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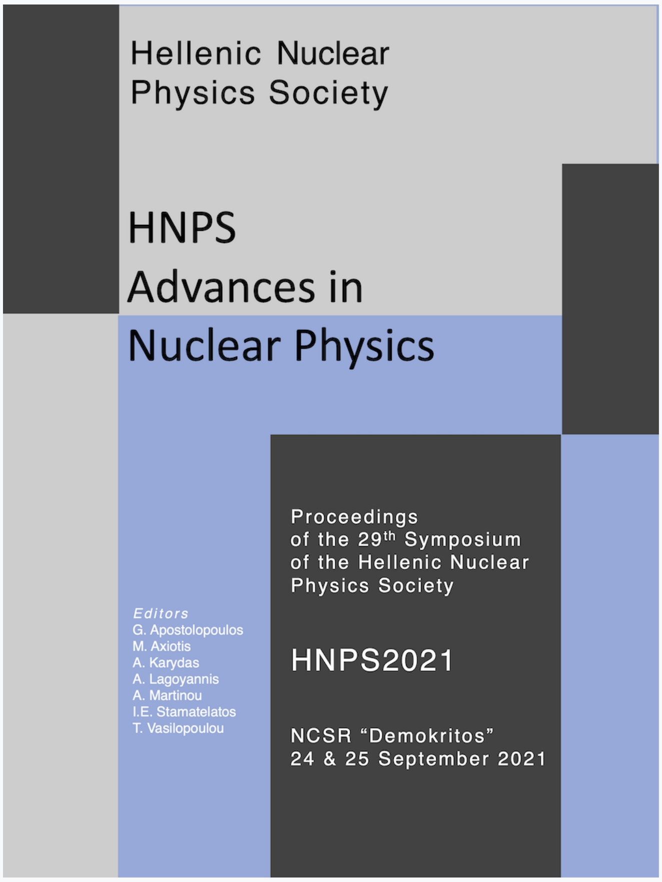

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The Giant Monopole and Dipole Resonances within the Constrained Molecular Dynamics (CoMD) Framework

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Abstract The Constrained Molecular Dynamics (CoMD) model is used to describe the collective motion of various nuclear systems. A CoMD-inspired phenomenology for the GDR is developed. In addition, the dependence of the GDR upon the effective interaction parameters is studied. Furthermore, both the monopole and dipole main and soft modes of ^{68}Ni are reliably reproduced. We conclude that a hard EoS with K=308 MeV increases the GDR energy, without altering the GMR energy. Thus, this EoS gives rather consistent results in both the monopole and dipole giant resonances.

Keywords giant resonances, nuclear equation of state, compressibility, constrained molecular dynamics

INTRODUCTION

The atomic nuclei are some of the most complicated many-body quantum systems in nature. Their nucleon components are tightly packed and strongly correlated by the nuclear interaction and the Pauli principle. Albeit their complexity, the nuclei present a significant level of organization. The nucleonic degrees of freedom can be excited under external perturbations in a collective manner. These collective motions are the well-known Giant Resonances (GRs). The GRs have a prominent role in the study of near-ground state dynamics. The characteristics of their spectra can constrain the various parameters of the nuclear interaction. Consequently, one can use the GR spectra to investigate the properties and Equation of State (EoS) of nuclear matter (NM) [1,2].

The aforementioned resonances contain a wide variety of collective motions. First and foremost, they can be categorized by the variation of the nuclear isospin as isoscalar ($\Delta\tau$=0) or isovector ($\Delta\tau$=1). Furthermore, the multipolar expansion of the total nuclear radius, characterizes the possible collective excitations as monopole, dipole, quadruple etc [2]. Additionally, the neutron rich systems present a soft mode for each GR. These soft modes correspond to oscillations of the neutron skin with respect to the symmetric nuclear core.

The purpose of this article is the study of the isovector Giant Dipole Resonance (IVGDR or GDR) and the isoscalar Giant Monopole Resonance (ISGMR or GMR), as well as their corresponding soft modes with the Constrained Molecular Dynamics (CoMD) model. The CoMD model is a semi-classical approach to the nuclear N-body problem, that is applied to a broad range of nuclear dynamics applications. Simulations of peripheral reactions at the Fermi level, near ground state properties, positron-electron pair production and fission [3-6] are just a few examples of the model applications to date.

