Anharmonic vibrations in nuclei

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In this letter, we show that the non-linearities of large amplitude motions in atomic nuclei induce giant quadrupole and monopole vibrations. As a consequence, the main source of anharmonicity is the coupling with configurations including one of these two giant resonances on top of any state. Two-phonon energies are often lowered by one or two MeV because of the large matrix elements with such three phonon configurations. These effects are studied in two nuclei, ^{40}Ca and ^{208}Pb.
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Many-body fermionic systems possess collective vibrational states which are well described as bosonic modes (phonons). The existence in atomic nuclei of such states, both low-lying and Giant Resonances (GR) is now well established up to the second quantum [1,2]. However, their properties such as energy and excitation probability are still open questions. From the experimental point of view the strong excitation cross section of two phonon states calls for the presence of large anharmonicities but up to now, all the theoretical estimates were pointing to weak deviations from a harmonic spectrum. To our knowledge, so far only the mixing of one- and two-phonon states has been considered in microscopic calculations, with two exceptions. In ref. [3] the coupling to some specific three-phonon configurations has been included as a mechanism generating the damping width of the Double Giant Dipole Resonance. In ref. [4] the fragmentation of the doubly excited low lying octupole states in ^{208}Pb has been studied by allowing the coupling to one- and three-phonon configurations with a low energy cut-off introduced to reduce the diagonalization space. For this reason monopole, (GMR) and quadrupole (GQR) contributions which, as we will see, play an important role, were neglected.

In the present paper we show that a correct description of the states for which the main component is a two-phonon configuration requires the inclusion of one- and three-phonon ones. We stress the essential role played by the breathing mode in the nuclear anharmonicity as an important novelty of the present analysis since volume modes are usually not considered in damping or coupling mechanisms. Moreover, we will show that the very collective GQR plays also an important role.

The starting point of our calculation is a mapping of the fermion particle-hole operators $a_p^\dagger a_h$ into boson operators $B_{ph}^\dagger$ as for example the one proposed in ref. [5]

$$a_p^\dagger a_h \rightarrow B_{ph}^\dagger + (1 - \sqrt{2}) \sum_{p'h'} B_{p'h'}^\dagger B_{p'h}^\dagger B_{ph'} + ... \quad (1)$$

$$a_p^\dagger a_{p'} \rightarrow \sum_h B_{ph}^\dagger B_{p'h} \ , \ \ a_h a_{h'}^\dagger \rightarrow \sum_p B_{ph}^\dagger B_{ph'} \quad (2)$$

where $a^\dagger$ (a) creates (annihilates) one nucleon in an occupied (h) or unoccupied (p) single particle state. The second term on the right hand side of eq.(1) is a correction that takes care of the Pauli principle. Then we construct a boson image of the Hamiltonian, truncated at the fourth order in the $B^\dagger$ and B operators. Introducing the Bogoliubov transformation for bosons:

$$Q_\nu^\dagger \equiv \sum_{p,h} (X_{ph}^\nu B_{ph}^\dagger - Y_{ph}^\nu B_{ph}) \quad (3)$$

and imposing that the quadratic part of the boson Hamiltonian in the new operators is diagonal, we obtain the usual Random Phase Approximation (RPA) equations for the X and Y amplitudes.

By inverting eq.(3) we can express H_B in terms of the collective $Q^\dagger$ and Q operators:

$$\begin{aligned}
H_B = {}& \mathcal{H}_{11} Q^\dagger Q + (\mathcal{H}_{21} Q^\dagger Q^\dagger Q + h.c.) + \mathcal{H}_{22} Q^\dagger Q^\dagger Q Q \\
& + (\mathcal{H}_{30} Q^\dagger Q^\dagger Q^\dagger + h.c.) + (\mathcal{H}_{31} Q^\dagger Q^\dagger Q^\dagger Q + h.c.) \\
& + (\mathcal{H}_{40} Q^\dagger Q^\dagger Q^\dagger Q^\dagger + h.c.) + \ldots
\end{aligned} \quad (4)$$

