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Regularization of Multi-Reference Energy Density Functional Calculations

M. Bender

Université Bordeaux, CNRS/IN2P3, Centre d'Etudes Nucléaires de Bordeaux Gradignan, CENBG, Chemin du Solarium, BP120, F-33175 Gradignan, France

T. Duguet

CEA, Centre de Saclay, IRFU/Service de Physique Nucléaire, F-91191 Gif-sur-Yvette, France
National Superconducting Cyclotron Laboratory and Department of Physics and Astronomy, Michigan State University, East Lansing, MI 48824, USA

P.-H. Heenen

PNTPM, CP229, Université Libre de Bruxelles, B-1050 Bruxelles, Belgium

D. Lacroix

GANIL, CEA et IN2P3, BP 5027, 14076 Caen Cedex, France

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We report the first application of a recently proposed regularization procedure for multi-reference energy density functionals, which removes spurious divergent or non-continuous contributions to the binding energy, to a general configuration mixing. As an example, we present a calculation that corresponds to the particle-number and angular momentum projection of axially symmetric time-reversal invariant quasiparticle vacua of different quadrupole deformation for the nucleus ^{18}O. The SIII parameterization of the Skyrme energy functional is used.

1. Introduction

Methods based on energy density functionals (EDF) currently provide the only set of fully microscopic theoretical tools that can be applied to all bound atomic nuclei in a systematic manner irrespective of their mass, isospin, and deformation.[1] Nuclear EDF methods coexist on two distinct levels. On the first level, traditionally called "self-consistent mean-field theory" or sometimes Hartree-Fock (HF) or Hartree-Fock-Bogoliubov (HFB) method, a single product state provides the normal and anomalous density matrices that enter the energy density functional. This type of method is referred to as a single-reference (SR) approach. On the second level, often called "beyond-mean-field methods", symmetry restoration and configuration mixing in the spirit of the Generator Coordinate Method (GCM) can be

achieved.[2,3] At that level, the many-body energy takes the form of a functional of the transition density matrices that are constructed from a set of several product states, the number of which might be on the order of 10^5 in the most advanced applications. Such a method, that encompasses the SR one by construction, is referred to as a multi-reference (MR) approach.

It has been pointed out that MR EDF calculations might be contaminated by unphysical contributions to the energy.[4,5,6] In what follows, we provide a summary of the analysis of this problem and of a regularization scheme to remove it.[7,8,9] Results for ^{18}O are used as an illustrative example. Configuration mixing calculations using projection and GCM techniques were originally introduced in a Hamilton-operator+wave-function based framework.[10,11] It has to be stressed that *none* of the problems discussed in the present paper appears when such calculations are performed without making *any* simplifying approximations.

2. SR and MR EDF in a nutshell

In the SR EDF framework, the effective interaction is set-up through an energy functional

$$\mathcal{E}_q^{\rm SR} \equiv \mathcal{E}_q^{\rm SR}[\rho_{qq}, \kappa_{qq}, \kappa_{qq}^*]\,, \tag{1}$$

that depends on various local or non-local densities, which themselves are functionals of the normal and anomalous density matrices of an auxiliary reference product state $|{\rm SR}_q\rangle$ labelled by some collective coordinate q

$$\mathcal{R}_{qq} \equiv \begin{pmatrix} \rho_{qq} & \kappa_{qq} \\ -\kappa_{qq}^* & 1-\rho_{qq}^* \end{pmatrix} \equiv \begin{pmatrix} \langle {\rm SR}_q|\hat{a}^\dagger\hat{a}|{\rm SR}_q\rangle^T & \langle {\rm SR}_q|\hat{a}\hat{a}|{\rm SR}_q\rangle^T \\ \langle {\rm SR}_q|\hat{a}^\dagger\hat{a}^\dagger|{\rm SR}_q\rangle^T & \langle {\rm SR}_q|\hat{a}\hat{a}^\dagger|{\rm SR}_q\rangle^T \end{pmatrix} = \mathcal{R}_{qq}^2\,. \tag{2}$$

