Consequences of self-consistency violations in Hartree-Fock random-phase approximation calculations of the nuclear breathing mode energy

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Abstract

We provide for the first time accurate assessments of the consequences of violations of self-consistency in the Hartree-Fock based random phase approximation (RPA) as commonly used to calculate the energy E_c of the nuclear breathing mode. Using several Skyrme interactions we find that the self-consistency violated by ignoring the spin-orbit interaction in the RPA calculation causes a spurious enhancement of the breathing mode energy for spin unsaturated systems. Contrarily, neglecting the Coulomb interaction in the RPA or performing the RPA calculations in the TJ scheme underestimates the breathing mode energy. Surprisingly, our results for the ^{90}Zr and ^{208}Pb nuclei for several Skyrme type effective nucleon-nucleon interactions having a wide range of nuclear matter incompressibility ($K_{nm} \sim 215 - 275$ MeV) and symmetry energy ($J \sim 27 - 37$ MeV) indicate that the net uncertainty ($\delta E_c \sim 0.3$ MeV) is comparable to the experimental one.

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The Hartree-Fock (HF) based random phase approximation (RPA) provides a microscopic description of the nuclear compressional modes. The most special of these compressional modes is the isoscalar giant monopole resonance (ISGMR) also referred to as the breathing mode. The centroid energy E_c of the ISGMR enables one to determine the value of nuclear matter incompressibility coefficient K_{nm} which plays an important role in understanding a wide variety of phenomena ranging from heavy-ion collision to supernova explosions. Recent experimental data [1] for the E_c in heavy nuclei have rather small uncertainties ($\sim 0.1 - 0.3$ MeV). Since, the uncertainty δE_c associated with E_c is approximately related to the uncertainty δK_{nm} in K_{nm} by,

$$\frac{\delta K_{nm}}{K_{nm}} = 2\frac{\delta E_c}{E_c}, \tag{1}$$

the value of δK_{nm} is only about 10 MeV, for $K_{nm} = 250$ MeV and $E_c = 14.17 \pm 0.28$ MeV for the ^{208}Pb nucleus. On the theoretical side, most of the results obtained within the HF-RPA theory, as employed for the determination of E_c, are plagued by the lack of self-consistency, see however, Ref. [2]. Self-consistency is violated due to the neglect of the spin-orbit and Coulomb terms in the particle-hole interaction used in the RPA calculations. Furthermore, some of the RPA calculations are performed in the TJ (isospin) scheme. Uncertainties in the value of E_c calculated in the HF-RPA approach arise also due to various numerical approximations such as the use of very small particle-hole excitation energies and the introduction of the smearing parameter Γ to smoothen the strength function. In Ref. [3], we have investigated in detail the effects of these numerical approximations and emphasized the need to perform a highly accurate calculation of the strength function. So, it is of utmost importance that in order to determine an accurate value of K_{nm} one must have an accurate knowledge of the effects of violations of self-consistency on the centroid energy of the ISGMR. We may also point out that modifying the particle-hole interaction in an ad hoc manner in such a way that the spurious state associated with the center of mass motion appears at zero energy [4] does not restore the self-consistency (see also Ref. [3]).

In this work we provide for the first time accurate assessments of the effects of violations of self-consistency on the constrained and the scaling energies,

$$E_{con} = \sqrt{\frac{m_1}{m_{-1}}}, \qquad \text{and} \qquad E_s = \sqrt{\frac{m_3}{m_1}}, \tag{2}$$

of the ISGMR. Here

$$m_k = \int_0^\infty \omega^k S(\omega) d\omega \tag{3}$$

is the energy moments of the strength function

$$S(\omega) = \sum_n |\langle n \mid f \mid 0 \rangle|^2 \delta(\omega - \omega_n), \tag{4}$$

for the monopole operator $f(r) = \sum_{i=1}^{A} r_i^2$.

