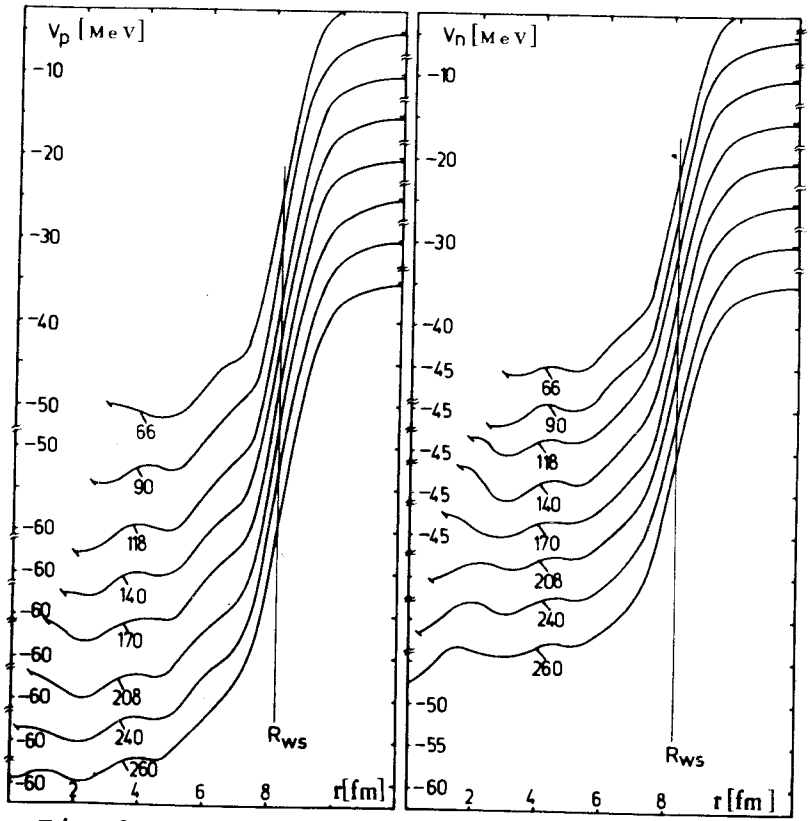

Fig.2. The statistically averaged self-consistent proton (to the left) and neutron (to the right) potentials in the nuclei ^{66}Zn, ^{90}Zr, ^{118}Sn, ^{140}Ce, ^{170}Yb, ^{208}Pb, and ^{240}Pu that are close to the valley of beta-stability. The values of mass number are shown near the curves. Variant II of the effective short-range forces from ref.[14] was used. Each curve is shifted with respect to its neighbour vertically by 5 MeV and horizontally till the coincidence of the half-minimum radius of the equivalent Woods-Saxon potential (the definition is given in the text) with the vertical straight line denoted as R_{WS}.

case of spherical symmetry the difference $\Delta\rho_r$ in this region contributes to the integral with a small weight and, as a result, the approximation to the density (6) is the poorest one in this region. In addition, the property of the exact density that its derivative over r vanishes on the symmetry axis is not built into the approximation (7).

To calculate the potentials shown in figs. 1 and 2 an approximation (7) was used with 14 parameters (R and a included, and d taken to be equal to zero). The self-consistent parameters vary smoothly over the whole Periodic Table. To accelerate the convergence of the self-consistency process the interpolated values of the self-consistent parameters were used as initial values in the neighboring nucleus.

Let us make it clear that the method of determination of the radial dependence described above is applicable to any nuclear shape. In particular, nuclei for which the spherical shape does not correspond to stable equilibrium are shown in fig.2. In contrast to the Hartree-Fock method, in our case there is no difficulty in calculating the potential for the nucleus with an unclosed subshell. In this connection it is interesting to compare our method with the rather artificial method of averaging over subshells used in ref. [24] for supplementing of the definition of the self-consistency procedure.

A variation of the potential with deformation was studied in the nucleus ^{240}Pu. The shape of the nucleus was taken to be a Cassinian oval with a distance between the foci specified by the parameter ϵ (see ref.[19] for details). The nucleon-nucleon interaction

was chosen as in spherical nuclei discussed in connection with fig.2. The parameter d was equal to 2.0 fm.

