Level Densities by Particle-Number Reprojection Monte Carlo Methods

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Abstract. A particle-number reprojection method is applied in the framework of the shell model Monte Carlo approach to calculate level densities for a family of nuclei using Monte Carlo sampling for a single nucleus. In particular we can also calculate level densities of odd-even and odd-odd nuclei despite a new sign problem introduced by the projection on an odd number of particles. The method is applied to level densities in the iron region using the complete \(pf + g_{9/2}\)-shell. The single-particle level density parameter \(a\) and the backshift parameter \(\Delta\) are extracted by fitting the microscopically calculated level densities to the backshifted Bethe formula. We find good agreement with experimental level densities with no adjustable parameters in the microscopic calculations. The parameter \(a\) is found to vary smoothly with mass and does not show odd-even effects. The calculated backshift parameter \(\Delta\) displays an odd-even staggering effect versus mass and is in better agreement with the experimental data than are the empirical values.

INTRODUCTION

The nucleosynthesis of heavy elements takes place by radiative capture of neutrons (\(s\) and \(r\) process) and protons (\(rp\) process) in competition with beta decay. In the statistical regime, neutron and proton capture rates are proportional to the level density of the corresponding compound nucleus [1]. Most theoretical models of level densities are based on the Fermi gas model, e.g., the Bethe formula [2], which describes the exponential increase of the many-particle level density with both excitation energy and mass number. In the backshifted Bethe Formula (BBF) (see, e.g. Ref. [3]), shell corrections and two-body correlations are taken into account empirically by introducing a backshift \(\Delta\) of the ground state energy. The BBF offers a good description of the experimentally determined level densities when both \(a\) and \(\Delta\) are fitted for each nucleus [4,5]. The overall systematics of \(a\) and \(\Delta\) were studied empirically but it is difficult to accurately predict these parameters for a particular nucleus.
The interacting shell model takes into account both shell effects and residual interactions and constitutes an attractive framework for calculating accurate level densities. However, conventional diagonalization methods are limited by the size of the model space. Full major shell calculations are presently restricted to nuclei with $A \lesssim 50$ (in the pf-shell) [6]. The development of quantum shell model Monte Carlo (SMMC) methods [7,8] allows the calculation of finite and zero-temperature observables in model spaces orders of magnitude larger than those that can be treated by conventional diagonalization techniques. Recently the SMMC method was successfully adapted to the microscopic calculations of nuclear level densities [9].

The applications of fermionic Monte Carlo methods are often limited by the so-called sign problem, which causes a breakdown of the method at low temperatures. A practical solution was developed in the nuclear case [8], but the resulting extrapolation errors were found to be too large for accurate calculations of level densities. Instead we have constructed good-sign interactions that include the dominating collective components of effective nuclear interactions [10] and were proven to be realistic for the calculation of level densities.

The SMMC method is based on a representation of the many-body imaginary-time propagator as a functional integral over one-body propagators in fluctuating auxiliary fields, known as the Hubbard-Stratonovich transformation [11]. The many-dimensional integration is then performed by Monte Carlo. The SMMC method is computationally intensive. In particular, level density calculations require computation of the thermal energy at all temperatures. If this procedure is to be repeated for a series of nuclei, the calculations quickly become very time-consuming. Recently we introduced a novel particle-number reprojec- tion method [12] with which we can calculate nuclear observables for a series of nuclei using the Monte Carlo sampling for a single nucleus. The weight function used in the sampling is proportional to the partition function of a fixed even-even or $N = Z$ nucleus. Thermal observables for neighboring nuclei are then calculated by reprojection on different particle numbers (both even and odd). This technique offers an economical way of calculating level densities for a large number of nuclei.

**THE SHELL MODEL MONTE CARLO METHODS**

A general many-body Hamiltonian containing up to two-body interactions can be written in the following quadratic form:

$$H = \sum_\alpha \epsilon_\alpha \hat{\rho}_\alpha + \frac{1}{2} \sum_\alpha v_\alpha \hat{\rho}_\alpha^2,$$

where $\hat{\rho}_\alpha$ are one-body densities. Using the Hubbard-Stratonovich transformation, the imaginary-time many-body propagator $e^{-\beta H}$ can be represented as

$$e^{-\beta H} = \int D[\sigma] G(\sigma) U_\sigma,$$
where $G(\sigma)$ is a Gaussian weight and $U_\sigma$ is a one-body propagator of non-interacting nucleons moving in fluctuating time-dependent auxiliary fields $\sigma(\tau)$. The canonical expectation value of an observable $\hat{O}$ at inverse temperature $\beta$ is calculated from

$$
\langle \hat{O} \rangle_A = \frac{\int D[\sigma] G(\sigma) \text{Tr}_A(\hat{O}U_\sigma)}{\int D[\sigma] G(\sigma) \text{Tr}_A U_\sigma},
$$

