CONFIGURATION MIXING OF MEAN-FIELD WAVE-FUNCTIONS PROJECTED ON ANGULAR MOMENTUM AND PARTICLE NUMBER; APPLICATION TO ^{24}Mg*

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We present in this talk the general framework of a method which permits to restore the rotational and particle number symmetries of wave functions obtained in Skyrme HF+BCS calculations. This restoration is nothing but a projection of mean-field intrinsic wave functions onto good particle number and good angular momentum. The method allows also to *mix* projected wave functions. Such a configuration mixing is discussed for sets of HF+BCS intrinsic states generated in constrained calculations with suitable collective variables. This procedure gives collective states which are eigenstates of the particle number and the angular momentum operators and between which transition probabilities are calculated. A test application to ^{24}Mg is presented with mean-field wave functions generated by axial quadrupole constraints. Theoretical spectra and transition probabilities are compared to the experiment. Some preliminary results for ^{32}Mg and ^{16}O are also reported.

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1. Introduction

The cranking method is widely used in nuclear structure calculations to describe high spin states [1]. In this method, a rotational band is generated by the rotation of a deformed intrinsic state. The aim of the method

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presented in this talk is to cure two of the main deficiencies of this intrinsically semi classical approach. First, cranking states are not eigenstates of angular momentum, and it is not straightforward to determine transition rates in nuclei which are not very well deformed. Approximations have been developed for transitions within a band, but they are only valid when the structure of the nuclear states are not affected by rotation.

A second limitation of the cranking model occurs in nuclei soft with respect to the variation of a collective variable. In this case, one expects that the interference of the zero-point vibrational mode with the rotational motion will lead to variations in the nuclear structure along the yrast line.

Our aim is to introduce a method in which rotations and vibrations are taken into account simultaneously in a general and consistent way.

The starting point of the approach is a set of many-body wave functions generated by constrained Skyrme HF+BCS calculations [2]. The discretization of these wave functions on a 3-dimensional Cartesian mesh enables to describe very general shapes of the nuclear density and to easily write the effect of a spatial rotation on the mean-field wave functions. This property permits to restore symmetries with respect to angular momentum [3] and to the proton and neutron particle numbers [4] in a systematic way.

We present below the general framework of our method together with a test on a light nucleus for which extensive calculations can be performed. In the first part, we show how to implement the projection on $\vec{J}$, N and Z, simultaneously. In the second part, we present a test application to the ^{24}Mg nucleus and compare our results with experimental data. We then show first results on ^{32}Mg and on the excited states of ^{16}O.

2. Angular momentum and particle number projections

2.1. Principle of the method

A detailed presentation of the method has already been presented in [5]. We recall here its main features.

The starting point of our method is a set of wave functions $|\Phi_\alpha\rangle$ generated by mean-field calculations with a constraint on a collective coordinate α. Wave functions with good angular momentum and particle numbers are obtained by restorations of symmetry on $|\Phi_\alpha\rangle$:

$$|\Phi, JM\alpha\rangle = \frac{1}{\mathcal{N}} \sum_K g_K^J \hat{P}_{MK}^J \hat{P}^Z \hat{P}^N |\Phi_\alpha\rangle\,, \tag{1}$$

where $\mathcal{N}$ is a normalization factor, $\hat{P}_{MK}^J$, $\hat{P}^N$, $\hat{P}^Z$ are, respectively, projectors onto angular momentum J with projection M along the laboratory z-axis, neutron number N and proton number Z.

In the applications shown in this paper, axial symmetry and time reversal invariance are imposed. Therefore, K can only be 0 and we shall omit the coefficient g^J_K.

A configuration mixing on the collective variable α is then performed for each angular momentum:

$$|\Psi, JM\rangle = \sum_\alpha f^{JM}_\alpha |\Phi, JM\alpha\rangle \,. \tag{2}$$

