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AN ADVERSE EFFECT OF THE HYPERSPHERICAL L_m APPROXIMATION

- APPLICATION TO ^6Li -

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Abstract

One shows in an application of the hyperspherical L_m approximation to ^6Li with soft core two body potentials that for nuclei A>4 it is necessary to replace the Schrödinger equation by at least two coupled equations in order to treat correctly an interaction including a Majorana exchange operator. Binding energies for ^6Li even parity states are calculated.

Key words : Hyperspherical Harmonics - L_m approximation - ^6Li even parity states.

Introduction

It has been shown [1,2] that the L_m approximation, in which only the first term of a hyperspherical harmonic (H.H.) expansion of the nuclear ground state wave function is taken into account, is very similar to a Hartree-Fock calculation performed with a harmonic oscillator (H.O.) Slater determinant in which the H.O. parameter is varied in order to obtain the minimum energy.

Our purpose is to analyze to what extend the L_m approximation leads to a rather reliable ground state wave function and whether one has actually the right to neglect the other terms of the expansion at least as a crude approximation.

The L_m approximation

When the interaction between the particles of a system composed of A fermions with coordinates $\vec{x}_i$ (i=1,...,A) is described by a potential U(r) of the collective hyperradial coordinate

$$r^2 = \frac{2}{A} \sum_{i,j>i}^{A} (\vec{x}_i - \vec{x}_j) = 2 \sum_{1}^{A} (\vec{x}_i - \vec{X})^2 \quad , \quad \vec{X} = \frac{1}{A} \sum_{1}^{A} \vec{x}_i , \qquad (1)$$

a fundamental theorem states that the grand orbital L takes its minimal value L_m for a ground state.

The ground state wave function is then the product of a hyperspherical harmonic $B_{L_m}(\Omega,s,t)$ of minimal order L_m,

suitably symmetrized, including the spin-isospin states (s,t) of the nucleons, and a function $\psi_0(r)$ of the collective coordinate :

$$\Psi_{g.s.} = B_{L_m}(\Omega,s,t)\psi_0(r) \qquad (2)$$

Ω is a set of 3A-4 angular coordinates after elimination of the center of mass $\vec{X}$.

The potential responsible for the binding of the nuclei is assumed to be a sum of mainly two body nucleon-nucleon interactions

$$V(r,\Omega,\vec{\sigma},\vec{\tau},) = \sum_{\substack{1\\ i,j>i}}^{A} V(\vec{x}_i-\vec{x}_j,\vec{\sigma},\vec{\tau}) \qquad (3)$$

in which $(\vec{\tau})$ $\vec{\sigma}$ are the (iso)spin operators. In the L_m approximation one assumes that the first term, which depends on r only, of the H.H. expansion of the potential is largely predominant in such a way that the fundamental theorem still holds.

In which case the gross properties of the ground state are described by the first term (2) of the H.H. expansion of the wave function. The ground state hyperradial wave function $\psi_0(r) = r^{-\frac{3A-4}{2}} u_0(r)$ is the regular solution of the differential equation

$$\left\{ -\frac{\hbar^2}{m}\left(\frac{d^2}{dr^2} - \frac{\mathcal{L}_m(\mathcal{L}_m+1)}{r^2}\right) + U(r) - E \right\} u_0(r) = 0 \qquad (4)$$

where $\mathcal{L}_m = L_m + \frac{3A-5}{2}$

and $U(r) = \langle B_{L_m}(\Omega,s,t) | V(r,\Omega,\vec{\sigma},\vec{\tau}) | B(\Omega,s,t) \rangle$

is the effective potential. E is the total binding energy.

Application to ^{6}Li

It has been shown in earlier works [3-7] how to obtain the effective potential in the L_m approximation. The aim of the present paper is to calculate the ground state wave function of ^{6}Li for various potentials which have already been used to solve the problem of ^{4}He in the L_m approximation [8] and to compare the binding energy of both nuclei.

