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On the non-Unitarity of the Bogoliubov Transformation due to the Quasiparticle Space Truncation

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Abstract. We show that due to the energy cutoff in the Hartree-Fock-Bogoliubov quasiparticle space, the Bogoliubov transformation becomes non-unitary. We propose a method of restoring the unitarity by introducing a truncated single-particle Hilbert space, in which the HFB equations are to be solved.

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1 Introduction

Skyrme energy density functionals are among the most commonly used in the self-consistent mean-field nuclear structure calculations. The pairing component of the functional usually corresponds to a zero-range interaction in the coordinate space [1], which is equivalent to a constant (infinite range) interaction in the momentum space. Therefore, an energy cutoff followed by a pairing strength refit is necessary to regularize the results, and the number of active quasiparticle states becomes finite. On the other hand, the dimension of the particle space is either infinite (coordinate representation) or truncated for reasons that are not related to the pairing regularization. This implies different dimensions of particle and quasiparticle spaces and, therefore, renders the Bogoliubov transformation non-unitary. As a result, the pairing tensor is no longer antisymmetric, but it acquires a finite symmetric component.

In this work, we propose a method of restoring the unitarity of the Bogoliubov transformation, while keeping the number of quasiparticle states limited. The method is based on a truncation of the particle space and solving the Hartree-Fock-Bogoliubov [2] (HFB) equations in this truncated Hilbert space. The proposed truncation scheme accommodates all the particle states that are needed within a given truncation of the quasiparticle space.

2 Method

By using the code HFBTHO [3], we perform the HFB calculations within the particle space of 20 harmonic oscillator shells, which leads to the single-particle energies of 200 MeV and above. When no truncation is performed in the quasiparticle space, the Bogoliubov transformation is unitary, and this guarantees that the pairing tensor κ is antisymmetric. This is no longer true for the finite energy cutoff. The inset in Fig. 1 shows the maximum matrix element of the symmetric and antisymmetric parts of the pairing tensor as functions of the cutoff energy E_c in the quasiparticle space. Typically, the former does not exceed 1% of the latter; however, a non-zero symmetric component means that the fermion quasiparticle state representing the HFB ground state does not exist. Usually one simply disregards this symmetric part in the Skyrme-HFB calculations. Our method ensures the antisymmetricity of the pairing tensor and, at the same time, keeps the number of quasiparticle states limited. The approach is based on finding an optimal truncated particle space, dictated by a given quasiparticle truncation, in which the HFB equations are solved without any further cutoff. Full-space diagonalization of the HFB equations is necessary only to provide the aforementioned optimal basis.

The Singular Value Decomposition (SVD) [4] is an algebraic method, which, by means of finding the so-called singular values, orders orthonormal basis states according to their importance for decomposition of a rectangular matrix into a sum of components. We use it to decompose the combined matrix $[B^* A^*]$, where B and A are the Bogoliubov matrices corresponding to a non-unitary transformation, and assemble the optimal basis by taking only those particle states which have the corresponding singular values above a certain SVD cutoff, v_c. Since for each value of the SVD cutoff the dimension of the result-

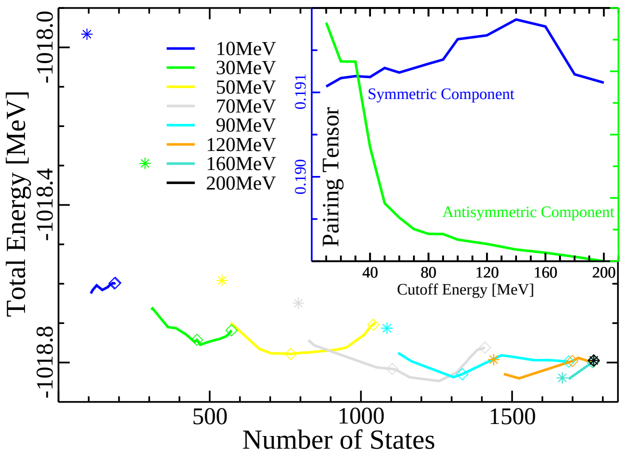

Fig. 1. Total energies of ^{120}Sn obtained for the Sly4 Skyrme functional and different values of the energy and SVD cutoffs. Stars correspond to the standard HFB solutions and diamonds to two values of the SVD cutoff: $v_c = 10^{-3}$ and 10^{-2}. The maximum matrix element of the symmetric (left scale) and anti-symmetric (right scale) parts of the pairing tensor are shown in the inset.

ing particle space is different, one has to refit the pairing strength as function of v_c. We do it so that the pairing gap is the same in both steps: in the full-space solution obtained for a given energy cutoff and in the truncated-space solution. Our calculations are carried out according to the following scheme:

a Self-consistent solution of the HFB equations in the full space.
b Singular Value Decomposition of the combined matrix $[B^* A^*]$ corresponding to the full-space solution.
c Defining the truncated particle space by keeping the SVD states that correspond to singular values above the SVD cutoff v_c.
d Self-consistent solution of the HFB equations in the truncated particle space.
e Fitting the pairing strength by repeating step (d) with different pairing strengths until the pairing gaps in the full and truncated spaces are equal.

3 Results

Figure 2 shows the number of states in the truncated particle spaces as functions of the SVD cutoff v_c for various cutoff energies E_c. For large v_c or E_c, these numbers are close to the numbers of quasiparticle states (shown by dotted lines); however, for small v_c, additional particle states are necessary to properly represent the kept quasiparticle states. Total energies obtained by solving the HFB equations in the truncated particle spaces are shown in Fig. 1. For cutoff energies above 30 MeV, the total energy is stable up to about 200 keV. For any fixed cutoff energy, the method is also very stable (<100 keV) with respect to the SVD cutoff. Therefore, our method allows

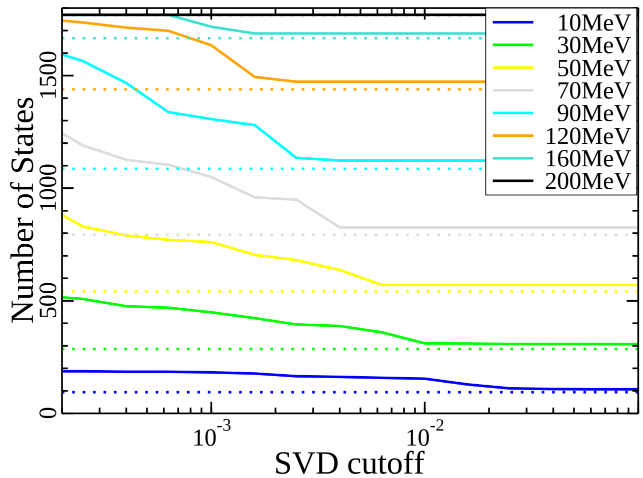

Fig. 2. Number of neutron particle states in ^{120}Sn in the truncated spaces (solid lines) and numbers of quasiparticle states below the cutoff energies (dotted lines) as functions of the SVD cutoff, for different values of the energy cutoff.

us to perform the HFB calculations with satisfying precision for relatively small cutoff energies and dimensions of the particle space. While the two-step character of the method, and necessity to refit the pairing strength, makes the method significantly more computationally extensive than the standard HFB approach, the procedure allows for usual interpretation in terms of Bogoliubov product states. In order to implement the pairing readjustments, one could use the Green-function regularization methods [5], which will be considered in future work.

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