with $\mathcal{H}_{11}^{\nu\nu'} = E_\nu \delta_{\nu\nu'}$. The $\mathcal{H}$ matrices are expressed in terms of the X and Y of transformation (3). The contributions to eq.(4) coming from the high order terms of the expansion (1) appear to be reduced by the number of configurations involved in the collective states and therefore can be neglected. In the case of closed shell nuclei, the RPA correlations are moderate. Therefore, the Y/X ratios are small. In eq.(4) we will neglect the $\mathcal{H}$ terms containing at least one Y amplitude. These two approximations leave unaffected only the first three terms of eq.(4) [6]. We will compare the spectra of ^{40}Ca and ^{208}Pb obtained by the diagonalization in the spaces containing up to two-phonon states and up to three-phonon states, respectively. In ref. [7] a similar analysis was done in the two level Lipkin model. It was found that this approximation is well justified and one gets good results in the larger space for the eigenstates which main component is a two-phonon configuration.

All calculations have been performed by using the SGII Skyrme interaction [8]. We include all natural parity

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RPA collective one-phonon states with angular momentum $J \leq 3$ which exhaust at least 5% of the EWSR and all two- and three-phonon configurations built with them, without any energy cut-off, with both natural and unnatural parity.

Let us start looking at the results for ^{40}Ca. In table I we show the one-phonon states taken into account. In table II we show some results of the diagonalization for a selected set of states. The energies obtained in the space up to two-phonons (see ref. [9]) are reported here for comparison. The so-calculated anharmonicity was limited to a few hundred keV. Let us now study the more complete calculation including the three phonon states.

As a general comment, one can say that the shift induced by the coupling to three-phonon states is fairly large, being in almost all the cases more than 1 MeV, and always downward. This can be understood in second order perturbation which, as can be seen from the table, gives a good estimate for the energies in most cases. In second order perturbation the correction to the energy is given by

$$\Delta E_i = <\varphi_i|V|\varphi_i> + \sum_{j \neq i} \frac{|<\varphi_j|V|\varphi_i>|^2}{E_i^0 - E_j^0} \qquad (5)$$

where $|\varphi_i>$ is the considered unperturbed state, $|\varphi_j>$ all the other states and E^0 the corresponding unperturbed energies. Since the diagonal, first order, contribution is small in most cases, the sign of the shift is that of the denominator in the second order term. Therefore, if $|\varphi_i>$ is a two-phonon state, the contributions from three-phonon configurations are negative in most cases since most of the three phonon states lye above the two phonon ones. Moreover, whenever a GMR is added on top of any state, the $\mathcal{H}_{21}$ terms (see eq.4) are large , of the order of 1 to 2 MeV in ^{40}Ca. The specific values can be found in the last three columns of table I. Indeed, in the coupling leading to the addition of one GMR on top of any state, the residual interaction between the underlying fermions is not truncated by conservation laws, because the particles and the holes involved in the GMR carry identical parity and spin quantum numbers (cf. ref. [10]). Phenomenologically, this strong coupling of all collective vibrations with the breathing mode comes from the fact that in a small nucleus like the ^{40}Ca any large amplitude motion affects the central density. Therefore, surface modes cannot be decoupled from a density variation in the whole volume as clearly seen in recent TDHF simulations ref. [11].