For ^{6}Li the grand orbital L_m=2 describes four nucleons in the 1s shell and two nucleons in the 1p shell. The effective potential has been calculated for the 1^+ ground state and the 0^+ excited state in which the two nucleons in the p shell coupled to a total angular momentum ℓ=0 are respectively in the triplet and singlet state.

The effective potential is [7]

$$U(r) = W(r) \pm \delta U(r) \tag{5}$$

$$W(r) = 5(U_0^{3+}+U_0^{1+}) - \frac{1}{3}(U_1^{3+}+U_1^{1+}) + \frac{1}{6}(U_2^{3+}+U_2^{1+}) + \frac{9}{2}U_0^{3-} + \frac{1}{2}U_0^{1-} - 3U_1^{3-} + \frac{1}{3}U_1^{-1} \tag{6}$$

$$\delta U(r) = \frac{1}{2}(U_0^{3+}-U_0^{1+}) - \frac{1}{3}(U_1^{3+}-U_1^{+1}) + \frac{1}{6}(U_2^{3+}-U_2^{1+}) \tag{7}$$

The multipoles U_N^α of the potential are expressed in terms of the two body potentials $V^\alpha(r_{ij})$ by

$$U_N^\alpha = (-1)^N \frac{4}{\sqrt{\pi}} \frac{N!\Gamma(L_m+\frac{D}{2})}{\Gamma(L_m+\frac{D-3}{2})} \int_0^{\pi/2} V^\alpha(r\cos\phi)\cos^2\phi \quad (8)$$

$$(\sin\phi)^{2L_m+D-4-N} P_N^{(L_m+\frac{D-5}{2}-N,\,\frac{1}{2})}(\cos 2\phi)\, d\phi$$

$$L_m = 2, \qquad D = 3(A-1) = 15$$

where $P_N^{(a,b)}$ is a Jacobi polynomial and the index $\alpha = 3^+, 1^+, 3^-, 1^-$ refer to the triplet even, singlet even, triplet odd and singlet odd potentials respectively. The sign + in (5) applies to the 1^+ ground state and - to the 0^+ excited state of ^{6}Li.

Eq. (7) shows that the difference between the singlet and triplet even potentials is responsible for the excitation energy of the 0^+ state.

The effective Coulomb interaction calculated in ref. (7) has been neglected in this work.

The investigated potentials are composed of a sum of gaussians

$$V^\alpha(r_{ij}) = \sum_k V_k^\alpha \, e^{-(\frac{r_{ij}}{\rho_k})^2}, \quad r_{ij}=|\vec{x}_i-\vec{x}_j|. \qquad (9)$$

One term is a short range repulsive soft core, the other ones attractive.

The triplet and singlet even potentials of the Volkov [9] (V_1), Brink-Boeker [10] (B_1) and Baker et al. [11] (B) interactions are the same and the odd potentials are neglected (Serber force).

On table I in the first and second column are shown the binding energies of the deuteron (d) and ^{4}He, and in the next column the difference $\Delta E = E_{^6Li} - E_{^4HE} - E_d$ between the binding energy of ^{6}Li and the sum of d+^{4}He. The r.m.s. radius of ^{4}He and the binding energy $E^w_{^6Li}$ of ^{6}Li calculated assuming a two body potential of pure Wigner nature are given in the two last columns.

A nearly exact calculation of the binding of ^{4}He by the method of ref.(8) shows that the energy neglected by the L_m approximation is 1.5±.5 MeV for the Volkov potentials. One notices that for any Serber potential

i) the binding of ^{6}Li is always weaker than the one of ^{4}He+d

ii) the smaller is the r.m.s. radius of ^{4}He the larger is the difference ΔE.

One concludes that from a variational point of view the part of the Hilbert space selected by the L_m approximation is smaller for ^{4}He in the 15-dimensional space used to treat ^{6}Li than in the 9-dimensional space suitable for the calculation of the α particle. In other words the deformation of the potential $\Sigma V(r_{ij})$ with respect to the hyperspherical symmetry is larger in the 15-dimensional space than in the 9-dimensional space otherwise the binding energy of ^{6}Li should be at least equal to the one of ^{4}He.

