Nuclear deformation in the configuration-interaction shell model

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Abstract. We review a method that we recently introduced to calculate the finite-temperature distribution of the axial quadrupole operator in the laboratory frame using the auxiliary-field Monte Carlo technique in the framework of the configuration-interaction shell model. We also discuss recent work to determine the probability distribution of the quadrupole shape tensor as a function of intrinsic deformation \(\beta, \gamma\) by expanding its logarithm in quadrupole invariants. We demonstrate our method for an isotope chain of samarium nuclei whose ground states describe a crossover from spherical to deformed shapes.

1. Introduction

Deformation is a central concept in understanding the physics of heavy nuclei [1]. However, since intrinsic deformation is introduced by invoking a mean-field approximation that breaks rotational symmetry, it is a challenge to determine the probability density of the intrinsic deformation in the configuration-interaction (CI) shell model, a framework that preserves rotational symmetry.

Here we review a recent technique we introduced to calculate the axial quadrupole distribution in the laboratory frame using the auxiliary-field Monte Carlo (AFMC) method [2, 3]. We found that this lab-frame distribution exhibits a model-independent signature of deformation. We then discuss recent work in which we used quadrupole invariants [4, 5] to model the quadrupole shape distribution in the intrinsic frame [6]. We demonstrate our method for an isotope chain of samarium nuclei, using the model space and interaction of Refs. [7, 8]. Quadrupole invariants were used to extract the effective intrinsic deformation within the framework of the CI shell model in lighter nuclei; see the recent examples in Refs. [9, 10] and references therein.

2. Auxiliary-field Monte Carlo method

AFMC, also known in the context of the nuclear shell model as the shell model Monte Carlo (SMMC) method [11, 12, 13], is based on the Hubbard-Stratonovich (HS) transformation [14]. The Gibbs operator \(e^{-\hat{H}/T}\) of a nucleus described by the Hamiltonian \(\hat{H}\) at temperature \(T\) is represented as a superposition of non-interacting propagators \(\hat{U}_\sigma\) of nucleons moving in auxiliary fields \(\sigma = \sigma(\tau)\) that depend on imaginary time \(\tau\)

\[
e^{-\hat{H}/T} = \int D[\sigma] \, G_\sigma \hat{U}_\sigma,
\]

(1)
where $G_\sigma$ is a Gaussian weight. The thermal expectation value of an observable $\hat{O}$ can then be written as

$$
\langle \hat{O} \rangle = \frac{\text{Tr} \left( \hat{O} e^{-\hat{H}/T} \right)}{\text{Tr} e^{-\hat{H}/T}} = \frac{\int \mathcal{D}[\sigma] G_\sigma(\hat{O}) \sigma \text{Tr} \hat{U}_\sigma}{\int \mathcal{D}[\sigma] G_\sigma \text{Tr} \hat{U}_\sigma},
$$

where $\langle \hat{O} \rangle_\sigma \equiv \text{Tr} (\hat{O} \hat{U}_\sigma)/\text{Tr} \hat{U}_\sigma$. The integrands in Eq. (2) can be calculated using matrix algebra in the single-particle space, and the integration over the large number of auxiliary fields $\sigma(\tau)$ is carried out by Monte Carlo methods. Canonical expectation values at fixed number of protons and neutrons are calculated using a discrete Fourier representation of the particle-number projection [15, 16].

3. Quadrupole distribution in the laboratory frame

The lab-frame distribution $P(q)$ of the axial quadrupole $\hat{Q}_{20}$ at temperature $T$ is defined by

$$
P(q) = \text{Tr} \left[ \delta(\hat{Q}_{20} - q) e^{-\hat{H}/T} \right] / \text{Tr} e^{-\hat{H}/T}.
$$

Using complete sets of many-particle eigenstates $|e_m\rangle$ and $|q_n\rangle$ of $\hat{H}$ and $\hat{Q}_{20}$, respectively, we have (note that $[H, \hat{Q}_{20}] \neq 0$)

$$
P(q) = \sum_n \delta(q - q_n) \sum_m \langle q_n | e_m \rangle^2 e^{-\epsilon_m/T}.
$$

In the CI shell model, the spectrum of $\hat{Q}_{20}$ is discrete, but for a heavy nucleus it becomes a quasi-continuum.