The weight functions f^{JM}_α are found by requiring that the expectation value of the energy:

$$E^{JM} = \frac{\langle \Psi, JM|\hat{H}|\Psi, JM\rangle}{\langle \Psi, JM|\Psi, JM\rangle}\,, \tag{3}$$

is stationary with respect to an arbitrary variation δf^{JM}_α. This prescription leads to the discretized Hill–Wheeler equation [6]:

$$\sum_\alpha (\mathcal{H}^{JM}_{\alpha,\alpha'} - E^{JM}_k \mathcal{I}^{JM}_{\alpha,\alpha'}) f^{JM,k}_{\alpha'} = 0\,, \tag{4}$$

in which the Hamiltonian kernel $\mathcal{H}^{JM}$ and the overlap kernel $\mathcal{I}^{JM}$ are defined as

$$\mathcal{H}^{JM}_{\alpha,\alpha'} = \langle \Phi JM\alpha|\hat{H}|\Phi JM\alpha'\rangle\,, \quad \mathcal{I}^{JM}_{\alpha,\alpha'} = \langle \Phi JM\alpha|\Phi JM\alpha'\rangle\,. \tag{5}$$

Since the Hamiltonian is rotationally invariant and conserves the number of particles, one has to restore the symmetries on only one of the two wave functions entering in each matrix element like Eq. (5). The kernels are obtained by integration on a single Euler angle, because of axial symmetry, and two gauge angles of the matrix elements between rotated wave functions.

Besides these kernels, we will calculate transition probabilities between different eigenstates of the Hill–Wheeler equation. This requires the calculation of the matrix elements of a tensor of order L, $\hat{T}^M_L$, between projected states.

Such a secular problem based on the configuration mixing defined by Eq. (2) amounts to a variation after projection in a many-body Hilbert space built on a limited set of states obtained for different values of the collective variables α's.

2.2. Calculation of multipole moments and transition probabilities

The determination of transition probabilities requires the calculation of the matrix element of a tensor of order L, $\hat{T}^M_L$, between eigenstates of the angular momentum operator.

In the case of electric quadrupole transitions, the diagonal matrix element takes the form:

$$\begin{aligned}
&\langle JM=0,\Phi|\hat{Q}_{20}|JM=0,\Phi\rangle \\
&= \langle J020|J0\rangle^2 \times \frac{\left[\int \sin\beta\, d\beta\, d^J_{00}(\beta)\langle\Phi|\mathrm{e}^{i\beta\hat{J}_y}\hat{Q}_{20}|\Phi\rangle\right]}{\left[\int \sin\beta\, d\beta\, d^J_{00}(\beta)\langle\Phi|\mathrm{e}^{i\beta\hat{J}_y}|\Phi\rangle\right]} \\
&= \frac{(J+1)J}{(2J+3)(2J-1)} \times \frac{\left[\int \sin\beta\, d\beta\, d^J_{00}(\beta)\langle\Phi|\mathrm{e}^{i\beta\hat{J}_y}\hat{Q}_{20}|\Phi\rangle\right]}{\left[\int \sin\beta\, d\beta\, d^J_{00}(\beta)\langle\Phi|\mathrm{e}^{i\beta\hat{J}_y}|\Phi\rangle\right]}. \qquad (6)
\end{aligned}$$

The transition matrix elements between GCM states are obtained as the weighted sums of the contributions of the different basis states.

3. Application to ^{24}Mg

The results shown in this section have been obtained using the HF+BCS wave functions generated with an axial quadrupole constraint. The Lipkin–Nogami prescription has been used to improve the treatment of pairing correlations. It has indeed been shown that this prescription permits to generate wave functions which give reasonable approximations of the energies obtained by a variation after projection on the good particle number [7]. In this way, the lack of a complete variation after projection should be partly compensated. The mean-field results, which we will present below, correspond to these HF+BCS+LN calculations.

We have performed calculations with the Sly4 Skyrme parameterization which has given satisfactory results in the description of rotational bands in well deformed nuclei [8]. The pairing interaction is a zero range interaction similar to the ones used in previous studies of nuclei far from stability [9]. We have slightly decreased the strength of the density-dependent pairing force from $G = 1250\,\mathrm{MeV\,fm^3}$ to $G = 1000\,\mathrm{MeV\,fm^3}$ to take into account that more correlations are included in the wave functions by the configuration mixing and the symmetry restorations.

The variation of the energy as a function of prolate and oblate deformations is plotted in Fig. 1. The mean-field curve presents a well deformed prolate minimum corresponding to a mass quadrupole moment of approximately 1b and a shoulder at an oblate deformation around 0.5 b.

The energies obtained by projecting each of the mean-field wave functions on good particle number and angular momentum are also shown in the left part of Fig. 1. The abscissa of the projected energies correspond to the quadrupole moment of the intrinsic wave function. The spherical configuration is a pure 0^+ state and contributes only to the 0^+ projected curve.