MR EDF calculations rely on the extension of the SR EDF to non-diagonal energy kernels. There is a set of rules and minimal requirements[12] based on symmetry arguments and specific limits of configuration mixing calculations that is usually agreed on when constructing the MR EDF. It is common practice to proceed by formal analogy with the expressions obtained when applying the generalized Wick theorem[13] (GWT) to the non-diagonal matrix element of a Hamilton operator between two product states.[14] In such a scheme, the MR EDF corresponding to a state characterized by a set of quantum numbers μ becomes a weighted sum over EDF kernels $\mathcal{E}_{qq'}^{\rm MR}$ between all possible combinations of SR states entering the MR calculation

$$\mathcal{E}_\mu^{\rm MR} = \frac{\sum_{q,q'} f_\mu^*(q)\, \mathcal{E}_{qq'}^{\rm MR}[\rho_{qq'}, \kappa_{qq'}, \kappa_{qq'}^*]\, f_\mu(q')}{\sum_{q'',q'''} f_\mu^*(q'')\, \langle {\rm SR}_{q''}|{\rm SR}_{q'''}\rangle\, f_\mu(q''')}\,. \tag{3}$$

Each EDF kernel $\mathcal{E}_{qq'}^{\rm MR}$ is constructed by replacing the density matrices entering the SR EDF $\mathcal{E}_q^{\rm SR}$ by their homologue *transition* density matrices

$$\mathcal{R}_{qq'} \equiv \begin{pmatrix} \rho_{qq'} & \kappa_{qq'} \\ -\kappa_{q'q}^* & 1-\rho_{qq'}^* \end{pmatrix} \equiv \begin{pmatrix} \frac{\langle {\rm SR}_q|\hat{a}^\dagger\hat{a}|{\rm SR}_{q'}\rangle}{\langle {\rm SR}_q|{\rm SR}_{q'}\rangle}^T & \frac{\langle {\rm SR}_q|\hat{a}\hat{a}|{\rm SR}_{q'}\rangle}{\langle {\rm SR}_q|{\rm SR}_{q'}\rangle}^T \\ \frac{\langle {\rm SR}_q|\hat{a}^\dagger\hat{a}^\dagger|{\rm SR}_{q'}\rangle}{\langle {\rm SR}_q|{\rm SR}_{q'}\rangle}^T & \frac{\langle {\rm SR}_q|\hat{a}\hat{a}^\dagger|{\rm SR}_{q'}\rangle}{\langle {\rm SR}_q|{\rm SR}_{q'}\rangle}^T \end{pmatrix} \tag{4}$$

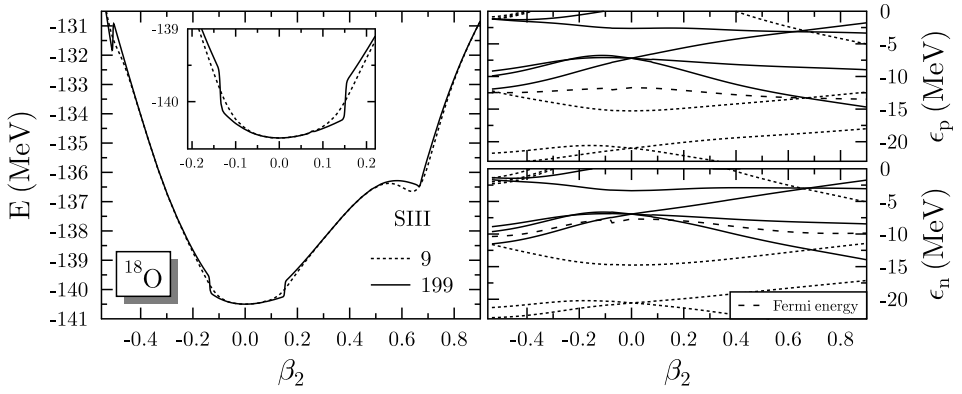

Fig. 1. Left: Particle-number-projected deformation energy surfaces of ^{18}O as a function of the axial quadrupole deformation, one calculated with $L = 9$ discretization points of the integrals over gauge angles, the other with $L = 199$. The inset in the right panel magnifies the region at small deformation. Right: corresponding Nilsson diagram of protons (upper right) and neutrons (lower right). Anomalies in the deformation energy appear when either a proton or neutron single-particle level crosses the respective Fermi energy, but they are resolved only when using an excessively large number of discretization points for the gauge-space integrals.