(3)

where $\text{Tr}_A$ is a canonical trace in the subspace of fixed particle number $A$. In practice we project on both neutron and proton number, $N$ and $Z$, respectively, so $A$ denotes the pair $(N, Z)$. Introducing the notation

$$
\langle X \rangle_W \equiv \frac{\int D[\sigma] W(\sigma) X_\sigma}{\int D[\sigma] W(\sigma)},
$$

(5)

where $W(\sigma)$ is positive-definite. The $\sigma$-fields are sampled according to $W(\sigma)$ and thermal observables are calculated from (4).

**THE PARTICLE-NUMBER REPROJECTION METHOD**

We assume that the Monte Carlo sampling is done for a nucleus with particle number $A$. The ratio $Z_{A'}/Z_A$ between the partition function of another nucleus with particle number $A'$ and that of the original nucleus $A$ is written as

$$
\frac{Z_{A'}(\beta)}{Z_A(\beta)} \equiv \frac{\text{Tr}_{A'} e^{-\beta H}}{\text{Tr}_A e^{-\beta H}} = \langle \frac{\text{Tr}_{A'} U_\sigma}{\text{Tr}_A U_\sigma} \rangle_W.
$$

(5)

The expectation value of an observable $\hat{O}$ for nucleus with $A'$ particles is calculated from

$$
\langle \hat{O} \rangle_{A'} = \frac{\langle \frac{\text{Tr}_{A'} \hat{O} U_\sigma}{\text{Tr}_{A'} U_\sigma} \frac{\text{Tr}_A U_\sigma}{\text{Tr}_A U_\sigma} \rangle}{\langle \frac{\text{Tr}_{A'} U_\sigma}{\text{Tr}_A U_\sigma} \rangle W}.
$$

(6)

The Monte Carlo sampling is carried out using the weight function $W(\sigma)$ which is proportional to the partition function of nucleus $A$, and Eq. (6) is used to calculate the same observable for nuclei with $A' \neq A$.

In the calculations of level densities we used the Hamiltonian [9]

$$
H = \sum_a \epsilon_a \hat{n}_a + g_0 P^{(0,1)^\dagger} \cdot \bar{P}^{(0,1)} - \chi \sum_{\lambda=2}^4 k_\lambda O^{(\lambda,0)} \cdot O^{(\lambda,0)},
$$

(7)

where
\[ P^{(\lambda,T)} = \frac{\sqrt{4\pi}}{2^{2A+1}} \sum_{a\beta} \langle j_a | Y_\lambda | j_b \rangle [a_j^\dagger \times a_{j_b}^{\dagger}]^{(\lambda,T)}, \]

\[ O^{(\lambda,T)} = \frac{1}{\sqrt{2A+1}} \sum_{a\beta} \langle j_a | \frac{dV}{dr} Y_\lambda | j_b \rangle [a_j^\dagger \times a_{j_b}^{\dagger}]^{(\lambda,T)}. \]

The modified annihilation operator is defined by \( \tilde{a}_{j,m,m_t} = (-1)^{j-m+\frac{1}{2}-m_t} a_{j,-m,-m_t} \), and a similar definition is used for \( P^{(\lambda,T)} \). The single-particle energies \( \epsilon_a \) are calculated in a central Woods-Saxon potential \( V(r) \) plus spin-orbit interaction. \( g_0 \) is a monopole pairing interaction strength determined from experimental odd-even mass differences. The quadrupole, octupole and hexadecupole interaction terms in (7) are obtained by expanding a separable surface-peaked interaction \( v(r,r') = -\chi (dV/dr)(dV/dr') \delta(r-r') \) [13] whose strength \( \chi \) is determined self-consistently. The parameters \( k_2 = 2, k_3 = 1.5 \) and \( k_4 = 1 \) are renormalization constants that take into account core polarization effects. Both the pairing and the surface-peaked interactions are attractive and therefore have a good sign [8].

