Spin projection in the shell model Monte Carlo method and the spin distribution of nuclear level densities

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We introduce spin projection methods in the shell model Monte Carlo approach and apply them to calculate the spin distribution of level densities for iron-region nuclei using the complete $(pf + g_{9/2})$-shell. We compare the calculated distributions with the spin-cutoff model and extract an energy-dependent moment of inertia. For even-even nuclei and at low excitation energies, we observe a significant suppression of the moment of inertia and odd-even staggering in the spin dependence of level densities.

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The spin distribution of level densities are important for the calculation of statistical nuclear reaction rates such as those in thermal stellar reactions. Knowledge of the spin distribution is also required for the determination of total level densities from measured neutron or proton resonances, since the latter are subjected to spin selection rules.

The microscopic calculation of the spin distribution of level densities in the presence of correlations is a difficult problem. It is often assumed that the spin distribution follows the spin-cutoff model, obtained in the random coupling model of uncorrelated spins of the individual nucleons or excitons. The spin-cutoff distribution is determined by a single parameter, an effective moment of inertia. The latter is often set to its rigid-body value and occasionally determined empirically.

The interacting shell model takes into account both shell effects and correlations and thus provides a suitable framework for the calculation of level densities. However, in mid-mass and heavy nuclei, the required model space is many orders of magnitude larger than spaces in which conventional diagonalization methods can be applied. This problem was overcome by using the shell model Monte Carlo (SMMC) approach to calculate level densities. SMMC level densities in the iron region were found to be in good agreement with experimental data without any adjustable parameters.

In the SMMC approach, thermal averages are taken over all possible states of a given nucleus, and thus the computed level densities are those summed over all possible spin values. Here we introduce spin projection methods within the SMMC approach that enable us to calculate thermal observables at constant spin. We first discuss projection on a given spin component $J_z$, and then use it to calculate spin-projected expectation values of scalar observables.

We apply the method to the spin distribution of level densities in the iron region, and compare the results with the spin-cutoff model. We also extract from the spin distribution an energy-dependent moment of inertia. Such moments of inertia are required for the calculation of statistical nuclear reaction rates, e.g., at fixed number $Z, N$ of protons and neutrons, unless otherwise stated. The Monte Carlo method is based on the Hubbard-Stratonovich (HS) transformation $e^{-\beta H} = \int D[\sigma] G_{\sigma} U_{\sigma}$, where $G_{\sigma}$ is a Gaussian weight and $U_{\sigma}$ is the imaginary-time propagator of non-interacting nucleons moving in auxiliary fields $\sigma$. Using the HS representation, the probability to find a state with a given spin projection $M$ at temperature $\beta^{-1}$ is

$$Z_M(\beta) = \frac{\langle X_{\sigma} U_{\sigma} \Phi_{\sigma} \rangle_W}{\langle \Phi_{\sigma} \rangle_W},$$

where we have introduced the notation $\langle X_{\sigma} \rangle_W = \int D[\sigma] W(\sigma) X_{\sigma} / \int D[\sigma] W(\sigma)$, and $W(\sigma) = G_{\sigma} |\text{Tr} U_{\sigma}|$ is a positive-definite function used for the Monte Carlo sampling. $\Phi_{\sigma} = \text{Tr} U_{\sigma} / |\text{Tr} U_{\sigma}|$ in (2) is the Monte Carlo sign.

In general $U_{\sigma}$ is not rotationally invariant, and the $M$-projected partition $\text{Tr} M U_{\sigma}$ can be calculated by $J_z$ projection. To this end, we use the identity

$$\text{Tr} \left( e^{i\phi J_z} U_{\sigma} \right) = \sum_{M=-J_z}^{J_z} e^{i\phi M} \text{Tr} M U_{\sigma},$$
where $J_\alpha$ is the maximal many-particle spin in the model space and $\varphi_k$ assumes a discrete set of values. Using the $2J_\alpha + 1$ quadrature points $\varphi_k \equiv \pi_{J_\alpha + \frac{1}{2}} (k = -J_\alpha, \ldots, J_\alpha)$, the set of discrete functions $\chi_M(\varphi_k) \equiv (2J_\alpha + 1)^{-1/2} e^{i\varphi_k M}$ is orthonormal, $\sum_{k=-J_\alpha}^{J_\alpha} \chi_M(\varphi_k) \chi_M^*(\varphi_k) = \delta_{MM'}$. This orthogonality relation can be used to invert

$$\text{Tr}_M U_\sigma = \frac{1}{2J_\alpha + 1} \sum_{k=-J_\alpha}^{J_\alpha} e^{-i\varphi_k M} \text{Tr} \left( e^{i\varphi_k J_\alpha} U_\sigma \right). \quad (4)$$