3.1. Projection on the axial quadrupole

To carry out the projection in AFMC, we represent the $\delta$ function as a Fourier integral

$$
\delta(\hat{Q}_{20} - q) = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\varphi e^{-i\varphi q} e^{i\varphi \hat{Q}_{20}},
$$

and use this in (3) together with the HS transformation (1) for $e^{-\hat{H}/T}$. For each configuration $\sigma$ of the auxiliary fields, we replace the Fourier integral by a discrete Fourier transform. Choosing an interval $[-q_{\text{max}}, q_{\text{max}}]$, dividing it into $2M + 1$ intervals of equal length $\Delta q = 2q_{\text{max}}/(2M + 1)$, and defining $q_m = m\Delta q$, we have

$$
\text{Tr} \left[ \delta(\hat{Q}_{20} - q_m) \hat{U}_\sigma \right] \approx \frac{1}{2q_{\text{max}}} \sum_{k=-M}^{M} e^{-ik\varphi_k q_m} \text{Tr}(e^{i\varphi_k \hat{Q}_{20}} \hat{U}_\sigma),
$$

where $\varphi_k = \pi k/q_{\text{max}}$ ($k = -M, \ldots, M$). Since $\hat{Q}_{20}$ is a one-body operator, we can calculate the grand-canonical traces on the r.h.s. of (6) in terms of the matrices $\hat{Q}_{20}$ and $\hat{U}_\sigma$ representing, respectively, $\hat{Q}_{20}$ and $\hat{U}_\sigma$ in the single-particle space, i.e., $\text{Tr}(e^{i\varphi_k \hat{Q}_{20}} \hat{U}_\sigma) = \det(1 + e^{i\varphi_k \hat{Q}_{20}})$.  

3.2. Angle averaging

When using the usual Metropolis algorithm, we find that for a deformed nucleus, the distribution $P(q)$ and its moments are slow to thermalize and have a large decorrelation length. We resolved this problem by averaging over a specific set of rotation angles $\Omega_j$

$$
\langle e^{i\varphi \hat{Q}_{20}} \rangle_\sigma \rightarrow \frac{1}{N_\Omega} \sum_{j=1}^{N_\Omega} \langle e^{i\varphi \hat{Q}_{20}} \rangle_{\sigma,\Omega_j},
$$

(7)
where \( \langle e^{i\varphi \hat{Q}_{20}} \rangle_{\sigma, \Omega} = \text{Tr} \left( e^{i\varphi \hat{Q}_{20}} \hat{R}\sigma \hat{R}^\dagger \right) / \text{Tr} \left( \hat{R}\sigma \hat{R}^\dagger \right) \), with \( \hat{R} = \hat{R}(\Omega) \) being the rotation operator with angles \( \Omega \). We note that any rotation of \( \hat{Q}_{20} \) in (5) does not affect the distribution \( P(q) \) since the Hamiltonian \( \hat{H} \) is invariant under rotations. The angles \( \Omega_j \) are chosen such that \( \hat{Q}_{m}^{20} \) is proportional to the invariant of order \( m \) up to a given order \( n \). We have determined a set of 6 angles for \( n = 2 \) and a set of 21 angles for \( n = 3 \) \([3]\). All calculations shown here are based on a 21-angle average. We used a time slice of \( \Delta \beta = 1/64 \text{ MeV}^{-1} \) in a discretized version of the HS transformation (1) and \( \sim 5000 \) auxiliary-field configurations for each temperature.