and multiplying with the norm kernel $\langle \mathrm{SR}_q | \mathrm{SR}_{q'} \rangle$

$$\mathcal{E}^{\mathrm{SR}}_q[\rho_{qq}, \kappa_{qq}, \kappa^*_{qq}] \rightarrow \mathcal{E}^{\mathrm{MR}}_{qq'}[\rho_{qq'}, \kappa_{qq'}, \kappa^*_{q'q}] \, \langle \mathrm{SR}_q | \mathrm{SR}_{q'} \rangle \, . \tag{5}$$

The weights $f_\mu(q)$ entering Eq. (3) are either determined by symmetries that are restored, or by solving the so-called Hill-Wheeler-Griffin equation, or by a combination of both.[3,10,11]

Over the years it has been realized, however, that in spite of the many successes of MR EDF calculations the energy functional (3) is ill-defined. As an example Fig. 1 shows a particle-number projected deformation energy curve as a function of axial mass quadrupole deformation $\beta_2 = \sqrt{5/16\pi}\,(4\pi/3R^2A)\,\langle \mathrm{SR}_q | 2z^2 - y^2 - x^2 | \mathrm{SR}_q \rangle$ of the underlying SR states, where $R = 1.2\,A^{1/3}$ fm. At some deformations, the MR energy does not converge when increasing the number L of discretization points in the gauge-space integral, although all operator matrix elements are converged already using 5 points in this case. Instead, with increasing number of discretization points the energy curve slowly develops discontinuities, which coincide with the deformations at which single-particle levels cross the Fermi energy.

First indications for this problem came from an analysis of particle-number projection that demonstrated that the contribution of a pair of exactly half-filled levels to the particle-number projected energy diverges when direct, exchange and pairing terms do not recombine in a particular manner.[5] The same divergence has been pointed out to appear in approximations that are tempting to be made for separable forces in a Hamiltonian- and wave function based framework.[15,16] A more recent thorough analysis[6] in a strict EDF framework indicates that the divergences are just the tip of the iceberg of a much larger problem hidden beneath.

One of the key features of all contemporary successful EDFs used in nuclear structure physics is that in one way or the other the Pauli principle is sacrificed for the sake of a simple and efficient description of the in-medium interaction.[a] This might concern just a density dependence, or using different functionals for the particle-hole and particle-particle parts of the interaction, or neglecting certain (even all) exchange terms, or any combination of the above. Such a feature of energy functionals is known to generate spurious "self-interaction" in the literature on density functional theory (DFT) for electronic systems, and there exists a vast literature on the subject.[18] All early analyses[5,6,15,16] point to some violation of the Pauli principle as a prerequisite for the appearance of the pathologies observed in configuration mixing calculations. The contamination of the EDF with a spurious self-interaction as such, however, does *not* lead to the pathologies visible in Fig. 1. The problem is that the contribution of self-interaction (and in addition those of spurious "self-pairing"[8] that might appear in calculations with pairing) to the MR EDF is multiplied with an ill-defined *weight factor* when the MR EDF is defined in analogy to the GWT along the lines of Eq. (3). This can be shown when constructing the same energy kernels in analogy to the standard Wick theorem in a suitable basis.[7] Indeed, the results inspired from the two Wick theorems differ in the weight factors that multiply self-interaction and self-pairing terms. It has to be stressed that there is nothing wrong with the GWT when used to evaluate matrix elements of operators, for which there are no such self-interaction terms.

