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COLLECTIVE 1⁻ EXCITATIONS WITH SKYRME FORCES

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1. Introduction

This work is a natural continuation of the article [1] where Wigner function moments method was used to calculate energies and excitation probabilities of 3^- and 2^- states with Skyrme forces.

The system of dynamical equations for Cartesian tensors of the 3d rank was derived there. This tensors are collective variables of the method. By evident combinations one can divide the system to the separate subsystems for irreducible tensors of 3,2 and 1st multipolarity.

The last subsystem occurred to be most complicate. It allows to study collective 1⁻ excitations of both the kindes - isovector and isoscalar. There is giant dipole resonance among them, evidently. Calculations performed for it are interesting mostly from the methodical point of view. It is important for us to show that our method works not worse than other approaches - both fenomenological [2] and self-consistent ones [3].

The studying of the isoscalar 1^- excitations is interesting due to recent experiment of the Holland group [4], where low lying dipole isoscalar excitations were discovered. We shall also pay attention to the high lying isoscalar dipole modes, which were detected experimentally not so long ago, hence, there is some uncertainty in the data [5]-[7].

2. Center of mass motion

The needed definitions and detailed derivation of dynamical equations for cartesian tensors of the 1st and 3d rank (they are also called virial equations) are given in [1] and [8].

Here we shall consider only the center of mass motion problem, which must be treated in a proper way by any theory pretending to describe correctly 1^- excitations. In the strict sence, it is not a real problem in our method of moments. The reason is that the center of mass coordinates are the collective variables of the method and there are dynamical equations for them. Let us adduce their derivation.

One can obtain virial equations of the 1st order by integrating continuity equation

$$\frac{\partial n_q}{\partial t} + div(n_q \vec{u}_q) = 0 \tag{1}$$

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and the Euler equation

$$\frac{\partial}{\partial t}(n_{q}u_{qi}) + \frac{n_{q}}{m}\frac{\partial W_{q}}{\partial x_{i}} +$$

$$+\sum_{s}\frac{\partial}{\partial x_{s}}(\frac{1}{m}P_{qis} + n_{q}u_{qi}u_{qs}) = 0$$
(2)

over nuclear volume with x_i and 1 weights correspondingly. Here $n_q(\vec{r})$ is nucleon density, $u_q(\vec{r})$ is their mean velocity, q is index distinguishing protons and neutrons, $P_{q\,is}$ is pressure tensor, $W_q(\vec{r})$ is mean field, m is nucleon mass and i, s are indexes of the Cartesian system of coordinates. By integrating the last terms in both equations by parts we obtain:

$$\frac{d}{dt}\mathcal{J}_{q\,i}-\mathcal{P}_{q\,i}=0,\tag{3}$$

$$\frac{d}{dt}\mathcal{P}_{q\,i} + \frac{1}{m}\int n_q \frac{\partial W_q}{\partial x_i} d\vec{r} = 0, \qquad (4)$$

where $\mathcal{J}_{qi} = \int x_i n_q d\vec{r}$ is a proton or neutron center of mass coordinate, $\mathcal{P}_{qi} = \int n_q u_{qi} d\vec{r}$ is a corresponding momentum. The integral of the last term in (2) is equal to zero due to boundary condition. $n_q(\pm \infty) =$ $P_{qis}(\pm \infty) = 0$. Equation (4) describes the dynamics of protons or neutrons momentum. Without external fields the sum of the equations (4) for neutrons and protons is just the conservation law for nucleus momentum $\mathcal{P}_i = \mathcal{P}_{ni} + \mathcal{P}_{pi}$. In this case integral $\int (n_p \frac{\partial W_p}{\partial x_i} + n_n \frac{\partial W_n}{\partial x_i}) d\vec{r}$ is nothing else than a sum of all the internal forces in nucleus and must be equal to zero. It should be mentioned that this equality is true only in the case of self-consistent mean field $W_q(\vec{r})$. The sum of equations (3) for neutrons and protons describes linear uniform motion of the nucleus.

