PROCEEDINGS

of the Union of Scientists - Ruse

Book 5

Mathematics, Informatics and Physics

Volume 13, 2016

RUSE

PROCEEDINGS
OF THE UNION OF SCIENTISTS - RUSE

Union of Scientists - Ruse
16, Konstantin Irechek Street
7000 Ruse
BULGARIA
Phone: (++359 82) 828 135,
(++359 82) 841 634
E-mail: suruse@uni-ruse.bg
web: suruse.uni-ruse.bg

Contacts with Editor
Phone: (++359 82) 888 738
E-mail: zzdravkova@uni-ruse.bg

PROCEEDINGS
of the Union of Scientists – Ruse

ISSN 1314-3077

The Ruse Branch of the Union of Scientists in Bulgaria was founded in 1956. Its first Chairman was Prof. Stoyan Petrov. He was followed by Prof. Trifon Georgiev, Prof. Kolyo Vasilev, Prof. Georgi Popov, Prof. Mityo Kanev, Assoc. Prof. Boris Borisov, Prof. Emil Marinov, Prof. Hristo Beloev. The individual members number nearly 300 recognized scientists from Ruse, organized in 13 scientific sections. There are several collective members too – organizations and companies from Ruse, known for their success in the field of science and higher education, or their applied research activities. The activities of the Union of Scientists – Ruse are numerous: scientific, educational and other humanitarian events directly related to hot issues in the development of Ruse region, including its infrastructure, environment, history and future development; commitment to the development of the scientific organizations in Ruse, the professional development and growth of the scientists and the protection of their individual rights.

The Union of Scientists – Ruse (US – Ruse) organizes publishing of scientific and popular informative literature, and since 1998 – the “Proceedings of the Union of Scientists- Ruse".

BOOK 5

"MATHEMATICS, INFORMATICS AND PHYSICS"

VOLUME 13

CONTENTS

BOOK 5

"MATHEMATICS, INFORMATICS AND PHYSICS"

VOLUME 13

web: suruse.uni-ruse.bg

NATURAL ORBITAL APPROACH AND LOCAL SCALE TRANSFORMATION METHOD FOR DESCRIPTION OF SOME GROUND AND MONOPOLE EXCITED STATE CHARACTERISTICS OF NUCLEI

Galina Krumova

Angel Kanchev University of Ruse

Abstract: *The extended Local-scale transformation method (LSTM) in combination with the Natural orbital representation is applied to investigate the nuclear ground state local density and momentum distributions. The 'breathing' monopole excitation mode is considered within this approach and the adiabatic limit of the Time-dependent Hartree-Fock theory (ATDHF).Numeric calculations for the nucleus* ^{16}***O*** *with the effective Skyrme forces have been carried out. The occupation numbers are determined, taking into account the experimental charge density distribution data.*

Keywords: *Natural orbitals, Local-scale transformation method, Fermi sea depletion.*

The Local-scale transformation method (**LSTM**) [10], [6] was extended by inclusion of ***N***scalarfunctions [4] and successfully applied to the nuclear 'breathing' monopole excitation mode within the adiabatic limit of the Time-dependent Hartree-Fock theory (**ATDHF**). The purpose of the present paper is to show the possibility of the above-mentioned approach in combination with the recently used Natural orbital representation method [5] to improve previously obtained results with respect to the monopole excitation energy, ground state local density and momentum distributions. Such an approach has the advantage of taking into account the nuclear charge density distribution experimental data.

Within the **LSTM** a given model many-particle wave function

$$\overline{\Phi}\left(\vec{r_1},\vec{r_2},\dots,\vec{r_A}\right)$$

is transformed to a new trial wave function, depending in a certain way on ***A*** scalar functions

$$f_i,(i=1,2,\dots,A)$$

$$\Phi_{\{f\}_A}\equiv\Phi\left(\vec{r_1},\vec{r_2},\dots\vec{r_A};[f_1,f_2,\dots,f_A]\right)=\left[\prod_{i=1}^{A}D_i(\vec{r_i})\right]^{\frac{1}{2}}\overline{\Phi}\left(\vec{\mathfrak{f}}_1(\vec{r_1}),\vec{\mathfrak{f}}_2(\vec{r_2}),\dots,\vec{\mathfrak{f}}_A(\vec{r_A})\right),$$

where

$$\vec{\mathfrak{f}}_i(\vec{r})=\vec{r_0}\,f_i(\vec{r}),\qquad \vec{r_0}=\frac{\vec{r}}{r}.$$

