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Collective modes in the generator coordinate method

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Abstract. Using the harmonic version of the generator coordinate method, and Skyrme interaction, the frequencies of the isoscalar breathing and quadrupole modes are related to the relevant incompressibility coefficients. The possibility of extending this to spin modes is also examined. It is found that a spin incompressibility coefficient is negative for a particular set of Skyrme parameter for ^{4}He. Other sets produce low positive values and these in turn could imply a relatively low lying $S = 2$, $T = 1$ state. The replacement of the three-body term by the density-dependent one, suggested by Chang provides a cure for this pathology.

Keywords. Collective modes; generator coordinate method; Skyrme interaction; isoscalar breathing; quadrupole mode; spin mode.

1. Introduction

The generator coordinate method (GCM) (Hill and Wheeler 1953; Griffin and Wheeler 1957) is a very flexible one for the description of collective modes in any many-body system. Being fully quantal it is particularly useful for nuclei (see Wong 1975).

The GCM wave function for a collective mode (CM) is taken as

$$\psi_{\text{GCM}} = \int f(\alpha)\, \Phi(\alpha)\, d\alpha, \tag{1}$$

where α is a set of real* collective generator coordinate (GC) and $\Phi(\alpha)$ is a many-body wave function which depends on all the relevant coordinates and on α. The weight function $f(\alpha)$ satisfies the Hill-Wheeler equation

$$\int [H(\alpha', \alpha) - E\, I(\alpha', \alpha)]\, f(\alpha)\, d\alpha = 0, \tag{2}$$

where $\begin{Bmatrix} H(\alpha', \alpha) \\ I(\alpha', \alpha) \end{Bmatrix} = \left\langle \Phi(\alpha') \middle| \begin{Bmatrix} H \\ 1 \end{Bmatrix} \middle| \Phi(\alpha) \right\rangle.$

The choice of α, in the past have been based on 'educated' guess and here also we take such a course. However we must call attention to some recent work by Reinhard and Goeke (1979) on this question and the path of integration in (1).

*In certain situations it is necessary to allow for complex GC (Brink and Weiguny 1968)

In the harmonic approximation of GCM (Brink and Weiguny 1968) one assumes that

$$I(\alpha', \alpha) \approx \exp\,[-(\alpha-\alpha')^2/2\,\Gamma], \tag{3}$$

$$H(\alpha', \alpha) \approx I(\alpha', \alpha)\,[H(0, 0) + \tfrac{1}{2}\,B\,(\alpha^2 + \alpha'^2) + C\,\alpha\,\alpha'], \tag{4}$$

with $$B = \frac{\partial^2}{\partial\alpha\,\partial\alpha'}\left[\frac{H(\alpha', \alpha)}{I(\alpha', \alpha)}\right]_{\alpha=\alpha'=0}, \qquad C = \frac{\partial^2}{\partial\alpha^2}\left[\frac{H(\alpha', \alpha)}{I(\alpha', \alpha)}\right]_{\alpha=\alpha'=0}.$$

Then the energies of the correlated ground state E_0 (correlation due to zero-point oscillation of the particular mode) and the corresponding 'single phonon' state energy E_1 are given by

$$E_0 = H(0, 0) + \tfrac{1}{2}\,(\omega - B), \tag{5}$$

$$E_1 - E_0 \equiv \hbar\,\omega = \Gamma\,(B^2 - C^2)^{1/2}. \tag{6}$$

In the above it is assumed that $H(\alpha, \alpha)$ is a minimum at $\alpha=0$. If the minimum is at some other non-zero value of α, then the definition of GC can be suitably modified so that the above results are valid.

In the following sections we identify the GC for the three cases and relate $\hbar\,\omega$ to the relevant incompressibility coefficients

Our inputs are

(*i*) $H = \sum_i p_i^2/2m - \left(\sum_i p_i\right)^2/\,2\,Am + V$

and V is taken to be the Skyrme interaction (Vautherin and Brink 1972)
(*ii*) $\Phi\,(\alpha)$ is made up of 'scaled' harmonic oscillator wave functions with the cm coordinate constrained to be at the origin (Khadkikar and Nair 1975).