In the particle-number reprojection method described above we have assumed that the Hamiltonian \( H \) is independent of \( A \). Suitable corrections should be made if some of the Hamiltonian parameters vary with \( A \). In the iron region we find that \( \chi \) depends only weakly on the mass number \( A \), and the pairing strength \( g_0 \) is constant through the shell. The largest variation in this mass region is that of the single-particle energies. The thermal energy of a nucleus with \( A' = (N',Z') \) can then be estimated from \( E_{A'}(\beta) \approx \sum_a [\epsilon_a(A') - \epsilon_a(A)] \langle n_a \rangle_{A'} + \langle H \rangle_{A'} \), where \( H \) is the Hamiltonian for a nucleus with \( A = (N,Z) \). This estimate for \( E_{A'} \) is an approximation since we are still using the propagator \( e^{-\beta H} \) with the Hamiltonian \( H \) for nucleus \( A \) (instead of \( A' \)). This is a good approximation if we reproject on nuclei with \( N' - Z' \) values close to \( N - Z \) (the Woods-Saxon potential depends on \( N - Z \)). In the applications below this leads to negligible errors in the level densities.

**APPLICATIONS AND RESULTS**

In this section we present applications of the particle-number reprojection method to nuclei in the iron region. Since we are interested in level densities around the neutron and proton resonance energies we use the complete \((pf + g_{9/2})\)-shell. This model space contains both positive and negative parity states.

We perform the direct Monte Carlo sampling for the even-even nucleus \(^{56}\text{Fe}\) and the \( N = Z \) nucleus \(^{54}\text{Co}\) (both have a good sign for the interaction (7)). The thermal energies of \(^{53-56}\text{Mn}\), \(^{54-58}\text{Fe}\) and \(^{54-60}\text{Co}\) were reprojected from \(^{56}\text{Fe}\), while those of \(^{50-52}\text{Mn}\) and \(^{52,53}\text{Fe}\) were reprojected from \(^{54}\text{Co}\). The calculations were done for \( \beta \) values up to 2.5 MeV\(^{-1}\). At small \( \beta \) (< 1) the calculations were done in a smaller step of \( \Delta \beta = 1/16 \). At larger \( \beta \) points, the Monte Carlo calculations become more time-consuming, and we doubled our step size to \( \Delta \beta = 1/8 \). For each \( \beta \) point we took about 4000 independent samples. The reprojected energies usually have larger statistical error at large values of \( \beta \). To calculate reliable ground
state energies we performed direct Monte Carlo runs for some of the reprojected nuclei at several values of $\beta$ between 1.75 and 2.5. For $\beta > 2.5$ the statistical error for the thermal energy of an odd-even nucleus becomes too large to be useful. Since the thermal energy of an odd-even nucleus is already close to its asymptotic value at these large $\beta$ values, we could extract the ground state energy to within an accuracy of $\sim 0.3$ MeV.

Fig. 1 shows the SMMC thermal energies versus $\beta$ for manganese isotopes. The staggering observed in the spacings of the thermal energies at large $\beta$ is a pairing effect. The inset of Fig. 1 shows the SMMC thermal energies of $^{54}$Mn (diamonds with error bars) at large values of $\beta$. It demonstrates the procedure we used to extract the ground state energy.

The level density is related to the partition function by an inverse Laplace transform

$$\rho_{A'}(E) = \int_{-i\infty}^{i\infty} \frac{d\beta}{2\pi i} e^{\beta E_{A'} Z_{A'}(\beta)}. \tag{9}$$

The partition function $Z_{A'}(\beta)$ is computed from the SMMC thermal energies by integrating the thermodynamic relation $-\partial \ln Z_{A'} / \partial \beta = E_{A'}(\beta)$. The average level density is then calculated by evaluating (9) in the saddle point method

$$\rho_{A'} = (2\pi \beta^{-2} C_{A'})^{-1/2} e^{S_{A'}}, \tag{10}$$

where $S_{A'} = \beta E_{A'} + \ln Z_{A'}$ and $C_{A'} = -\beta^2 dE_{A'}/d\beta$ are the canonical entropy and heat capacity, respectively.
FIGURE 2. The SMMC level densities of the $^{50-56}$Mn isotopes. The solid lines are the fit of the calculated level densities to the BBF (11).

