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Deformation inside and outside the nuclear molecules

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We investigate the interrelation of the clusterization and quadrupole deformation of atomic nuclei, as well as the role of the deformation of the clusters. In our study we incorporate both the energetic preference, and the effect of the Pauli-exclusion principle. The ^{40}Ca nucleus is considered as an illustrative example. The applied methods can be generalised to heavy nuclei, and to ternary clusterization, too.

Keywords: Cluster models; group theory.

Se investiga la relación entre la formación de cúmulos y la deformación cuadrupolar de núcleos atómicos, así como la importancia de la deformación de los cúmulos mismos. En el presente trabajo se incorporan tanto a la preferencia energética como al principio de Pauli. Se considera al núcleo ^{40}Ca como un ejemplo ilustrativo. Los métodos usados pueden extenderse a núcleos pesados y a sistemas de tres cúmulos.

Descriptores: Modelos de cúmulos; teoría de grupos.

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1. Introduction

Clusterization is an important phenomenon both in light and in heavy nuclei. The two basic natural laws governing the clusterization (just like the composition of nuclei from nucleons) are the minimum-energy principle, and the Pauli-exclusion principle. In a fully microscopic description of clusterization both aspects are taken into account. This kind of description, however, is limited to the domain of light nuclei.

Many interesting aspects of the clusterization, like e.g. the appearance of exotic cluster-configurations, show up only in heavy nuclei. Phenomenologic approaches are applied both to light and to heavy nuclei, on an equal footing, but these models do not really contain the effects of the antisymmetrization, or it is not under control, what aspects of the exclusion principle are incorporated.

In this paper we present an approach, which involves both the energetic preference and the exclusion principle. We present the method for two-cluster systems, but it is easy to generalise to ternary clusterization, or even to multi-cluster configurations. The antisymmetrization is not carried out explicitely, it is treated in an approximate way, but it is done microscopically in a well-controlled manner, and consistency-check measures, how effective it is.

We calculate the energetic preference of different clusterizations both on the basis of simple binding-energy-

arguments [1], and from the Dinuclear System Model (DNS) [2], including Coulomb as well as nuclear interactions. The potential energy is calculated both for the usual pole-to-pole configuration, and for those more compact configurations, which turn out to be allowed from the microscopic viewpoint.

The exclusion principle is treated by the application of a selection rule, related to the microscopic structure. For light nuclei it is based on the real $U(3)$ symmetry [3], and it is exact to the extent to which the leading term representation is valid. In heavy nuclei it is based on the quasidynamical, or effective $U(3)$ symmetry [4]. Its validity is shown by the consistency of the quadrupole deformation of the cluster state and the state of the parent nucleus.

In these considerations the deformation of the clusters are taken into account, too. Therefore, we investigate the interrelation of the quadrupole deformation and the clusterization from two aspects. On the one side, looking at the possible clusterizations of states with different quadrupole deformation of the parent nucleus, we tend to determine the deformation-dependence of various cluster-configurations. On the other side, we can investigate the role of the cluster-deformation inside the cluster (or molecular) nuclear states; *i.e.* figure out, how the relative orientation of deformed clusters can build up different states of the same nucleus.

In this contribution we apply the above methods to the ^{40}Ca nucleus, which is investigated also in the framework of the Antisymmetrised Molecular Dynamics (AMD) [5], thus we can compare our results with those of a fully microscopic treatment. This is interesting for the special case of the ^{40}Ca nucleus, too, at the same time, however, it can be considered as a test of our method, which we apply also to heavy nuclei [6–8].

^{40}Ca seems to be an ideal tool for this kind of investigation, not only because it is around the upper end of the domain of applicability of the fully microscopic cluster models, but also due to the fact that its superdeformed band has experimentally been observed [9], and theoretically studied by different methods [5, 10].

The structure of this paper is as follows. In Sec. 2 the methods of calculation are presented, in Sec. 3 we present our results for the ground and superdeformed bands of ^{40}Ca, as well as for its hypothetical hyperdeformed states, finally in Sec. 4 some conclusions are drawn.