Pathologies introducing discontinuities into MR EDF calculations are easiest to identify for pure particle-number restoration but they appear for *any* configuration mixing. The gauge-angle integration contained in particle-number projection can be transformed into a contour integral in the complex plane.[6,8] Then, the total energy is proportional to the sum of the residues of poles at the interior of the integration contour. All operator matrix elements have only one pole at $z = 0$. Two of the pathologies of the MR EDF, are connected to the appearance of unphysical poles in the EDF at finite $z_\mu^\pm = \pm i\,|u_\mu|/|v_\mu|$ in the complex plane, one for each pair of conjugated single-particle states in the canonical basis.[6,8] *Divergences* might appear at certain deformations whenever the integration contour hits a pole at finite $z_\mu^\pm$. The divergences are accompanied by a *finite step*, i.e. at some deformation the continuation of the energy surface on one side does not match the energy surface on the other side. The difference is connected to a pole being either inside the integration contour (thereby contributing to the energy) or outside (and thereby not contributing). In rare cases where two or more poles cross the Fermi energy simultaneously (for example at β_2 values around 0.7 in Fig. 1), one observes a sudden change in the slope of the energy surface instead of a finite step.

Divergences and steps appear whenever the set of MR states contains at least one pair of orthogonal states, $\langle \mathrm{SR}_q | \mathrm{SR}_{q'} \rangle = 0$. In particle-number projection this

[a]Some widely used and in general very successful many-body techniques, such as RPA for example, violate the Pauli-principle by construction even when a genuine Hamiltonian is used.[11,17]

always happens for half-filled single-particle levels with $u_\mu^2 = v_\mu^2 = 1/2$ at gauge angle $\pi/2$. There, the denominator of the transition densities, Eq. (4), becomes zero, which explains why the steps in Fig. 1 coincide with single-particle levels crossing the Fermi energy. For other configuration mixings, or when combining particle-number projection with other mixings, there is no such simple intuitive rule for the appearance of orthogonal states. However, such situation is known to appear when mixing quasiparticle vacua with two-quasiparticle states,[4] in angular-momentum projection of cranked HFB states,[20] or in combined angular-momentum and isospin projection,[21] and the possible appearance of spurious contributions to the MR EDF has been reported on all occasions.

The finite steps can appear in MR EDF calculations with any non-trivial functional, whereas divergences require at least one term in the EDF that is of higher than second order in normal and/or anomalous density matrices of a given isospin.[9] For this reason, there are no divergences towards $\pm\infty$ in Fig. 1, as the combination of SIII and a "volume"-type pairing functional gives a functional that contains only terms up to second order in each isospin.[8] Having steps, however, indicates that there are also spurious contributions to the total energy that are present even though no divergence occurs.

There is a third pathology related to the integration contour hitting branch cuts of the EDF in the complex plane,[6,9] which will not be discussed here. It appears when using density dependencies that become multi-valued functions when extended into the complex plane. Again, this might happen for any configuration mixing which leads to complex transition densities. For certain restricted configuration mixings, this problem can be suppressed using partially projected densities for the density dependencies instead of transition densities. This is done, for example, in recent configuration mixing calculations using the density-dependent Gogny force,[19] where this strategy together with the painstaking calculation of *all* exchange terms suppresses any visible signs of the pathologies discussed here. Such scheme, however, cannot be expected to work for all imaginable configuration mixings.[12]

In projection after variation (PAV) calculations, all of these problems are usually hidden as their unambiguous resolution requires a discretization of the deformation energy surfaces and of the integrals over gauge (or Euler) angles that is *much* finer than what is usually used, c.f. Fig. 1. By contrast, a variation after projection calculation is very much likely to find the divergences.[6] But also in a PAV framework, there is no guarantee that just using low resolution will suppress all consequences of the unphysical contribution to the MR EDF.

3. Regularization of the MR EDF

A general method to regularize MR EDF calculations for arbitrary mixing has been proposed by us.[7] The discussion of the formalism is beyond the scope of these proceedings, and we refer to the literature[7,8,22] for details. Instead, we will give

here a summary of the ideas and key concepts.