To calculate the nuclear excitation probabilities we use linear response theory in the form given by Lane [9]. The external field $W_q(\vec{r},t) = Q_q(r)e^{-iwt} + Q_q^{\dagger}(r)e^{iwt}$ is added to the Hamiltonian where $Q_q(\vec{r})$ is the operator with needed matrix elements. To conserve the nucleus momentum W_q must fulfill the following condition

$$\int (n_p \frac{\partial \mathcal{W}_p}{\partial x_i} + n_n \frac{\partial \mathcal{W}_n}{\partial x_i}) d\vec{r} = 0.$$
(5)

This condition permites to fix effective charges and other parameters of the external field. Thus for the dipole operator $Q_{q1\mu} = e_q r Y_{1\mu}$ exciting

GDR we have:

$$\sum_{q} e_{q} \int n_{q} \frac{\partial}{\partial x_{i}} (rY_{1\mu}) d\vec{r} \simeq$$

$$\sum_{q} e_{q} \frac{Z_{q}}{A} \int n \frac{\partial}{\partial x_{i}} (rY_{1\mu}) d\vec{r} = 0.$$
(6)

Here we used generally accepted approximation $n_q = \frac{Z_q}{A} \cdot n$, where $n = n_p + n_n$. Evidently integral in (6) is not equal to zero, hence:

$$\sum_{q} e_{q} \cdot Z_{q} = e_{p} \cdot Z + e_{n} \cdot N = 0.$$
⁽⁷⁾

It is easy to see that this condition can be satisfied by the well-known choice of the effective charges: $e_p = \frac{N}{A} \cdot e$, $e_n = -\frac{Z}{A} \cdot e$. In the case of electromagnetic (Coulomb) excitations, when $e_p = e$ and $e_n = 0$, or isoscalar excitations, when $e_p = e_n$, every term in (5) must be equal to zero, that can be achieved only by special choice of the operator. Usually one takes $Q_{g1\mu} = e_q(r^3 + \alpha r)$. Then one gets from (5) the following expression (after integration over angels):

$$\sum_{q} e_{q} \cdot \frac{Z_{q}}{A} \int \frac{\partial n}{\partial r} (r^{3} + \alpha r) r^{2} dr = 0.$$
(8)

The integral here must be equal to zero. It leads to known formula [3] for the constant α :

$$\alpha = -\frac{5}{3} \int nr^4 dr \, / \, \int nr^2 dr = -\frac{5}{3} \langle r^2 \rangle. \tag{9}$$

It is more convenient in calculations to deal with one equation obtained by substitution of (3) into (4):

$$\frac{d^2 \mathcal{J}_{q\,i}}{dt^2} + \frac{1}{m} \int n_q \frac{\partial W_q}{\partial x_i} d\vec{r} = 0.$$
⁽¹⁰⁾

Difference of the proton and neutron equations (10) describes, obviously, relative movement of proton and neutron mass centers. In principle that is enough for the studying giant dipole resonance in a Goldhaber-Teller

way. Due to the mean field W_q , however, equation (10) is linked with higher rank tensors. As a result it becomes possible to investigate centers of mass motion together with more complicate nucleon motions of compressional and rotational type (which are characteristic feature of Steinwedel-Jensen model). The natural unification of these models takes place in such a way. Earlier, similar unification has been performed phenomenologically [2] using the "droplet" model.

3. Numerical results

The calculated dipole excitation energies E_{ν} are shown in Fig.1 as a function of the mass number A. They are obtained from the characteristic equation of the system of dynamical equations for different tensors of multipolarity $\lambda = 1$, which was derived in [1]. This equation is a polynomial of degree seven: thus seven 1⁻ levels are expected. This is the case for the most nuclei, but the figure shows that only five real solutions are found in the region of rare earth and also for light nuclei. This fact is still puzzling.