2. Method of calculation

2.1. Exclusion principle

The structural selection rule we apply, is based on the $U(3)$ symmetry, what is known to be a good approximate symmetry of light nuclei [3], and its role in the clusterization was also observed in the early studies [11], followed by the understanding of its importance from different aspects of clusterization [12]. The simple $U(3)$ selection rule reads:

$$[n_1 n_2 n_3] = [n_1^{(1)} n_2^{(1)} n_3^{(1)}] \otimes [n_1^{(2)} n_2^{(2)} n_3^{(2)}] \otimes [n^{(R)} 00] \quad (1)$$

where $[n_1 n_2 n_3]$ is the set of (approximate) $U(3)$ quantum numbers of the parent nucleus, the superscript (i) stands for the ith cluster, and (R) indicates relative motion.

Please note that the shape of the nuclei (or clusters) is determined by the $U(3)$ irreducible representation $[n_1, n_2, n_3]$, which includes spherical, prolate, oblate, as well as triaxial shapes. When generalising this selection rule to ternary cluster-configurations, one has a product of five terms on the right-side, three characterising the clusters, and two standing for two independent relative motions.

In medium and heavy nuclei, the $U(3)$ symmetry is not valid in its original form, due to the importance of the symmetry-breaking interactions, like spin-orbit and pairing. Nevertheless, it was found [4] that in spite of the strong symmetry-breaking interactions a generalised $U(3)$ symmetry, called effective, or quasi-dynamical $U(3)$ symmetry, may survive even for heavy nuclei. Then the energy-eigenstates are:

$$\psi_{\alpha KJM} = \Sigma_{\xi\lambda\mu} C_{\alpha\xi\lambda\mu K} \phi_{\xi\lambda\mu KJM}, \quad (2)$$

where $\phi_{\xi\lambda\mu KJM}$ is a basis vector for an $SU(3)$ irrep, and ξ stands for all the quantum numbers not belonging to the $SU(3)$ group [13]. Please, note that the $C_{\alpha\xi\lambda\mu K}$ coefficients of the linear combination are independent of JM, i.e. within a band the contribution of different $SU(3)$ basis states are the same. In particular the matrix elements of the $SU(3)$ generators between these states may approximate the matrix elements of an exact representation. In such a case we speak about an approximate embedded representation, and related to it, about an approximate quasidynamical or effective $SU(3)$ symmetry.

The effective $U(3)$ symmetry provides us with effective (or average) $U(3)$ quantum numbers, and based on that a selection rule can be formulated. Due to the average nature of these quantum numbers, however, the effect of the selection rule is different from that of the real $U(3)$ selection rule. It gives information on the matching, or mismatching of the average nucleon distributions in the cluster-configuration and in the shell-model-state. Therefore, it acts like a self-consistency check of the quadrupole deformation and the clusterization.

In Ref. 13 a method is developed for the determination of the effective $U(3)$ quantum numbers of the heavy nuclei, based on the occupation of the asymptotic Nilsson orbits. The procedure, which was originally invented for the large prolate deformation was extended in [14] for the oblate shape and small deformations as well, based on the expansion of single-particle orbitals in terms of asymptotic Nilsson-states.

The concept of effective symmetry is applicable also to light nuclei, and when the simple leading representation approximation is valid, the real and effective $U(3)$ quantum numbers usually coincide [14].

When a cluster configuration is forbidden, we can characterise its forbiddenness quantitatively in the following way [15]. The distance between a $U(3)$ reaction channel and the irrep of the parent nucleus is defined as: $min(\sqrt{(\Delta n_1)^2+(\Delta n_2)^2+(\Delta n_3)^2})$, where $\Delta n_i = |n_i - n^c_{i,k}|$. Here n_i refers to the $U(3)$ representation of the parent nucleus, while $n^c_{i,k}$ stands for the $U(3)$ representation of channel c , obtained from the right-hand-side of Eq.(1), with the k index distinguishing the different product-representations. Based on this quantity we determine, for reasons of convenience, the reciprocal forbiddenness S in such a way, that $0 \leq S \leq 1$:

$$S = \frac{1}{1 + min(\sqrt{(\Delta n_1)^2+(\Delta n_2)^2+(\Delta n_3)^2})}. \quad (3)$$

Then $S = 0$, and $S = 1$ correspond to completely forbidden and allowed clusterizations, respectively.

