Particle-Number Reprojection in the Shell Model Monte Carlo Method: Application to Nuclear Level Densities

Y. Alhassid,[1] S. Liu,[1] and H. Nakada[2]
[1]*Center for Theoretical Physics, Sloane Physics Laboratory, Yale University, New Haven, Connecticut 06520*
[2]*Department of Physics, Chiba University, Yayoi-cho, Chiba 263-8522, Japan*
(Received 16 August 1999)

We introduce a particle-number reprojection method in the shell model Monte Carlo that enables the calculation of observables for a series of nuclei using a Monte Carlo sampling for a single nucleus. The method is applied to calculate nuclear level densities in the complete $(pf + g_{9/2})$-shell using a good-sign Hamiltonian. Level densities of odd-A and odd-odd nuclei are reliably extracted despite an additional sign problem. Both the mass and the T_z dependence of the experimental level densities are well described without any adjustable parameters. The odd-even staggering observed in the calculated backshift parameter follows the experimental data more closely than do empirical formulas.

PACS numbers: 21.10.Ma, 21.60.Cs, 21.60.Ka, 27.40.+z

The interacting shell model has successfully described a variety of nuclear properties. However, the size of the model space increases rapidly with the number of valence nucleons and/or orbits, and exact diagonalization of the nuclear Hamiltonian in a full major shell is limited to nuclei with $A \lesssim 50$ [1,2]. The development of quantum Monte Carlo methods for the nuclear shell model allowed realistic calculations of finite- and zero-temperature observables in model spaces that are much larger than those treated by conventional diagonalization techniques [3,4].

The Monte Carlo method was successfully adapted to the microscopic calculation of nuclear level densities [5]. Accurate level densities are needed for estimating nuclear reaction rates, e.g., neutron and proton capture rates. The nucleosynthesis of many of the heavy elements proceeds by radiative capture of neutrons (s and r processes) or protons (rp process) in competition with beta decay [6,7]. Theoretical approaches to level densities are often based on the Fermi gas model, i.e., the Bethe formula [8], which describes the many-particle level density in terms of the single-particle level density parameter a. Shell corrections and two-body correlations are taken into account empirically by defining a fictitious ground state energy. In the backshifted Bethe formula (BBF) the ground state energy is shifted by an amount Δ. This formula describes well the experimental level densities of many nuclei if both a and Δ are fitted for each individual nucleus [9]. While these parameters have been discussed in terms of their global systematics, it is difficult to predict their values for particular nuclei.

The nuclear shell model offers an attractive framework for calculating level densities, but the model space required to calculate level densities at excitation energies in the neutron resonance regime is usually too large for conventional diagonalization methods. We have recently developed a method [5] to calculate exact level densities using the shell model Monte Carlo (SMMC) approach, and applied it to calculate the level densities of even-even nuclei from iron to germanium [10]. Fermionic Monte Carlo methods are usually hampered by the so-called sign problem, which causes a breakdown of the method at low temperatures. A practical solution in the nuclear case was developed in Ref. [4] but the associated extrapolation errors are too large for reliable calculations of level densities. In Ref. [5] the sign problem was overcome by constructing a good-sign interaction in the $(pf + g_{9/2})$-shell that includes correctly the dominating collective components of realistic effective interactions [11]. The SMMC level densities are well fitted by the BBF, and both a and Δ can be extracted from the microscopic calculations.

The SMMC approach is computationally intensive. In particular, the SMMC level densities require calculation of the thermal energy at all temperatures. The weight function used in the random walk is temperature dependent, and a new Monte Carlo sampling is required at each temperature. Since this procedure must be repeated for each nucleus, the calculations are time consuming. In this paper we describe a particle-number reprojection method that allows us to calculate observables for a series of nuclei using Monte Carlo sampling for one nucleus only. The random walk is done with a weight function proportional to the partition function of a given even-even nucleus (which is positive definite for a good-sign interaction), and the thermal observables are then calculated for several nuclei by reprojection on different particle numbers (both even and odd). This method allows significantly more economical calculations of level densities. We apply the method in the full $(pf + g_{9/2})$-shell to study the systematics of a and Δ for even-even, odd-A, and odd-odd manganese, iron, and cobalt nuclei. A direct comparison with both experimental data and empirical formulas is presented. The agreement with the data is remarkably good with no adjustable

0031-9007/99/83(21)/4265(4)$15.00

parameters in the microscopic calculations. Furthermore, we find that the SMMC values follow the data more closely than do the empirical values.