In the following the fully self-consistent and highly accurate values of the constraint energy, E_{con}, and the scaling energy, E_s, are obtained by calculating the energy moments m_k for $k = -1, 1$ and 3 using the constrained HF (CHF), the double commutator and the generalized scaling approaches, respectively [5]. The self-consistent values of E_{con} and E_s are then compared with those obtained within the HF-RPA approach [3, 4] in order to assess the effects of each type of violation of self-consistency. It may be pointed out that very recently in Ref. [6] some preliminary attempts are made to estimate the effects of self-consistency violation on the value of E_{con}. However, E_s was not considered and the different components contributing to the self-consistency violations are not dealt separately. We show here that the appropriate knowledge of the effects of each of these components on the ISGMR energies are instrumental in validating the HF-RPA calculations.

We consider here the HF solution for the Hamiltonian,

$$H = \sum_{i=1}^{A} T_i + \frac{1}{2} \sum_{i,j=1}^{A} V_{ij} + \frac{1}{2} \sum_{i,j=1}^{Z} V_{ij}^C, \tag{5}$$

where T is the kinetic energy operator, V^C is the Coulomb interaction and V is the effective two-body interaction of the Skyrme type [7],

$$\begin{aligned}
V_{12} &= t_0 \left(1 + x_0 P_{12}^\sigma\right) \delta(\mathbf{r}_1 - \mathbf{r}_2) \\
&+ \frac{1}{2} t_1 \left(1 + x_1 P_{12}^\sigma\right) \times \left[\overleftarrow{k}_{12}^2 \delta(\mathbf{r}_1 - \mathbf{r}_2) + \delta(\mathbf{r}_1 - \mathbf{r}_2) \overrightarrow{k}_{12}^2 \right] \\
&+ t_2 \left(1 + x_2 P_{12}^\sigma\right) \overleftarrow{k}_{12} \delta(\mathbf{r}_1 - \mathbf{r}_2) \overrightarrow{k}_{12} \\
&+ \frac{1}{6} t_3 \left(1 + x_3 P_{12}^\sigma\right) \rho^\alpha \left(\frac{\mathbf{r}_1 + \mathbf{r}_2}{2}\right) \delta(\mathbf{r}_1 - \mathbf{r}_2) \\
&+ i W_0 \overleftarrow{k}_{12} \delta(\mathbf{r}_1 - \mathbf{r}_2)(\overrightarrow{\sigma_1} + \overrightarrow{\sigma_2}) \times \overrightarrow{k}_{12}, \tag{6}
\end{aligned}$$

where P_{12}^σ is the spin exchange operator, $\overrightarrow{\sigma}_i$ is the Pauli spin operator, $\overrightarrow{k}_{12} = -i(\overrightarrow{\nabla}_1 - \overrightarrow{\nabla}_2)/2$ and $\overleftarrow{k}_{12} = -i(\overleftarrow{\nabla}_1 - \overleftarrow{\nabla}_2)/2$. Here, the right and left arrows indicate that the momentum operators act on the right and on the left, respectively. The parameters of the Skyrme force t_i, x_i, α and W_0 are obtained by fitting the HF results to the experimental data for the bulk properties of finite nuclei.

Once the HF equations are solved, the m_1 and m_3 can be expressed in terms of the ground state density ρ, kinetic energy density τ and spin density $\mathbf{J}$. The value of m_1 can be obtained from the corresponding double commutator [8] and is given as,

$$m_1 = 2\frac{\hbar^2}{m}\langle r^2 \rangle, \tag{7}$$

where,

$$\langle r^2 \rangle = \int r^2 \rho(r) d\mathbf{r}. \tag{8}$$

The cubic moment m_3 can be evaluated in the generalized scaling approach and it is given by[5, 9],

$$
\begin{aligned}
m_3 = \ & \frac{1}{2}\left(\frac{2\hbar^2}{m}\right)^2 [2T + 6E_\delta + 20(E_{fin} + E_{so}) + \\
& (3\alpha + 2)(3\alpha + 3)E_\rho],
\end{aligned}
\tag{9}
$$