The structure of this paper is as follows. Firstly, we describe the theoretical framework of our study, the CoMD model, the EoS and the GDR phenomenology. Afterwards, we present the details of our computations. Finally, we discuss the basic results and their implications to the EoS and effective interaction's parameters. Our efforts to include a spin-orbit coupling (SO) term are also discussed.

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THEORETICAL FRAMEWORK

Basic Principles of Constrained Fermionic Dynamics

The effective interaction functional forms the basis of every model and CoMD is no exception. As is described in [7,8], the potential component of the CoMD Hamiltonian is of the Skyrme type and is given by $\hat{V} = \sum_{i<j} \hat{V}_{ij}$, with $\hat{V}_{ij} = \hat{V}^{vol} + \hat{V}^{surf} + \hat{V}^{coul} + \hat{V}^{sym} + \hat{V}^{(3)}$. The volume, surface, coulomb, symmetry and three body terms are respectively given by

$$\hat{V}^{vol} = \frac{T_0}{\rho_0} \delta(\vec{r}_i - \vec{r}_j), \tag{1}$$

$$\hat{V}^{surf} = \frac{C_s}{\rho_0} \vec{\nabla}^2_{\langle \vec{r}_i \rangle} \delta(\vec{r}_i - \vec{r}_j), \tag{2}$$

$$\hat{V}^{coul} = \frac{e^2}{\|\vec{r}_i - \vec{r}_j\|}, \tag{3}$$

$$\hat{V}^{sym} = \frac{a_{sym}}{\rho_0} \left(2\delta_{\tau_i,\tau_j} - 1\right) \delta(\vec{r}_i - \vec{r}_j), \tag{4}$$

$$\hat{V}^{(3)} = \frac{2T_3 \rho_{ij}^{\sigma-1}}{{\rho_0}^{\sigma}(\sigma+1)} \delta(\vec{r}_i - \vec{r}_j). \tag{5}$$

The ρ_0 is the saturation density of nuclear matter (NM), a_{sym} is the symmetry parameter, T_0 is the volume coefficient, C_s is the surface parameter, while T_3 and σ are the three body parameters.

Nucleons are represented by gaussian wave packets, parametrized by their phase-space centroids. The corresponding Wigner transformed one-body distributions are given by the formula

$$f_i(\vec{r}, \vec{p}) = \frac{1}{\left(2\pi\sigma_r\sigma_p\right)^3} e^{-\frac{(\vec{r} - \langle \vec{r}_i \rangle)^2}{2\sigma_r^2}} e^{-\frac{(\vec{p} - \langle \vec{p}_i \rangle)^2}{2\sigma_p^2}} \tag{6}$$

where σ_r, σ_p are the widths and $\langle \vec{r}_i \rangle$, $\langle \vec{p}_i \rangle$ are centroids in the phase-space. By assuming that the entire time dependence of the nucleons is included in within the centroids, the Time Dependent Variational Principle gives the Hamilton's equations of motion for the system.

The Pauli principle is enforced implicitly on the nucleons. The occupation probability of a phase-space hyper-cube with volume h^3 is constrained by the Pauli-Blocking of nucleon-nucleon (NN) scattering. The constraint is given by the formula

$$\bar{f}_i \equiv \sum_{j \in L} \delta_{\tau_i,\tau_j} \delta_{s_i,s_j} \int_{h^3} f_j(\vec{r}, \vec{p}) d^3\vec{r} d^3\vec{p} \leq \frac{paulm}{128} \tag{7}$$

where L is the ensemble of j nucleons in in the proximity of i. The free parameter $paulm$ is inverse of the strength of the Pauli correlations. Its higher values correspond to a less strict enforcement of the Pauli constraint and thus weaker correlations.