The trace on the r.h.s. of (4) is a canonical trace at a fixed particle number $\mathcal{A}$ (in practice we need to project on both $N$ and $Z$), and is calculated from the grand-canonical traces by a particle-number projection

$$\text{Tr} \left( e^{i\varphi_k J_\alpha} U_\sigma \right) = \frac{1}{N_\sigma} \sum_{n=1}^{N_\sigma} e^{-i\varphi_k A} \text{det}(I + U_{\sigma}^{(n,k)}) \quad (5)$$

Here $\chi_n = \pi n/2N_\sigma$ are quadrature points, and $U_{\sigma}^{(n,k)} \equiv e^{-i\varphi_k J_\alpha} U_{\sigma}$ is the $N_\sigma \times N_\sigma$ matrix representing the many-particle propagator $e^{-i\varphi_k J_\alpha} U_{\sigma}$ in the $N_\sigma$-dimensional single-particle space. In particular, $e^{-i\varphi_k J_\alpha}$ is a diagonal matrix with elements $e^{i\varphi_k m_a}$ ($m_a$ is the magnetic quantum number of orbital $a$). The canonical $M$-projected partition $\text{Tr}_M U_\sigma$ is calculated from Eqs. (4) and (5).

Similarly, the canonical expectation value of an observable $O$ at fixed $M$ is calculated from

$$\langle O \rangle_M = \frac{\text{Tr}_M (O e^{-\beta H})}{\text{Tr}_M e^{-\beta H}} = \left( \frac{\langle \text{Tr}_M (OU_\sigma) \rangle_{\Phi_\sigma}}{\text{Tr}_M U_\sigma \langle \Phi_\sigma \rangle_{\Phi_\sigma}} \right)_W \quad (6)$$

where $\text{Tr}_M U_\sigma$ is given by (4), and

$$\text{Tr}_M (OU_\sigma) = \frac{1}{2J_\alpha + 1} \sum_{k=-J_\alpha}^{J_\alpha} e^{-i\varphi_k M} \text{Tr}(e^{i\varphi_k J_\alpha} U_\sigma) \quad (7)$$

The canonical trace on the r.h.s. of (7) can be calculated by particle-number projection. For example, for a one-body operator $O = \sum_{ab} \langle a|O|b \rangle a_k^a b_k^b$ we find an expression similar to (5), but each term in the sum includes the additional factor

$$\frac{\text{Tr}(a_k^a b_k^b e^{i\varphi_k A} e^{i\varphi_k J_\alpha} U_{\sigma})}{\text{Tr}(e^{i\varphi_k A} e^{i\varphi_k J_\alpha} U_{\sigma})} = \left( \frac{I}{I + U_{\sigma}^{(n,k)}} \right)_{ab} \quad (8)$$

where here the traces are grand-canonical.

The spin-projected partition function at fixed total spin $J$ is defined by $Z_J(\beta) \equiv \text{Tr}_J e^{-\beta H} = \sum_M \langle \alpha JM | e^{-\beta H} | \alpha JM \rangle = \sum_M e^{-\beta E_{\alpha J}}$ and is independent of $M$. The $J$-projected partition can be expressed as a difference of corresponding $M$-projected partitions

$$\text{Tr}_J e^{-\beta H} = \text{Tr}_{M=J} e^{-\beta H} - \text{Tr}_{M=J+1} e^{-\beta H} \quad (9)$$

