Extrapolation Method for Shell Model Calculations with Projected Deformed Basis

Takahiro Mizusaki,
Institute of Natural Sciences, Senshu University, Jimbocho 3-8, Kanda, Chiyoda-ku, Tokyo, 101-8425, Japan.

An investigation for numerical algorithms for large-scale shell model problems has been one of long-standing and central issues in nuclear structure physics. Recently we have developed new extrapolation method in shell model calculations with spherical basis [1,2] and deformed basis [3], which have succeeded in enlarging the feasibility of large-scale shell model calculations. A crucial point of the present extrapolation method is to derive the extrapolation formula in a non-empirical way. The extrapolation method is based on a scaling property between the energies and energy variances of approximated wave functions. For a series of systematically approximated wave functions, energies are linear (with slight quadratic correction [2]) as a function of energy variance. By this relation, we can estimate *exact* energy by taking zero-variance limit.

In Ref. [1,2], we applied this extrapolation method to shell model calculations with spherical basis. However, within spherical basis, truncation often becomes quite severer in larger shell model calculations. For such a case, optimized deformed basis with angular momentum projection becomes a suitable approximation. Therefore we have developed extrapolation for such a deformed basis in Ref. [3].

In Fig. 1, an example for ^{60}Zn is shown where two kinds of extrapolation are shown and, in the zero-variance limit, agreement of extrapolated energies is quite nice for ground and first excited states. Its complete shell model space has about two billion dimension, while, in the deformed basis, we can get *exact* energy from one Slater determinant with angular momentum projection. Its details are shown in Ref. [3].

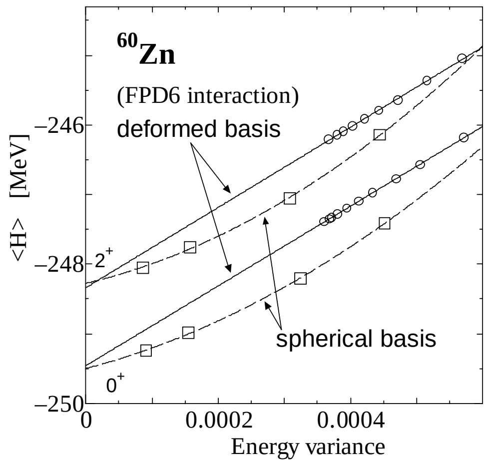

Figure 1: Ground and first excited state energies are shown as a function of energy variance for ^{60}Zn with FPD6 interaction. Two kinds of extrapolations are shown.

Recently the N=Z nuclei with medium mass (around 80) becomes interesting because of coexistence of various shapes, various types of isomers and various alignments at high spins [4]. However, the relevant shell model spaces become quite huge. Therefore the present extrapolation method with deformed basis can make an essential contribution for such large-scale shell model problems.

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[2] T.Mizusaki and M.Imada, Phys. Rev. **C67**, 041301R (2003).
[3] T.Mizusaki, Phys. Rev. C**70**, 044316 (2004).
[4] M. Hasegawa, K.Kaneko and T. Mizusaki, Phys. Rev. C**70** 031301R (2004).