At this point, two comments are in order. First, the calculations are performed with a spherical shape for nuclei in the ground state [10]. This could be the main reason for the reduction of the number of real solutions in the region of well deformed rare-earth nuclei. Second, there is a lack of general self-consistency in the calculations. On the one side, the ground-state matter density is described by Fermi functions with the same parameters for the whole periodic table, and on the other side the simple Thomas-Fermi approximation is used for the kinetic energy density. Both approximations (called "Fermi density" - FD) can work successfully for the description of relatively rough observables such as giant resonances, especially in heavy nuclei, but they obviously may lead to noticeable discrepancies in light nuclei. One should mention that dipole excitations are especially sensitive to the self-consistency because the separation of center of mass motion can be correctly performed only in self-consistent calculations (Thouless theorem [11]).

To understand the nature of each of these (seven or five) 1^- resonances, one has to calculate the probability of their excitation by different kinds of operators.



Fig.1.

Energies of 1^- excitations as a function of the mass number. Calculations are done for the nuclei on the beta-stability line, with the SkM^* interaction in the FD approximation. Solid points correspond to experimental values for GDR centroids from refs. [16] and [12].



Fig.2

Part of Fig.1

Dashed line : centroid of E_4 and E_5 weighted with their B(E1)-factors (eq.30).

Dotted line : GDR centroid calculated with a simpler version of the method (with first rank tensors only).

The first operator under consideration concerns the giant dipole resonance (GDR):

$$\hat{O}_1 = e(\delta_{q,n} \frac{Z}{A} - \delta_{q,p} \frac{N}{A}) \ rY_{1\mu}$$
(11)

The results are shown for ²⁰⁸Pb in Table 1: the first column gives the centroid of the excitation energy and the second column gives the B(E1) factor, i.e. $|\langle \nu | \hat{O}_1 | 0 \rangle|^2$ which, in agreement with the linear response theory [9], comes from the function:

$$F_1(E_{\nu}) = \lim_{E \to E_{\nu}} (E - E_{\nu}) \int \delta n \ \hat{O}_1 \ d^3r$$
(12)

However, it turns out that this definition leads to negative values for some of the E_{ν} , as can be seen in the table. That means, that this levels are not excited by operator \hat{O}_1 They are expected to have a very small probability B(E1) in self-consistent calculations (see also the discussion concerning the tables 2 and 3).

The whole energy weighted sum rule (EWSR) of the GDR is practically exhausted by two levels, at $E_4 = 11.3 MeV$ and $E_5 = 17.3 MeV$, the contribution of the other levels being negligible, or questionable when negative. The centroid E_x of these two levels, calculated by:

$$E_x = \frac{E_4 \ B_4(E1) + E_5 \ B_5(E1)}{B_4(E1) + B_5(E1)}$$
(13)

is located at $E_x = 13.48 MeV$ and practically coincides with the experimental value $E_x = 13.46 MeV$ [12] for the GDR centroid in ²⁰⁸Pb.

The value of this centroid is shown in Fig.2 by the dashed curve, as a function of the mass number: a good agreement with experimental data is found for all nuclei.

For comparison, the results obtained with simplified calculations [13] are shown in the same figure by the dotted curve: in this case, only the first rank tensors are taken into account, which corresponds to the Goldhaber-Teller model [14]. In this latter simplified calculation, only one value E_x is found and an effect of the third rank tensors is to split the resonance at energy E_x into two branches at energies E_4 and E_5 : this is exactly what occurs with RPA calculations [15],[3]. Very likely, including tensors of higher and higher rank would give more and more fragmented GDR.

