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What can we learn from recent non-relativistic mean field calculations ?

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In the present contribution, we discuss the relevance of fully self-consistent HF plus RPA (or HF-BCS plus QRPA) calculations based on Skyrme effective forces, and their impact on our present knowledge of basic properties of the nuclear equation of state, like the incompressibilty and the symmetry energy. Finally, we address the problem whether correlations beyond mean field can alter the picture obtained at the (Q)RPA level. Throghout the paper, the comparison with the results obtained using Gogny forces, or RMF Lagrangians, will be emphasized.

1. Introduction

The self-consistent mean field models (with their extensions) are the only possible microscopic framework which is available, at present, to study the structure of the medium-heavy nuclei (for a recent review, cf. Ref. [1]). These calculations are performed either in the non-relativistic or in the relativistic framework. The recent progress within the Relativistic Mean Field (RMF) is described, within this volume, in the paper by P. Ring [2]. The non-relativistic calculations can be based either on the finite-range Gogny effective force [3], which has the advantage that the pairing channel can be treated on the same footing as the mean field, or on the zero-range Skyrme force which is usually supplemented by a simple density-dependent pairing force (see below). Computer codes based on the Skyrme interactions are more common, since they are, as a rule, computationally less demanding. In recent years, many approximations inherent in the practical implementation of the Skyrme calculations have been released, and a detailed confrontation with the results of Gogny and RMF calculations has been carried out. These issues, as well as the problem of how the mean field models should be extended to include further correlations, lie at the basis of the discussion of the present contribution.

The different mean field models can be seen as alternative formulations of an effective Density Functional Theory (DFT) for atomic nuclei. Within this framework, one tries to construct the best possible approximation for the energy functional $E[\rho]$ where ρ is the matter density (in practice, different kinds of densities must be introduced, that is, spin and isospin densities, kinetic energy density, abnormal density). Usually, the parameter sets which characterize the functionals are fitted on nuclear matter properties (like the empirical saturation point) and on the experimental binding energies and charge radii of

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a few magic nuclei. Recently, the behavior of many of these functionals has been studied on a much larger scale: some of them have been tested against, or constrained to, the systematics of nuclear masses [4], while others have been tested against, or constrained to, realistic calculations of pure neutron matter [5]. In fact, the aim should be to go towards universal functionals which are able to account for as many experimental observables as possible. This program has just started but it is of paramount importance if reliable predictions for unstable isotopes are required.

In fact, the most difficult part to fix (within the nuclear energy functional) is probably the one which is associated with the neutron-proton (n-p) asymmetry. Since in nuclei we have neutron and proton densities ρ_n and ρ_p, we can re-write $E[\rho_p, \rho_n]$ as a function of the total (or isoscalar) density ρ and of the isovector density $\rho_- = \rho_n - \rho_p$. The energy functional can be re-written as a part which depends only on ρ, plus the rest which depends on ρ_-, that is,

$$E = E_0[\rho] + S(\rho) \left(\frac{\rho_-}{\rho} \right)^2 . \quad (1)$$

This equation defines the so-called *symmetry energy* $S(\rho)$. In this paper, we define $J = S(\rho_0)$ (sometimes, this quantity is called a_τ or a_4).

The different energy functionals (non-relativistic or relativistic ones) have uncontrolled forms for $S(\rho)$, especially at densities far from the saturation density ρ_0 [6]. This fact has evidently consequences for nuclei far from the stability valley but also for the properties of neutron stars [7].

The present paper is organized as follows. In Sec. 2, we briefly mention our implementation of a fully self-consistent (Q)RPA, with a few tests and examples. In Sec. 3, we discuss what we have recently learnt about the extraction of the nuclear incompressibility coefficient (K_∞) from the giant monopole resonance. Since it will be concluded that, among the rest, mainly the density dependence of $S(\rho)$ plays a role in the residual uncertainity on the value of K_∞, we touch in Sec. 4 upon the problem of the relation between the symmetry energy and the isovector giant dipole resonance energy. Finally, we discuss in Sec. 5 the role of correlations which go *beyond* the mean field, and we draw our conclusions in Sec. 6.

2. Fully self-consistent RPA and QRPA calculations

We have recently implemented a fully self-consistent (Q)RPA scheme. For the case of the charge-exchange excitations, this implementation and the first results have been published in Ref. [8], and further work is in progress. We discuss in what follows the usual, non charge-exchange modes. All the terms of the residual two-body interaction are included: in particular, the two-body spin-orbit and Coulomb terms. These terms have been neglected in all the Skyrme RPA calculations performed until recently. Only in the recent calculations of Refs. [9,10] they have been taken into account.