If the state is a two-phonon one, then the matrix elements coupling it to the state obtained by exciting a breathing mode on top of it are about 3 MeV (up to 5.5 MeV) when the less (more) collective component of the ^{40}Ca GMR is considered. Even larger matrix elements are obtained, when the states connected by $\mathcal{H}_{21}$ involve several GMR. In that case a Bose enhancement factor

appears and no Clebsch-Gordan coefficients enter in the calculation. Thus the matrix element between the double and the triple GMR located at 18.25 MeV, M_1, is $\sqrt{6}$ times larger than between the single and the double M_1. That gives a matrix element of -5.22 MeV, giving a contribution of -1.49 MeV to the second order energy correction of the double M_1 state. An even larger value comes out in the case of the double GMR located at 22.47 MeV, M_2, and the triple M_2, namely a matrix element of -9.69 MeV giving a -4.18 MeV contribution to the energy shift of the double M_2. This is due to the fact that M_2 is more collective than M_1 in ^{40}Ca.

Something similar, but less strong, happens also for the matrix elements connecting some state with that built by adding one GQR phonon. We quote two examples. The low-lying component of the Giant Dipole Resonance $|D_1>$ has a matrix element of the residual interaction with the states $|D_1 \otimes M_1>$, $|D_1 \otimes M_2>$ and $|D_1 \otimes Q_1>$ equal to -1.38 MeV, -2.12 MeV and -1.25 MeV respectively. Another example, with total $J=1$, is given by the matrix elements between $|D_1 \otimes Q_1>$ and $|(M_1 \otimes D_1)_1 \otimes Q_1>$, $|(M_2 \otimes D_1)_1 \otimes Q_1>$ and $|(Q_1)_2^2 \otimes D_1>$ equal to -2.74 MeV, -4.61 MeV and -1.41 MeV respectively.

These findings clearly indicate that large amplitude motions are strongly coupled both to surface and volume oscillations, the latter being more important in ^{40}Ca. It is worthwhile stressing that such large corrections to the energy of two-phonon states are obtained despite the quite large absolute values of the energy difference between the coupled states. Therefore, introducing an energy cut-off in the three-phonon states included in the calculation may lead to erroneous results. Let us consider for example the case of the 0^+ member of the multiplet of double low-lying octupole states. At first order perturbation, it is shifted up by 2.24 MeV. The second order correction coming from the single GMR states is -0.93 MeV. These two contributions, leading to a total shift of +1.31 MeV, dominate the effects of the coupling with one- and two-phonon states as confirmed by the result of the diagonalization in this subspace. When three-phonon states are included, one gets a further shift down of 1.86 MeV coming from the configuration including a GMR on top of the two octupoles. This contribution is absent in ref. [4] because the energy cut-off introduced there in order to reduce the number of three-phonon configurations was too low. The same happens for the other members of the multiplet as well as for the double D_1 or D_2, the double Q_1 and the D_1 or $D_2 \otimes Q_1$ states.

The results for ^{208}Pb are shown in tables III and IV. The same general remarks already made for ^{40}Ca apply also in this case. The most relevant difference is that the role played by the GMR and the GQR in ^{40}Ca is now inverted, the latter being dominant in ^{208}Pb. This reduced importance of the GMR may come from the fact that in large nuclei the surface vibrations can occur without

changing the volume. Concluding about the energy of the two-phonon states one can see that the inclusion of the three phonon configurations induces an anharmonicity of more than 1 MeV in ^{40}Ca but only of a few hundred keV in ^{208}Pb. Because of the location at high energy of the three phonon states, the observed shift is systematically downward. It is important to stress that the considered residual interaction only couples states with a number of phonon varying at maximum by one unit. Therefore, the energy variation of the two-phonon spectrum induced by inclusion of four and more phonon states would be small since it corresponds to a third order perturbation involving two large energy differences in the denominator.

If we now analyze the splitting of the two-phonon multiplets we can see that it remains small for giant resonances (about a few hundred keV) while it may go up to 1 MeV for low lying states in ^{40}Ca. Comparing the splitting and the ordering of the states obtained in first order perturbation and in the full calculation we can see that they remain almost unchanged. Therefore, the diagonal matrix elements of the residual interaction are responsible for this splitting and ordering.