where,

$$T = \int \frac{\hbar}{2m}\tau d\mathbf{r}, \tag{10}$$

$$E_\delta = \int \left[\frac{3}{8}t_0\rho^2 - \frac{1}{4}t_0(x_0 + \frac{1}{2})\rho_1^2\right] d\mathbf{r} \tag{11}$$

$$E_{fin} = \int \left[a_0\rho\tau + a_1\rho_1\tau_1 + c(\nabla\rho)^2 + d(\nabla\rho_1)^2\right] d\mathbf{r} \tag{12}$$

$$E_\rho = \int \left[\frac{3}{48}t_3\rho^{\alpha+2} - \frac{1}{24}t_3(x_3 + \frac{1}{2})\rho^\alpha\rho_1^2\right] d\mathbf{r} \tag{13}$$

$$E_{so} = -\frac{1}{2}W_0 \int \left[\rho\nabla \cdot \mathbf{J} + \rho_p\nabla \cdot \mathbf{J}_p + \rho_n\nabla \cdot \mathbf{J}_n\right] d\mathbf{r} \tag{14}$$

with $\rho_1 = \rho_n - \rho_p$, $\tau_1 = \tau_n - \tau_p$, $a_0 = \frac{1}{16}(3t_1 + (5 + 4x_2)t_2)$, $a_1 = \frac{1}{8}t_2(x_2 + \frac{1}{2}) - t_1(x_1 + \frac{1}{2})$, $c = \frac{1}{64}(9t_1 - (5 + 4x_2) + t_2)$ and $d = -\frac{1}{32}(3t_1(x_1 + \frac{1}{2}) + t_2(x_2 + \frac{1}{2}))$. As described in detail in Ref. [5], m_{-1} can be evaluated via the CHF approach and is given as,

$$m_{-1} = \frac{1}{2}\frac{d}{d\lambda}\langle r_\lambda^2 \rangle\Big|_{\lambda=0} = \frac{1}{2}\frac{d^2}{d\lambda^2}\langle H_\lambda \rangle\Big|_{\lambda=0} \tag{15}$$

where, $\langle O_\lambda \rangle = \langle \Phi_\lambda | O | \Phi_\lambda \rangle$, with Φ_λ being the HF solution for the constrained Hamiltonian, $H_\lambda = H - \lambda f$.

The corresponding HF-RPA values of m_k are obtained from Eq. (3) using,

$$S(\omega) = \frac{1}{\pi}Im\left[Tr(fG(\omega)f)\right] \tag{16}$$

with $G(\omega)$ being the RPA Green's function [3, 4]. The differences between the values of m_k and consequently the difference

$$\delta E = E(RPA) - E(SC), \qquad (17)$$

between the energies obtained within the HF-RPA and the self-consistent (SC) values obtained within the HF approach are due to the violation of self-consistency in the HF-RPA. Since we are unable to obtain a fully self-consistent value for m_0, we only provide the value of the centroid energy

$$E_c = \frac{m_1}{m_0}, \qquad (18)$$

obtained within the HF-RPA. Thus we use δE_{con} and δE_s as measures of δE_c. We point out that we find $E_c \approx E_{con}$.

Before we present the main results, some remarks about the numerical accuracies are in order. We carry out the HF calculations using a box of 18 fm and a mesh size of $\delta r = 0.02$ fm. To determine m_{-1} given by Eq. (15) with an accuracy of 0.1% we calculate the first derivative of $\langle r_\lambda^2 \rangle$ using a five-point formula with the increment $\delta\lambda = 0.02$. In order to limit the spurious enhancement in m_k (particularly m_3), due to the Lorentzian smearing of the RPA Green's function, to below 0.2%, we carry out the continuum RPA (CRPA) and the discretized RPA (DRPA) calculations using the very small smearing parameter of $\Gamma/2 = 5 \times 10^{-2}$ MeV and the maximum energy of $4E_c$ in the integral of Eq. (3). In Ref. [3] we show that in order to calculate the centroid energy accurate to within 0.1 MeV, one must set the cut-off for the p-h excitations $E_{ph}^{max} > 400$ MeV. In what follows, we shall present our DRPA results obtained with $E_{ph}^{max} = 950$ MeV.