In our case, we start by solving the HF equations in coordinate space. In the case of open-shell systems, the BCS equations are considered in a restricted configuration space. A zero-range, density-dependent pairing force is employed, whose strength is obtained by requiring a reasonably good agreement between the theoretical and empirical values of the pairing gaps Δ along the whole series of isotopes under study. When the ground state is obtained, together with the quasi-particle states lying within the pairing window, a number of unoccupied states (which have occupation factors v^2 strictly equal to zero) are calculated by using box boundary conditions. For every value of (l, j), we calculate unoccupied states with Δn increasing values of the radial quantum number n, up to a given particle cutoff energy. The stability of results against the dimension of the model space is carefully checked. In this space, the (Q)RPA matrix equation are solved and from this, one obtains the energies E_λ of the vibrational states as well as the strength associated with a given operator $\hat{O}$.

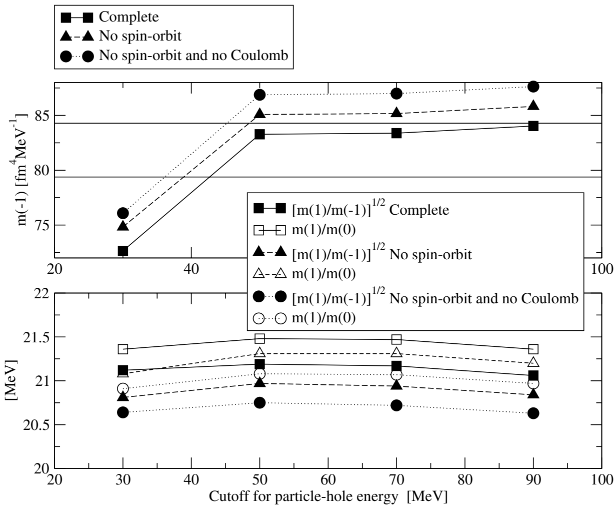

Figure 1. Monopole $m(-1)$ sum rules and centroid energies obtained in ^{40}Ca by using the force SLy4. The results of the complete RPA calculation are compared with those obtained within different approximations. The two horizontal lines in the upper panel define the CHF result.

The accuracy of our scheme can be checked by looking, e.g., at appropriate sum rules $m(k) = \sum_\lambda |\langle\lambda|\hat{O}|0\rangle^2 E_\lambda^k$. In fact, $m(1)$ can be compared with the well-known double commutator sum rule, and $m(-1)$ with the results of constrained Hartree-Fock (CHF) calculations by means of the so-called dielectric theorem [11]. In Fig. 1 we show our results for the monopole centroid energies in the case of ^{40}Ca (obtained by employing the force SLy4 [5]). The results are shown as a function of the energy cutoff for the particle-hole configurations. In the upper panel the CHF value for $m(-1)$, with a numerical error bar, is marked by the two horizontal lines. Only the calculation with the full residual interaction (labelled by “Complete”) lies within this range. When the two-body Coulomb and spin-orbit terms in the residual particle-hole force are omitted, the $m(-1)$ sum rule is overestimated. This effect is not constant for different nuclei as it is discussed in detail in [10]. In the case of ^{208}Pb, with the interaction SGII in a box of 20 fm, the value of $m(-1)$ from RPA is 226.32 fm^4/MeV, in excellent agreement with result from CHF which is 225.92 fm^4/MeV. When the residual Coulomb and spin-orbit interactions are neglected in RPA, the change in the $m(-1)$ value produces a significant effect on the energy $\sqrt{m(1)/m(-1)}$ of the ISGMR (see next Section).

Table 1
Results for the low-lying 2^+ state in ^{208}Pb using the force Sly4.