3.3. Application to samarium isotopes

In Fig. 1 we show AFMC distributions \( P(q) \) for an isotope chain of samarium nuclei \( ^{148−154}\text{Sm} \) at low, intermediate and high temperatures. We observed that the low-temperature distribution for \( ^{154}\text{Sm} \), whose Hartree-Fock-Bogoliubov (HFB) ground state is deformed, is skewed and in qualitative agreement with the distribution for a prolate rigid rotor (dashed line). In contrast, the low-temperature distribution for the spherical nucleus \( ^{148}\text{Sm} \) is close to a Gaussian. We conclude that the axial quadrupole distribution in the lab frame is a model-independent signature of deformation. At low temperatures, we observe a crossover from a spherical to a prolate shape as we increase the number of neutrons. In the isotopes that are deformed at low temperature \( (^{150−154}\text{Sm}) \), we observe a crossover to a spherical shape as we increase \( T \).

![Figure 1. AFMC distributions \( P(q) \) vs. \( q \) (blue circles) for an isotope chain of samarium nuclei at high, intermediate and low temperatures. The dashed lines are rigid-rotor distributions. The red solid lines are the distributions obtained from (12) (see Sec. 4.2). Adapted from Ref. [3].](image)

4. Quadrupole distribution in the intrinsic frame

In physical applications, we are interested in the intrinsic deformation of the nucleus. Information on intrinsic deformation can be extracted without invoking a mean-field approximation by using quadrupole invariants which are frame-independent.

4.1. Quadrupole invariants and their relation to moments of \( \hat{Q}_{20} \)

A quadrupole invariant is a linear combination of products of the components \( \hat{Q}_{2\mu} \) that is invariant under rotations. These invariants can be constructed from tensor products of the
second-rank quadrupole tensor $\hat{Q}_{2\mu}$ \cite{4, 5}. For any given order $2 \leq n \leq 4$, these invariants are unique and their expectation values can be expressed in terms of the corresponding moments of $\hat{Q}_{20}$:

$$
\langle \hat{Q} \cdot \hat{Q} \rangle = 5\langle \hat{Q}^2_{20} \rangle, \quad \langle (\hat{Q} \times \hat{Q})^{(2)} \cdot \hat{Q} \rangle = -5\sqrt{\frac{7}{2}}\langle \hat{Q}^3_{20} \rangle, \quad \langle (\hat{Q} \cdot \hat{Q})^2 \rangle = \frac{35}{3}\langle \hat{Q}_{20}^4 \rangle.
$$

(8)

For given values $q_{2\mu}$ of the quadrupole tensor, we define dimensionless quadrupole deformation parameters $\alpha_{2\mu}$ as in the liquid drop model, i.e., $q_{2\mu} = \frac{3}{\sqrt{5\pi}} r_0^2 A^{5/3} \alpha_{2\mu}$, where $r_0 = 1.2$ fm and $A$ is the mass number of the nucleus. For each set of deformation parameters $\alpha_{2\mu}$, we define an intrinsic frame whose orientation is characterized by Euler angles $\Omega$, and in which the deformation parameters $\tilde{\alpha}_{2\mu}$ are given by

$$
\tilde{\alpha}_{20} = \beta \cos \gamma, \quad \tilde{\alpha}_{21} = \tilde{\alpha}_{2,-1} = 0, \quad \tilde{\alpha}_{22} = \tilde{\alpha}_{2,-2} = \text{real} = \frac{1}{\sqrt{2}} \beta \sin \gamma.
$$

(9)

The parameters $\beta, \gamma$ are known as the Hill-Wheeler parameters. The metric of the transformation from the lab-frame variables $\alpha_{2\mu}$ to the intrinsic-frame variables $\beta, \gamma, \Omega$ is given by

$$
\prod_{\mu} d\alpha_{2\mu} = \frac{1}{2} \beta^4 |\sin(3\gamma)| d\beta d\gamma d\Omega.
$$

(10)

Quadrupole invariants can also be constructed from $\alpha_{2\mu}$, and up to fourth order, they are given by

$$
\alpha \cdot \alpha = \beta^2, \quad [\alpha \times \alpha]_2 \cdot \alpha = -\sqrt{\frac{7}{5}} \beta^3 \cos(3\gamma), \quad (\alpha \cdot \alpha)^2 = \beta^4.
$$

(11)