Eq. (9) holds since $e^{-\beta H}$ is a scalar operator. Using the HS representation for both $M = J$ and $M = J + 1$, we find

$$\frac{Z_J(\beta)}{Z(\beta)} = \frac{\left( \frac{\langle \text{Tr}_{M=J} (OU_\sigma) \rangle_{\Phi_\sigma}}{\text{Tr}_{M=J} U_\sigma \langle \Phi_\sigma \rangle_{\Phi_\sigma}} \right)_W}{\left( \frac{\langle \text{Tr}_{M=J+1} (OU_\sigma) \rangle_{\Phi_\sigma}}{\text{Tr}_{M=J+1} U_\sigma \langle \Phi_\sigma \rangle_{\Phi_\sigma}} \right)_W}, \quad (10)$$

where $\text{Tr}_M U_\sigma$ are calculated as before. It is also possible to apply the HS transformation directly in $Z_0$ and obtain $Z_J(\beta)/Z(\beta) = (\langle \text{Tr}_J U_\sigma \rangle / \langle \text{Tr}_J U_\sigma \rangle \langle \Phi_\sigma \rangle_{\Phi_\sigma})_W$. This relation is not equivalent to Eq. (10) since $U_\sigma$ is not rotationally invariant and $\text{Tr}_J U_\sigma \neq \text{Tr}_{M=J} U_\sigma - \text{Tr}_{M=J+1} U_\sigma$. However, the calculation of $\text{Tr}_J U_\sigma$ requires a full spin projection and is considerably more time-consuming than the $M$ projection required in (10).

To calculate the spin-projected expectation value $\langle O \rangle_J = \text{Tr}_J (O e^{-\beta H}) / \text{Tr}_J e^{-\beta H}$ of a scalar observable $O$ (e.g., the energy), we note that $\text{Tr}_J (O e^{-\beta H}) = \text{Tr}_{M=J} (O e^{-\beta H}) - \text{Tr}_{M=J+1} (O e^{-\beta H})$. Applying the HS transformation, we find

$$\langle O \rangle_J = \frac{\left( \frac{\langle \text{Tr}_{M=J} (OU_\sigma) \rangle_{\Phi_\sigma}}{\text{Tr}_{M=J} U_\sigma \langle \Phi_\sigma \rangle_{\Phi_\sigma}} \right)_W}{\left( \frac{\langle \text{Tr}_{M=J+1} (OU_\sigma) \rangle_{\Phi_\sigma}}{\text{Tr}_{M=J+1} U_\sigma \langle \Phi_\sigma \rangle_{\Phi_\sigma}} \right)_W}, \quad (11)$$

where $M$-projected quantities are calculated as before.

For a good-sign interaction, $U_\sigma$ is time-reversal invariant. Since $e^{i\varphi_k J_\alpha}$ is always time-reversal invariant, so is $e^{i\varphi_k J_\alpha} U_\sigma$, and its grand-canonical trace is always positive (since the eigenvalues of the single-particle matrix $e^{i\varphi_k J_\alpha} U_\sigma$ come in complex conjugate pairs). When projected on an even number of particles, $\text{Tr}(e^{i\varphi_k J_\alpha} U_\sigma)$ remains almost always positive. In Eq. (11) we are summing positive numbers with coefficients $e^{-i\varphi_k M}$, leading to $M$-projected partition $\text{Tr}_M U_\sigma$ that can be non-positive, with the exception of the $M = 0$ case. However, this sign problem becomes severe only above a certain $\beta$, and typically occurs at smaller values of $\beta$ as $M$ gets larger. We encounter a similar situation for the $J$ projection with the $J = 0$ projection having no sign problem. In practice, the level density at higher spin values becomes appreciable only at higher excitations, and meaningful spin distributions can be extracted except for very low excitations.

We used the spin projection method to calculate the spin distribution of the partition function and level density in the presence of correlations. In particular we calculated such spin distributions for $^{56}$Fe (an even-even nucleus), $^{54}$Fe (odd-even), and $^{60}$Co (odd-odd) in the complete $(pf + 0g_{9/2})$-shell, and for $\beta$ in the range from 0 to $\sim 2$ MeV$^{-1}$ using the Hamiltonian of Ref. [7]. The SMMC results for $Z_J/Z$, calculated from Eq. (11), are shown in Fig. 1. For temperatures $T = \beta^{-1} \leq 1.5$ MeV, an odd-even staggering is observed in the even-even nucleus $^{56}$Fe. In particular, $Z_{J=\alpha}/Z$ is significantly enhanced as $T$ decreases. No odd-even spin staggering effect is observed in the odd-even and odd-odd nuclei.
We calculated spin-projected thermal energies \( \langle H \rangle_M \) and \( \langle H \rangle \) as a function of \( \beta \) and used the method of Refs. [5, 6, 8] to obtain the level densities \( \rho_M(E_x) \) and \( \rho_J(E_x) \) as a function of excitation energy \( E_x \). The total level density \( \rho(E_x) \) was found from \( \langle H \rangle \), so we could determine the spin distribution \( \rho_J/\rho \) at fixed values of the excitation energy. In Fig. 2 we show the spin distribution of \( \rho_J/\rho \) at several excitation energies for \(^{56}\)Fe (middle panels), \(^{55}\)Fe (left panels), and \(^{60}\)Co (right panels). The solid squares are the SMMC results, while the solid lines describe fits (at fixed \( E_x \)) to the spin-cutoff model