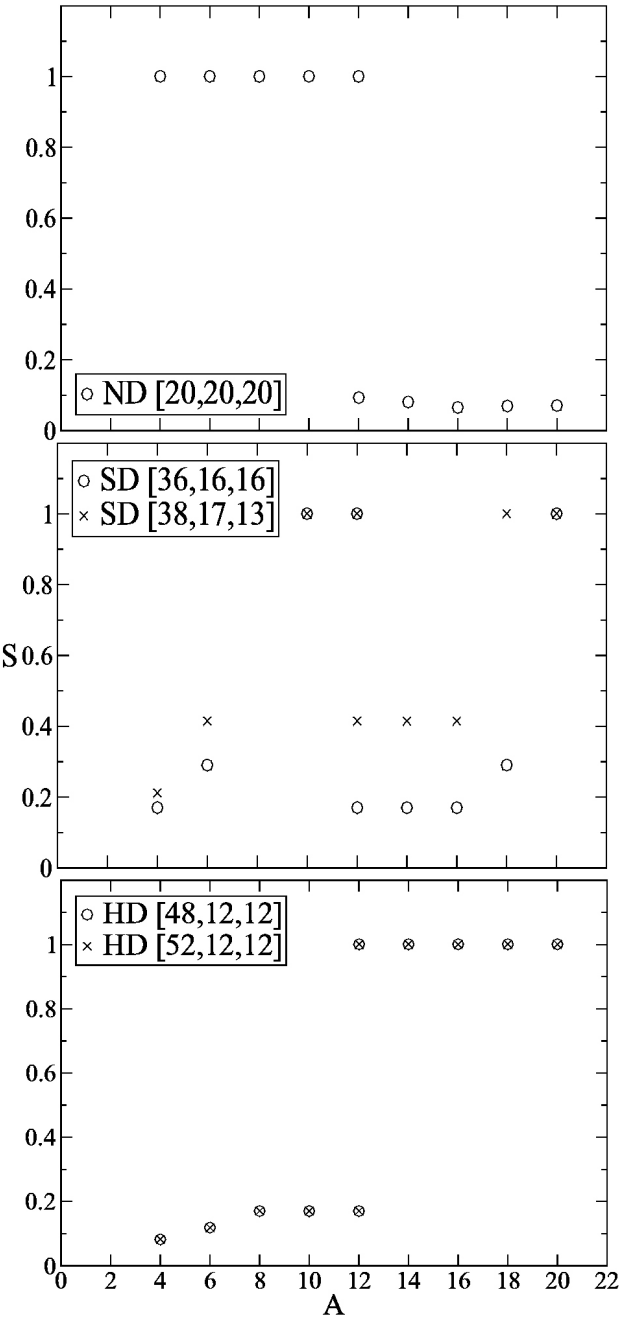

FIGURE 1. Reciprocal forbiddenness for the ^{40}Ca clusterizations. ND stands for the normal deformed (ground) state, while SD and HD indicate super and hyperdeformed states, respectively.

2.2. Energy preference

The criterium of maximal stability [1], requires the largest value of the summed differences of the measured binding energies and the corresponding liquid drop values:

$$D(1,2) = [B(1) - B_L(1)] + [B(2) - B_L(2)], \quad (4)$$

where $B(i)$ is the experimental binding energy of the ith cluster [16], while $B_L(i)$ stands for liquid drop value.

In the generalised version of the method, as we apply it here, a further condition is also taken into account, which is called dipole constraint [1]. It is based on the observation that electric dipole transitions are very weak, therefore, the decomposition $A_T \rightarrow A_1 + A_2$ is expected to be close to satisfying the constraint:

$$\frac{Z_1}{A_1} \approx \frac{Z_T}{A_T} \approx \frac{Z_2}{A_2}. \quad (5)$$

A more detailed calculation of the energetic preference can be carried out within the Dinuclear System Model. According to this description the clusterization process involves the motions in charge $\eta_Z = (Z_1 - Z_2)/(Z_1 + Z_2)$ $(Z = Z_1 + Z_2)$ and mass $\eta = (A_1 - A_2)/(A_1 + A_2)$ $(A = A_1 + A_2)$ asymmetry coordinates, where Z_1 (A_1) and Z_2 (A_2) are the charge (mass) numbers of the heavy and light nuclei of the dinuclear system (DNS) [2, 17] formed by two touching nuclei or clusters, and in the relative separation coordinate R between the centers of mass. The charge (mass) asymmetry η_Z (η) is the relevant collective variable describing the partition of nucleons between the nuclei forming the DNS. The wave function in η_Z can be thought as a superposition of the mononucleus configuration with $|\eta_Z|$=1 and different cluster-type configurations. The relative contribution of each cluster component to the total wave function is ruled by the potential $U(\eta_Z, I)$ which is the DNS potential energy for $|\eta_Z| < 1$ [18–21]

