Physics Letters B 679 (2009) 214–218

Contents lists available at ScienceDirect

Physics Letters B

www.elsevier.com/locate/physletb

Shell-model Hamiltonian from self-consistent mean-field model: $N = Z$ nuclei

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ARTICLE INFO

Article history:
Received 6 April 2009
Received in revised form 9 July 2009
Accepted 15 July 2009
Available online 22 July 2009
Editor: W. Haxton

PACS:
21.60.Cs
21.60.Jz
21.60.-n
21.10.-k

Keywords:
Nuclear shell model
Skyrme Hartree–Fock
$N = Z$ nuclei

ABSTRACT

We propose a procedure to determine the effective nuclear shell-model Hamiltonian in a truncated space from a self-consistent mean-field model, e.g., the Skyrme model. The parameters of pairing plus quadrupole–quadrupole interaction with monopole force are obtained so that the potential energy surface of the Skyrme Hartree–Fock + BCS calculation is reproduced. We test our method for $N = Z$ nuclei in the fpg- and sd-shell regions. It is shown that the calculated energy spectra with these parameters are in a good agreement with experimental data, in which the importance of the monopole interaction is discussed. This method may represent a practical way of defining the Hamiltonian for general shell-model calculations.

Nuclear structure study is usually carried out with two major groups of microscopic approaches: the self-consistent mean-field (SCMF) method [1] and the shell model (SM) method [2]. Both approaches have their advantages and disadvantages. The SCMF method has a wide applicability across the nuclear chart for global properties of the ground state, such as the binding energy, nuclear size, and surface deformation. However, it does not give detailed spectra of excited states and wave functions. Beyond mean-field approximations, the angular momentum and particle number projection method has been applied; but it has been pointed out that there are some conceptual problems and numerical difficulties [3,4]. On the other hand, the SM method has the advantage that excited energy levels and wave functions are described properly with many-body correlations included. However, in the SM approach, the shell model Hamiltonian is required to accord with each truncated model space, and single-particle energies and interaction matrix elements must be specific to the mass region. It is not very clear how to determine these quantities microscopically. There have been attempts along this line by Brown and Richter [5] and by Alhassid, Bertsch, and collaborators [6,7]. In the former attempt, the SCMF was used to determine single-particle energies of the SM Hamiltonian, while in the latter, a procedure for mapping the SCMF onto the SM Hamiltonian, which includes monopole pairing and quadrupole–quadrupole (QQ) interactions, was proposed. Very recently, a novel way of determining parameters of the interacting boson model (IBM) Hamiltonian has been proposed by Nomura et al. [8] by using the potential energy surfaces (PESs) of the SCMF model.

A realistic SM Hamiltonian can in principle be derived from the free nucleon–nucleon force, and in fact, such microscopic interactions have been proposed for the pf shell [9,10]. However, they fail to reproduce excitation spectra, binding energies, and transitions if many valence nucleons are involved. To overcome this defect, considerable effort has been put forward on effective interactions with empirical fit to experimental data [11–13]. On the other hand, realistic effective interactions in nuclei are expressed in terms of multipole pairing, multipole particle–hole, and monopole interactions, the dominant parts of which are the monopole pairing and quadrupole–quadrupole interactions with monopole terms (PQQM) [14]. This has actually been confirmed for a wide range of $N \approx Z$ nuclei in a series of calculations with an extended PQQM interactions including additional terms (the quadrupole pairing and the octupole–octupole term) [15,16]. This extended PQQM model has

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0370-2693/$ – see front matter
doi:10.1016/j.physletb.2009.07.041

