Giant resonances in ^{238}U within the quasiparticle random-phase approximation with the Gogny force

S. Péru,[1,*] G. Gosselin,[1] M. Martini,[1] M. Dupuis,[1] S. Hilaire,[1] and J.-C. Devaux[2]

[1] *CEA/DAM/DIF, F-91297 Arpajon, France*

[2] *ENSIIE, 1 square de la résistance, F-91025 Evry Cedex, France*

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Fully consistent axially-symmetric deformed quasiparticle random-phase approximation (QRPA) calculations have been performed, using the same Gogny D1S effective force for both the Hartree-Fock-Bogolyubov mean field and QRPA matrix. New implementation of this approach leads to the applicability of QRPA to heavy deformed nuclei. Giant resonances and low-energy collective states for monopole, dipole, quadrupole, and octupole modes are predicted for the heavy deformed nucleus ^{238}U and compared with experimental data.

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I. INTRODUCTION

The development of a generic approach suitable to describe the excited states of all nuclear systems with the same accuracy is still a challenge for theoretical nuclear physics. Models based on the random-phase approximation (RPA) [1] are well suited in magic and semimagic nuclei as they describe on the same footing both individual and collective excited states. This formalism has been found to be successful in predicting low-lying multipole vibrations as well as giant resonances [2]. Pairing correlations have been included within quasiparticle RPA (QRPA) formalism to describe excited states of open-shell nuclei [3,4] and deformed (Q)RPA models have been developed [5–9]. In order to avoid inconsistencies [10], many calculations are now performed using the same effective nucleon-nucleon interaction for the mean field ground state and the (Q)RPA excited states [9–17]. The only parameters of these fully self consistent Hartree-Fock (-Bogolyubov)+(Q)RPA [HFB+QRPA] approaches are those of the effective interaction. Till now such calculations have been applied to light and medium mass nuclei and to some heavy spherical nuclei. Heavy deformed nuclei still remain an open challenge because of the huge configuration space required to perform a consistent calculation. Recently dipole responses of some heavy deformed nuclei have been theoretically studied [18] but by using the approximation of a separable RPA formalism. The aim of this work is to present the first application of the fully consistent axially-symmetric deformed HFB+QRPA approach using a finite-range force—namely the D1S Gogny force [19,20]—to the description of multipole responses of ^{238}U. These predictions are quite relevant for the study of the low-energy collective states as well as of the fission decay of giant resonances. Furthermore, they could provide a solution to the longstanding issue related to the theoretical underestimation of the neutron-induced ^{238}U neutron emission cross section [21–23].

In order to apply QRPA calculations to such a system, a new implementation of the numerical code, based on parallel computation, is needed. It is described in Sec. II. Multipole responses for ^{238}U are presented and discussed in Sec. III. Conclusions and perspectives are given in Sec. IV.

II. FORMALISM AND NUMERICAL CODE

In the present work, the QRPA matrix is expressed in terms of the two-quasiparticle (2qp) states obtained from HFB calculations at the minimum of the axially deformed potential energy surfaces. Since the 2qp states are expanded on a basis composed of harmonic oscillator (HO) states, the continuum is discretized. The effective force we employ is the D1S Gogny interaction [19,20], which is known to give reasonable spectroscopy within the five-dimension collective Hamiltonian (5DCH) approach over the entire nuclear map [24,25]. The use of the same force in the HFB and QRPA calculations ensures a full consistency of our method once the whole 2qp configuration space is considered. More details about the formalism of the present approach can be found in a previous publication [9].