Table 1

E_{ν}	\mathcal{F}_1/\sum_1	\mathcal{F}_3/\sum_3				
MeV	iv (%)	em~(%)	iv (%)	is (%)		
8.1	0	5.4	0.1	10.0		
8.6	-7.1	3.1	0	4.2		
		(9.8 exp)		(14.7 exp)		
10.0	-26.7	0.1	0.7	-0.3		
11.3	78.8	1.6	1.9	0.1		
17.3	71.1	0	-1.2	0.3		
24.8	0	26.1	7.1	74.2		
37.4	0.1	63.6	102.6	0.2		
	$\sum_{1} = 116$	$\sum_{3} = 99.9$	$\sum_{3} = 111.2$	$\sum_{3} = 89$		

1⁻ excitation energies E_{ν} for ²⁰⁸*Pb* and corresponding functions $\mathcal{F}_i(E_{\nu})/\sum_i$, calculated for operators \hat{O}_i , i = 1, 3.

$$\hat{O}_1 = e(\delta_{q,n}\frac{Z}{A} - \delta_{q,p}\frac{N}{A})rY_{1\mu}, \quad \hat{O}_3 = e(r^3 + \alpha r)Y_{1\mu},$$

 \sum_{i} - energy weighted sum rule for operator \hat{O}_{i} ,

$$\mathcal{F}_i(E_\nu) \equiv \lim_{E \to E_\nu} (E - E\nu) \int \delta n \, \hat{O}_i \, d\vec{r}.$$

According to the linear response theory the function $\mathcal{F}_i(E_{\nu})$ must be equal to the reduced probability B(E1) (see section 4). em – electromagnetic, is – isoscalar, iv – isovector kinds of excitation. The calculations are done in the FD approximation with SkM^* force.

As can be seen in Fig.2, the inclusion of third rank tensors, that means discarding of the long wave approximation in treating GDR, is needed in order to improve the agreement with experiment (dashed curve as compared to dotted curve). It must also be added that the energy gap between the levels E_4 and E_5 is in good agreement with the experimental GDR widths.

The second operator under consideration allows to study compressional modes [3]:

$$\hat{O}_3 = e (r^3 + \alpha r) Y_{1\mu},$$
 (14)

where the constant α is given by the condition of a fixed center of mass:

$$\alpha = -\frac{5}{3} \langle r^2 \rangle$$

and for any function x(r), the mean value stands for:

$$\langle x \rangle = \frac{1}{A} \int n(r) x(r) d^3 r$$

The probabilities of the different levels to be excited by this operator are given in Table 1 for ^{208}Pb . The contributions to the electromagnetic (em) energy weighted sum rule:

$$S(E1) = \frac{3}{4\pi} \frac{\hbar^2}{2m} e^2 Z \left[11 \langle r^4 \rangle - \frac{25}{3} \langle r^2 \rangle^2 + \frac{m}{2\hbar^2} (t_+ - \frac{t_-}{2} \frac{Z}{A}) \cdot (11 \langle nr^4 \rangle + 10\alpha \langle nr^2 \rangle + 3\alpha^2 \langle n \rangle) \right]$$
(15)

is shown in the third column and the contributions to the isovector (iv) and isoscalar (is) sum rules:

$$S(\tau = 1, \lambda = 1) = S(\tau = 0, \lambda = 1) = \frac{3}{4\pi} \frac{\hbar^2}{2m} e^2 A \cdot$$
(16)

$$\cdot \left[11 \langle r^4 \rangle - \frac{25}{3} \langle r^2 \rangle^2 + \frac{m}{2\hbar^2} (t_+ - \frac{t_-}{2} \frac{Z^2 + N^2}{A^2}) \cdot (11 \langle nr^4 \rangle + 10\alpha \langle nr^2 \rangle + 3\alpha^2 \langle n \rangle) \right]$$

are in the two last columns. The largest contribution to the isovector energy weighted sum rule comes from the highest level $(E_7 = 37.4 MeV)$: it

thus can be called the compressional isovector dipole resonance, although no experimental information about it is yet available.

The isoscalar EWSR is mainly exhausted by the sixth level ($E_6 = 24.8 MeV$), which thus can be called the compressional isoscalar dipole resonance. Quite similar results (E = 25.9 MeV with a contribution of 58%) were obtained in RPA calculations using the SGII interaction [3]. The same resonance is found experimentally at about 22 MeV with a EWSR contribution in the range 44% - 90% [5],[6],[7] which overlaps our value 74.2%.