The parameters of the effective interaction are determined by the saturation property of NM in the equilibrium density. Their values depend on the compressibility of NM, that is given by [9]

$$K = 9\rho_0^2 \frac{\partial^2 E/A}{\partial \rho^2}\bigg|_{\rho_0} = 9T_3 \frac{\sigma(\sigma-1)}{\sigma+1} - 2\bar{\varepsilon}_F \tag{8}$$

where $\bar{\varepsilon}_F$ is the mean Fermi energy. An additional characteristic of the NM is the effective mass. It is well-known [10] that the finite range of the nuclear interaction can be modeled via a momentum dependent potential. In the CoMD model, we are using a gaussian momentum dependent term in the low energy limit. That term corresponds to an effective nucleon mass smaller than the bound mass i.e., $m^* \leq m$. In the present version of the code, the effective mass ratio m^*/m is decoupled from the compressibility and thus is a free parameter.

As a final point, we note that so far, the CoMD model does not contain an inherent SO term. Recently, we instigated the inclusion of a possible microscopic 2-body SO term that is consistent with fermionic dynamics. Following the guidelines of Vaidya [11], we propose a term of the following form

$$\hat{V}^{so} = W_0 \left\{ \vec{\nabla}_{\langle \vec{r}_i \rangle} \rho_{ij} \times \frac{1}{\hbar} \left[\langle \vec{p}_i \rangle - \langle \vec{p}_j \rangle \right] \right\} \cdot \left[\langle \vec{\sigma}_i \rangle + \langle \vec{\sigma}_j \rangle \right] \tag{9}$$

where W_0 is the SO coefficient, $\langle \vec{\sigma}_i \rangle$ is the expectation value of the spin vector for the i nucleon and ρ_{ij} is the interaction density of the pair of i and j nucleons.

Phenomenology of the GDR

The GDR corresponds to an off-phase oscillation of the proton against the neutron quantum fluid, while its soft mode, the Pygmy resonance (PGR), corresponds to an off-phase oscillation of the neutron skin against the inner symmetric core. The spectrum of the resonance is strongly dependent on the effective interaction's parameters. In order to understand these dependencies, we have derived a simplified oscillatory model for the collective motion, based on the CoMD formalism. The GDR can be induced by a position space perturbation. This perturbation corresponds to an off-phase transformation of the initial z-axis centroids of protons and neutrons. This transformation is given by

$$\langle z_i \rangle \rightarrow \langle z_i \rangle \pm d_{n/p} \tag{10}$$

where $d_{n/p}$ is the time-dependent perturbation for neutrons, with a positive sign and for protons with a negative sign. The sum of these perturbations is the GDR oscillation amplitude $D = d_p + d_n$, the corresponding computational parameter of our simulation. This is connected to the neutron/proton perturbations in order for the total nuclear center of mass to remain stationary, $d_p = \frac{N}{A} D$ and $d_n = \frac{Z}{A} D$.

To quantify the effect of the GDR perturbation to the system, we have to consider its effect on the Hamiltonian. We assume, up to a first approximation, that the external disturbance affects mostly the symmetry term, whose expectation value is

$$U_{sym} = \frac{a_{sym}}{2\rho_0}\left(\rho_{pp} + \rho_{nn} - 2\rho_{np}\right) \tag{11}$$

where ρ_{pp}, ρ_{nn} and ρ_{np} are the total interaction densities of all proton-proton, neutron-neutron and neutron-proton pairs respectively. By introducing the aforementioned transformation to the z-axis centroids, the neutron-proton interaction density is altered and thus the symmetry energy near the ground state minimum is transformed as

$$U_{sym} \to U'_{sym} = \frac{a_{sym}}{2\rho_0}\left(\rho_{pp} + \rho_{nn} - 2\rho'_{np}\right) = U_{sym} + \frac{1}{2}\left(\frac{\rho_{np}a_{sym}}{2\rho_0\sigma_r^2}D^2\right) + O(D^3) \tag{12}$$

Consequently, the potential component of the GDR perturbation energy can be recognized to be

$$\Delta U_{sym} = \frac{1}{2}\left(\frac{\rho_{np}a_{sym}}{2\rho_0\sigma_r^2}\right)D^2 \tag{13}$$

