Shell model Monte Carlo approach: the heavy nuclei

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Abstract. The auxiliary-field Monte Carlo (AFMC) method, also known as the shell model Monte Carlo (SMMC), enables us to calculate microscopically statistical and collective properties of nuclei in the presence of strong correlations. These calculations can be carried out in shell model spaces that are many orders of magnitude larger than spaces that can be treated with conventional diagonalization methods. A recent major development has been the extension of the AFMC approach to heavy nuclei. Such applications to heavy nuclei have been a major challenge. On the conceptual level, a crucial question is whether a truncated spherical shell model Hamiltonian can describe the proper collectivity observed in heavy nuclei and, in particular, the rotational character of strongly deformed nuclei. On the technical level, the low excitation energies make it necessary to perform calculations down to much lower temperatures. At such low temperatures the propagator becomes ill-conditioned and requires the introduction of stabilization methods.

1. Introduction

The microscopic derivation of nuclear properties from the underlying nuclear forces is a major challenge in nuclear theory. These nuclear properties are required in the modeling of astrophysical processes such as nucleosynthesis and supernovas. Microscopic theories are also necessary for the interpretation of data from new radioactive beam facilities.

Much progress has been made in applications of ab initio methods such as the Green function Monte Carlo (GFMC) method [1] and the no core shell model (NCSM) [2]. However, both GFMC and NCSM are limited to light nuclei. Density functional theory (DFT) has been successful in the global treatment of nuclei [3, 4], but the inclusion of correlations beyond the mean field and the description of excitations require extensions of DFT [5, 6].

A promising approach is the configuration-interaction (CI) shell model method, in which the correlated state is expressed as a coherent superposition of a large number of uncorrelated configurations. The CI approach is widely used in atomic, molecular and nuclear physics, as well as in finite-size condensed matter systems (e.g., quantum dots). It accounts for both shell effects and correlations, and has been very successful in describing the low-energy spectroscopy of nuclei up to $A \sim 52$ using a single major valence shell [7]. However, applications of the CI method in medium-mass and heavy nuclei are limited as the dimensionality of the model space becomes prohibitively large for conventional diagonalization methods.

This difficulty was overcome in part through the use of the auxiliary-field Monte Carlo (AFMC) method, also known in nuclear physics as the shell model Monte Carlo (SMMC)
approach [8, 9, 10]. Fermionic Monte Carlo methods are often limited by the so-called sign problem. However, the dominating collective components of effective nuclear interactions [11] have a good sign. Consequently, certain nuclear properties can be calculated with good-sign interactions [12, 13]. Furthermore, interactions containing small terms that have a bad sign can be treated by an extrapolation method [9]. AFMC enables us to carry out calculations in model spaces that are many orders of magnitude larger than those that can be solved by conventional methods.

The AFMC method has proven to be a very powerful tool in calculating the statistical properties of nuclei [14, 15, 16, 17]. However, most of the AFMC calculations carried out to date were limited to medium-mass nuclei whose deformation is not large. In such even-even nuclei the gap to the first excited state is of the order of 1-2 MeV and the ground state can be reached with modest values of the inverse temperature $\beta$. The situation is very different in heavy nuclei (e.g., the rare-earth region) where the deformation can be large and the first excitation energy is of the order of 100 keV. This leads to major technical difficulties in extending AFMC to heavy deformed nuclei. Furthermore, well-deformed nuclei are characterized by rotational bands. A central issue is whether it is possible to describe this rotational behavior in the framework of a truncated spherical shell model.

We have recently extended the AFMC approach to such heavy deformed nuclei [18]. In Sec. 2 we discuss the AFMC and its extension to heavy nuclei and in Sec. 3 we demonstrate its applications to a typical heavy deformed rare-earth nucleus, $^{162}\text{Dy}$.

2. Auxiliary-field Monte Carlo (AFMC) approach

We briefly outline the AFMC method and then discuss technical aspects that arise in heavy nuclei.

2.1. AFMC method

The AFMC method is based on a Hubbard-Stratonovich (HS) transformation [19], a representation of the imaginary-time many-particle propagator as a functional integral over propagators of non-interacting particles moving in external time-dependent auxiliary fields.

In the HS representation, the Gibbs operator $e^{-\beta \hat{H}}$ of a nucleus describes by the Hamiltonian $\hat{H}$ at inverse temperature $\beta = 1/T$ is decomposed as

$$e^{-\beta \hat{H}} = \int D[\sigma] G_\sigma U_\sigma ,$$

(1)

where $G_\sigma$ is a Gaussian weight and $U_\sigma$ is the propagator of non-interacting nucleons moving in time-dependent auxiliary fields $\sigma(\tau)$.

The integrand in Eq. (1) describes a one-body propagator and is relatively easy to calculate using matrix algebra in the single-particle space. However, the number of auxiliary fields to be integrated over is very large. In AFMC, this integration is carried out by Monte Carlo methods that select the most important configurations.