Let us now investigate the mixing induced by the residual interaction. In tables II and IV the mixing coefficients of the two main components in each state are presented. First we can see that there is always one component that remains very large, explaining the success of the perturbation approach. The important point is that in general we observe large mixing coefficients, namely about 0.2 to 0.4 or more in ^{40}Ca and 0.15 to 0.3 in ^{208}Pb. This may have very important consequences in the excitation process as we will investigate in a forthcoming work.

It is worthwhile mentioning that, in some cases, a three-phonon component appears with a large amplitude in the wave function of a (mainly) two-phonon state, despite the fact that the residual interaction does not couple directly these configurations together. In a few cases, indeed, this is the second main component as can be seen for ^{40}Ca in table II (the $|(D_1)^2_0>$ and $|M_2 \otimes Q_1>$ states) and for ^{208}Pb in table IV (the $|(M_1)^2>$ state). This happens because the diagonal matrix elements of the Hamiltonian in the two-phonon and three-phonon configurations are close and the matrix elements coupling the latter with other configurations are large. A similar situation has been found in ^{208}Pb for two one-phonon (mainly) states which have a three-phonon configuration as second important component, even though our Hamiltonian does not couple directly states which numbers of phonons differ by more than one. This is the case for the state which main component is $|M_1>$, with amplitude $c_0 = -0.79$, and for which the second most important component is $|(3^-)^2_2 \otimes 2^+>$ with $c_1 = 0.55$. Both components have large matrix elements with the two-phonon state $|(3^-)^2_0>$. How this mixing of the monopole resonance may affect the monopole response, and so the usual conclusion about the compressibility, is now un-

der study. The other case is the single high energy octupole resonance $|O>$ which is strongly mixed with the states $|(2^+ \otimes 3^-)_J \otimes Q_1>$. The energy of these states are, however, shifted by less than 100 keV. This is coherent because the strong mixing is coming from a quasi degeneracy of the considered states.

Summarizing, the spectrum of two-phonon states is strongly modified by their coupling to the three-phonon ones. All of the states appear mixed with the excitation of a GMR and GQR on top of it. This is due to the fact that most of the matrix elements of $\mathcal{H}_{21}$ coupling a phonon with the same phonon plus a GMR or a GQR are large. Moreover, because of the Bose enhancement factors, the effect of $\mathcal{H}_{21}$ between the two and three phonon states is even larger. It is also to be noted that many of the important three-phonon states are higher in energy than the two-phonon ones. Therefore, they induce a systematic shift down of the two phonon states as the sum of several quite large negative contributions. This unexpected finding can be understood as a modification of the central density in large amplitude motion leading to an excitation of the breathing mode. The case of the GQR seems to be related to the extreme collectivity of this state leading to a strong quadrupole response to the quadrupole component of the non-linearities of the mean-field. We also want to stress that, because of the perturbative nature of the observed phenomenon, the possible introduction of four-phonon states should not modify the above conclusions about two phonon states. Of course, our findings imply that in order to get a correct three-phonon spectrum one should further enlarge the space up to four-phonons. This is a formidable task which is beyond the scopes of the present paper.

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TABLE I. RPA one-phonon basis for ^{40}Ca. For each state, spin, parity, isospin, energy and percentage of the EWSR are reported. In the following columns, V_{M_1} stands for the matrix element $<\nu|V|\nu \otimes M_1>$, where ν is the one phonon in the 1st column, the same for V_{M_2} and V_{Q_1}.