In order to deal with heavy deformed nuclei, the axially symmetric, deformed QRPA code has been ported and extended on a massively parallel computer. Calculating the QRPA matrix for heavy nuclei in a HO basis with 13 major shells is a big numerical challenge. It implies the calculations of symmetrical matrices whose sizes range from 23 000 to 26 000, that is, a total of around 3×10^8 elements for each matrix. As each element requires a few seconds of CPU time, a sequential algorithm is no longer an option. Therefore a massively parallel master-slave algorithm has been developed to calculate all the matrix elements. The master process dispatches individual matrix elements to each slave process and receives and stores the results in the right place in the matrix before sending another job to the slave process. This parallelization scheme has the benefit that only the master process requires knowledge of the whole matrix, thereby considerably reducing the total memory requirements. As each slave spends a few seconds to perform its calculation, the master process has sufficient time to deal with up to a thousand slaves simultaneously in a completely scalable scheme.

The matrix is split into three parts depending of the isospin of 2qp configurations: proton-proton, proton-neutron, and

*sophie.peru-desenfants@cea.fr

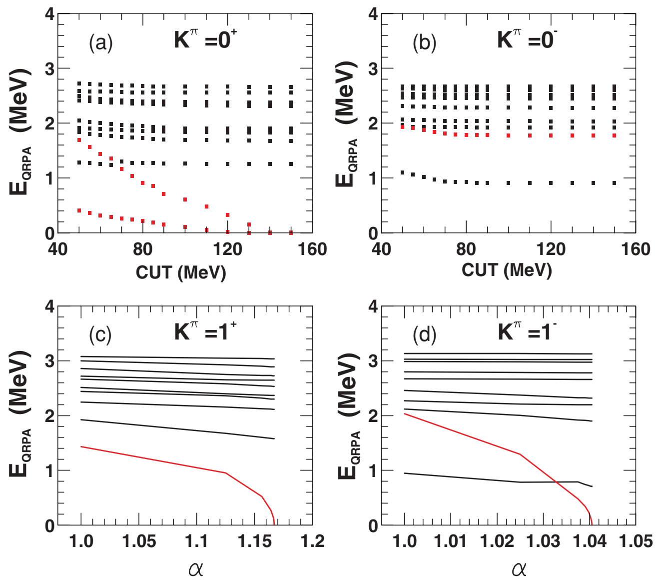

FIG. 1. (Color online) Evolution of the first 10 QRPA eigenvalues obtained in ^{238}U for (a) $K^\pi = 0^+$ and (b) $K^\pi = 0^-$ with different values of the cut in energy in the 2qp configuration basis. The "CUT" variable is defined as the maximal energy above which the 2qp states are not taken into account. Evolution of the first 10 eigenvalues for (c) $K^\pi = 1^+$ and (d) $K^\pi = 1^-$ as a function of the α renormalization factor (see text). Identified spurious states are plotted in red.

neutron-neutron. For each part, only the relevant terms of the interaction are calculated, thus negating the time-consuming requirement to check whether the term has to be calculated, as for instance the Coulomb term.

Calculating the eigenvalues and the eigenvectors is a three-step procedure as detailed in [9]. The internal diagonalizations and the matrix multiplications have been parallelized with functions from the ScaLAPACK library [26]. An extraction procedure also allows us to diagonalize smaller matrices tagged by the cut in energy, in order to check the convergence of the QRPA spectrum. This is illustrated in Figs. 1(a) and 1(b), which show the first 10 QRPA eigenvalues obtained in ^{238}U as a function of the cut in energy of the 2qp configuration space for $K^\pi = 0^+$ and 0^-. Here K represents the projection of the angular momentum onto the nucleus symmetry axis, and π the parity. Let us note that the maximum energy that can be reached with the current 13-major-shell HO basis is 145, 155, 135, and 145 MeV for $K^\pi = 0^+$, 0^-, 1^+ and 1^-, respectively, and that calculations are quite well converged for a cut of 80 MeV. For $K^\pi = 0^+$, the two spurious states related to the restoration of the particle number dive to zero value and can be easily disentangled from the physical spectrum. Other multipolarities require more analysis. Related wave functions of low-energy QRPA bosons have been checked to identify spurious states (rotation and translation) and to clean the spectrum. As shown in Figs. 1(c) and 1(d), we can introduce a small renormalization factor α of the residual interaction, which affected only the spurious components. Then the spurious state of translation is identified to be second eigenstates for $K^\pi = 1^-$, while the spurious state of rotation is the first eigenstate for $K^\pi = 1^+$. For $K^\pi = 0^-$, the spurious state of translation has been identified with the same procedure to be the second eigenstate. Let us mention that calculations performed in a larger base with 15 major shells, for $K^\pi = 0^-$ multipolarity, have confirmed the convergence of the present results.