In particular, $\Phi_{\{f\}_N}$ denotes the wave function, in which $N\ (N\le A)$ scalar **LST** functions $f_\alpha,(\alpha=1,2,\dots,N)$ are included in a certain way. Obviously,

$$\Phi_{\{f\}_A}=\Phi_{\{f\}_{N=A}}.$$

The expectation value of the Hamiltonian with respect to the many-particle function $\Phi_{\{f\}_N}$ becomes an energy functional of the unknown **LST** functions f_α. They are determined through the Euler-Lagrange equations system

$$\frac{\delta E_N[\{f\}]}{\delta f_\alpha(\vec{r})} = 0, \quad f_\alpha(\vec{r}) \in F, \qquad (\alpha = 1, 2, \dots, N)$$

with

$$E_N[\{f\}] = \langle \Phi_{\{f\}_N} | \widehat{H} | \Phi_{\{f\}_N} \rangle.$$

We consider one-determinant model wave function, built on harmonic oscillator single-particle wave functions, suitable for investigation of light nuclei. The number of scalar **LST** functions corresponds, for instance, to the number of shells in the Hartree-Fock method.

Using the effective Skyrme forces [8] in the Hamiltonian, the energy functional takes the form

$$E[\{f\}] = \int \mathcal{H}(\vec{r}) d\vec{r},$$

where $\mathcal{H}(\vec{r})$ is the energy density functional [9]. It has quite simple form in the case of even-even spherical nuclei with ***N=Z***[11]:

$$\mathcal{H}(\vec{r}) = \frac{\hbar^2}{2m}(A-1)A^{-1}\tau + \frac{3}{8}t_0\rho^2 + \frac{1}{16}t_3\rho^{\sigma+2} + \frac{1}{16}(3t_1+5t_2)\rho\tau + \frac{1}{64}(9t_1-5t_2)(\nabla\rho)^2,$$

where $t_0, t_1, t_2, t_3, \quad \sigma$ are the Skyrme force parameters; ρ and τ – the local and kinetic energy densities, expressed by means of the model basis and the **LST** functions $f_\alpha, \quad (\alpha = 1, 2, \dots, N)$. The Coulomb interaction has been neglected.

Assuming a pure scale transformation

$$f_i(\vec{r}) = \alpha_i r, \qquad (i = 1, 2, \dots, N),$$

one has to minimize the energy density functional within the class of **LST** functions, instead of solving the variational equations. (In this way, the optimal values of the parameters α_i^0 are obtained).

In the framework of the adiabatic **TDHF** limit the classical Hamiltonian is presented in terms of the collective time-dependent variables $\alpha_i(t)$ [2]:

$$H = \frac{m}{2}\sum_{i,j} m_{ij}\,\dot{\alpha}_i\dot{\alpha}_j + E(\alpha_1, \alpha_2, \dots, \alpha_N), \qquad (i,j = 1, 2, \dots, N).$$

m_{ij} are the matrix elements of the mass-tensor, the second term on the right-hand side is the collective potential energy. Within the harmonic approximation m_{ij} are calculated at the equilibrium point $(\alpha_1^0, \alpha_2^0, \dots, \alpha_N^0)$. The potential energy is expanded in series of $\alpha_i - \alpha_i^0$ up to second order terms. After the corresponding procedure of diagonalization and quantization [3], [12] of the collective Hamiltonian, the normal coordinates and the normal modes excitation energies are obtained. This approach affords an opportunity for studying the 'breathing' monopole mode. **LSTM** enables a natural introduction of collective variables, namely, the oscillator frequencies within the present approach.