	Energy [MeV]	B(E2) [e^{2}fm^4]
No Coulomb and no spin-orbit	5.77	3728
No Coulomb	5.11	4547
Complete calculation	5.23	3864
Experiment	4.10	3200

In Table 1 we show the results for the low-lying 2^+ state in ^{208}Pb, calculated with the SLy4 interaction. One can see that the discrepancy between theory and experiment is reduced when the whole residual interaction is taken into account, in agreement with the case of the Gogny force [12]. With Skyrme forces, the full self-consistency seems to be more crucial in the case of low-lying density modes than for giant resonances: the spin-orbit residual interaction, in particular, enforces the components in the wavefunction with opposite spins. Without the residual spin-orbit force the wavefunction reads

$$\begin{aligned} |\Psi(old)\rangle \;=\;& 0.69|\nu i_{13/2}-g_{9/2}\rangle + 0.65|\pi h_{11/2}-f_{7/2}\rangle + 0.16|\pi h_{11/2}-h_{9/2}\rangle - \\ & 0.11|\pi h_{11/2}-j_{15/2}\rangle - 0.10|\pi g_{9/2}-i_{13/2}\rangle, \end{aligned} \tag{2}$$

while including it the wavefunction becomes

$$\begin{aligned} |\Psi(new)\rangle \;=\;& 0.66|\nu i_{13/2}-g_{9/2}\rangle + 0.63|\pi h_{11/2}-f_{7/2}\rangle + 0.27|\pi h_{11/2}-h_{9/2}\rangle - \\ & 0.13|\pi h_{11/2}-j_{15/2}\rangle - 0.12|\pi g_{9/2}-i_{13/2}\rangle - 0.11|\pi f_{7/2}-i_{11/2}\rangle. \end{aligned} \tag{3}$$

3. Applications: the monopole resonance and the nuclear incompressibility

Around the saturation point of symmetric nuclear matter, one has

$$E(\rho) = E(\rho_0) + \frac{1}{18}K_\infty\left(\frac{\rho-\rho_0}{\rho_0}\right)^2 + \ldots \tag{4}$$

where

$$K_\infty = 9\rho_0^2\frac{d^2(E/A)}{d\rho^2}\Big|_{\rho_0} \tag{5}$$

is the (nuclear) incompressibility. The knowledge of an accurate value for K_∞ is needed to extend our knowledge of the nuclear EOS in the vicinity of the saturation point, and has strong impact on the study of heavy ion collisions, neutron stars and supernovae.

There have been many attempts over the years to determine the value of K_∞, but eventually there has been consensus on the idea that the most sensitive method is based on the comparison of accurate experimental data on the strength function of the isoscalar giant monopole resonance (ISGMR), or of the isoscalar giant dipole resonance (ISGDR), with the results of the microscopic, self-consistent RPA. The main experimental tool for studying these resonances is inelastic α-particle scattering: the most recent developments in this area of investigation made it possible to measure the centroid energies E_0 of the ISGMR with an error $\delta E_0 \sim 0.1 - 0.3$ MeV [13].

Since the original works of Ref. [14,15], a clear correlation has been shown to exist between the monopole energy in ^{208}Pb and the value of K_∞ associated with a given functional; however, until a few years ago, the extraction of the empirical value of K_∞ was plagued by a critical model dependence, as the functions defining the correlation between E_0 and K_∞ were different for different families of functionals (Skyrme, Gogny or RMF). In [16], it was shown that this discrepancy between Skyrme and Gogny results does not exist, once the effect of the self-consistency violations (the neglect of Coulomb and spin-orbit residual terms discussed above) has been taken into account. Fully self-consistent Skyrme calculations do not point any more to the value of about 210 MeV quoted in [14], but to about 235 MeV in clear agreement with the Gogny result.

To make a proper comparison between the predictions of the relativistic [17] and the non-relativistic models, a systematic analysis has been made in Ref. [18]. A large set of new Skyrme forces has been generated, built with the same protocol used for the Lyon forces [5] and spanning a wide range of values for K_∞, for the symmetry energy at saturation J and its density dependence. The monopole energies, and consequently the extracted value of K_∞, depend on a well-defined parameter (K_{sym}), which controls the slope of the symmetry energy curve as a function of density. In fact, it is has been shown that there is a correlation between the values of the symmetry energy at saturation J and its slope. The Skyrme forces having a density dependence characterized by an exponent α=1/6, like SLy4, predict K_∞ around 230-240 MeV. If this exponent is increased to values of the order of 1/3, and consequently the slope of the symmetry energy curve is made stiffer, one can produce forces which are compatible with K_∞ around 250-260 MeV. This result has been independently found in Ref. [19]. It must be stressed that a further increase of α, and accordingly of K_∞, would become difficult to obtain since the effective mass m^* would become too small. One thus can make the clear and strong conclusion that the difference in the values of K_∞ obtained in the relativistic and non-relativistic models is not due to model dependence. It is mainly due to the different behavior of the symmetry energy within these models (cf. also [20]). One can quote a value of 240 MeV$\pm$20 MeV which is somewhat larger than what was previously advocated.