Although the contribution of the two first levels $E_1 = 8.1 MeV$ and $E_2 = 8.6 \ MeV$ is much weaker, they appear to be now of increasing interest because of recent experimental data of a dutch group [4]. In this work, the reaction $(\alpha, \alpha' \gamma_0)$ has been studied at zero angle with ^{208}Pb , ^{90}Zr , ^{58}Ni and ^{40}Ca targets. The inelastically scattered α -particles are measured in coincidence with the gamma-decay towards a 0^+ ground state: the characteristics of the $\alpha - \gamma$ angular correlation allow a unique identification of the multipolarity of the excited intermediate states. As a result, the experiment confirms and improves previous data and also a number of new levels are identified. For ^{208}Pb , seven 1⁻ levels are found in an energy range of 5.3 to 7.28 MeV with a total contribution to the isoscalar EWSR of $14.7 \pm 0.3\%$ and a contribution to the electromagnetic sum rule of $9.82 \pm 0.14\%$. As can be seen in Table 1, these values are close to the contribution to the same sum rules of our two lowest 1⁻ levels ($E_1 = 8.1$ and $E_2 = 8.6 MeV$). However, the quality of the agreement is not the same for the energies: the calculated energy centroid (at 8.23 MeV is 2.3 MeV higher than the experimental one (at 5.94 MeV). In this connection, the extreme sensitivity of the low lying levels to all details of calculation must be pointed out. For example, if the quantum corrections to Vlasov equation are neglected (column II in Table 2), the energy of this centroid is lowered by 2MeV, while all the other levels are only slightly changed. This sensitivity suggests that self-consistent calculations could be an effective improvement. In addition, more realistic interactions could also help for a better agreement with experimental energies.

Table 2 shows the calculated energy levels and their contribution to the GDR sum rule with different approximations in the interaction. In particular, if the Coulomb interaction is neglected (column III) two roots

Table 2

$E_{\nu} (MeV)$					\mathcal{F}_1 / \sum_1 (%)						
I	II	III	IV	v	VI	I	II	III	IV	v	VI
8.1	6.2	8.2	-	7.0	9.0	0	0	-0.8	-	0	-5.2
8.6	8.4	8.8	-	7.9	9.5	-7.1	-5.8	-1.9	-	-0.2	-14.9
10.0	9.7		9.5	10.9	10.8	-26.8	-7.5	-	-0.7	0.3	34.0
11.3	11.2		10.6	12.5	12.1	78.8	48.1	-	9.6	27.0	31.1
17.3	16.9	17.3	17.4	15.9	18.9	71.1	81.4	22.4	40.0	72.7	68.7
24.8	25.4	25.6	24.6	24.6	28.8	0.	0	-0.3	-0.3	0	0
37.4	37.8	38.3	37.2	36.9	39.2	-0.1	-0.1	0.1	-0.2	0.2	0

1⁻ excitation energies E_{ν} for $208^{P}b$ and corresponding functions $\mathcal{F}_{1}(E_{\nu})/\sum_{1}$, (see explanation to Table 1) for different approximations in the interaction W_{q} . Column I : SkM^{*} , same as Table I. Column II : same as column I but without quantum corrections. Column III : same as column I but without Coulomb interaction. Column IV : same as column I but ground state pressure tensor is calculated in TF approximation. Column V : local SkM^{*} ($t_{1} = t_{2} = 0$) interaction. Column VI : SkIII force.