The Monte Carlo method is based on the Hubbard-Stratonovich representation of the imaginary-time propagator, $e^{-\beta H} = \int D[\sigma] G(\sigma) U_\sigma$, where $G(\sigma)$ is a Gaussian weight and U_σ is the propagator of noninteracting nucleons moving in fluctuating auxiliary fields σ which depend on imaginary time. The canonical thermal expectation value of an observable O is given by $\langle O \rangle_{\mathcal{A}} = \int D[\sigma] G(\sigma) \times \mathrm{Tr}_{\mathcal{A}}(OU_\sigma) / \int D[\sigma] G(\sigma) \mathrm{Tr}_{\mathcal{A}} U_\sigma$, where $\mathrm{Tr}_{\mathcal{A}}$ denotes a trace in the subspace of a fixed number of particles $\mathcal{A}$. In actual calculations we project on both neutron number N and proton number Z, and in the following $\mathcal{A}$ will denote (N, Z). We rewrite

$$\langle O \rangle_{\mathcal{A}} = \langle \mathrm{Tr}_{\mathcal{A}}(OU_\sigma) / \mathrm{Tr}_{\mathcal{A}} U_\sigma \rangle_W , \tag{1}$$

where we have introduced the notation

$$\langle X_\sigma \rangle_W \equiv \frac{\int D[\sigma] W(\sigma) X_\sigma}{\int D[\sigma] W(\sigma)} , \tag{2}$$

and $W(\sigma) \equiv G(\sigma) \mathrm{Tr}_{\mathcal{A}} U_\sigma$. For an even number of particles with a good-sign interaction, $W(\sigma)$ is positive definite. In the Monte Carlo method we choose M samples (each denoted by σ_k) according to the weight function $W(\sigma)$, and estimate $\langle X_\sigma \rangle_W \approx \sum_k X_{\sigma_k} / M$.

We assume that the Monte Carlo sampling is done for a nucleus with particle number $\mathcal{A}$, and consider the ratio $Z_{\mathcal{A}'} / Z_{\mathcal{A}}$ between the partition function of a nucleus with $\mathcal{A}'$ particles and the partition function of the original nucleus. In the notation of Eq. (2),

$$\frac{Z_{\mathcal{A}'}(\beta)}{Z_{\mathcal{A}}(\beta)} \equiv \frac{\mathrm{Tr}_{\mathcal{A}'} e^{-\beta H}}{\mathrm{Tr}_{\mathcal{A}} e^{-\beta H}} = \left\langle \frac{\mathrm{Tr}_{\mathcal{A}'} U_\sigma}{\mathrm{Tr}_{\mathcal{A}} U_\sigma} \right\rangle_W . \tag{3}$$

Similarly, the expectation value of an observable O for the nucleus with $\mathcal{A}'$ particles can be calculated from

$$\langle O \rangle_{\mathcal{A}'} = \frac{\langle (\frac{\mathrm{Tr}_{\mathcal{A}'} O U_\sigma}{\mathrm{Tr}_{\mathcal{A}'} U_\sigma}) (\frac{\mathrm{Tr}_{\mathcal{A}'} U_\sigma}{\mathrm{Tr}_{\mathcal{A}} U_\sigma}) \rangle_W}{\langle \frac{\mathrm{Tr}_{\mathcal{A}'} U_\sigma}{\mathrm{Tr}_{\mathcal{A}} U_\sigma} \rangle_W} . \tag{4}$$

The Monte Carlo walk is carried out by projection on a fixed $\mathcal{A}$, and Eqs. (3) and (4) are then used to calculate the partition functions and observables for a family of nuclei with $\mathcal{A}' \neq \mathcal{A}$.