We intend to find out which is the part of the potential responsible for the difference ΔE. The small discrepancy of about 1.5 MeV between the exact and approximate binding of ^{4}He for the Volkov potentials cannot explain the 3-6 MeV energy gap ΔE.

For this purpose the problem will be studied with a two body harmonic oscillator (H.O.) potential of Serber exchange nature

$$V_{H.O}(r_{ij}) = (-V_0 + 2\pi^2 m\omega^2 r_{ij}^2) \frac{1+P_{ij}^M}{2} \qquad (10)$$

where P_{ij}^M is the Majorana exchange operator acting between the nucleons (i) and (j). The multipoles given by (8) lead for the L_m approximation to an effective potential

$$U(r) = -10\ V_0 + \frac{64}{19}\pi^2 m\omega^2 r^2$$

The ground state binding energy and m.s. radius of ^{6}Li are

$$E_{^6Li} = -10V_0 + 4\sqrt{19}\ \hbar\omega \qquad a^2_{^6Li} = \frac{2}{3}\left(\frac{19}{16}\right)^{3/2} \frac{\hbar^2}{m}\frac{1}{\hbar\omega} \qquad (11)$$

One reminds that the binding energies and m.s. radii of the deuteron, the trinucleon and the α particle for the same H.O. potential are [12]

$$E_d = -V_0 + \frac{3}{\sqrt{2}}\ \hbar\omega \qquad (12)$$

$$E_{^3H} = -3V_0 + 3\sqrt{3}\ \hbar\omega \qquad a^2_{^3H} = \frac{1}{\sqrt{3}}\frac{\hbar^2}{m}\frac{1}{\hbar\omega} \qquad (13)$$

$$E_{^4He} = -6V_0 + 9\hbar\omega \qquad a^2_{^4He} = \frac{9}{16}\frac{\hbar^2}{m}\frac{1}{\hbar\omega} \qquad (14)$$

ΔE is given in terms of the binding energy and m.s. radius of ^{4}He by

$$\Delta E = E_{^6Li} - E_{^4He} - E_d = \frac{1}{2}E_{^4He} + \frac{9}{16}\left(4\sqrt{19} - \frac{27+3\sqrt{2}}{2}\right)\frac{\hbar^2}{m a^2_{^4He}} \qquad (15)$$

The effects i) and ii) still appear for the H.O. interaction. The numerical values obtained by using the experimental data for $P_{^4He}$ and $a_{^4He}$ are shown on the line H.O. of table I.

ΔE is close to the values procured by the Volkov and Brink-Boeker potentials.

The binding energy for a Wigner H.O. potential is

$$E^W_{^6Li} = -15V_0 + 19\sqrt{\frac{3}{2}}\hbar\omega = \frac{5}{2}E_{^4He} + (19\sqrt{\frac{3}{2}} - \frac{45}{2})\frac{9}{16}\frac{\hbar^2}{ma^2_{^4He}}$$

Using the experimental data one obtains $E^W_{^6Li} = 62.4$ MeV which is quite similar to the numbers resulting from the Volkov and Brink-Boeker potentials.

It is clear from the comparison between the binding energies of ^6Li for a Serber and a Wigner H.O. interaction that the particular behaviour of ΔE originates from the Majorana exchange operator.