The time evolution of the neutron and proton perturbations are connected to the kinetic component of the GDR perturbation Hamiltonian

$$T = \sum_{i\in p}\frac{1}{2}m^*\dot{d}_p^2 + \sum_{i\in n}\frac{1}{2}m^*\dot{d}_n^2 = \frac{1}{2}m^*\frac{NZ}{A}\dot{D}^2 \tag{14}$$

With the use of the aforementioned results, the perturbation Lagrangian can be written as follows

$$L = T - \Delta U_{sym} = \frac{1}{2}m^*\frac{NZ}{A}\dot{D}^2 - \frac{1}{2}\left(\frac{\rho_{np}a_{sym}}{2\rho_0\sigma_r^2}\right)D^2 \tag{15}$$

The Lagrangian has the form of a Harmonic oscillator with “mass” $M = m^*\frac{NZ}{A}$ and “spring constant” $k = \frac{\rho_{np}a_{sym}}{2\rho_0\sigma_r^2}$. The collective equations of motion are then given by the application of the Euler-Lagrange equations to the Lagrangian of eq. (15). To simulate the damping effect of the nucleon-nucleon (NN) scatterings, we can introduce a damping first order term of the form $Mb\dot{D}$, where $b = \Gamma/\hbar$ is connected to the width of the resonance. The equations of motion can thus be rewritten as

$$\ddot{D} + b\dot{D} + \omega_0^2 D = 0 \tag{16}$$

where ω_0 is the principal frequency of the GDR motion. This is described by the formula

$$\omega_0 = \sqrt{\frac{k}{M}} = \sqrt{\frac{\rho_{np}a_{sym}}{2m^*\rho_0\sigma_r^2}\frac{A}{NZ}} \tag{17}$$

The solution of the equations of motion yields a damped oscillatory waveform and a Lorentzian Fourier transform. These functional forms are the functional forms that we use to fit the CoMD data.

COMPUTATIONAL DETAILS

The computational procedure via the CoMD model consists of three steps: initialization, evolution and data processing. First, the collection of the initial values of the centroids for each nucleon is calculated. These collections are termed as 'initial configurations and a whole set of these is produced by a Simulated Annealing algorithm. Afterwards a globally optimized configuration from the whole set is chosen with a dedicated algorithm. This procedure is the initialization step [8].

After an initial configuration is chosen, the nuclear system is perturbed in either the position or momentum space. The momentum space perturbations correspond to a temperature and are used for the simulation of the GMR and PGR, while r-space perturbation induces the GDR. Afterwards, the nucleus evolves according to the Hamiltonian equations. To account for the approximate character of the interaction, the centroids are randomly rotated in the phase space before the evolution. This rotation conserves the total energy, linear and angular momentum of the system. The time evolution of each rotated system corresponds to a different 'event'.

The final step of processing the resulting data depends on the nuclear phenomenon that is studied. Firstly, the trajectories the nucleons are properly averaged for each event and the various characteristics are calculated. For the study of the GRs, a Fourier transform is applied to the evolution of either the radius (GMR) or the relative distance of the neutron-proton fluids (GDR/PDR). This process is performed by a Fast Fourier Transform (FFT) code and produces the corresponding spectrum.

The results of a CoMD study depend heavily upon the characteristics of the effective interaction. Here, we use two different EoS, the 'Standard' and the 'Hard'. The 'Standard' EoS is characterized by $\mathrm{K} = 254$ MeV, $m^*/m = 1$ and $a_{sym} = 32$ MeV, while the 'Hard' EoS has $\mathrm{K} = 308$ MeV, $m^*/m = 0.9$ and $a_{sym} = 38$ MeV. Unless stated otherwise, it is assumed that our calculations were performed with the Standard EoS and $\rho_0 = 0.165$ fm^{-3}, $C_s/\rho_0 = -1$ and $\sigma_r = \hbar/\sigma_p = 1.30$ fm.