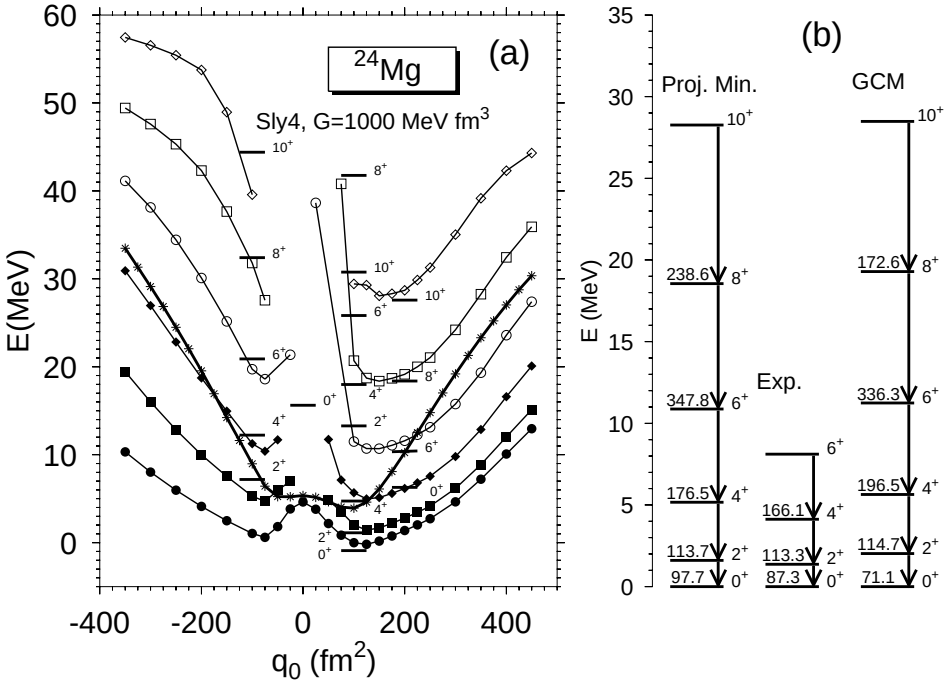

Fig. 1. (a) Projected energies for ^{24}Mg as a function of the axial quadrupole moment. The thick line with asterisks corresponds to the HF+BCS+LN energies. The energies obtained by projecting on angular momentum (from 0^+ to 10^+) intrinsic wave functions are plotted in full line as a function of the quadrupole moment of the intrinsic wave function. The first three energies obtained for each angular momentum in the configuration mixing calculation are represented by horizontal bars centered at the value of q_0 where the respective collective wave functions are maximum. (b) B(E2) transition probabilities (in e^2fm^4) for ^{24}Mg. Transition probabilities between the configurations corresponding to the minimum of the projected energy curves of Fig. 3 are shown on the left-hand-side of this figure and between the yrast collective states obtained in the GCM calculation (right-hand-side). In the central part are shown the experimental values [10].

The energy gained by projection in this case is due to the difference between the Lipkin–Nogami approximation of the energy gain due to projection on particle number, $-\lambda_2 \Delta N^2$, and the exact gain. It is of the order of 1 MeV.

The projection on angular momentum increases the energy difference between the spherical configuration and the minimum of the $J = 0^+$ curve by 3 to 4 MeV. The intrinsic wave function leading to the minimum of this curve has a quadrupole moment slightly larger than the one corresponding to the mean-field minimum. For higher angular momenta, the minima are shifted to higher quadrupole moments.

The full projection creates an oblate minimum at the position of that shoulder for J values ranging from 0^+ to 6^+. For greater values of J, the weights of the intrinsic wave functions for deformations below -2 b are very small. Consequently, the projected energy curves do not exhibit any oblate minima. However, the J=0^+ to 6^+ minima are probably not stable against triaxial deformations, since a calculation including triaxial deformations indicates that the shoulder in the intrinsic curve is a maximum with respect to γ.