As is well-known, the natural orbitals have been defined as the orthonormal basis $\varphi_\alpha(\vec{r})$ which diagonalizes the one-body density matrix [5]

$$\rho(\vec{r},\vec{r}') = \sum_\alpha n_\alpha \varphi^*_\alpha(\vec{r})\ \varphi_\alpha(\vec{r}'),$$

where n_α is the occupation number in the stateα, $0 \le n_\alpha \le 1$ and

$$\sum_\alpha n_\alpha = A.$$

Such representation assumes a certain depletion of the Fermi sea. The local density and momentum distributions have the following form [1]:

$$\rho(\vec{r}) = \sum_\alpha n_\alpha |\varphi_\alpha(\vec{r})|^2,$$

$$n(\vec{k}) = \sum_\alpha n_\alpha |\varphi_\alpha(\vec{k})|^2$$

with $\varphi_\alpha(\vec{k})$ - the Fourier transforms of $\varphi_\alpha(\vec{r})$. The form of the above equations is quite simple for a system with spherical symmetry. One can assume φ_α to be the local-scale transformed harmonic oscillator single-particle wave functions depending on the collective parameters $\alpha_i, (i = 1, 2, \dots, N)$. The expressions for the local density and momentum distributions are expanded in series of $\alpha_i - \alpha_i^0$ up tosecond order terms. In this way, dynamical corrections to these quantities are taken into account within the **ATDHF** approach, as it is described above. The occupation numbers n_α are determined by means of a self-consistent procedure, fitting the nuclear charge density to the experimental one and accounting for the ground state energy minimization. Within this approach the nuclear density and momentum distributions can be reproduced as well as the root-mean-square radius and the 'breathing' monopole mode excitation energy.

For example, let us consider the nucleus of $^{16}O$by means of one dynamical variable α and restrict the number of shells to four - $1s, 1p, 1d and 2s$. The fitting procedure leads to 7,2% depletion of the Fermi sea for the Skyrme type force modification **SkM***. The obtained results are presented in Table 1. They refer to the optimal value of α,the energy and root-mean-square radius of the one-phonon excited state for the fitted occupation number values in comparison with the same quantities in the case of occupation numbers 1 and 0.

As the results show, the depletion of the Fermi sea leads to a lower excitation energy and optimal value of α , while, as expected, the root-mean-square radius increases.

The nuclear local density distribution of the ^{16}O-ground state shows an obvious tendency of flattering inside the nucleus, due to the Fermi sea depletion. The last causes a slight shift (of about one order) of the nucleon momentum distribution tail.

*Table 1. Occupation numbers, equilibrium value of α , one-phonon excitationenergy E_1-E_0, excitedstate root-mean-square radius r_{11} and isoscalar energy-weighted sum rules (**EWSR**) estimate of the excited state contribution. The occupation numbers in the second column are fitted to reproduce the experimental charge density of ^{16}Onucleus; calculations are performedfor the Skyrme force modification **SkM****

States	Occupation numbers	
1s	1.000	1
1p	0.940	1
1d	0.038	0
2s	0.098	0
α^0, fm^{-1}	0.558	0.561
E_1-E_0, ***MeV***	26.712	27.256
r_{11}, ***fm***	2.853	2.751
EWSR, %	100	96.388

An interesting approach allowing calculation of the natural occupation numbers of ***N=Zsp-*** and ***sd-*** shell nuclei is developed in [7]. It is based on the correlated one-body density matrix. Central correlations of Jastrow type have been considered in a proper approximation. The short-range correlations effect on the natural orbitals, natural occupation numbers and the Fermi sea depletion is analyzed. The authors find a higher value of the Fermi sea depletion in closed shell nuclei compared to open shell ones. The same quantity is lower compared to the nuclear matter case. A comparison with the Mean field approximation is presented. It is found that the harmonic oscillator and natural orbital wave functions differ mainly for states above the Fermi level. This affects the high momentum components of the momentum distribution.