Phonons	J^π T	$E(MeV)$	$\%EWSR$	$V_{M_1}(MeV)$	$V_{M_2}(MeV)$	$V_{Q_1}(MeV)$
M_1	0^+ 0	18.25	30	-2.13	-2.36	$-$
M_2	0^+ 0	22.47	54	-2.03	-3.96	$-$
D_1	1^- 1	17.78	56	-1.38	-2.12	-1.25
D_2	1^- 1	22.03	10	-1.48	-2.16	$+0.73$
Q_1	2^+ 0	16.91	85	-1.36	-2.49	-0.36
Q_2	2^+ 1	29.59	26	-1.70	-2.85	-0.00
3^-	3^- 0	4.94	14	-1.74	-2.60	-0.07
O_1	3^- 0	9.71	5	-1.42	-2.28	-0.43
O_2	3^- 0	31.33	25	-1.69	-2.72	-0.31

TABLE II. Results for ^{40}Ca. In the first column, the states are labelled by their main component in the eigenvector and their unperturbed energy (in parentheses). In the second column, the amplitude of the main component c_0. Then for each total angular momentum J, we show the results of the calculation in the basis up to 2 phonon states, the present results for the basis extended to 3 phonon states, the corresponding first order perturbation theory energy, and the second order one. The last two columns contain the 2nd main component in the eigenstates and the corresponding amplitude c_1. The subindex in the two-phonon configurations denotes J. All energies are given in MeV.

Main component	c_0	J^π	$\leq 2ph$	$\leq 3ph$	1st order	2nd order	$2^{nd}{}_{main}$ component	c_1
$3^-\otimes 3^-$ (9.88)	-0.91	0^+	10.96	9.27	12.12	9.20	M_1	0.21
	-0.96	2^+	10.63	8.89	10.66	8.75	$(3^-)^2_2 \otimes M_2$	-0.21
	-0.96	4^+	9.85	8.10	9.86	7.96	$(3^-)^2_4 \otimes M_2$	-0.21
	-0.96	6^+	10.88	9.12	10.88	8.99	$(3^-)^2_6 \otimes M_2$	-0.21
$D_1\otimes D_1$ (35.56)	-0.92	0^+	35.27	33.71	35.25	33.59	$(3^-)^2_0 \otimes M_2$	-0.22
	-0.96	2^+	35.10	33.66	35.06	33.59	$(D_1)^2_2 \otimes M_2$	-0.17
$D_1\otimes Q_1$ (34.69)	0.95	1^-	34.83	33.35	34.72	33.24	$(M_2\otimes D_1)_1\otimes Q_1$	0.19
	0.96	2^-	34.56	33.22	34.56	33.16	$(M_2\otimes D_1)_1\otimes Q_1$	0.19
	-0.96	3^-	34.67	33.13	34.67	33.02	$(M_2\otimes D_1)_1\otimes Q_1$	-0.19
$Q_1\otimes Q_1$ (33.82)	-0.87	0^+	33.88	32.47	33.83	32.27	$(Q_1\otimes 3^-)_3\otimes O_1$	0.32
	0.84	2^+	33.82	32.47	33.82	32.26	$(Q_1\otimes 3^-)_5\otimes O_1$	-0.38
	0.90	4^+	34.02	32.61	34.02	32.44	$(Q_1\otimes 3^-)_5\otimes O_1$	-0.32
$M_2\otimes D_1$ (40.25)	-0.89	1^-	40.26	38.14	40.05	37.65	$(M_2)^2_0 \otimes D_1$	0.26
$M_2\otimes Q_1$ (39.38)	-0.73	2^+	39.62	37.34	39.35	36.80	$(O_1)^2_2 \otimes M_1$	0.40
$M_2\otimes M_2$ (44.94)	0.67	0^+	45.60	42.76	44.87	41.18	$(O_1)^2_0 \otimes M_2$	-0.55

TABLE III. Same as table I for the nucleus ^{208}Pb.