$$U(\eta_Z, I) = V(R = R_m, \eta_Z, I) + B_1(\eta_Z) + B_2(\eta_Z) - B. \quad (6)$$

Here R_m is the (touching) distance of the two clusters, which depends on their deformation and relative orientation.

Since the mode responsible for the N/Z-equilibrium in the DNS is the fast one (η_Z is slow in comparison with the ratio η_Z/η), the potential energy U is minimized with respect to the mass asymmetry η for each fixed charge asymmetry η_Z. The quantities B_1 and B_2, which are negative, are the binding energies of the clusters forming the DNS at a given η, and B is the binding energy of the parent nucleus. The experimental ground state masses and quadrupole deformation parameters [16, 22] are used in the present calculations. Due to the normalization by B in Eq. (6), $U(|\eta_Z| = 1, I = 0) = 0$.

TABLE I. Orientation of clusters in ^{40}Ca. The abbreviations for the shape are: s: spherical, p: prolate, o: oblate, t: triaxial; while the meaning of the symbols for the orientation are: a: symmetry axis; *: ^{32}S middle axis: x, larger axis in yz plane (closer to y); **: ^{28}Si symmetry axis close to z; ***: ^{20}Ne (C_1) symmetry axis in xy plane at 45^o; +: ^{28}Si symmetry axis in zy plane (closer to z); ++: ^{24}Mg middle axis: x, other two in zy plane, larger axis closer to z; +++: ^{20}Ne (C_1) symmetry axis in xy plane at 45°.

^{40}Ca state	C_1	Shape	Ratio	Position	C_2	Shape	Ratio	Position
ground	^{36}Ar	o	1.27 : 1	$a:z$	^{4}He	s	1	–
[20, 20, 20]	^{32}S	t	1.5 : 1.33 : 1	$y>x>z$	^{8}Be	p	2 : 1	$a:x$
$\beta_2=0$	^{28}Si	o	1.66 : 1	$a:z$	^{12}C	o	1.66 : 1	$a:z$
superdeformed	^{32}S	t	1.5 : 1.33 : 1	$*$	^{8}Be	p	2 : 1	$a:z$
[36, 16, 16]	^{28}Si	o	1.66 : 1	$**$	^{12}C	o	1.66 : 1	$a:y$ (or x)
$\beta_2=0.50$	^{20}Ne	p	1.57 : 1	$***$	^{20}Ne	p	1.57 : 1	$a:y$ (or x)
hyperdeformed	^{28}Si	p	1.55 : 1	$+$	^{6}C	o	1.66 : 1	$a:y$ (or x)
[48, 12, 12]	^{24}Mg	t	1.75 : 1.25 : 1	$++$	^{16}O	s	1	–
$\beta_2=0.86$	^{20}Ne	p	1.57 : 1	$+++$	^{20}Ne	p	1.57 : 1	$a:z$

TABLE II. Energetic preferences of different cluster configurations in ^{40}Ca. $D(1,2)$ stands for the binding-energy difference of Eq.(4), thus the larger value corresponds to more probable appearance. U means potential energy, calculated from the dinuclear system model, therefore, smaller values correspond to more stable cluster-configurations. pp indicates the pole-to-pole configuration, typical in DNS calculations, while m stands for the orientation corresponding to the microscopic consideration. All values are in MeV. (n), (s), and (h) refer to normal, superdeformed, and hyperdeformed states.