From the results shown in fig.3 it follows that the conclusion drawn earlier for the spherical nuclei that the potential in good approximation may be considered to be a universal function of only the distance from the surface is also valid for the deformed nucleus. It is seen from fig.3 that this function varies very weakly with deformation. It should be noted, however that the accuracy of the approximation, which can be measured as a mean squared deviation $\Delta\rho_r$ (see sect.2) is slowly deteriorating with deformation, especially for protons.

As a hypothesis, let us say that such a deviation of the proton density $\rho_p(\vec{r})$ from the averaged value $\rho_p^{av}(\ell)$ (see sects.2 and 3) is connected with the distortion of the nuclear field by the Coulomb potential inasmuch as the latter has less deformed equipotential surfaces that the former.

One may get some improvement of the approximation by introducing different surface shapes for the protons and neutrons ; however this point has not been studied quantitatively. The noticeable diminution of the oscillation of the potentials as functions of z , if $0 \leq z \leq 4$ fm, r is small and ϵ is close to 0.5 (see fig.3), is a consequence of the fact that in this domain the distance between a point and the nuclear surface is almost independent of the position of the point.

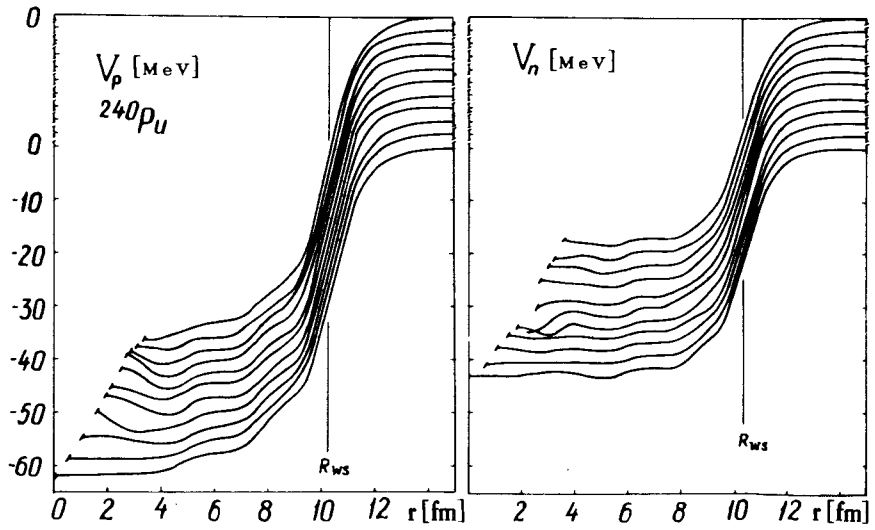

Fig.3. The statistically self-consistent proton (to the left) and neutron (to the right) potentials in ^{240}Pu . The cuts of the potential along the z-axis at very small r ($r \approx 0.5$ fm, the lower five curves) and along the r -axis at very small z ($z \approx 0.5$ fm, the upper five curves) are shown. Each curve corresponds to different deformation which changes within each transition from the lower curve to the upper one at first from $\epsilon = 0.5$ through 0.0 with a 0.1 step and then from 0.1 through 0.5 with the same step. Each curve is shifted with respect to its neighbour vertically by 2.5 MeV and horizontally till the coincidence of the nuclear border (denoted by vertical straight line and symbol R_{WS} in the figure). The deviation of the neutron spherical potential (the central curve to the right) from the universal functional form is connected with the inaccuracy in the approximation to the density near the nuclear centre, which is discussed in sect.4.

5. CONCLUSION

A method for definition of the radial dependence of a nuclear force potential has been described, which permits the fixing of the surface shape and a study of only the radial variations of the potential. A definition is given for the radial dependence in a deformed nucleus (see sect.2).

The potential is consistent with statistically averaged nucleon density which is further averaged over the angular variables with the least-square-fit method (see sects. 2 and 3). The so defined radial dependence of the potential is shown to be almost the same (except for the small region around the nuclear centre) for a number of spherical nuclei and only weakly changes with deformation (see sect.4). The potential is expected to be useful for calculations by the Strutinsky method of nuclear masses, surface shapes and fission barriers.

However, the effective nucleon-nucleon interactions used in the present paper should be slightly re-adjusted to reproduce accurately the global features of the potential.

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