As already mentioned, the origin of the divergences and steps is that postulating the MR EDF as a functional of normal and anomalous transition densities multiplies contributions to the EDF that violate the Pauli principle by ill-defined weight factors. These weight factors turn out to be different (and well-behaved) when postulating the MR EDF in analogy with operator matrix elements computed on the basis of the standard Wick theorem (SWR).[7] As a matter of fact, the weights of self-interaction and self-pairing terms are the *only* ones in the EDF which are different when comparing a GWT-motivated definition of the MR EDF with the SWT-motivated one. Obviously the SWT and GWT are strictly equivalent when evaluating an operator matrix element.

The basic idea of the regularization procedure is to define the MR EDF in analogy to operator matrix elements computed from the SWT. However, two technical difficulties arise when trying to do so. The first one is that the SWT can be applied to the evaluation of non-diagonal matrix elements only in carefully chosen bases. By contrast, the GWT can be used in any basis, or even when using two different bases, one for each of the two states entering a matrix element,[14] which of course explains the GWT's use as the standard procedure in symmetry restoration and GCM-type calculations. A basis allowing the use of the SWT is provided by the canonical basis of the Bogoliubov transformation between the two quasiparticle bases that provide the "left" and "right" product states entering the non-diagonal matrix element.[7] This Bogoliubov transformation between two quasiparticle bases is not related to pairing correlations, but it has the same formal properties as the Bogoliubov transformation in HFB theory. The Bloch-Messiah-Zumino (BMZ) factorization of this Bogoliubov transformation, which provides the canonical basis that permits to use the SWT, can be done, but in general turns out to be non-trivial.[22] Pure particle-number projection has the advantage that this canonical basis can be analytically constructed: the original "left" and "right" bases and the canonical one of the transformation between them differ by state-dependent phase factors only. This simplification made particle-number projection the testing ground for first applications of the regularization procedure.[8] Once a procedure for BMZ factorization of a general Bogoliubov transformation has been set up, however, it allows for the regularization of any MR EDF calculation.[22]

A second difficulty with setting up the MR EDF in analogy to the SWT is that doing this directly would lead to difficulty in handling the expression of the functional. The contributions from specific combinations of single-particle states have to be taken out from the energy, which prohibits to write the energy as a functional of one-body densities at all. A more efficient strategy is to set-up the basic EDF through one-body transition densities in analogy to the GWT as usual, and to subtract a *correction* that is defined as the difference between the expressions obtained when defining the MR EDF in analogy to the GWT or the SWT, respectively.

As mentioned above, in the case of pure particle-number restoration, divergences and steps in the deformation energy surfaces are intimately connected to the ap-

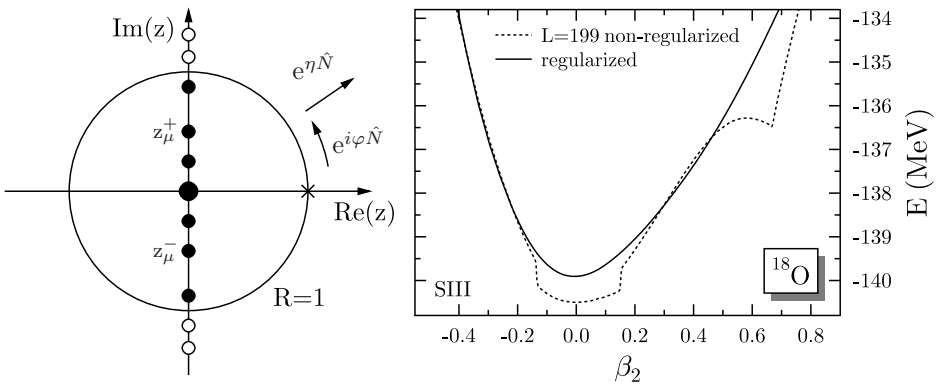

Fig. 2. Left: Schematic view of the analytical structure of the energy kernels entering the particle-number restored EDF over the complex plane. Poles marked with filled circles are within the standard circular integration contour of radius $R = 1$, whereas those outside are marked with open circles. The cross marks the location of the SR EDF at $z = 1$. The operator $e^{i\varphi\hat{N}}$ produces a rotation in gauge space, whereas $e^{\eta\hat{N}}$ scales the integration contour. Right: Non-regularized (dotted line) and regularized (solid line) particle-number-projected deformation energy for ^{18}O, calculated with $L = 199$ discretization points of the integrals in gauge space. The regularized energy curve is independent on L for $L > 5$, whereas the non-regularized one is not, cf. Fig. 1.