Fig. 2 shows the level densities for the manganese isotopes of Fig. 1 as a function of excitation energy. These densities are fitted to a modified version of the BBF [3]

$$\rho(E_x) \approx \sqrt{\pi} a^{-\frac{3}{2}} (E_x - \Delta + t)^{-\frac{5}{4}} e^{2\sqrt{a(E_x-\Delta)}}. \tag{11}$$

Here $t$ is a thermodynamic temperature determined by the relation $E_x - \Delta = at^2 - t.$ Eq. (11) differs from the usual BBF in the term $t$ which appears in the pre-exponential factor, and gives a better fit to the SMMC level densities at lower excitation energies. The solid lines in Fig. 2 are the fitted BBF level densities of Eq. (11). The fitting is done in the energy range $E_x < 20$ MeV and is usually good down to $\sim 1$ MeV for even-even nuclei (for which $\Delta$ is positive), or even below 1 MeV for odd-$A$ nuclei. The reduced pairing correlations in odd-odd nuclei are clearly observed in the level densities of Fig. 2. The backshift parameter $\Delta$ for the odd-odd nucleus $^{54}$Co is lower than $\Delta$ for the odd-even nucleus $^{55}$Co, leading to a higher level density for $^{54}$Co despite its smaller mass.

The level density parameters $a$ and $\Delta$ were extracted by fitting Eq. (11) to the microscopic SMMC level densities, and are shown in Fig. 3 versus mass number $A.$ The SMMC results (solid squares) are compared with the experimental data (×’s) quoted in Refs. [4] and [5]. The solid lines describe the empirical formulae of Refs. [14]. The SMMC values of $a$ depend smoothly on the mass $A,$ unlike the values predicted by the empirical formulae. The pairing effects are clearly reflected in the staggering behavior of $\Delta$ versus $A$ as seen on the right column of Fig. 3. In the empirical formulae, $\Delta$ is close to zero for odd-even nuclei, positive for even-even nuclei and negative for odd-odd nuclei. However, we see that both
FIGURE 3. The single-particle level density parameter \( a \) (left column) and the backshift parameter \( \Delta \) (right column) for Mn, Fe and Co isotopes. The solid squares are the SMMC values (obtained by fitting the SMMC level densities to the BBF (11)). The ×’s are the experimental results taken from the compilations of [4] (assuming rigid body moment of inertia), except for \(^{58}\text{Co}\) and \(^{59}\text{Co}\) where we used the values quoted in [5]. The solid lines are the empirical formulae of [14]. Taken from Ref. [12].

the experimental and SMMC values of \( \Delta \) can differ significantly from zero for the odd-even nuclei. The SMMC values of \( a \) and particularly \( \Delta \) are generally in better agreement with the experimental results than the empirical values. For some of the odd-odd manganese isotopes we observe discrepancies between the SMMC values of \( a \) and the experimental data. However, the lower values of \( a \) for these manganese isotopes are compensated by corresponding lower values of \( \Delta \). Consequently, the discrepancies in the level densities themselves are less significant for \( E_x \lesssim 10 \text{ MeV} \).

To demonstrate the \( T_z \)-dependence of level densities we show in Fig. 4 the level densities of two odd-odd \( A = 54 \) (Mn and Co) and three odd-even \( A = 55 \) nuclei (Mn, Fe and Co). The empirical formulae predict similar level densities for the two odd-odd nuclei as well as for the three odd-\( A \) nuclei: the values of \( a \) are similar if the mass \( A \) is the same; \( \Delta \sim 0 \) for odd-\( A \) nuclei; and \( \Delta \) are approximately the same for odd-odd nuclei. However the SMMC level densities of these nuclei (symbols) are seen to be quite different from each other. We also see that the experimental level densities (dashed lines) are in good agreement with the SMMC densities.

In conclusion, we have described a particle-number reprojection method in the shell model Monte Carlo method. With this reprojection technique we can calculate the thermal properties for a series of nuclei using Monte Carlo sampling for a single nucleus. Level densities of odd-\( A \) and odd-odd nuclei are calculated despite a new sign problem introduced by the projection on an odd number of particles.
FIGURE 4. The level densities of two odd-odd $A = 54$ nuclei: $^{54}\text{Mn}$ and $^{54}\text{Co}$ (left), and three odd-even $A = 55$ nuclei: $^{55}\text{Mn}$, $^{55}\text{Fe}$ and $^{57}\text{Co}$ (right). The symbols are the SMMC level densities and the dashed lines are the experimental level densities.

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