2. Breathing mode

The idea of using the oscillator length parameter b as a GC was considered earlier by Pal *et al* (1971). We use its scaling version by defining $b=b_0\,c^{\alpha}$ and α is then the GC (Khadkikar and Nair 1975); it was shown in this paper that for $N=Z$ closed shell nuclei, the inputs described above and (6) leads to

$$\hbar\,\omega_B = (\hbar^2\,\Gamma\,K_B\,A/m\,b_0^2)^{1/2}, \tag{7}$$

where the bulk incompressibility coefficient K_B is defined as

$$K_B = \frac{1}{A}\,b_0^2\,\frac{\partial^2}{\partial b^2}\,H(b, b)\bigg|_{b=b_0}. \tag{8}$$

We have now checked the validity of this result for $N \neq Z$ and partially closed (subshell closure) nuclei where the spin-orbit part of the Skyrme interaction gives a nonzero contribution. Since many experimental searches for the breathing mode have been on ^{208}Pb (Wambach *et al* 1977, Youngblood *et al* 1977) this is particularly relevant. Instead of working with ^{208}Pb, we take a simple model case of ^{8}He, with 2 protons occupying the $1s_{1/2}$ shell and 6 neutrons filling completely the $1s_{1/2}$ and $1p_{3/2}$ levels. From the point of view $N \neq Z$ and partial shell closure this example is very similar to ^{208}Pb. For this case we have the following results:

$$\Gamma = 2/29$$

$$B = \frac{\hbar^2}{\Gamma m b_0^2} + \frac{3}{4}\frac{S_0}{b_0^3} + \frac{15}{4}\frac{(S_1+S_2+S_3)}{b_0^5} + 6\,\frac{S_4}{b_0^6}, \tag{9}$$

$$C = \frac{15}{4}\frac{S_0}{b_0^3} + \frac{35}{4}\frac{(S_1+S_2+S_3)}{b_0^5} + 12\frac{S_4}{b_0^6},$$

$$K_B = \frac{1}{A}\left[\frac{3\hbar^2}{\Gamma m b_0^2} + \frac{12 S_0}{b_0^3} + \frac{30(S_1+S_2+S_3)}{b_0^5} + 42\frac{S_4}{b_0^6}\right], \tag{10}$$

and the self consistency condition

$$\frac{\partial}{\partial b} H(b, b) = 0,$$

implies
$$\frac{\hbar^2}{\Gamma m b_0^2} + \frac{3S_0}{b_0^3} + \frac{5(S_1+S_2+S_3)}{b_0^5} + \frac{6S_4}{b_0^6} = 0, \tag{11}$$

where
$$S_0 = \frac{t_0}{(2\pi^3)^{1/2}}\left(\frac{41}{3} - \frac{5}{3}X_0\right), \quad S_1 = \frac{91}{8(2\pi^3)^{1/2}}\,t_1,$$

$$S_2 = \frac{20\,t_2}{3(2\pi^3)^{1/2}}, \qquad S_3 = W_0/2,$$

$$S_4 = \frac{216}{81(3)^{1/2}}\frac{t_3}{\pi^3}.$$

In the above t_0, t_1, t_2, t_3, X_0 and W_0 are the Skyrme parameters (Vautherin and Brink 1972). Using these, the validity of the relation between the frequency and K_B is easily established.

Of the four sets of Skyrme parameters with nonzero t_3 term it is found that SIV gives the smallest K_B (Beiner *et al* 1975). For this set we list the values of $\hbar\omega_B$ for ^{16}O, ^{40}Ca and ^{208}Pb in table 1, column 1. Column 2 gives the values of $\hbar\omega_B$ calculated by a numerical solution of (2) with the same scaled $\Phi(\alpha)$. For comparison we also quote in column 3 the results of another study (Flocard and Vautherin 1976).

Table 1. Breathing mode energies (MeV)

Nucleus	1	2	3
^{16}O	33·35	31·35	30·24
^{40}Ca	29·7	28·3	27·22
^{208}Pb	17	16	—

The experimental value of $\hbar\omega_B$ for $^{208}Pb \approx 14$ MeV (Wambach *et al* 1977; Youngblood *et al* 1977). It was shown by Faessler's group (Krewald *et al* 1976) that a combination of ρ and $\rho^{2/3}$ dependent terms (instead of the three body term) can lower K_B sufficiently, and agree with the above experimental result. For ^{40}Ca our results give a value of 22·9 MeV as compared to Faessler *et al*'s result using ρ and $\rho^{2/3}$ dependent term which give 20·73 MeV. Faessler *et al* used a more elaborate constrained Hartree-Fock solution for $\Phi(\alpha)$, compared to our simple scaling approach. So the closeness of our results is gratifying.