One of the main interests of a restoration of rotational symmetry is the possibility to calculate transition probabilities without the approximation involved in a cranking calculation. On the right part of Fig. 1, the transition probabilities along the yrast line obtained in the GCM calculation and by considering only the minima of projected energy curves are compared to the experimental data [10]. The transition probability between the configurations minimizing the projected energy curves is very close to the experimental value. The configuration mixing causes a spreading of the collective wave function on the quadrupole moment and decreases slightly the value of the B(E2). This effect is similar to the effect of quadrupole vibrations that is sometimes included phenomenologically [11] in the determination of transition probabilities from intrinsic wave functions. Since for spin different from 0, the wave functions do not have components at low quadrupole moment, the configuration mixing does not affect significantly the transition probabilities. The agreement between both the calculations and experimental data is excellent in these cases.

4. Applications to ^{32}Mg and ^{16}O

Experimentally, it is now well established that ^{32}Mg is a well deformed nucleus: the energy of the first 2^+ state is much lower than in heavier $N = 20$ isotones and the B(E2) transition probability to the ground state is very large and compatible with a strong deformation. The description of the disappearance of the $N = 20$ shell closure is a major challenge for theory, the difficulty being to account for the changing behavior of this shell closure as a function of the proton number.

In Fig. 2 are shown the results obtained with the same mean field and pairing interactions as for ^{24}Mg. The projection and the configuration mixing are clearly not sufficient to cure the deficiencies of the pure mean field calculation. The excitation energy of the first 2^+ state is largely overestimated. However, the dynamical deformations of both the 0^+ and the 2^+ are large and lead to a B(E2) value which is around 40% of the experimental one.

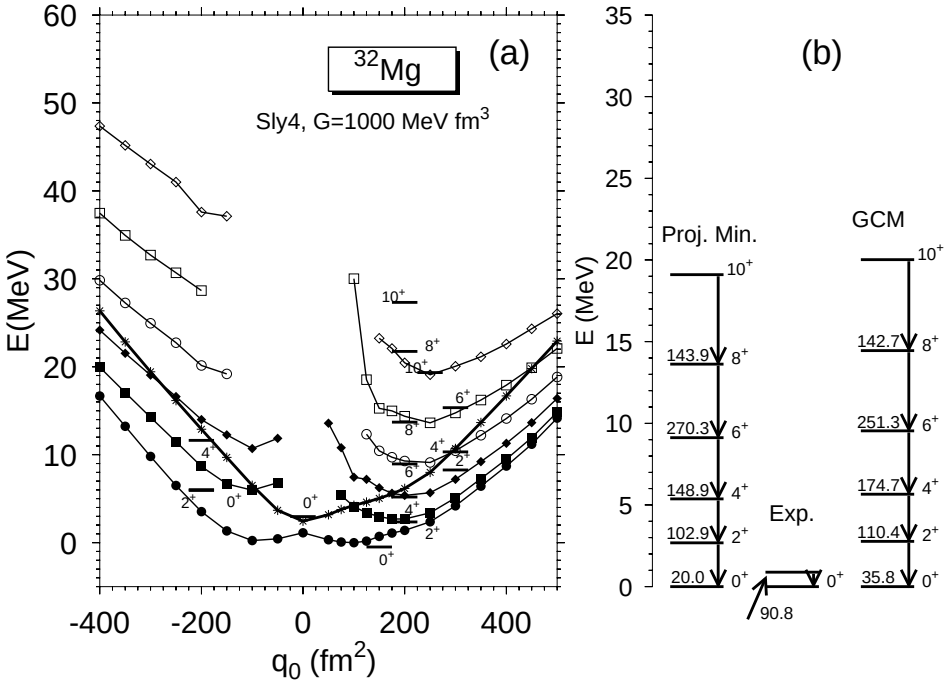

Fig. 2. Same as Fig. 1, but for ^{32}Mg. The experimental values are from [10].

The spectrum of ^{32}Mg is very sensitive to the details of the interactions that are used in both the mean field and the pairing channel. In Fig. 3, we show the results obtained with the Skyrme Skm* [12] parametrization and a volume pairing leading to pairing energies similar to the surface pairing. The excitation energy of the 2^+ state is now much more realistic (1.2 MeV) and the B(E2) value is around 75% of the experimental one. This result is encouraging and gives hope that the study of this mass region will help to improve our knowledge on the nuclear interaction. However, much work still remains to be done, the Skm* interaction having a very bad behaviour as a function of the isospin.