In Table I we demonstrate the accuracy of our calculations by employing a simplified Skyrme interaction [3] with $t_0 = -1800$ MeVfm^3, $t_3 = 12871$ MeVfm^4 and $\alpha = 1/3$. We consider the ^{80}Zr nucleus and keep the spin-orbit and the Coulomb interactions switched off in the HF as well as in RPA calculations, so that the HF-RPA calculations are fully self-consistent. Self-consistent (SC) values of m_k and the energies E_{con} and E_s shown in the first row of this table are obtained using Eqs. (2), (7), (9) and (15). These values are accurate to within 0.1%. We compare these highly accurate results with the corresponding ones obtained within the HF-RPA approach. The CRPA and DRPA results presented in Table I are calculated by integrating the RPA strength function appearing in Eq. (3) up to the different values of the maximum energy ω_{max}. One can easily verify that the CRPA as well as

DRPA results are quite close to the highly accurate SC results (first row). For instance, the maximum uncertainty is associated with the E_s and it is about 0.3% for $\omega_{max} = 100$ MeV. Since, the RPA energies E_{con}, E_c and E_s obtained by integrating Eq. (3) up to $\omega_{max} = 100$ and 120 MeV are very close, we shall adopt in the following the value of $\omega_{max} \approx 4E_c$ for the RPA calculations.

Having demonstrated in Table I the high accuracy of our numerical calculations, we now consider the effects of the violations of self-consistency. To investigate effects of each of the components contributing to the self-consistency violations, we carry out the calculations for some specific nuclei using several interactions [10, 11, 12, 13]. We denote by $\theta_{ls}(\theta_c) = 0$ or 1 that the spin-orbit (Coulomb) interaction is turned off or on in the HF calculations. In the RPA calculations the p-h spin-orbit and Coulomb interactions are always absent. Thus, the HF-RPA calculations for symmetric nuclei (N = Z) with $\theta_{ls} = \theta_c = 0$ are fully self-consistent. The effects of ignoring the p-h spin-orbit interaction on the ISGMR energies can be singled out by carrying out the calculations for symmetric nuclei with $\theta_{ls} = 1$ and $\theta_c = 0$. Similarly the effects due to the neglect of p-h Coulomb interaction can be estimated by performing the calculations for the cases with $\theta_{ls} = 0$ and $\theta_c = 1$. The HF-RPA calculations for asymmetric nuclei with $\theta_{ls} = \theta_c = 0$ yields the effect of working in the TJ scheme. In Table II we present the results obtained using the SGII interaction [10] for several nuclei for different combinations of θ_{ls} and θ_c. Results for other Skyrme interactions exhibit similar features. The ^{40,60}Ca and ^{80,110}Zr nuclei considered here are spin saturated systems. But, ^{56}Ni and ^{100}Sn are spin unsaturated nuclei having $1f_{7/2}$ and $1g_{9/2}$ orbits as the last occupied ones, respectively. As seen in Table I, it is once again evident that the fully self-consistent HF-RPA calculations for the ^{40}Ca and ^{80}Zr nuclei ($\theta_{ls} = \theta_c = 0$ case) yield small values for δE_{con} and δE_s (< 0.1 MeV). Considering the results for the cases with $\theta_{ls} = 1$, we find that for the spin saturated nuclei the ISGMR energy do not get altered much even if the p-h spin-orbit interaction is not included. However, in case of the spin unsaturated nuclei, the effect of the neglect of the p-h spin-orbit interaction in the RPA leads to a significant spurious enhancement of the ISGMR energy. Following Eq. (1), one can easily verify that such enhancements in the ISGMR energies are equivalent to overestimating the value of K_{nm} by about 30-40 MeV, which is unreasonably large in view of the current accuracy of the experimental data. Let us now focus on the results obtained for ^{60}Ca and ^{110}Zr nuclei with $\theta_{ls} = \theta_c = 0$ and ^{40}Ca and ^{80}Zr nuclei with $\theta_{ls} = 0$ but $\theta_c = 1$. Compilation of these

results enables us to investigate the effects of working in the TJ scheme as well as the neglect of the Coulomb term in the p-h interaction used in the RPA calculations. One can conclude from Table II that both of these factors, contributing to the violation of self-consistency, tend to underestimate the ISGMR energy compared with its SC value.