3. Quadrupole mode

Flocard and Vautherin (1976) solved (2) numerically with the following scaled Φ

$$b_x = be^{\alpha}, \quad b_y = be^{\alpha}, \quad b_z = b\, e^{-2\alpha}.$$

The above results in a volume conserving quadrupole deformation.

Again with α as the GC, the results quoted in § 1 lead for ^4He to the following

$$\Gamma = 2/9,$$

$$B = \frac{2\hbar^2}{\Gamma m b_0^2} - \frac{3S_0}{b_0^3} - \frac{9S_1}{b_0^5} - \frac{6S_3}{b_0^6}, \tag{12}$$

$$C = \frac{3S_0}{b_0^3} + \frac{21\, S_1}{b_0^5} + \frac{6\, S_3}{b_0^6},$$

$$K_q \equiv \frac{1}{A}\frac{\partial^2}{\partial \alpha^2} H_q(\alpha, \alpha)\bigg|_{\alpha = 0} = \frac{1}{A}\left[\frac{18\,\hbar^2}{m b_0^2} + \frac{24\, S_1}{b_0^5}\right], \tag{13}$$

and the self consistency condition with reference to b gives

$$\frac{\hbar^2}{\Gamma m b_0^2} + \frac{3\, S_0}{b_0^3} + \frac{15\, S_1}{b_0^5} + \frac{6\, S_3}{b_0^6} = 0. \tag{14}$$

$$S_0 = \frac{3 \quad t_0}{(2\pi^3)^{1/2}} \quad S_1 = \frac{3 \quad t_1}{2(2\pi^3)^{1/2}} \quad S_3 = \frac{4 \quad t_3}{3(3)^{1/2}\, \pi^3}.$$

We also note that $\frac{\partial}{\partial a} H_q (a, a) = 0$. On substituting (12), (13) and (14) in (6) we arrive at the result.

$$\hbar\, \omega_q = \left(\frac{\hbar^2\, \Gamma\, K_q\, A}{2mb_0^2}\right)^{1/2}, \tag{15}$$

$$= (2)^{1/2}\, \hbar\, \omega \left(1 + \frac{6\, S_1\, \Gamma\, m}{\hbar^2\, b_0^3}\right)^{1/2},$$

$$\approx (2)^{1/2}\, \hbar\, \omega\, (1 + 0{\cdot}076). \tag{16}$$

The last approximate result is for the SIII set of Skyrme interaction. For other sets, the corrections are slightly larger. The approximate result that $\hbar\omega_q = (2)^{1/2}\, \hbar\omega$ was obtained several years ago by Mottelson (1958), Suzuki (1973) and recently by Golin and Zamick (1975) by different methods. The exact result in (15) was also obtained earlier using the sum rule method by Brink and Leonardi (1976) and by Bohigas *et al* (1979). From general arguments, earlier Bohigas *et al* (1976) had shown that a version of the sum rule method in RPA and the scaled version of the harmonic GCM give identical results. Hence our GCM result in (16) is only to be expected. Though we have demonstrated explicitly here for ^{4}He, (15) is of general validity.

We have included it here for completeness as well as to bring out a certain kind of universality in relationship between $\hbar\,\omega_c$ and the relevant K, in the scaling version of GCM. As we shall see in the next section, for spin modes as well we could expect a similar result.

4. A spin mode

There is a good deal of interest currently in the study of the properties (position, width, etc) of giant $M1$ resonance in ^{208}Pb and in other nuclei. Though we have not yet identified the relevant GC for $M1$ mode, we have studied a possible spin-dependent mode in ^{4}He as an illustrative example. Here we use a spin-dependent scaling parameter as the GC. The $\Phi\,(a)$ is taken as

$$\Phi\,(a) = \frac{1}{(4!)^{1/2}}\, \mathscr{A}\, \{\phi_p\,(r_1, b_+) \uparrow \phi_p\,(r_2, b_-) \downarrow \phi_n\,(r_3, b_+) \uparrow \phi_n\,(r_4, b_-)\}, \tag{17}$$

where $\mathscr{A}$ is the usual antisymmetrisation operator and $\downarrow$ and $\uparrow$ stand for $m_s = \frac{1}{2}$ and $m_s = -\frac{1}{2}$ spin states. Also,

$$\phi\,(r_1, b_+) = \frac{2}{((\pi)^{1/2}\, b_+^3)^{1/2}} \exp\,(-r_1^2/2\, b_+^2) \tag{18}$$