⁴⁰ Ca				²⁰⁸ Pb				
$E_{\nu}(MeV)$		\mathcal{F}_1/\sum_1 (%)		$E_{\nu}(MeV)$		\mathcal{F}_1/\sum_1 (%)		
F.D.	H.F.	F.D.	H.F.	F.D.	H.F.	F.D.	H.F.	
10.5	14.9	-0.1	0.05	3.5	5.7	-0.01	-0.14	
11.4	16.6	5.0	0.06	8.2	9.0	0.09	2.1	
13.6	22.5	0.7	39.0	11.5	14.4	1.5	38.3	
15.9	24.5	0.6	0.23	13.6	15.4	40.5	22.4	
19.4	31.8	90.5	59.1	15.8	21.7	55.7	30.8	
25.5	57.3	0.2	0	27.8	38.4	-0.17	0.07	
40.3	64.4	3.2	1.6	37.6	54.1	2.4	6.5	

Table 3

1⁻ excitation energies E_{ν} and corresponding functions $\mathcal{F}_1(E_{\nu})/\sum_1$, (see explanation to Table 1) for $208^P b$ and $40^C a$. Calculations are done with local *SkIII* force $(t_1 = t_2 = 0)$ within the FD approximation or within the HF approximation for the densities and pressure tensor.

of the characteristic equation disappear. The same effect, i.e. less than seven solutions, occurs when TF approximation instead of equilibrium conditions (see ref. [1]) is used to calculate ground state pressure tensor (column IV). In the case of a local Skyrme interaction (namely SkM^* with $t_1 = t_2 = 0$) the lowest root of characteristic equation becomes negative. So we have in this case six levels. It is interesting to note that one can obtain seven levels changing the parameters of this simple interaction. Also we should stress that contrary to the case of nonlocal potential only one negative contribution to the sum rule appears (column V) and it is very small: - 0.2%. That means evidently that nonlocal potential requires more careful treatment (self-consistency). In the calculation with the SkIII force (column VI) the resonance splits into three branches with a centroid at $E_x = 15.2MeV$.

In Table 3, the results of self-consistent calculations for ${}^{40}Ca$ and ^{208}Pb are compared to the previous FD approximation values. Till now, only a local Skyrme interaction SkIII (with $t_1 = t_2 = 0$) was used in order to evaluate the changes due to self-consistent densities. The results are clearly far above the previous calculations using Fermi shape densities (which were in a good agreement with experiment) nevertheless they show the role played by self-consistency in our approach. The largest changes take place, as it was expected, in the light nucleus. The energies change by a factor of about 1.5 and the isovector strength is radically redistributed amongst the levels. The fact that three of four levels which had previously negative (although small -0.1%, -0.2%) contributions to the sum rule now give also small but positive values is rather encouraging (the negative value for the lowest level in ^{208}Pb requires the additional investigation). On these grounds, we can expect that Hartree-Fock calculations for densities and pressure tensors and a more realistic non-local Skyrme force could provide reliable probability values.

4 Summary and conclusions

Virial equations of the first and third order derived in [1] were applied to describe dipole excitations of spherical nuclei with Skyrme forces. Summarizing our results we should say that our theory gives seven 1^- resonances in the interval 7 - 40 MeV.

Analyses of their excitation probabilities shows that:

1. Two resonances represent splitted GDR with the energy distance between them corresponding to experimentally observed GDR width. Their centroid coincides practically with the corresponding experimental value.

2. The highest two resonances are the isoscalar and isovector compressional modes. The energy and contribution to the sum rule of the isoscalar excitation are rather close to the experimental data, although for the better agreement it is necessary to choose more suitable interaction. We did not come across any experimental data on the isovector resonance yet.

3. The lowest two resonances can be interpreted as a compressional isoscalar excitations. Their joint contribution to the electromagnetic (Coulomb) and isoscalar sum rules agrees very good with recent experimental results [4].

Our investigation demonstrates great sensitivity of dipole excitations (especially low lying) to the all fine points of the calculation. Hence, there is the great sense to repeat the calculations with Hartree-Fock densities and pressure tensor. The next step will be to use more realistic interactions in both the densities and the dynamic equations and to allow for deformed ground-state when necessary.

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