III. MULTIPOLE RESPONSES FOR ^{238}U

We have predicted monopole, dipole, quadrupole, and octupole responses for the heavy nucleus ^{238}U. This nucleus is well deformed with a prolate shape and self-consistent HFB calculation gives for the ground state a deformation parameter $\beta = 0.279$ [27] (where the definition of β is also given in [25]). Therefore seven separated calculations have been performed to generate all QRPA bosons for $K^\pi = 0^+$, 0^-, 1^+, 1^-, 2^+, 2^-, and 3^-.

In Fig. 2 theoretical transition probabilities for dipole modes are plotted and compared with experimental data of photoabsorption [28] (in which the dipole QRPA response is folded with a 2-MeV-width Lorentzian distribution). As for lighter nuclei, the dipole response is found to be split into two components: The $K^\pi = 0^-$ component is located at an energy lower than the $|K^\pi| = 1^-$ one, as expected for a prolate shape [9] and as already illustrated in early works [29,30] using a long-range correlation model. Predictions overestimate by 2 MeV the energy of the dipole response, a value expected to be correlated with particle-vibration coupling [31], which is neglected here. Nonnegligible dipole strengths are predicted (for $\alpha = 1$) at low energy: 2.03 MeV for $K = 0$ and 2.12 MeV for $K = 1$ with transition probabilities $B(E1; 0_{\rm GS} \rightarrow 1^-) = 0.102$ and 4.207 e^2 fm^2, respectively.

The monopole response is displayed in Fig. 3(a). The observed splitting is due to the coupling with the $K = 0$ quadrupole strength [Fig. 3(b)]. High strength is also predicted between 20 and 30 MeV, exhausting 20% of the $B(E0)$ energy-weighted sum rule (EWSR). The mean excitation

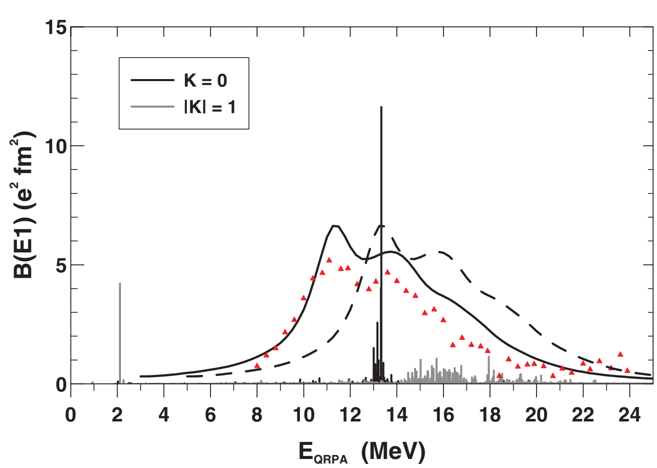

FIG. 2. (Color online) Dipole responses for ^{238}U. Transition probabilities $B(E1)$ are given in e^2 fm^2. The Lorentzian distribution of 2-MeV-width folding of the QRPA prediction (full line) shifted by 2 MeV with respect to the simple folding (dashed line) is plotted in order to compare with photoabsorption data (red triangles).