C_1+C_2			D(1,2)	U(pp)	U(m)
^{4}He	+	^{36}Ar	9.64	-3.3	-3.4
^{8}Be	+	^{32}S	5.58	3.8	3.8
^{12}C	+	^{28}Si	6.61	2.8	1.3 (n,s)
					2.8 (h)
^{16}O	+	^{24}Mg	3.83	8.6	8.6
^{20}Ne	+	^{20}Ne	-0.79	12.9	11.9 (s)
					14.3 (h)

The nucleus-nucleus potential [21]

$$V(R,\eta_Z,I)=V_C(R,\eta_Z)+V_N(R,\eta_Z)+V_{rot}(R,\eta_Z,I) \quad (7)$$

consists of the Coulomb V_C, centrifugal $V_{rot}=\hbar^2 I(I+1)/(2\Im(\eta_Z))$ and nuclear interaction V_N potentials. $\Im(\eta_Z)=0.85(j_1+j_2+\mu R^2)$ is the moment of inertia of the DNS, where μ is the reduced mass, $j_{1,2}$ are the rigid body moments of inertia of the clusters with respect to the axes parallel to the rotational axis and passing trough the centers of mass of the clusters. The factor 0.85 was suggested in Ref. 23 and used in Refs. 18 to 20. The nuclear part $V_N(R)$ of nucleus-nucleus potential is taken in the double-folding form:

$$V_N(R,\eta_Z)=\int \rho_1(\mathbf{r_1})\rho_2(\mathbf{R}-\mathbf{r_2})F(\mathbf{r_1}-\mathbf{r_2})d\mathbf{r_1}d\mathbf{r_2}.$$

The well-known two-parameter Woods-Saxon function for nuclear densities

$$\rho_i(\mathbf{r})=\frac{\rho_{00}}{1+\exp(|\mathbf{r}-\mathbf{R_i}|/a_{0_i})},$$

is used, where $\mathbf{R_i}$ is the radius vector of the nuclear surface of the cluster i in the direction of $\mathbf{r}$. Here, ρ_{00}=0.17 fm^{-3} is a saturation nucleon density of nucleus, r_{0_i}=1.16 fm apart from alpha particle, where r_0=1.0 fm, are nuclear radius parameters, and a_{0_i} denotes the diffuseness depending on the mass number of the nucleus. We use in our calculation a_0 =0.48, 0.51, 0.53, and 0.55 fm for alpha particle, Be, C, and nuclei with $Z>6$, respectively. The simplified Skyrme-type nucleon-nucleon forces

$$F(\mathbf{r_1}-\mathbf{r_2})=C_0\left(F_{in}\frac{\rho_0(\mathbf{r_1})}{\rho_{00}}+F_{ex}\left(1-\frac{\rho_0(\mathbf{r_1})}{\rho_{00}}\right)\right)\times\delta(\mathbf{r_1}-\mathbf{r_2}),$$

$$F_{in,ex}=\zeta_{in,ex}+\zeta'_{in,ex}\frac{A_1-2Z_1}{A_1}\frac{A_2-2Z_2}{A_2},$$

depend on the density of nuclei because $\rho_0(\mathbf{r_1})=\rho_1(\mathbf{r_1})+\rho_2(\mathbf{R}-\mathbf{r_2})$. We used the following constants $\zeta_{in}=0.09$, $\zeta_{ex}=-2.59$, $\zeta'_{in}=0.42$, $\zeta'_{ex}=0.54$, $C_0=300$ MeV·fm^3 from Ref. [24] where they were tested for nuclear structure purposes. The Coulomb potential for two deformed nuclei U_C is calculated with the following analytical formula [25]:

$$V_C(R,\eta_Z)=\frac{e^2Z_1Z_2}{R}+\sqrt{\frac{9}{20\pi}}\frac{e^2Z_1Z_2}{R^3}\sum_{i=1,2}R_{0i}^2\beta_i P_2(\cos\theta_i),$$

where $P_2(\cos\theta_i)$ is Legendre polynomial and θ_i is the angle between the symmetry axis and the axis z connecting the centers of clusters. In the first order in β_i this expression is valid for any mutual orientation of the nuclei.

The DNS potential energy as a function of η_Z (η) has minima corresponding to some clusterizations of the system.

3. Application to ^{40}Ca

The superdeformed band of the ^{40}Ca nucleus has recently been observed experimentally [9] with spins $0^+ \dots 16^+$. First a $\beta_2 = 0.59$ value was determined for its quadrupole deformation, then it was confirmed in more detailed experimental studies for the high spin states, while for low-J values $\beta_2 = 0.40$ was found. The same band has been detected in an independent measurement up to $J^\pi = 12^+$ [26].