These conclusions have been drawn based on the case of ^{208}Pb. Results for Sn isotopes are discussed in the contribution by U. Garg, and need to be critically studied in order to decide whether they challenge the understanding reached so far.

4. The dipole resonance and the symmetry energy

In the previous Section, the problem of the density dependence of the symmetry energy has been introduced. One would imagine that the isovector giant dipole resonance (IVGDR) is the best mode for constraining the symmetry energy. However, already in Ref. [21] it has been shown that the IVGDR centroid energy cannot be simply correlated with J. The parameter which governs the value of the dipole centroid is rather

$$F_D = (f_1 \cdot J \cdot f_2)^{1/2}, \tag{6}$$

where $f_1 \sim t_1(1+\frac{x_1}{2})+t_2(1+\frac{x_2}{2})$ is proportional to the so-called enhancement factor of the classical sum rule κ (which arises from the velocity dependence of the force and cannot be strongy constrained, being empirically between 0.25 and 0.5), while $f_2 \sim \alpha\frac{m^*}{m} + \beta$ is a linear function of the effective mass which has been shown to parametrize efficiently the ratio between the surface and volume symmetry energy. This result is not surprising, since the IVDGR is known to be neither a pure volume, nor a pure surface oscillation (from its empirical mass dependence).

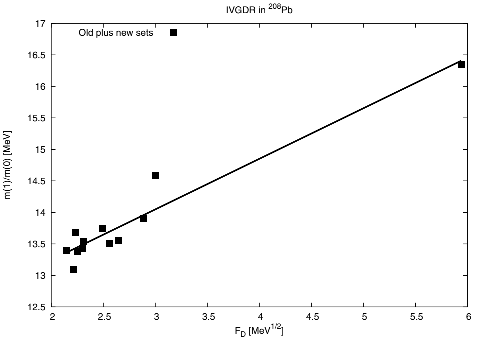

Figure 2. IV dipole centroid energies $m(1)/m(0)$ obtained in ^{208}Pb by using both the forces already considered in Ref. [21] and some of the new Skyrme parametrizations built with the Lyon protocol. The correlation with the parameter F_D defined in the text shows the same quality as in Ref. [21].

In view of the renewed interest concerning the symmetry energy, we have checked with our new RPA code that the correlation explored in Ref. [21] remains true, once new Skyrme parameter sets are introduced (at the time, no force of the type of SLy4 was available). The result is shown in Fig. 2 and agrees with expectations. On the other hand, it also indicates that the IVDGR data in a single nucleus are not enough to fix the value of J. Probably, a combined effort is needed to fix the symmetry energy and its dependence from different observables. A discussion on this issue is available in Ref. [22].

5. The dipole states calculated beyond the mean field approximation

All the previous considerations are done at HF+RPA or HFB+QRPA level (that is, mean field). It is well known that these theories are not able to describe completely the nuclear response. In particular, the giant resonances possess a conspicuous spreading width $\Gamma^{\downarrow}$, of the order of several MeV, which is due to the coupling of the simple particle-hole (or two quasi-particles) configurations with more complex ones.

In fact, in atomic nuclei the mean field defines a surface which can vibrate leading to the spectrum of the collective low-lying excitations. The coupling of the nucleons to these dynamical vibrations, a process which goes beyond mean field, can strongly renormalize the single-particle motion by changing the energy and the occupancy of the levels around the Fermi energy, and, eventually, by providing a single-particle spreading width $\Gamma^{\downarrow}_{\text{s.p.}}$. In keeping with the fact that the giant resonances can be viewed as correlated particle-hole, or two quasi-particles, states, the very same mechanism will produces their spreading width $\Gamma^{\downarrow}$. Recently, we have implemented a nuclear structure model which takes this process into account. The formalism is described in Refs. [23,24]. We have called it (Q)RPA-PC, that is, (Q)RPA plus phonon coupling.