In Fig. 4 is plotted the HF+BCS and the $J = 0$ curve obtained for ^{16}O. As expected, the mean field curve shows a very steep minimum at the spherical point, with a shoulder around 15 MeV at a mass quadrupole moment around 100 fm^2. The curve projected on $J = 0$ is not more structured and does not give any indications on excited 0^+ states. The interesting result is obtained when a mixing on the axial quadrupole moment is performed. The ground state is dominated by the spherical configuration, but two excited states appear with dominant contributions from very deformed state. The energy and the quadrupole moment of the dominant intrinsic configuration

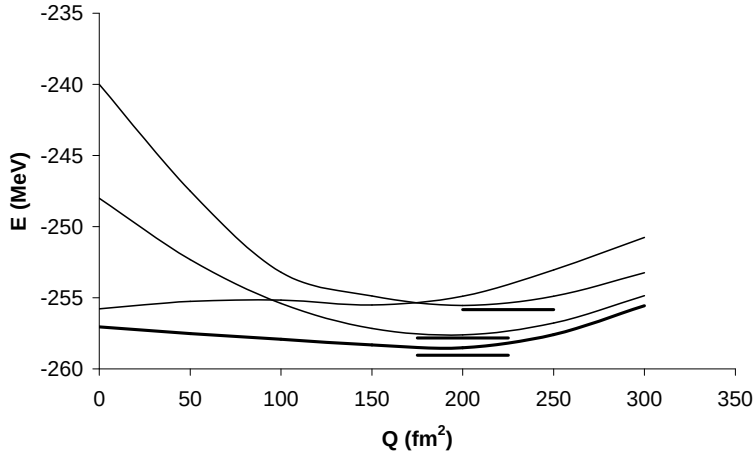

Fig. 3. Same as the left part of Fig. 1, but for ^{32}Mg and the Skm* interaction and a volume pairing.

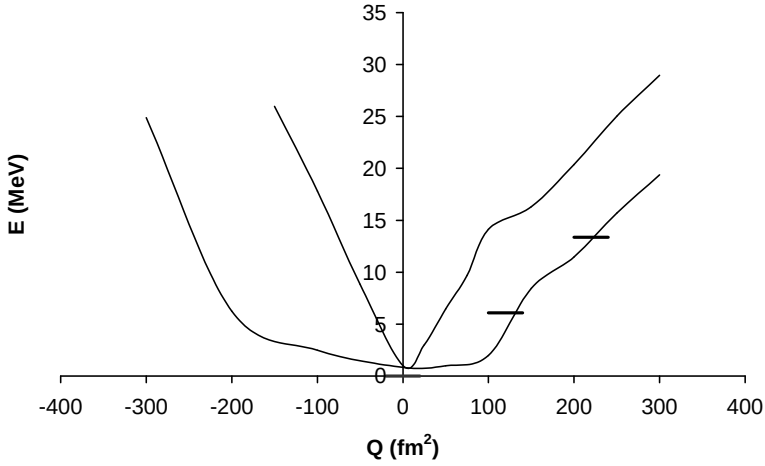

Fig. 4. HF+BCS and $J = 0$ energy curves obtained for ^{16}O. The three first 0^+ states obtained in the configuration mixing calculation are indicated by bars.

of the first state agrees very well with the first excited 0^+ state, located at 6.05 MeV and to which a dominant $4p$–$4h$ configuration is generally attributed. The characteristics of our second excited 0^+ state makes it a good candidate for a linear alpha chain configuration. These results obtained for ^{16}O indicate that our method seems to be well adapted to describe excited configurations whose structure is very different from the ground state.

5. Conclusion

In this paper, we have presented and tested a method to introduce correlations beyond mean-field on HF+BCS wave functions. The tests performed on the ^{24}Mg nucleus show that the method works with reasonable computing time.

The first and natural generalization from BCS to full Bogoliubov–Valatin transformations is under progress. It will allow a better treatment for pairing correlations. If no significant improvements for even–even nuclei close to the stability line are to be expected, HFB is essential to treat correctly nuclei near the drip lines.

The generalization to many-body wave functions breaking time reversal invariance is a necessary next step towards a description of odd nuclei. It will also make possible to project wave functions generated for each spin by cranking calculations. As it has already been shown theoretically [1], the use of cranking wave functions is the first order of a variation after projection on angular momentum. Numerical applications [3] have confirmed that the projection of cranking wave functions improves the energy obtained for each angular momentum and compresses the spectra. Such an effect would correct the too spread spectra obtained in the present study.

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