and similarly for $\phi\,(r_2, b_-)$ with

$$b_\pm = b_0 \exp^{(\pm a)}.$$

By explicit operation with spin and isospin raising or lowering operators it is easy to see that the above $\Phi(\alpha)$ has a component with $S=2$, $m_s=0$ and $T=1$ and $T_z=0$ quantum numbers for $\alpha \neq 0$. For $\alpha=0$ of course it has S=0 and T=0. Proceeding along identical lines as before, we have

$$\Gamma = 2/9,$$

$$B = \frac{\hbar^2}{\Gamma m b_0^2} + \frac{t_0}{4(2\pi^3)^{1/2} b_0^3}(-21 + 15 X_0) - \frac{27}{8}\frac{t_1}{(2\pi^3)^{1/2} b_0^5} + \frac{6}{(2\pi^3)^{1/2}}\frac{t_2}{b_0^5} - \frac{40}{9(3)^{1/2}}\frac{t_3}{\pi^3 b_0^6},$$

$$C = \frac{t_0\, 15(1+X_0)}{4(2\pi^3)^{1/2} b_0^3} + \frac{105}{8(2\pi^3)^{1/2}}\frac{t_1}{b_0^5} + \frac{32}{9(3)^{1/2}}\frac{t_3}{\pi^3 b_0^6}, \tag{19}$$

$$K_S = \frac{1}{A}\frac{\partial^2}{\partial \alpha^2} H_S(\alpha, \alpha)\Big|_{\alpha=0},$$

and the same self consistency condition as in § 3 with reference to b $\left(\text{again } \frac{\partial}{\partial\alpha} H_S(\alpha, \alpha) = 0\right)$ lead to

$$\hbar\omega_S = \left(\frac{\hbar^2 \Gamma A K_S (1 + S_{12})}{m b_0^2}\right)^{1/2}, \tag{20}$$

$$S_{12} = \frac{3\Gamma m (t_1 + t_2)}{(2\pi^3)^{1/2}\hbar^2 b_0^3}.$$

S_{12} is negligibly small for the sets SII, SIII and SVI.

So the scaling version of harmonic GCM seems to result in the same kind of relationship as the one for the adiabatic speed of ordinary sound in terms of the bulk modulus. This is the kind of universality we were referring to in § 3.

We list in table 2 the values of K_S for the four sets of Skyrme parameters. We see that K_S is in general small and for the set SVI it is even negative and this implies that there is no minimum for $H(\alpha, \alpha)$ at α=0. This is reminiscent of the results of Chang

Table 2. Spin mode incompressibility coefficients and energies (MeV)

1	2		3	
	K_S	$E=\hbar\omega_S$	K_S	$E=\hbar\omega_S$
SII	57·9	30·7	122	44·6
SIII	19	17·5	113·8	43
SIV	127	45	161·5	51·3
SVI	−15·5	—	100	40·5

in his study of the binding energies of the ground state ($S=1$) of ^{14}N and a spin polarised state of ^{16}O. Even when K_S is positive, the small values imply a relatively low lying state for the set II in addition to set III. From Chang's study SII was considered good (free from this pathology). But here from the point of view of predicting a relative low $S=2$, $T=1$ state also seems not very satisfactory. We must here mention that so far there has been no experimental evidence for such states. However very recently a 2^+ resonance at 40 MeV has been discovered in $^3H(p, \gamma)\,^4He$ and $^4He(e, ^3H)\,pe'$ reaction (McBroom *et al* 1980). Perhaps radiative capture of deutrons by deutrons ($d(d, ^4He)\,\gamma$) is another way to look for a $S=2$ state in ^4He. Being a very light nucleus, the harmonic approximation for the excitation energy may not at all be reliable and so our study have of ^4He has only an illustrative value.

A possible cure for the above pathological result of being negative is the replacement of the three-body terms in the Skyrme interaction by a linear density dependent one (Chang 1975). In column (3) of table 2 we list the corresponding values of K_S. Though K_S is small, it is no longer negative. A good test of the above cure would be to study $M1$ mode with the density-dependent replacement in the three body term. In the GCM since we need off-diagonal densities as well *i.e.* $\rho(a', a)$, we may have to approximate it by say, an averaged density $\rho\left(\frac{a'+a}{2}, \frac{a+a'}{2}\right)$.

It is also worth exploring the possibilities of scaling or other simple versions of $\Phi(a)$ for the description of other nuclear collective modes like $E1$, $E3$, etc. If such relations as (7) emerges, we would have achieved a real unification of simple but strictly quantal descriptions of collective modes in nuclei.

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