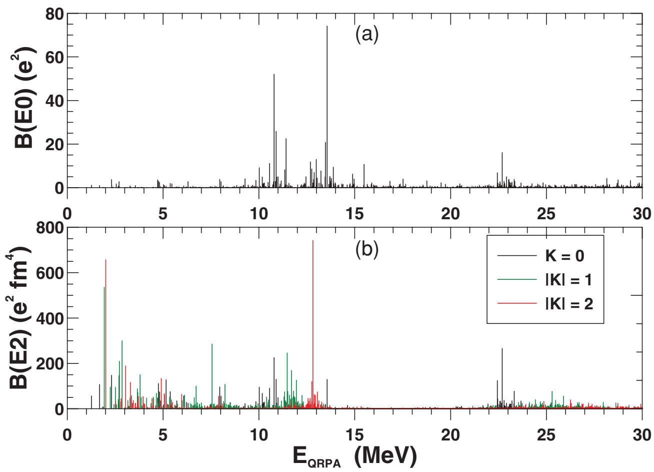

FIG. 3. (Color online) (a) Monopole transition probabilities $B(E0)$ for ^{238}U. (b) Quadrupole transition probabilities $B(E2)$ in e^2 fm^4 for ^{238}U.

energy values of the first and second peaks are 10.7 and 13.4 MeV, respectively, in good agreement with values extracted from ^{238}U (α, α' fission) [32,33] and ^{238}U (e, e' fission) [34] reactions studies. The peak related to the coupling of the quadrupole mode is the first one, according to the results shown in Fig. 3(b). As is well known, the theoretical description of the giant monopole resonance is crucial for the determination of the value of the incompressibility modulus of infinite nuclear matter K$_{nm}$ [35]. The value corresponding to D1S (K$_{nm}$ = 209 MeV) is a little bit low with respect to the admitted range (220–230 MeV) and the original D1 one (K$_{nm}$ = 228 MeV) and to the new parameter sets D1N (K$_{nm}$ = 230 MeV) [36] and D1M (K$_{nm}$ = 225 MeV) [37]. The mean value of the giant monopole resonance (GMR) (12.4 MeV when integrated in a range going from 8.5 to 16.5 MeV) predicted here with D1S is expected to be underestimated by less than 5% [16]. With spurious states being extracted, a physical 0^+ collective state still remains at 1.26 MeV. This state could be identified with one of the two experimental states measured at 927.21 and 997.23 keV. The first one decreases with $E2$ to the first 2^+ excited state while the second one decreases with $E0$ directly to the ground state. Consequently, we associate the first predicted monopole state to the experimental one at 997.23 keV. An experiment-theory discrepancy of roughly 260 keV can be considered as satisfactory for a microscopic approach.

Figure 3(b) shows the quadrupole response, which is very fragmented with many collective states predicted below 10 MeV. Let us note that the first $K^\pi = 0^+$ state at 1.26 MeV also contributes to the quadrupole response with a transition probability $B(E2) = 56\ e^2$ fm^4. Rotational bands, which are well reproduced by 5DCH using the same Gogny mean field [25], cannot be described with the present approach. Only the first 2^+ $K = 1^+$ QRPA state at 1.92 MeV [$B(E2; 0_{\rm GS} \to 2^+) = 535\ e^2$ fm^4] and second 2^+ $K = 2^+$ one at 2.00 MeV [$B(E2; 0_{\rm GS} \to 2^+) = 657\ e^2$ fm^4] can be compared with the bandhead state at 1.060 MeV [$B(E2) = 1330\ e^2$ fm^4]. As expected for a prolate shape nucleus, three major strengths between 10 and 14 MeV are found to be ordered by increasing K [9]. As in the monopole case, a nonnegligible strength is located above 20 MeV. The centroid is still ordered by K. In this region the fragmentation increases with K, broadening the $K = 2$ peak.