So far we have seen in a systematic manner how the inconsistency in implementing the HF-RPA approach introduces uncertainty in the ISGMR energy. Considering the results of Tables II, one may expect that the total effects of the self-consistency violation on the ISGMR energy may be smaller. Because, the absence of p-h spin-orbit interaction tends to increase the ISGMR energy while working in TJ scheme or ignoring the Coulomb term in p-h interaction used in the RPA tends to underestimate the ISGMR energy. As an illustration, we present in Table III the results for ^{90}Zr and ^{208}Pb nuclei which are widely used to extract the value of K_{nm} from the ISGMR energies. These calculations are carried out for several Skyrme interactions such as SGII, SkM*, SLy4, SK255 and SK272 [10, 11, 12, 13]. The choice of these interactions cover a wide range of incompressibility coefficient $K_{nm} = 214-272$ MeV, symmetry energy coefficient $J = 27 - 37$ MeV and the spin-orbit strength $W_0 = 95 - 130$ MeVfm^5. We see that in the case of ^{90}Zr, the ISGMR energy E_{con} obtained in DRPA agrees with the corresponding self-consistent values to within 0.3 MeV. For the ^{208}Pb nucleus, we have $\mid \delta E_{con} \mid \leq 0.4$ MeV. For both nuclei, the behaviour of δE_s is similar to that of δE_{con} except for the fact that former one is larger by about 0.2 MeV. Thus, the net uncertainties in the ISGMR energies due to the self-consistency violations are reasonably small for the ^{90}Zr and ^{208}Pb nuclei and are comparable to that attained in recent experiments. Of course, this may not be the case for spin saturated nuclei near the drip line; the inconsistency in the HF-RPA calculations introduced by the Coulomb interaction and the asymmetry in these nuclei may overshadow the effect of neglecting the p-h spin-orbit interaction.

In summary, we have investigated in detail the effects of the violations of the self-consistency in the HF-RPA calculation of the ISGMR energies E_{con} and E_s. In particular, we considered the self-consistency violations caused by ignoring the spin-orbit and Coulomb terms in the p-h interaction and by carrying out the RPA calculations in the TJ scheme. We performed the HF-RPA calculations for the ISGMR energies for several nuclei with the SGII Skyrme interaction and demonstrated that ignoring the spin-orbit term in the p-h interaction gives rise to a spurious enhancement in the values of E_{con} and E_s for spin unsaturated nuclei. On the contrary, neglect of the Coulomb term in the p-h interaction and performing

the RPA calculations in the TJ scheme underestimates the ISGMR energies. Finally, we calculated the ISGMR energies for the ^{90}Zr and ^{208}Pb nuclei for the five different Skyrme interactions SGII, SkM*, SLy4, SK255 and SK272 and show that in these nuclei, widely used to extract the value of K_{nm}, the various elements contributing to the self-consistency violations tend to counterbalance their effects leading to an uncertainty of about $0.1 - 0.4$ MeV in the values of ISGMR energies, which is quite acceptable in view of the accuracy of the experimental data currently available.

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TABLE I: Comparison of self-consistent (SC) values of the moments m_k (in $\mathrm{MeV}^k\mathrm{fm}^4$) and the ISGMR energies (in MeV) for the $^{80}\mathrm{Zr}$ nucleus calculated in the HF approach with the ones obtained within the continuum and discretized RPA using the smearing parameter $\Gamma = 0.01$ MeV. The RPA values are obtained by integrating Eq. (3) over the energy range $0 - \omega_{max}$ (in MeV). The calculations are performed using a simplified Skyrme interaction with $t_0 = -1800$ MeVfm^3, $t_3 = 12871$ MeVfm^4 and $\alpha = 1/3$.