RESULTS AND DISCUSSION

The Effective Interaction and the GDR

The value of the GDR energy can constrain the parameters of the effective interaction. First of all, the resonance energy increases with increased compressibility. This can be seen in fig. 1 (a), for ^{40}Ar, ^{64}Ni and ^{86}Kr. This can be explained by accounting the neutron-proton interaction densities ρ_{np}. A more compressed system has higher densities and thus the interaction between proton-neutron pairs is more prominent [4] and the nuclear response appears in higher frequencies. This tendency correlates the 3-body interactions with the dipole frequency. Interestingly, higher 3-body correlations result in a more bound system and higher GDR energies.

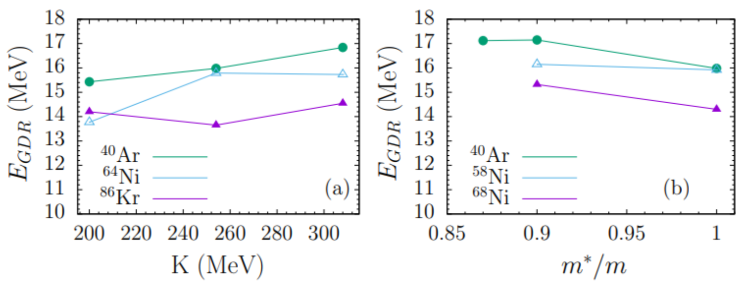

Fig. 1. *Effect of the compressibility (a) and effective mass (b) to the GDR energies. The calculations were performed with the standard EoS, for different isotopes according to the key.*

Another interesting characteristic is the effect of the momentum dependence. In fig. 1 (b), the energy of the main GDR peaks is plotted against the corresponding values of their effective mass ratios, for ^{40}Ar, ^{58}Ni and ^{86}Kr. We confirm the increment of the GDR energy with decreased effective masses, that is also discussed in [10]. This can be reasoned by the presence of the effective mass in the denominator of the dipole frequency in eq. (17). The effective mass is decoupled from the compressibility in the current version of the model and is treated as a free parameter. This is reason that our study favors a hard EoS, while other studies [12] prefer a softer EoS with $K = 250$ MeV. This feature is under investigation and we plan to construct an EoS with effective mass coupled with K.

We also state our preliminary results in the study of the spin-orbit coupling interaction. In fig. 2, the GDR spectra of ^{64}Ni for $W_0 = 0$ MeV fm^{-5} (a) and $W_0 = 30$ MeV fm^{-5} are shown. We note that the inclusion of a SO potential term decreases the total cross section and increases the centroid energy by ~1 MeV. The effect of SO coupling is presently under systematic investigation.

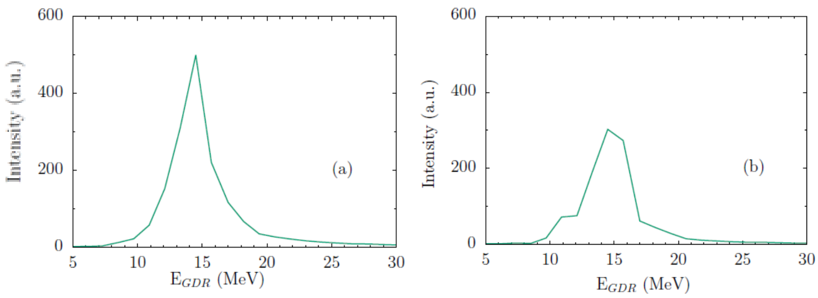

Fig. 2. *Effect of spin-orbit interaction to the GDR. The GDR spectra of ^{64}Ni with $W_0 = 0$ MeV fm^{-5} (a) and $W_0 = 30$ MeV (b), were calculated with the standard EoS.*

The dipole response of neutron rich systems usually exhibits the soft PDR mode. Such a system is the interesting ^{68}Ni nuclide. We present both its GDR (a) and the PDR (b) spectra in fig. 3. The main peak at ~15 MeV corresponds to the GDR and has a discrepancy of 2 MeV from the experimental value, of 17.84 MeV [13]. On the contrary, the secondary peak of panel (b) is identified as the PDR at ~12 MeV, which is closely reproduces the experimental value of 11 MeV [13].