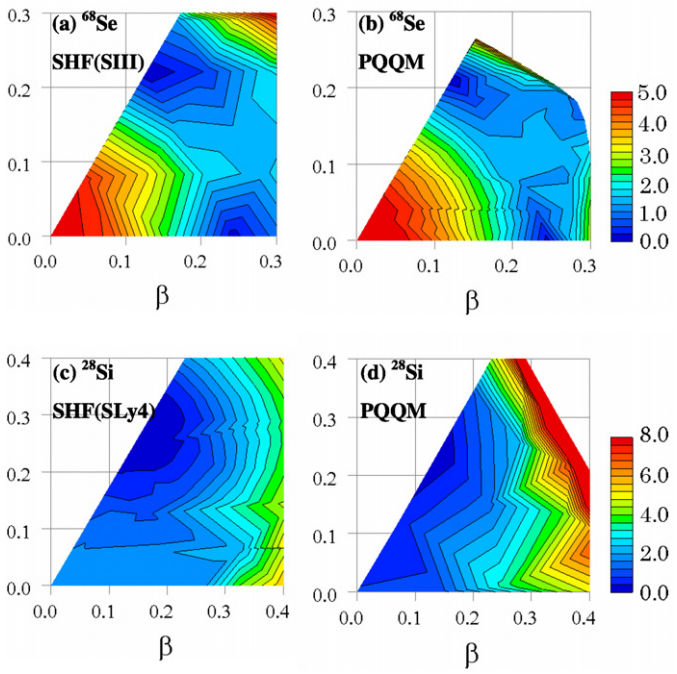

Fig. 1. (Color online.) PESs for ^{68}Se and ^{28}Si in the SHF calculation (a) and (c) and the PQQM shell-model calculation (b) and (d). The PQQM parameters are determined so that the PQQM PES reproduces approximately that of the SHF. Contour spacings are 0.2 MeV and 0.4 MeV for upper and lower graphs, respectively.

been successfully applied to different nuclei, as for instance those in the fp-shell region [15] and the fpg-shell region [16]. The model has only several parameters, far less than the number of realistic interaction matrix elements usually contained in shell model calculations. However, its capability is very much comparable to that of realistic effective interactions. Thus, the extended PQQM model is not a mere schematic model, but is a kind of realistic shell model calculation applicable to a large body of nuclei.

In general, defining an effective SM Hamiltonian, especially for heavier nuclei where truncation in the shell model space is necessary, is a very difficult task. It is desired that a SM Hamiltonian is determined at a more fundamental level, which can not only locally fit excitation spectra, but also be consistent with a global description of the ground state properties. It has been claimed [17] that within the SCMF method, the Skyrme force contains correct QQ and monopole components, and is able to describe both low- and high-energy quadrupole excitations. The Skyrme force including pairing interaction contains QQ and pairing, as well as monopole components. It is the purpose of the present Letter that based on the Skyrme SCMF, we propose the Hamiltonian for the truncated shell model by performing a global PES mapping. We note that for a shell model using realistic effective interactions, it may be very difficult to obtain a unique result when such a global PES mapping is performed because there are too many interaction matrix elements in the model. However, our PQQM model Hamiltonian has only few parameters, namely, the g_0, χ, and monopole strengths (see Eq. (1) below). Therefore, the PQQM type of interaction is particularly suitable for a global PES mapping.

Fig. 1a and c show PESs on the β–γ plane calculated by the constrained Skyrme Hartree–Fock + BCS method (hereafter denoted as SHF), which is imposed by the triaxial degrees of freedom using the mass quadrupole moments. The plotted energy ranges are up to 5 MeV for ^{68}Se and 8 MeV for ^{28}Si above the respective energy minimum. For ^{68}Se, we employ the SIII parameter set [18] of the Skyrme interaction for the mean-field channel, which has been successful in describing systematically the ground-state quadrupole deformations in proton- and neutron-rich Kr, Sr, Zr, and Mo isotopes [19]. For ^{28}Si, we use the SLy4 [20] interaction. We use the ev8 code [21] with pairing interaction of the δ-function type with the strength $V_0 = 1000$ MeV fm^3. For ^{68}Se, the long-standing prediction of a stable oblate deformation was confirmed by the observation of the oblate ground state band in ^{68}Se [22]. Determination of shape was inferred indirectly from the study of rotational bands, while direct quadrupole measurement is difficult for these short-lived states. It has been suggested by various theoretical approaches [23–27] that the oblate configuration coexists with a prolate rotational band, which constitutes a clear example of oblate–prolate shape coexistence. It can be seen from Fig. 1 that the PES of the current SCMF calculation with SIII interaction (Fig. 1a) indeed yields two separate minima at the oblate and prolate side with deformation $\beta \approx 0.24$. For ^{28}Si, the PES (Fig. 1c) has a minimum at the oblate side with deformation $\beta \approx 0.33$, corresponding to the experimental spectroscopic quadrupole moment $Q_s = 16\ e\,\mathrm{fm}^2$.