Three nuclei were considered, and we were able to reproduce nicely the experimental data for the IVGDR (including the width). In fact, using the Skyrme force SIII [25], we obtain for the IVGDR peak energy (width) the following values in MeV: 13.1 (3.7) in ^{208}Pb, to be compared with the experimental values 13.46 (3.9), 15.7 (5.3) in ^{120}Sn against 15.4 (4.9), and 15.5 (5.8) in ^{132}Sn where the very recent experimental values are 16.1 (4.7) [26]. This kind of agreement is encouraging. In the low-lying energy region, strength is obtained in all three nuclei. In ^{208}Pb, we can compare it with the experimental data of Ref. [27]. Our total integrated strength up to 8 MeV provides a total B(E1) equal to 1.27 e^{2}fm^2, the experimental number being 0.8 e^{2}fm^2. In ^{120}Sn, only a kind of smooth background is found. Finally, in ^{132}Sn, we obtain four definite peaks lying below 10 MeV. In this case, the calculated ratio of the photoneutron cross section in the low-lying region (with respect to the IVGDR region) is 0.04, to be compared with the experimental finding which is 0.03(2). In Fig. 3, the theoretical result (dashed line) is folded with the response of the detector (full line) and compared with the experimental finding (shaded histogram).

In our calculation, the states below 10 MeV in ^{132}Sn are mainly single-particle excitations, and the absence of collective states in the low-energy region is rather clear. This is confirmed by the transition densities associated to the different dipole states. For example, whereas the one of the IVGDR peak at 13.7 MeV displays the expected shape of collective type, the one of the low-lying state at 9.7 MeV has many nodes. The low-lying transition densities are dominated by the neutron contribution at the surface, and this fact is of course relevant for excitation by direct reactions. The neutron character of the low-lying states at the surface is even more pronounced in the complete calculation, than in the simple RPA.

This absence of collective motion in the low-energy region obtained in our model, is somehow at variance with the outcome of relativistic RPA study [29]. However, this absence is quite consistent with the discussion carried out in Ref. [30], where it is argued that the soft dipole strength, observed in halo nuclei like ^{11}Li, should decrease in skin nuclei like ^{132}Sn, due to the coupling to the IVGDR (screening effect).

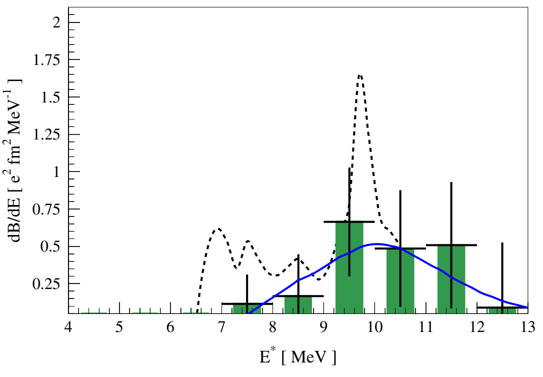

Figure 3. Comparison of the theoretical RPA-PC result for the low-lying dipole strength in ^{132}Sn (dashed line), and of the same result folded with the experimental detector response (full line), with experiment (shaded histogram with error bars) [28]. We stress that the strength below the neutron threshold (about 7.5 MeV) cannot be detected in the experiment.

As a by-product of these dipole calculations, we observe (cf. Table 2 of Ref. [24]) that the centroid energies $m(1)/m(0)$ obtained within our (Q)RPA-PC vary, with respect to simple (Q)RPA, only by at most few hundreds of keV. This means that the considerations made in the previous Sections should not be altered significantly.

6. Conclusions

Several groups are currently performing fully self-consistent RPA or QRPA calculations. It has been indeed verified that the inclusion of the full residual interaction is crucial either for the low-lying states, or when high accuracy is called for, as for the monopole response.

In fact, the centroid of the ISGMR should be determined within few hundreds of keV, if one aims to extract from this number a value for the nuclear incompressibility K_∞. In recent years, since the first Comex conference, some consensus between theoreticians has been reached about the extraction of K_∞ and the remaining uncertainity. Skyrme and Gogny functionals both point to about 230-240 MeV, but if the density dependent part of the effective interaction is made stiffer, the outcome of RMF, namely a value of K_∞ in the range 250-270 MeV, can be mimicked. In general, the ansatz for the density dependence of the energy functional (especially the part which is associated with the neutron-proton unbalance, that is, the symmetry part) is still somehow unconstrained by observables. Fixing this problem, which has considerable impact on the physics of exotic nuclei and on nuclear astrophysics, is one of the next challenges for nuclear theorists. In the present contribution we have pointed out that the IVGDR data alone are not able to solve this puzzle.

Finally, since all these considerations are done at the mean field level, we have discussed the problem of the inclusion of correlations beyond mean field. While a careful consideration of their contribution is called for, if a proper description of the lineshape of the nuclear response is required, it seems that their effect on the centroid of the resonances is not large.

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