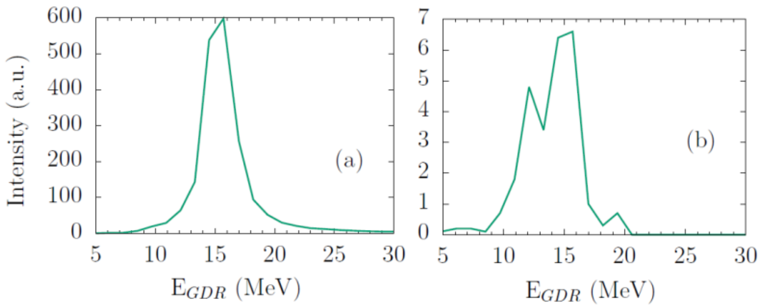

Fig. 3. *The GDR (a) and PDR (b) spectra of ^{68}Ni, calculated with the 'hard' EoS. We identify the soft Pygmy mode at ~12 MeV and the main GDR at ~15 MeV of the spectrum (b).*

Mass and Isospin dependence of the IVDGR

As discussed in [10] the GDR energy is independent of the total isospin of the nucleus. To study this effect, we introduce the asymmetry parameter $m_\chi = (N - Z)/A$. The energies of the main GDR peak are plotted against m_χ in fig. 4 (left), for the isobaric chains with A = 40, 68 and 100. We confirm the aforementioned invariance, up to ±1 MeV. On the contrary, we have shown in an earlier work [4] that the other important isovector parameter of neutron skin has a linear dependence on m_χ. The invariance of the GDR can be understood in the terms of the principal contribution of the symmetric core's interaction ρ_{np} density to the collective frequency, eq. (17).

In Fig. 4 (right), we also show the variation of E_{GDR} with respect to the nuclear mass. The red dashed curve corresponds to an experimental parametrization [10], while the green and cyan curves correspond to CoMD results with the 'standard' and 'hard' EoS respectively.

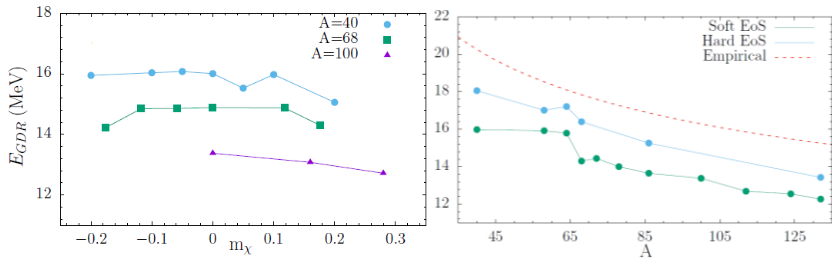

Fig. 4. *Dependence of the GDR energy on the asymmetry parameter (left) and mass number (right). The left plot presents calculations with the standard EoS for different isobaric chains, according to the key. In the right plot, the dashed line corresponds to an experimental parametrization from [10], the green curve to the standard EoS and the cyan curve to the 'hard' EoS.*

As it is known [10], effective interactions without momentum dependence underestimate the GDR energies. This is reflected in fig. 4, as the standard EoS results show a 3-4 MeV discrepancy. The use of a decoupled lower effective mass with the hard EoS, partially remedies the situation, giving results with 1-2 MeV discrepancies.

Simulation of the Monopole Modes

The monopole resonances are, in their own right, some of the most important studied phenomena in nuclear dynamics. They comprise the most prominent experimental constrain on the compressibility of NM. Here, we present our study of the monopole response of the ^{x}Ni, x = 58, 64 and 68 nuclides. In fig. 5, the GMR spectra of ^{58}Ni (a) and ^{64}Ni (b) isotopes are presented, while in fig. 6 (a) the ^{68}Ni spectrum is shown. All these calculations were performed with the standard K=254 MeV EoS.