H.H. dependence of the H.O. interaction including exchange operators

The total interaction for a Serber H.O. potential can be written

$$V_{H.O.}(r,\Omega) = \sum_{\substack{1\\ i,j>i}}^{A} V_{H.O.}(r_{ij}) = -\frac{1}{2}\left[\frac{A(A-1)}{2} + \sum_{i,j>i} P^M_{ij}\right]V_0$$

$$+2\pi m\omega^2\left(\frac{A}{2} + \frac{1}{A-1}\sum_{i,j>i} P^M_{ij}\right)r^2 + 2\pi^2 m\omega^2 \sum_{i,j>i}\left[(\vec{x}_i-\vec{x}_j)^2 - \frac{r^2}{A-1}\right] P^M_{ij} \qquad (16)$$

The term in r^2 is the hypercentral part of the potential but each component of the last term is an homogeneous polynomial of the coordinates $\vec{x}_i$ solution of the Laplace equation

$$\sum_{k=1}^{A} \nabla_k^2 [(\vec{x}_i - \vec{x}_j)^2 - \frac{r^2}{A-1}] = 0$$

The term

$$\sum_{i,j>i} [(\vec{x}_i - \vec{x}_j)^2 - \frac{r^2}{A-1}] P_{ij}^M = r^2 \; T_2(\Omega, \vec{\sigma}, \vec{\tau})$$

is therefore the product of r^2 and an operator $T_2(\Omega, \vec{\sigma}, \vec{\tau})$ of the spin-isospin space which is a H.H. of grand orbital 2 in the hyperspace. The potential (16) is no longer hypercentral and the operator T applied to the H.H. of minimal order $B_{L_m}(\Omega,s,t)$ generates a H.H. $B_{L_m+2}(\Omega,s,t)$ of grand orbital L_m+2.

All together the H.H. B_{L_m} and B_{L_m+2} constitute the two elements of the optimal subset (12,13,14) for a H.O. interaction including the Majorana exchange operator P_{ij}^M.

The treatment of the Schrödinger equation with an exchange H.O. potential using an H.H. expansion of the wave function restricted to the optimal subset requires the solution of a system of two coupled equations, one for each of the two H.H. components. The equation originating from the B_{L_m+2} component brings an additional binding energy which balances the effect i). This can be infered from an analysis of eq.(14) : when the strength ω of the H.O. vanishes the coupling between the two differential equations and the related additional binding disappear, but the difference ΔE becomes negative leading to

an asymptotic ^{6}Li binding energy $E_{^6Li}(\omega=0)=\frac{3}{2} E_{^4He}+E_d < E_{^4He}+E_d$. On the other hand from the identity

$$\sum_{i,j>i} [(\vec{x}_i-\vec{x}_j)^2 - \frac{r^2}{A-1}] = 0 \qquad \text{(see eq.1)}$$

it appears that the operator T_2 does not give any contribution when it is applied to a set of four spin-isospin saturated space states like for ^{4}He. Therefore only a single equation is required for solving exactly ^{4}He with a Serber H.C. interaction but two equations are needed in order to obtain a similar result (at the accuracy of the optimal subset) for heavier nuclei. This conclusion is still valid for weak soft core potentials and explains the occurrence of the effect i) for the Volkov interaction. This effect is more pronounced when the soft core becomes stronger like for the Brink B_1 potential.

The even parity excited levels of ^{6}Li

Assuming that the sequences and energies of the excited states of ^{6}Li with respect to the ground state are not drastically changed by the introduction of the coupled equations needed in order to solve accurately the Schrödinger equation we have calculated the levels of ^{6}Li with a few potential ajusted to the nucleon-nucleon phase shifts $^1S_0$ and $^3S_1$.

An analysis of the contribution of the odd central potentials has been done with the realistic Gogny-Pirès-de Tourreil potential [15].

Table I gives the results obtained assuming a Serber potential constituted by half the sum of the singlet and triplet even potentials for the Afnan-Tang [16] (S_1), Eikemeier-Hackenbroich [17] (S_4) and Gogny-Pirès-de Tourreil (GPDT) interactions. The tensor force is not an ingredient of the two first potentials for which the deuteron binding energy has been calculated with the triplet even potential.

The binding energy E_d given by the GPDT potential is too small because the tensor force has not been included in our calculation.

The weak binding of ^{4}He and the large value ΔE originate from the repulsive core which is stronger than in the Volkov potentials.