Early (shell model, and Hartree-Fock) calculations prior to the experimental observation predicted these states to have 8-particle 8-hole character [10], and more recent cranked relativistic mean field studies confirmed this conclusion [9]. The ab initio type AMD calculations also resulted in a band with 8p-8h nature corresponding to $\beta_2 = 0.40$ [5].

In the present considerations first we have determined the reciprocal forbiddenness for different binary cluster-configurations in the ground, superdeformed, and hyperdeformed state of ^{40}Ca, and then calculated their energetic preference, both from the simple binding-energy method, and from the dinuclear system model.

As for the superdeformed state, we have started from the joint conclusion of the experimental and previous theoretical investigations, and accepted its 8p-8h nature. The corresponding real $U(3)$ symmetry is $[36, 16, 16]$ (which indicates $\beta_2 = 0.50$). The effective $U(3)$ quantum numbers, belonging to the $\beta_2 = 0.59$ deformation (and having also an 8p-8h configuration) are $[38, 17, 13]$. For the symmetry of the hyperdeformed state we have two candidates from simple shell model considerations, which correspond to 12p-12h $[48, 12, 12]$, or 16p-16h excitations $[52, 12, 12]$, and to quadrupole deformations of $\beta_2 = 0.86, 0.93$, respectively.

The result is shown in Fig. 1. In the ground state the asymmetric cluster-configurations are preferred, in the hyperdeformed state the symmetric ones, while the superdeformed state has a situation in between. This finding is completely in line with the case of the ^{36}Ar nucleus [6]. Except for the $A = 18$ the allowed or forbidden nature of a cluster in the superdeformed state does not depend on the fact if we apply real or effective $U(3)$ symmetry. In the hyperdeformed state the two candidates result in the same cluster-picture. It is remarkable that the ^{12}C cluster is allowed both in the ground and in the super- and hyperdeformed states, though the complementer ^{28}Si nucleus is oblate in the two less-deformed states, and it is prolate in the hyperdeformed one. (This nucleus sits right in the middle of the sd-shell, and it is known to have a shape-coexistence.)

The geometrical configurations are shown in Table I for the alpha-like allowed clusterizations. We showed one of the possible geometrical configurations (usually it is the simplest one), but they are not necessarily the only possible ones, since the antisymmetrization may wash out the difference between different arrangements.

The energetic preferences for the alpha-like configurations (which are the more prefered ones) are given in Table II. It is interesting that the simple binding energy arguments, and the more detailed potential energy-calculations within the DNS framework give the same preferences for the different clusterizations, and it does not depend (qualitatively) on the fact either, if the nuclear molecule is in the pole-to-pole configuration, or in the one, preferred by the microscopic arrangement, shown in Table I. This situation is also similar to that of the ^{36}Ar nucleus [27]. A further remarkable observation is that the microscopically prefered orientations result in equal or less values of the potential energy than the pole-to-pole ones.

4. Summary and conclusions

In this paper we have considered the binary clusterizations of the ground, superdeformed and hyperdeformed states of ^{40}Ca. The clusters were considered to have deformation, like the free nuclei, and we applied no constraint for their relative orientation. We incorporated in our studies both the exclusion principle, and the energetic prefererence. The previous one was taken into account via a selection rule, based on the microscopic structure, the latter one was calculated phenomenologically.

We have found that the ground state prefers asymmetric cluster-configurations, the hyperdeformed state symmetric ones, while the superdeformed state shows a more complicated picture. It is interesting, that the ^{12}C+^{28}Si clusterization is allowed in each state. Nevertheless, they correspond to different geometrical configurations, since the relative orientation of the deformed clusters are different.

From the energetic viewpoint this clusterization is halfway between the energetically most preferred and least preferred alpha-like configurations. The energetic preference turned out to be similar from the simple binding-energy consideration and from the detailed potential-energy calculations.

Our finding is very much in line with that of the fully microscopic AMD calculations [5], which concluded that the superdeformed state has an ^{12}C+^{28}Si character. Furthermore, the coupling of the clusters is strong in both descriptions. This similarity can be considered as a check of our method with respect to the fully microscopic description, which seems to be very promising from the viewpoint of the more extensive applications to heavy nuclei.

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