2.2. The heavy nuclei

The extension of AFMC to heavy nuclei has required to overcome several major challenges that are summarized below.

- **AFMC in proton-neutron formalism.** In heavy nuclei, protons and neutrons occupy different shells. This has required the major task of rewriting the AFMC code in proton-neutron formalism. A different formulation based on isospin $T_z$ projection was used in Ref. [20]. Our formulation, however, is much more efficient since the matrices representing the auxiliary-field have the dimension of either the proton or neutron single-particle space rather than the combined dimension.
• **Stabilization at low temperatures.** The first excitation in even-even rare-earth nuclei is about an order of magnitude smaller than in medium-mass nuclei. To calculate ground-state observables it is then necessary to propagate to much longer imaginary time \( \beta \sim 20 \). At large \( \beta \), the propagator becomes ill-conditioned, i.e., the ratio between its largest and smallest eigenvalues becomes very large.

In strongly correlated electron systems a similar problem was resolved by stabilization methods in the grand-canonical ensemble [21], keeping the small and large scales separated in the propagation. The method is based on a singular value decomposition (SVD) or a modified Gram-Schmidt (MGS) decomposition of the propagation matrix. We have used the MGS decomposition of a matrix \( M = LDV \) or \( M = UDR \) where \( L \) (\( R \)) is a lower (upper) triangular matrix with diagonal elements 1 and \( D \) is a diagonal matrix. The MGS decomposition can be up to \( \sim 20 \) times faster than SVD [22].

We extended the stabilization methods to the canonical ensemble by stabilizing separately each term in the Fourier series of particle-projected observables.

• **Choice of model space.** It is necessary to use a sufficiently large model space to describe the rotational character of deformed nuclei. To determine the required spherical orbitals we consider a deformed Woods-Saxon plus spin-orbit mean-field potential and determine the average occupation of the spherical orbitals. We include in our model space all spherical orbitals whose occupation probabilities are between 0.1 and 0.9. The effect of other orbitals is taken into account by the renormalization of the effective interaction.

We find that the proton \( 1f_{7/2} \) orbital with an occupation probability of 0.15 is the only orbital above the \( Z = 82 \) gap that has an occupation probability larger than 0.1. For example, the occupation probability of the proton \( 0h_{9/2} \) orbital is only 0.03. We therefore choose the proton model space to include the \( 50 - 82 \) shell plus the \( 1f_{7/2} \) orbital. Similarly we determine the neutron model space to be the \( 82 - 126 \) shell plus the \( 0h_{11/2} \) and \( 1g_{9/2} \) orbitals.

• **Discretization effects.** In practice, the HS transformation is calculated by dividing \( \beta \) into a finite number of small time slices \( \Delta \beta \). This results in a systematic discretization error in observables, such as the thermal energy. We calculate observables at several values of \( \Delta \beta \) and then extrapolate linearly to \( \Delta \beta = 0 \). Above a certain value of \( \beta \) we find weak dependence on \( \Delta \beta \) and take instead an average.

• **Particle-number projection.** The stabilized calculations, required at larger values of \( \beta \), are time-consuming. We have implemented an approximate particle-number projection that uses a smaller number of quadrature points but is sufficiently accurate for the AFMC calculations. Time-reversal symmetry of the propagators for good-sign interactions can also be used to halve the computational time.

The single-particle Hamiltonian is taken from a Woods-Saxon plus spin-orbit potential. For the interaction we use the dominant components of realistic effective nuclear interactions: multipole-multipole interactions (quadrupole, octupole and hexadecupole) and a monopole pairing interaction [18]. These interaction components are attractive and have a good Monte Carlo sign.

3. Results

In this section we discuss AFMC results for a typically heavy deformed nucleus \(^{162}\)Dy.

3.1. **Thermal signatures of rotational collectivity**

While AFMC enables us to overcome the model’s size problem, it has its own limitations. AFMC is a method for calculating thermal and ground-state observables but it is not suitable for extracting a detailed spectrum. Since the particular collective character of a nucleus is often
identified by characteristic patterns of its spectrum, one has to rethink how various collectivity types manifest in statistical observables.

In AFMC we measure observables at a given temperature (canonical ensemble), while experiments in nuclei provide information on nuclear properties at fixed energy (microcanonical ensemble). However, it is relatively easy to transform the microcanonical results to the canonical ensemble. This requires the experimental knowledge of a complete set of levels and their spins, and is therefore limited to low excitation energies.

A thermal observable that can be used to distinguish between different types of collectivity is \( \langle J^2 \rangle \), where \( J \) is the total angular momentum of the nucleus. Assuming a nucleus characterized by a ground-state rotational band with moment of inertia \( I_g \), we have at sufficiently low temperatures \( T \)

\[
\langle J^2 \rangle \approx 2I_g T.
\] (2)

This result can also be derived by applying the equipartition theorem for the nuclear rotation.