	ω_{max}	m_{-1}	m_0	m_1	m_3	E_{con}	E_c	E_s
SC		185.1		96346	54490227	22.81		23.78
CRPA	80	185.0	4189	96229	53549803	22.80	22.97	23.59
CRPA	100	185.1	4190	96289	54024448	22.81	22.98	23.69
CRPA	120	185.1	4190	96303	54182661	22.81	22.98	23.72
DRPA	80	185.4	4194	96359	53721598	22.80	22.97	23.61
DRPA	100	185.4	4196	96426	54292408	22.80	22.98	23.73
DRPA	120	185.4	4196	96449	54544736	22.81	22.99	23.78

TABLE II: Comparison between the SC and DRPA results for the ISGMR energies (in MeV) for several nuclei obtained for the SGII interaction [10]. The notation $\theta_{ls}(\theta_c) = 1$ or 0 indicates that the HF calculations are performed with or without the inclusion of the spin-orbit (Coulomb) interaction. Note that the p-h interaction used in the RPA calculations does not include the spin-orbit and Coulomb terms.

| Nucleus | θ_{ls} | θ_c | DRPA | | | SC | | | |
			E_{con}	E_c	E_s	E_{con}	E_s	δE_{con}	δE_s
^{40}Ca	0	0	22.53	22.76	23.85	22.60	23.92	-0.07	-0.07
	1	0	22.31	22.63	23.96	22.58	23.93	-0.27	0.03
	0	1	20.97	21.24	22.44	21.38	22.69	-0.41	-0.25
^{80}Zr	0	0	19.57	19.69	20.26	19.60	20.32	-0.03	-0.06
	1	0	19.49	19.65	20.36	19.58	20.33	-0.09	0.03
	0	1	17.38	17.54	18.20	17.81	18.63	-0.43	-0.43
^{56}Ni	1	0	23.14	23.35	24.44	21.49	22.41	1.65	2.03
^{100}Sn	1	0	20.16	20.27	20.95	19.04	19.57	1.12	1.38
^{60}Ca	0	0	16.08	16.81	19.13	17.32	19.57	-1.24	-0.44
^{110}Zr	0	0	15.64	16.04	17.35	16.33	17.52	-0.69	-0.17

TABLE III: Comparison between the SC and the DRPA results for the ISGMR energies (in MeV) for the ^{90}Zr and ^{208}Pb nuclei. The DRPA results are obtained using the smearing parameter $\Gamma = 0.01$ MeV and the values of $\omega_{max} = 70$ and 50 MeV for the ^{90}Zr and ^{208}Pb nuclei, respectively. Note that the values of δE_{con} are comparable to the experimental uncertainties.

| Nucleus | Int. | DRPA | | | SC | | δE_{con} | δE_s |
		E_{con}	E_c	E_s	E_{con}	E_s		
^{90}Zr	SGII	17.93	18.05	18.70	17.70	18.30	0.23	0.40
	SkM*	17.72	17.85	18.55	17.43	18.00	0.29	0.55
	SLy4	18.19	18.33	19.07	17.86	18.46	0.33	0.61
	SK255	18.83	18.97	19.64	18.87	19.57	- 0.04	0.07
	SK272	19.55	19.70	20.45	19.49	20.28	0.06	0.17
^{208}Pb	SGII	13.53	13.64	14.22	13.42	13.94	0.11	0.28
	SkM*	13.46	13.61	14.31	13.36	13.88	0.10	0.43
	SLy4	14.04	14.16	14.80	13.68	14.22	0.36	0.58
	SK255	13.83	13.98	14.65	14.26	14.88	- 0.43	-0.23
	SK272	14.42	14.58	15.28	14.73	15.42	- 0.31	-0.14