REFERENCES

[1] Antonov, A. N., P. E. Hodgson, I. Zh. Petkov. Nuovo Cim. A97, 1987, p. 117.
[2] Baranger, M., M. Vénéroni. Ann. Phys.114, 1975, p. 123.
[3] Brack, M., W. Stocker. Nucl. Phys. A406, 1983, p. 413.
[4] Krumova, G. Z., I. Zh. Petkov, M. V. Stoitsov. Bulg. J. Phys. 14 (6), 1987, p. 501.
[5] Löwdin, P. O. Phys. Rev. 97, 1955, p. 1474.
[6] Petkov, I. Zh., M. V. Stoitsov, E. S. Kryacko. Int. J. Quantum Chem., 29, 1986, p. 149.
[7] Psonis, V. P., Ch. C. Moustakidis, S. E. Massen. Int. J. Mod. Phys. E22, 1350047, 2013.
[8] Skyrme, T. H. R. Nucl. Phys. 9, 1959, p. 615.
[9] Vautherin, D., D. M. Brink. Phys. Rev. C5, 1972, p. 626.
[10] Петков, И. Ж., М. В. Стоицов. ТМФ, 55, 1983, с. 407.
[11] Петков, И. Ж., М. В. Стоицов.Препринт ОИЯИ Р4-85-785, Дубна, 1985.
[12] Эллиот, Дж., П. Добер. Симметрия в физике, т. 1, Москва, „Мир“, 1983.

CONTACT ADDRESS
Assoc. Prof. Galina Zaharieva Krumova, PhD
Department of Physics, Faculty of Transport
Angel Kanchev University of Ruse
8 Studentska Str.,
7017 Ruse, Bulgaria
Phone: (++359 82) 888 215
E-mail: [gal@ uni-ruse.bg](mailto:gal@uni-ruse.bg)

ПРЕДСТАВЯНЕТО НА ЕСТЕСТВЕНИТЕ ОРБИТАЛИ И МЕТОДЪТ НА ЛОКАЛНО-МАЩАБНО ПРЕОБРАЗОВАНИЕ ЗА ОПИСАНИЕ НА НЯКОИ ХАРАКТЕРИСТИКИ НА ОСНОВНОТО И МОНОПОЛНИ ВЪЗБУДЕНИ СЪСТОЯНИЯ В ЯДРАТА

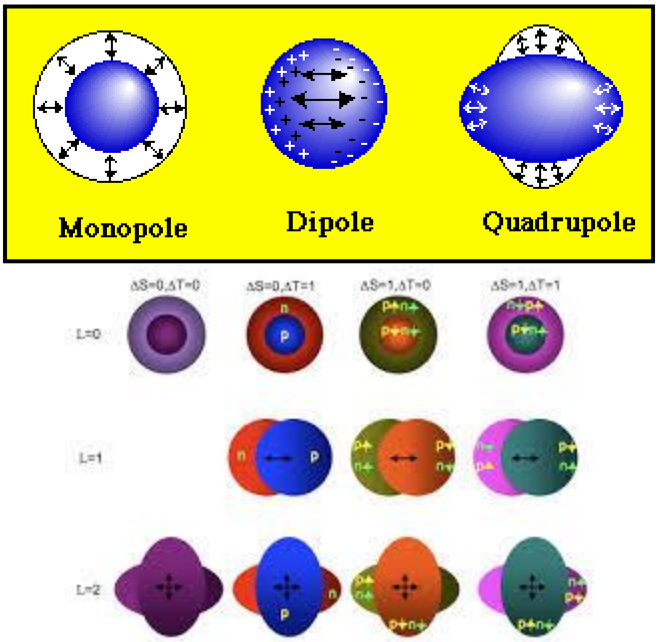
Галина Крумова

Русенски университет„Ангел Кънчев”

Резюме: *Разширеният метод на локално-мащабното преобразование (МЛМП) и Представянето на естествените орбиталисе прилагат за изследване на локално-плътностното и импулсното разпределения на основното състояние на ядрото. Разглежда се 'дихателният' монополен мод на възбуждане в рамките на Адиабатичната зависеща от времето теория на Хартри-Фок. Представени са числени резултати за ядрото на* ^{16}***O*** *с използване на ефективните сили на Скирм. Числата на запълване са определени в съответствие с експерименталните данни за разпределението на зарядовата плътност.*

Ключови думи: *Естествени орбитали, Метод на локално-мащабното преобразование, изпразване на морето на Ферми.*

DIFFERENT TYPES OF NUCLEAR VIBRATIONS



ISSN 1314-3077

9 771314 307000