pearance of unphysical poles at $z_\mu^\pm = \pm i\,|u_\mu|/|v_\mu|$ in the complex plane, see Fig. 2 for a schematic sketch, and to their evolution with deformation. The correction, however, does not only (entirely) remove the contribution of the unphysical poles, but also an unphysical contribution from the physical pole at $z = 0$. The latter is impossible to identify without having the comparison of SWT- and GWT-based expressions. Removing only the contribution from the poles at $z_\mu^\pm$ would lead to unphysical results, as their contribution can grow far beyond any physical scale in the nucleus.[6,8] It is the removal of both types of contributions that leads to a meaningful correction; individually both contributions are very large, of opposite sign, and nearly cancel. Eventually, the total correction remains smaller than the energy gain from particle-number restoration as it should.[8]

The regularization, however, is strictly limited to EDFs that depend on integer powers of the normal and anomalous density matrices only.[9] This excludes its application to almost all currently used functionals of acceptable predictive power. One of the few regularizable Skyrme interactions found in the literature is SIII,[23] which we use here for the particle-hole part of the strong interaction.

As pairing interaction we use a pairing functional of "volume" type of strength 300 MeV fm^{-3}. The widely used Slater approximation to the Coulomb exchange term, however, falls into the category of multi-valued density-dependent terms. To obtain a regularizable functional, we keep only the direct term of the Coulomb energy functional and neglect the approximate exchange term that was considered in the fit of SIII. As a consequence, nuclei will be underbound by a few MeV, but

this is of no importance for the purpose of the present article. The trilinear part of SIII has the particular property that all its terms are bilinear in densities of one nuclear species and linear in the other. As an important consequence, there are no divergences in the non-regularized results shown here, only finite steps as already pointed out.

4. Results for ^{18}O

4.1. *Pure particle-number restoration*

The comparison of the non-regularized and regularized particle-number projected deformation energy curve is presented in Fig. 2 for ^{18}O. First of all, the regularization removes the steps that appeared in the non-regularized particle-number restored deformation energy surface of Fig. 1. For ^{18}O, it even removes all structure from the deformation energy in the interval shown, including the pronounced shoulder at $\beta_2 \approx 0.7$. Second, the correction varies from several hundreds of keVs up to about 1 MeV depending on the deformation, which is small compared to the total binding energy but sometimes accounts for a substantial percentage of the energy gain from particle-number restoration. The regularized EDF converges numerically in the same manner as operator matrix elements when changing the discretization of MR EDF calculations. By contrast non-regularized calculations in general do not, and in fact cannot, converge at all deformations. The regularized EDF fulfills the sum rules known for particle-number projected operator matrix elements, whereas the non-regularized EDF might provide zero and negative particle numbers with non-zero energies.[8] The regularized EDF is also *shift invariant* (as are operator matrix elements), i.e. the energy is independent under a $e^{\eta \hat{N}}$ transformation that corresponds to a change of the radius of the integration contour in the complex plane.[8] By contrast, the non-regularized EDF might change by *many orders of magnitude* when varying the radius of the integration contour.[6,8] Altogether, this provides strong evidence that the regularized MR EDF is as well-behaved as operator matrix elements.