4.2. Landau-like expansion

The distribution $P(T, \alpha_{2\mu})$ of the quadrupole deformation $\alpha_{2\mu}$ at temperature $T$ is a rotational invariant and therefore it depends only on the intrinsic parameters $\beta, \gamma$. Using a Landau-like expansion \cite{17}, we expand the logarithm of $P$ in the quadrupole invariants up to fourth order

$$
P(T, \beta, \gamma) = N(T)e^{-a(T)\beta^2 - b(T)\beta^3 \cos(3\gamma) - c(T)\beta^4},
$$

(12)

where $a, b, c$ are temperature-dependent coefficients and $N$ is a normalization constant determined from $4\pi^2 \int d\beta d\gamma \beta^4 |\sin(3\gamma)| P(T, \beta, \gamma) = 1$. The parameters $a, b, c$ are determined by matching the expectation values [calculated with the distribution (12)] of the three quadrupole invariants as expressed in (11) with their AFMC values, which can be computed from the corresponding moments of $P(q)$ using Eqs. (8).

4.3. Validation of the Landau-like expansion

To test the validity of (12), we construct the lab-frame distribution $P(T, \alpha_{2\mu})$ by expressing the quadrupole invariants in terms of the lab-frame deformation $\alpha_{2\mu}$ [see Eq. (11)]. We then integrate over all $\alpha_{2\mu}$ with $\mu \neq 0$ to find the lab-frame distribution of $\alpha_{20}$, or equivalently $P(q)$, and compare it with the AFMC distribution. The distributions $P(q)$ calculated from the model (12) are shown by the solid red lines in Fig. 1 and are in excellent agreement with the AFMC distributions (open blue circles).

4.4. Application to samarium isotopes

Figure 2 shows the calculated shape distributions $P(T, \beta, \gamma)$ defined in (12) vs. $\beta, \gamma$ for the samarium isotopes at the same temperatures as in Fig. 1. The maxima of the distributions (12) mimic the shape transition observed in the HFB mean-field approximation but in the
Figure 2. Intrinsic shape distributions $P(T, \beta, \gamma)$ at low, intermediate and high temperatures for the even-mass samarium isotopes $^{148-154}$Sm. Adapted from Ref. [6].

Figure 3. Definition of a spherical, prolate and oblate shape regions in the $\beta - \gamma$ plane. These regions are used in presenting the results of Fig. 4. Taken from Ref. [6].

framework of the CI shell model [18]. As a function of neutron number we observe a transition from a spherical to prolate shape, while nuclei that are deformed in their ground state make a transition from deformed to spherical shape as a function of temperature.

To simplify the presentation of our results we divide the $\beta - \gamma$ plane into the three regions as shown in Fig. 3, which we choose to represent spherical, prolate and oblate shapes. For each region, we then define $P_{\text{shape}}(T)$ to be the probability to find the nucleus in the corresponding region, i.e., $P_{\text{shape}}(T) = 4\pi^2 \int_{\text{shape}} d\beta d\gamma |\beta|^4 |\sin 3\gamma| P(T, \beta, \gamma)$. In Fig. 4 we show these probabilities as a function of temperature $T$ for the four even-mass samarium isotopes. In the spherical $^{148}$Sm, the spherical region dominates at all temperatures, while in the deformed $^{152,154}$Sm isotopes, the prolate region has a probability close to 1 at low temperatures and the spherical region becomes the most probable above a certain temperature. The transitional nucleus $^{150}$Sm exhibits an intermediate behavior.
Figure 4. Probabilities of spherical (red open circles), prolate (green solid circles), and oblate (blue pluses) regions as a function of $T$ for $^{148-154}$Sm isotopes. Adapted from Ref. [6].

5. Conclusion and outlook

We discussed a method we recently introduced to calculate lab-frame and intrinsic shape distributions within the CI shell model without invoking a mean-field approximation. Using the saddle-point approximation, it is also possible to convert the finite-temperature intrinsic shape distribution (12) to level densities $\rho(E_x, \beta, \gamma)$ as a function of excitation energy $E_x$ and intrinsic deformation $\beta, \gamma$ [6]. Deformation-dependent level densities are useful in the modeling of nuclear shape dynamics, such as fission.

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