We identify the main GMR peak at ~21.5 MeV, which is close to the experimental value, of 21.9 MeV [14]. Furthermore, the neutron rich ^{68}Ni shows a minor peak at 14.5 MeV. We may identify this as the soft monopole mode, that corresponds to the breathing mode of the neutron skin against the symmetric core. Our result is in close proximity to the corresponding experimental value of 12.9 ± 1 MeV [14].

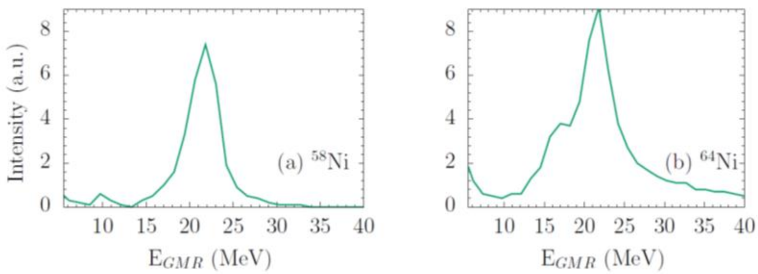

Fig. 5. *The GMR spectra of ^{58}Ni (a) and ^{64}Ni (b). The calculations were performed with the standard K=254 EoS, with a p-space perturbation. The main peaks are identified at ~21.5 MeV.*

Finally, in fig. 6 (b), we show the GMR spectrum of ^{68}Ni with the hard K=308 MeV EoS. Interestingly, the centroid of the main peak is increased only by ~1 MeV and its total cross section, as well as its width are also increased. On the contrary, the secondary soft monopole peak appears to retain its strength and centroid energy

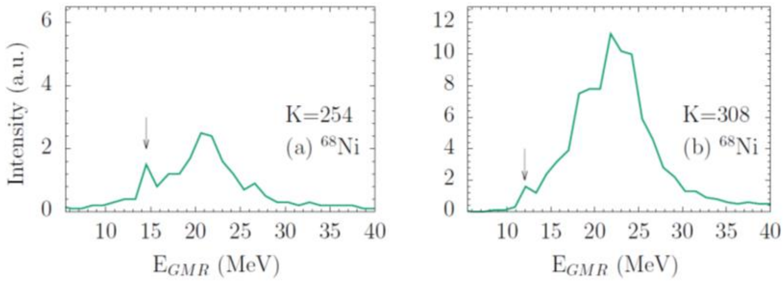

Fig. 6. *The GMR spectra of ^{68}Ni calculated with the standard EoS (a) and the 'hard' EoS (b). The soft monopole modes (indicated by arrows) appear at ~14.5 MeV.*

CONCLUSIONS

In this work, we extensively used the microscopic CoMD model to study the Giant Monopole and Dipole Resonances. First, we developed a simplified GDR phenomenology based on the usual CoMD formalism. Afterwards, we studied the effect of some important parameters of the effective nuclear interaction to the GDR spectrum.

We found that the increased compressibilities and decreased effective masses result in increased GDR energies. In addition, we started investigating the inclusion of a 2-body spin orbit potential to the model. Our results so far, suggest that the spin-orbit coupling slightly increases the GDR energy, while it significantly reduces its cross section. Additionally, we observed that a 'hard' EoS with $\mathrm{K} = 308$ MeV, $m^*/m = 0.9$ and $a_{sym} = 38$ MeV reproduces more reliably the experimental dipolar data, up to 1-2 MeV. Furthermore, we confirmed that, in contrast to the isovector neutron skin parameter, GDR is invariant with respect to the asymmetry ratio m_χ, in isobaric conditions. We also reproduced in a satisfactory manner the main and soft dipole peaks of ^{68}Ni.

Finally, our study concluded with the monopole GMR resonance and the corresponding soft mode. We calculated the monopole spectra of the ^{x}Ni, x = 58, 64, 68 isotopes. Our results were in the proximity of the experimental values. The calculation of the ^{68}Ni spectrum was also performed with the K=308 EoS and yielded consistent results with the experimental data. Our work points to the construction of a new EoS with effective mass compatible with the compressibility and a more thorough investigation of the spin-orbit coupling effect. We plan to focus our future studies on these directions.

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