In Fig. 1 we show \( \langle J^2 \rangle \) versus \( T \) for the well-deformed rare-earth nucleus \( ^{162}\text{Dy} \). The solid circles with error bars are the stabilized AFMC results at low temperature while the solid straight line is a fit to Eq. (2). We find a moment of inertia of \( I_g = 35.8 \pm 1.5 \) MeV\(^{-1} \), in agreement with the experimental value of \( I_g = 37.2 \) MeV\(^{-1} \) (determined by the excitation energy, 80.7 keV, of the first excited \( 2^+ \) state). The dashed line is calculated using the experimentally known lowest five experimental rotational bands. The dashed-dotted line is a fit assuming a vibrational nucleus. The good agreement of the AFMC results with Eq. (2) confirms the rotational character of \( ^{162}\text{Dy} \) within the truncated spherical model space discussed in Sec. 2.2.

The excitation energy of a rotational nucleus at low temperatures is given by

\[
E(T) = E_0 + T,
\] (3)

where \( E_0 \) is a ground-state energy. Fig. 2 shows the AFMC thermal energy of \( ^{162}\text{Dy} \) as a function of \( T \). The solid line is a fit to Eq. (3) with \( E_0 = -375.387 \pm 0.019 \) MeV. The good agreement with the AFMC results is consistent with the rotational character of this nucleus.

3.2. Level density

The level density is related to the partition function by an inverse Laplace transform. The average level density is obtained in the saddle-point approximation [23]

\[
\rho(E) \approx \frac{1}{\sqrt{2\pi T^2C}} e^{S(E)},
\] (4)

where \( S(E) \) is the canonical entropy and \( C \) is the canonical heat capacity.

In AFMC we calculate the thermal energy \( E(\beta) \) versus inverse temperature \( \beta \) and integrate the thermodynamic relation \( -\partial \ln Z/\partial \beta = E(\beta) \) to find the canonical partition function \( Z(\beta) \). The entropy and heat capacity are then calculated using \( S(E) = \ln Z + \beta E \) and \( C = -\beta^2 \partial E/\partial \beta \).

Fig. 3 shows the AFMC thermal energy as a function of the inverse temperature \( \beta \) up to \( \beta = 20 \) MeV\(^{-1} \). The dot-dashed line is the thermal Hartree-Fock-Bogoliubov (HFB) energy. The AFMC results give a correlation energy of \( E_{\text{HFB}} - E_0 \) of about 3.12 MeV (\( E_{\text{HFB}} \) is the ground-state energy in the HFB approximation).

The state density of \( ^{162}\text{Dy} \) is shown in Fig. 4. The solid blue circles are the AFMC results using Eq. (4) while the dot-dashed line is the HFB state density. The latter describes the intrinsic level density, while the AFMC state density includes the contribution from rotational bands. Thus, the ratio between the AFMC and HFB densities provides a microscopic estimate of the rotational enhancement factor \( K_{\text{rot}} \).

We used several experimental data sets to determine the experimental level density. At low energies, i.e., below \( \sim 2 \) MeV, there is a complete set of experimental levels [24, 25] (solid
Figure 1. \( \langle J^2 \rangle \) versus \( T \) for \( ^{162}\text{Dy} \). The solid circles with error bars are the AFMC results. The solid line is a fit to Eq. (2), while dot-dashed line is a fit to a vibrational model. The dashed line is obtained from the lowest experimentally known five rotational bands. From Ref. [18].

Figure 2. Thermal energy \( E(T) \) versus \( T \) for \( ^{162}\text{Dy} \). The solid circles are the AFMC results and the solid line is a fit to Eq. (3). The dashed line is calculated from the lowest five rotational bands of \( ^{162}\text{Dy} \). From Ref. [18].

Figure 3. Thermal energy \( E(\beta) \) versus inverse temperature \( \beta \) for \( ^{162}\text{Dy} \) and \( \beta > 2 \) MeV\(^{-1}\). The dashed line is the HFB energy. The inset shows the complete set of AFMC energies versus \( \beta \).

Figure 4. State density of \( ^{162}\text{Dy} \). The solid blue circles are the AFMC results and the dot-dashed line is the HFB state density. Also shown are three data sets (level counting, Oslo data and neutron resonance data) and the experimentally determined composite formula (dashed line). After Ref. [18].

histograms in Fig. 4). At intermediate energies below \( \sim 7 \) MeV there is the (renormalized) data set obtained by the Oslo method [26, 27] (open squares), and at \( E_x = 8.196 \) MeV we have the neutron resonance data [28] (red triangle). The dashed line in Fig. 4 is a composite level density formula [29] fitted to all three experimental data sets. This composite formula describes
a constant temperature level density formula below a matching energy of $E_M = 1.752$ MeV and a backshifted Fermi gas formula above $E_M$. We observe that the AFMC level density is in very good agreement with the experimentally determined composite formula.

4. Conclusion

The AFMC method enables us to calculate the statistical and collective properties of nuclei in very large model spaces. We discussed an extension of the method to heavy deformed nuclei. In particular, we find that the rotational character of such nuclei can be reproduced in a truncated spherical shell model approach.

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