To connect these SHF results with SM results, we start with the PQQM model Hamiltonian [27,28]

$$H = \sum_{\alpha} \varepsilon_a c_\alpha^\dagger c_\alpha - \frac{g_0}{2} P_0^\dagger \cdot P_0 - \frac{\chi}{2} Q_2^\dagger \cdot Q_2 + V_{\mathrm{m}}, \tag{1}$$

where ε_a is single-particle energy. The second term in Eq. (1) is the monopole pairing interactions with P_0 being the $T = 1$, $J = 0$ pair operator, and the third term is the QQ interaction with Q_2 the $T = 0$ quadrupole operator. The last term V_{m} is the monopole force. Due to isospin-invariance, each of these terms in Eq. (1) contains the p–n components which play important roles in $N = Z$ nuclei. The quadrupole-pairing, the octupole–octupole, and the average monopole terms employed in the previous papers [27,28] are neglected for simplicity because they do not affect the current conclusion.

The SM calculation [27,28] is performed by the SM code [29] for the fpg- and sd-SM spaces, for which we assume a closed ^{56}Ni- and ^{16}O-core, respectively. Since the Hamiltonian (1) is isospin-invariant, single-particle energies are taken as the same for protons and neutrons. For the fpg-shell space, the single-particle energies for the $2p_{3/2}$, $1f_{5/2}$, $2p_{1/2}$, and $1g_{9/2}$ states can be read from the low-lying states of ^{57}Ni. We use the experimental values $\varepsilon_{p3/2} = 0.0$, $\varepsilon_{f5/2} = 0.77$, $\varepsilon_{p1/2} = 1.11$, and $\varepsilon_{g9/2} = 2.50$ (all in MeV), as in the previous paper [27]. For the sd-shell space, the single-particle energies for the $1d_{5/2}$, $2s_{1/2}$, and $1d_{3/2}$ states are employed from USD Hamiltonian [11]. Nuclear shapes including triaxiality are calculated by the constrained Hartree–Fock (CHF) method [30,31] and SM PES is defined as the expectation value $\langle H \rangle$ with respect to the CHF state in the β–γ plane.

We now sketch the procedure to determine the pairing, the quadrupole–quadrupole, and the monopole force strengths by taking ^{68}Se and ^{28}Si as examples. Fig. 2 shows the PESs as functions of axial deformation β and of triaxiality γ with fixed β at the deformation minimum. The PES results in solid curves are obtained by requiring that the interaction strengths in the PQQM Hamiltonian are set so as to reproduce the PESs of the SHF calculation. As one can see, the PESs of the PQQM calculation reproduce well those of the SHF with SIII for ^{68}Se and SLy4 for ^{28}Si. For large deformations with $|\beta| > 0.24$ in ^{68}Se and $|\beta| > 0.4$ in ^{28}Si, the PESs have the pronounced sharp wall as shown in Fig. 2. This seems to be a general trend and is probably due to the small truncated model space. We therefore neglect this sharp wall in the PES mapping. In this way, the PQQM parameters are uniquely determined.

It is known that the SHF PES pattern depends on the Skyrme parameterization. To show that the extracted PQQM Hamiltonian