Phonons	J^π T	$E(MeV)$	$\%EWSR$	$V_{M_1}(MeV)$	$V_{M_2}(MeV)$	$V_{Q_1}(MeV)$
M_1	0^+ 0	13.61	61	-1.87	-0.92	$-$
M_2	0^+ 0	15.02	28	-1.32	-1.16	$-$
D_1	1^- 1	12.43	63	-0.79	-0.59	-0.68
D_2	1^- 1	16.66	17	0.00	0.00	-0.64
2^+	2^+ 0	5.54	15	-0.11	0.07	-1.18
Q_1	2^+ 0	11.60	76	-0.64	-0.48	-0.74
Q_2	2^+ 1	21.81	45	-0.86	-0.63	-0.55
3^-	3^- 0	3.46	21	-1.13	-0.62	-0.90
O	3^- 0	21.30	37	-0.99	-0.74	-0.42

TABLE IV. Same as table II for the ^{208}Pb nucleus.

Main component	c_0	J^π	$\leq 2ph$	$\leq 3ph$	1st order	2nd order	$2^{nd}{}_{main}$ component	c_1
$3^-\otimes 3^-$ (6.93)	-0.95	0^+	7.88	6.96	8.06	6.90	$(3^-)^2_0 \otimes 2^+$	-0.17
	-0.92	2^+	7.31	6.57	7.33	6.52	2^+	-0.28
	-0.98	4^+	7.16	6.55	7.16	6.51	$(3^-)^2_4 \otimes M_1$	-0.15
	0.97	6^+	7.43	6.63	7.44	6.56	$(3^-)^2_6 \otimes M_1$	0.15
$3^-\otimes 2^+$ (9.01)	-0.94	1^-	9.20	8.26	9.21	8.02	$(2^+)^2_2 \otimes 3^-$	-0.23
	0.97	2^-	9.12	8.54	9.12	8.50	$(2^+)^2_2 \otimes 3^-$	0.17
	0.96	3^-	9.17	8.70	9.12	8.56	$(3^-)^3_2$	-0.17
	0.96	4^-	9.07	8.61	9.07	8.45	$(3^-)^3$	0.19
	-0.96	5^-	9.06	8.33	9.06	8.16	$(2^+)^2_2 \otimes 3^-$	-0.18
$2^+\otimes 2^+$ (11.09)	0.92	0^+	11.23	9.88	11.24	9.46	$(2^+)^3$	-0.31
	-0.94	2^+	11.27	10.78	11.12	10.61	$(3^-)^2_2 \otimes 2^+$	0.24
	0.94	4^+	11.25	10.39	11.25	10.13	$(2^+)^3$	0.24
$D_1\otimes D_1$ (24.87)	0.97	0^+	24.91	24.42	24.90	24.40	$(D_1)^2_0 \otimes M_1$	0.11
	0.96	2^+	24.68	24.29	24.68	24.27	$3^-\otimes O$	0.19
$D_1\otimes Q_1$ (24.03)	-0.96	1^-	24.07	23.73	24.02	23.71	$(3^-)_2 \otimes D_1$	0.17
	0.98	2^-	23.97	23.82	23.97	23.80	$(3^-)^2_2 \otimes D_1$	-0.16
	0.96	3^-	24.03	23.74	24.03	23.71	$(2^+)^2_2 \otimes D_1$	0.18
$Q_1\otimes Q_1$ (23.20)	-0.94	0^+	23.20	22.92	23.20	22.86	$(3^-)^2_2 \otimes Q_1$	-0.24
	0.95	2^+	23.23	23.17	23.18	23.14	$(3^-)^2_2 \otimes Q_1$	0.22
	-0.95	4^+	23.26	23.10	23.26	23.07	$(3^-)^2_2 \otimes Q_1$	-0.22
$M_1\otimes D_1$ (26.05)	-0.94	1^-	26.05	25.35	26.02	25.28	$(M_1)^2_0 \otimes D_1$	-0.20
$M_1\otimes Q_1$ (25.21)	-0.92	2^+	25.25	24.77	25.22	24.66	$(3^-)^2_2 \otimes M_1$	-0.20
$M_1\otimes M_1$ (27.22)	0.74	0^+	27.52	26.23	27.28	25.95	$(2^+)^2_0 \otimes M_2$	0.54