In taking into account the odd central forces (mainly repulsive) of the GPDT interaction in eq.(6) and (4) one weakens the binding of ^{6}Li by 2 MeV with respect to the result obtained when only even interactions are used. The effective potential U(r) related to the states of total orbital momentum ℓ=2 is obtained in changing the coefficient from 1/6 into 1/15 for the multipole U_2 in eq.(6) and (7). The sign ± refers respectively to the triplet (3^+ 2^+ 1^+, S=1, T=0) and the singlet (2^+, S=0, T=1) states.

The degeneracy of the triplet states is removed by the spin-orbit interaction. The center of the triplet can be calculated by writting

$$E(J) = E_{gs} + E_0 + [J(J+1)-\ell(\ell+1)-S(S+1)]\ \bar{U}_{\ell S} \qquad J = 1, 2, 3$$

where E_{gs} is the ground state energy $\bar{U}_{\ell S}$ an average value of the spin orbit potential and where $\ell=2$, $S=1$. A good agreement with the experimental energies [18] is obtained with $\bar{U}_{\ell S}=-.705$ MeV and $E_0=3.60$ MeV. It is the energy E_0 which is calculated when the spin-orbit interaction is neglected.

The tensor force of the GPDT potential acts between the two nucleons of the 1p shell in a triplet spin state. In order to be consistent with the potentials S_1 and S_4 which include this contribution we have to estimate the contribution of this force. It seems reasonable to estimate that the contribution of the tensor force to the binding energy of ^{6}Li is of the order of the difference between the binding energy of the deuteron calculated once with and once without tensor force. The GPDT potential overbinds the deuteron by about .4 MeV [15], we have to add therefore about -2.4 MeV to the ground state binding energy of ^{6}Li calculated without the tensor force.

There is no contribution of the tensor force for the singlet 0^+ and 2^+ states and we have neglected its contribution to the triplet $\ell=2$ excited state.

Table II gives the excitation energies obtained for the three investigated potentials and the last line refers to the ground state r.m.s. radius. In spite of the L_m approximation the realistic GPDT potential gives the binding energies and r.m.s. radius in a reasonable accord with the experimental data. One notices that by neglecting the tensor interaction in the triplet state $\ell=2$ one over estimates the energy E_0.

The order or the levels obtained for the GPDT potential is in agreement with other calculations [19].

Conclusion

Calculations of the ^{6}Li ground state in the L_m approximation with nearly hypercentral soft core Serber potentials show (by comparison with a Serber H.O. interaction) that in order to obtain a binding stronger than the one of ^{4}He it is necessary to include at least two components in the H.H. expansion of the wave function. The second component is generated by the exchange part of the potential.

This second component constituted by an H.H. of grand orbital L_m+2 appears in the treatment of ^{4}He (for which $L_m=0$) where the difference between the singlet and triplet even central potentials generates the so called mixed symmetry state. But in contrast to the difference between the triplet and singlet even potential which is rather weak and generates a mixed symmetry state representing only about 1% of the ground state wave function of ^{4}He, the Serber potential is strong and generates a second component which is expected to contribute largely to the wave function. The Majorana component appears for nuclei $A>4$ and must be included in any accurate treatment of the Schrödinger equation. It will be shown in another paper that the H.H. B_{L_m+2} can be written as a sum of determinants including spherical harmonics absent from the original determinant describing the H.H. of minimal order L_m [20]. In this respect it cannot be taken into account by a standard Hartree-Fock calculation using a single Slater determinant.

On the other hand a calculation with semi realistic potentials suggests that the energies of ^{6}Li excited states with

respect to the ground state should not be very much perturbed by the poor accuracy of the L_m approximation.