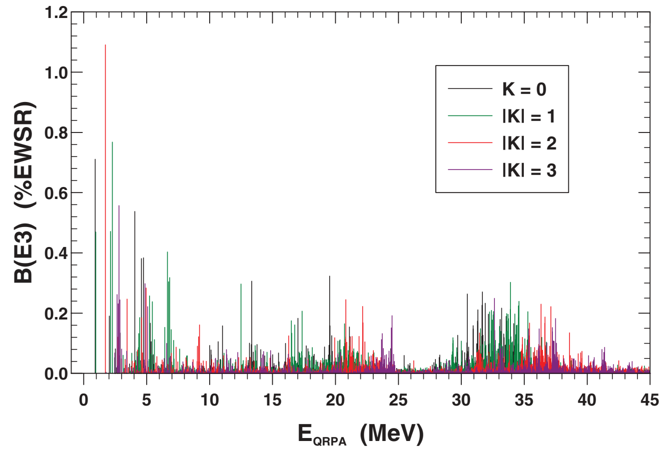

FIG. 4. (Color online) Octupole responses as percentage of the EWSR for ^{238}U.

The octupole response as function of percentage of the total EWSR is shown in Fig. 4. The high-energy octupole resonance (HEOR) is well identified between 30 and 40 MeV whereas the low-energy octupole resonance (LEOR) is very fragmented and spreads from very low energy values to 25 MeV with a large mixing between the different K projections. As in the quadrupole response, many states lie below 10 MeV. The two strengths observed below 1 MeV (for $K = 0$ and $K = 1$) are coupled with dipole modes. The lowest octupole states are predicted to be $K = 0$ at 911 keV, $K = 1$ at 949 keV, and $K = 2$ at 1.72 MeV with transition probabilities $B(E3; 0_{\rm GS} \to 3^-) = 46041$, 34613, and 44408 e^2 fm^6, respectively. This sequence is in agreement with the experimental bandhead one, i.e., $K = 0$ at 670 keV, $K = 1$ at 934 keV, and $K = 2$ at 1.128 MeV. The first octupole state for $K = 3$, which is experimentally unknown, is predicted with our approach to be at 1.772 MeV with a small value of $B(E3; 0_{\rm GS} \to 3^-) = 171\ e^2$ fm^6. This explains why no low-energy $K = 3$ state is reported experimentally. The second and third $K = 3$ states are predicted at 2.46 and 2.65 MeV, contributing with transition probabilities $B(E3; 0_{\rm GS} \to 3^-) = 1932$ and 6901 e^2 fm^6, respectively.

IV. CONCLUSION

A fully consistent microscopic axially-symmetric deformed QRPA approach using a finite-range Gogny force has been extended using a parallelized procedure on a supercomputer. This approach has been applied to the heavy deformed nucleus ^{238}U. Dipole, monopole, quadrupole, and octupole giant resonances as well as low-energy states have been described. The dipole response is predicted with the right envelope compared to experimental photoabsorption data but it is found to be a little bit high in energy. Results for the first 0^+, 2^+, and 3^- states have been analyzed and compared to literature-adopted levels. A prediction is given for the first

$K = 3$ octupole state. QRPA calculations offer a unique way to determine microscopically octupole vibrational headband states required in combinatorial level density predictions [38]. Indeed, if quadrupole vibrational states can be (and have been) systematically derived using the D1S interaction [25], phenomenological approximations are still used for octupole modes [38] and it would be certainly more accurate to extract such information from systematical QRPA studies.

Comparison with experimental data gives us enough confidence to use QRPA collective state wave functions as an input for microscopic reaction models used in direct inelastic scattering and preequilibrium studies [23] in order to obtain parameter-free cross sections. Until now a phenomenological procedure has been used to increase the neutron emission cross section and match scattering data [22]. Ad hoc vibrational collective states, which produce large inelastic cross sections, have been introduced in the ^{238}U spectrum in the excitation energy range between 0 and 5 MeV, even if such states have not yet been predicted in nuclear structure calculations. Such collective states are now predicted within our fully consistent microscopic approach and work is in progress to check their impact on direct reaction observables.

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