4.2. *Particle-number and angular-momentum restored GCM*

Now we turn to a more complex calculation that combines four different configuration mixings based on a set of axially symmetric time-reversal- and space-inversion-invariant quasiparticle vacua: particle-number restoration of $N = 10$ and $Z = 8$, i.e. the particle numbers constrained in the underlying SR calculations, angular-momentum projection, and GCM-type mixing of configurations with different (axial) shapes.[22] Results obtained from standard non-regularized calculations are compared with regularized ones in Fig. 3. The shoulder that appears at β_2 values around 0.7 in the non-regularized calculations of Fig. 2 leads to a very localized minimum in the $J = 0, 2$ and 4 curves. For higher angular momenta, the results become irregular. The regularized energy curves, however, are much smoother. In the non-regularized

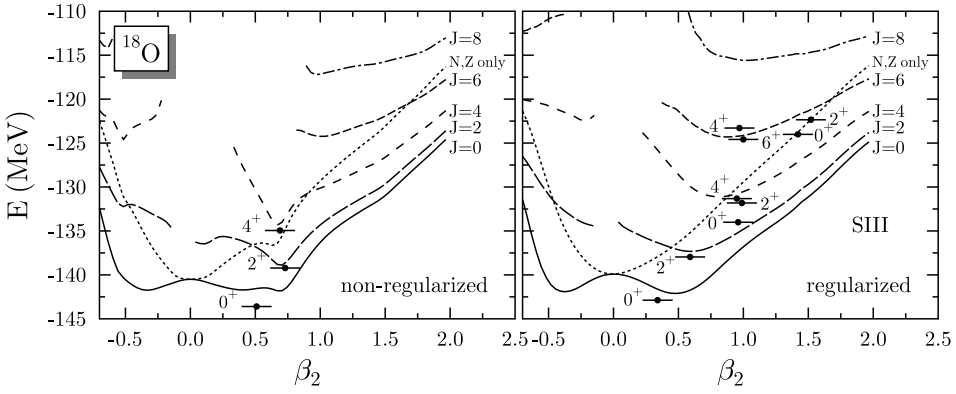

Fig. 3. Left: Non-regularized particle-number and angular momentum projected deformation energy curves for ^{18}O, calculated using $L = 9$ gauge angles and 20 Euler angles, together with the yrast states constructed by GCM-type mixing of configurations of different deformation up to $J = 4$, plotted at the average deformation of the intrinsic states they are constructed from. Right: Regularized particle-number and angular momentum projected deformation energy curves for ^{18}O, together with low-lying states obtained from GCM.

calculations, GCM states can be safely constructed up to $J = 4$ only. For higher values of J, and non-yrast states in general, the energies depend too sensitively on the selection of states entering the GCM, and the Hill-Wheeler-Griffin equation often gives spurious solutions. These difficulties almost disappear in the regularized calculations, where the complete low-lying spectrum can be constructed. It resembles the one of an anharmonic vibrator, which is in qualitative agreement with the data, where the low-lying states indeed suggest being such one- and two-phonon multiplets.[24] It has to be stressed that in the GCM mixing of axial quasiparticle vacua for such a small system as ^{18}O no more than about 8 sufficiently independent intrinsic configurations (i.e. of overlap sufficiently different from 1) can be found for $J = 0$, and even less for higher values of J. This is linked to the very small number of level crossings in the Nilsson diagrams of Fig. 2.

5. Discussion and Outlook

We have presented the first application of a regularization scheme for MR EDF calculation to a general configuration mixing. The impact of the regularization on the results obtained for ^{18}O is quite substantial. It gives "more regular" energy curves, and makes the Hill-Wheeler-Griffin equation much more stable. A much more detailed analysis of regularized MR EDF calculations of ^{18}O and other nuclei will be given in a forthcoming publication.[22] Already the example presented here shows that the regularization might become mandatory in many applications to detailed spectroscopy.

The nucleus ^{18}O discussed here is a relatively extreme example. The two single-particle levels crossing simultaneously the Fermi energy at β_2 values around 0.7,

which dominate many low-lying collective states, contaminates the most important energy kernels with large spurious contributions. For all other nuclei we have studied so far, the overall impact of the regularization on the spectrum of low-lying states is less dramatic.

Only energy density functionals which are strictly of integer power in normal and anomalous density matrices are regularizable. The construction of regularizable functionals of high quality is a priority for the near future. Eventually, it is likely that additional mathematical constraints on the functional form of the MR energy kernel must be derived based on group theoretical considerations to make symmetry restoration well formulated within the EDF context.[25,26]

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