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References

1) A.A. Sadovoi, I.K. Aver'yanov and A.I. Golubev, Sov. J. Nucl. Phys. 24 (1976) 581

2) J. Navarro, Phys. Letters 62B (1976) 22 and Ph. D. Thesis Universidad de Valencia (1976)

3) A.M. Badalyan, Yu. A. Simonov, Sov. J. Nucl. Phys.9 (1969) 42

4) A.M. Badalyan, F. Calogero and Yu. A. Simonov, Nuovo Cim. 68A (1970) 572

5) A.I. Baz', N.Y. Zhukov, Sov. J. Nucl. Phys. 11 (1970) 435

6) D. Levi, M. Moshinsky, Nuovo Cim. 20 (1974) 107

7) M. Fabre de la Ripelle,"Hyperspherical Harmonics and shell model", 3ème Session d'Etude La Toussuire, Feb. 1975, Ed. Elbaz IPN Villeurbanne

8) M. Fabre de la Ripelle, Sov. J. Nucl. Phys. 13 (1971) 279

9) A.B. Volkov, Nucl. Phys. 74 (1965) 33

10) D.M. Brink, E. Boeker, Nucl. Phys. A91 (1967) 1

11) G.A. Backer, J.L. Gammel, B.J. Hill, G.J. Wills, Phys. Rev. 127 (1962) 1754

12) M. Fabre de la Ripelle, Proceedings of the International School on Nuclear Theory Physics (Predeal 1969) Ed. Corciovei Inst. Atomic Phys. Bucarest

13) M. Fabre de la Ripelle, Session d'Etude La Toussuire (Feb. 1971) "Résolution du problème à N corps par le formalisme hypersphérique", Ed. Elbaz IPN Villeurbanne

14) J.L. Ballot, M. Beiner, M. Fabre de la Ripelle, Proceedings of the Symposium on Present Status and Novel Developments in the Many Body Problem, Roma 1972, Ed. F. Calogero and C. Ciofi degli Atti (Bologna 1974) Vol.1

15) D. Gogny, P. Pirès, R. de Tourreil, Phys. Letters 32B (1970) 591

16) I.R. Afnan, Y.C. Tang, Phys. Rev. 175 (1968) 1337

17) H. Eikemeier, H.H. Hackenbroich, Z. Phys. 195 (1966) 412

18) F. Ajzenberg-Selove and T. Lauritzen, Nucl. Phys. A227 (1974)

19) R. Ceuleneer, M. Erculisse and M. Gilles, Phys. Letters 65B (1976) 101

20) Yu. A. Simonov, Sov. J. Nucl. Phys. 7 (1968) 722

Table I

Pot	E_d	$E_{^4He}$	ΔE	$a_{^4He}$	$E^W_{^6Li}$
B	- .402	- 39.163	9.971	1.162	- 79.493
V_4	- .445	- 29.151	6.979	1.387	- 61.476
V_3	- .352	- 29.259	5.837	1.402	- 61.954
V_5	- .469	- 28.087	4.089	1.486	- 60.333
V_1	- .544	- 28.578	4.175	1.488	- 61.845
V_6	- .534	- 28.749	3.637	1.491	- 62.150
V_7	- .497	- 28.030	3.918	1.494	- 60.246
V_8	- .542	- 28.452	3.756	1.495	- 61.380
V_2	- .608	- 29.402	3.086	1.496	- 63.735
B_1	-1.010	- 29.292	4.932	1.497	- 63.504
H.O.		- 28.2	4.83	1.495	- 62.46
Exp	-2.22	- 28.2	- 1.47	1.495	
S_1	-2.169	- 16.156	12.156	1.535	
S_4	-2.131	- 18.572	10.581	1.548	
GPDT	- .233	- 14.198	8.772	1.651	

Table II

J^π	T	ℓ	$\bar{S}_4$	S_1	GPDT	exp.(17)
(g.s) 1^+	0	0	0	0	0	0
0^+	1	0	5.64	4.69	3.49	3.56
3^+ 2^+ 1^+	0	2	2.90	3.18	4.19	3.60
2^+	1	2	6.37	5.32	5.06	5.36
a (^{6}Li) (g.s.)			2.13	2.12	2.55	2.3±.1