\[
\rho_J(E_x) = \rho(E_x) \frac{(2J+1)}{2\sqrt{2\pi}\sigma^2} e^{-\frac{(J+1)^2}{2\sigma^2}},
\]

with an energy-dependent spin-cutoff parameter \( \sigma \) as the only fit parameter. The spin-projected density \( \rho_J(E_x) \) in [12] is normalized such that \( \sum_J (2J+1)\rho_J(E_x) \approx \rho(E_x) \). Equation (12) follows from the random coupling model, in which the distribution of the total spin vector \( J \) is Gaussian [1]. At intermediate and high excitation energies the spin-cutoff model seems to work well for all three nuclei. However, for the even-even nucleus \(^{56}\)Fe, we observe an odd-even (spin) staggering effect below \( E_x \sim 8 \) MeV that cannot be explained by the spin-cutoff model.

The energy-dependent spin-cutoff parameter \( \sigma^2(E_x) \), obtained by fitting \( \rho_J/\rho \) to Eq. (12), is shown (solid squares) versus \( E_x \) in the top panels of Fig. 3 for \(^{55}\)Fe, \(^{56}\)Fe, and \(^{60}\)Co. The quantity \( \sigma^2 \) can also be obtained from fits to \( \rho_M/\rho \) [in the spin-cutoff model \( \rho_M/\rho = (2\pi\sigma^2)^{-1/2} e^{-M^2/2\sigma^2} \)] but the results are similar. Despite the deviation from [12] at \( E_x \lesssim 8 \) MeV in \(^{56}\)Fe, the fitted \( \sigma^2(E_x) \) represents well the average behavior of \( \rho_J/\rho \).

There is not much data available regarding the spin-cutoff parameter. A few available experimental data points are shown for \(^{55}\)Fe [4]. The SMMC calculations are in general agreement with the experimental data. \( \sigma^2 \) is related to an effective moment of inertia \( I \) through

\[
\sigma^2 = \frac{IT}{\hbar^2},
\]

where \( T \) is the temperature. Using Eq. (13) we can convert the SMMC values of \( \sigma^2 \) to an energy-dependent moment of inertia \( I(E_x) \). The results are shown in the middle panels of Fig. 3 (solid squares). For comparison we also show the rigid-body value \( I/\hbar^2 = 0.0137A^{5/3} \) MeV\(^{-1} \) (dashed lines), and (for \(^{56}\)Fe only) half the rigid body value (long dashed lines) of the moment of inertia. In all three nuclei, \( I(E_x) \) is a monotonically increasing function of \( E_x \) and is close to the rigid-body value at intermediate and high excitations. However, for energies below \( \sim 8 \sim 10 \) MeV we observe a suppression that is particularly strong for the even-even nucleus \(^{56}\)Fe.

The energy dependence of the moment of inertia extracted from the spin distributions originates in pairing correlations. To demonstrate that we calculated the average number of \( J = 0 \) nucleon pairs \( \langle \Delta^1 \Delta \rangle \), where \( \Delta^1 = \sum_{a_m a_m} (-1)^{p_a-p_b} a_{p_a}^\dagger a_{-p_a}^\dagger a_{-p_b} a_{p_b} \). The SMMC results for proton (p-p), neutron (n-n) and proton-neutron (p-n) pairs are shown versus \( E_x \) in the bottom panels of Fig. 3. The rapid decrease of the number of p-p and n-n pairs for \(^{56}\)Fe is strongly correlated with the rapid increase observed of the moment of inertia. The correlation between \( I \) and the number of pairs suggests that
used them to calculate the spin distributions of level densities. The energy-dependent moment of inertia extracted from these distributions displays an odd-even effect that is a signature of the pairing correlations.

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