We applied the method to nuclei in the $(pf + g_{9/2})$-shell, using the Hamiltonian of Ref. [5]. The single-particle energies are computed in a central Woods-Saxon potential $V(r)$ plus spin-orbit interaction, while the two-body interaction includes a monopole isovector pairing of strength g_0 plus a separable surface-peaked interaction [12] $v(\boldsymbol{r}, \boldsymbol{r}') = -\chi (dV/dr)(dV/dr') \delta(\hat{\boldsymbol{r}} - \hat{\boldsymbol{r}}')$. The surface-peaked interaction is expanded into multipoles and only the quadrupole, octupole, and hexadecupole terms are kept. The strength χ is determined self-consistently and renormalized. The strength of the pairing interaction $g_0 \approx 0.2$ is determined from experimental odd-even mass differences. Both the pairing and the surface-peaked interactions are attractive and lead to a good-sign Hamiltonian. A repulsive isospin-dependent interaction leads to a sign problem, and was included perturbatively in recent level density calculations in sd-shell [13] and pf-shell [14] nuclei.

In the particle-reprojection method described above we have assumed that the Hamiltonian H is independent of $\mathcal{A}$. Suitable corrections should be made if some of the Hamiltonian parameters vary with $\mathcal{A}$. Since χ depends only weakly on the mass number A ($\propto A^{-1/3}$), and the pairing strength g_0 is constant through the shell, the largest variation is that of the single-particle energies of the orbit a, $\epsilon_a(\mathcal{A})$. To correct this variation we approximate the thermal energy of $\mathcal{A}' \equiv (N', Z')$ particles by

$$E_{\mathcal{A}'}(\beta) \approx \sum_a [\epsilon_a(\mathcal{A}') - \epsilon_a(\mathcal{A})] \langle n_a \rangle_{\mathcal{A}'} + \langle H \rangle_{\mathcal{A}'} , \tag{5}$$

where H is the Hamiltonian for a nucleus with $\mathcal{A}$ particles. In calculating the energy for $\mathcal{A}'$ particles from (5), we used in the propagator ($e^{-\beta H}$) the Hamiltonian H for nucleus $\mathcal{A}$ rather than $\mathcal{A}'$. To minimize the error we reproject on nuclei with $N' - Z'$ values close to $N - Z$ (the Woods-Saxon potential depends on $N - Z$). In the applications below we have checked that the resulting error in the level density is negligible.

We used the reprojection method to calculate the thermal energies versus β for $^{50-56}$Mn, $^{52-58}$Fe, and $^{54-60}$Co including odd-A and odd-odd nuclei. We sampled according to the even-even nucleus ^{56}Fe and reprojected onto $^{53-56}$Mn, $^{54-58}$Fe, and $^{54-60}$Co, while the nuclei $^{50-52}$Mn and ^{52,53}Fe were reprojected from Monte Carlo sampling of the odd-odd $N = Z$ nucleus ^{54}Co. The calculations were done for values of β between $\beta = 0$ and 1 MeV^{-1} in steps of $\Delta\beta = 1/16$, and between 1 and 2.5 in steps of $\Delta\beta = 1/8$. At each β we used about 4000 independent samples. Reprojected energy calculations typically have larger statistical errors at larger values of β. Therefore we also performed direct Monte Carlo runs (without reprojection) for the above nuclei at several values of β between 1.75 and 3.0 MeV^{-1}. For odd-A and odd-odd nuclei, a typical statistical error for the energy at $\beta \sim 2.5$ is $\sim$0.5 MeV, while for $\beta \gtrsim 3$ the error is too large for the data to be useful. This is just another manifestation of the sign problem for nuclei with an odd number of protons and/or neutrons. Fortunately, because of the high degeneracy in the vicinity of the ground state of these nuclei, the thermal energy is already close to its asymptotic value.

Figure 1 shows the calculated SMMC thermal energies versus β for a series of cobalt isotopes. The effect of pairing on the thermal energies at low temperatures (i.e., large β) is clearly seen in their uneven spacings. The inset of Fig. 1 shows the SMMC thermal energies (triangles with error bars) for ^{60}Co for the large values of β only.

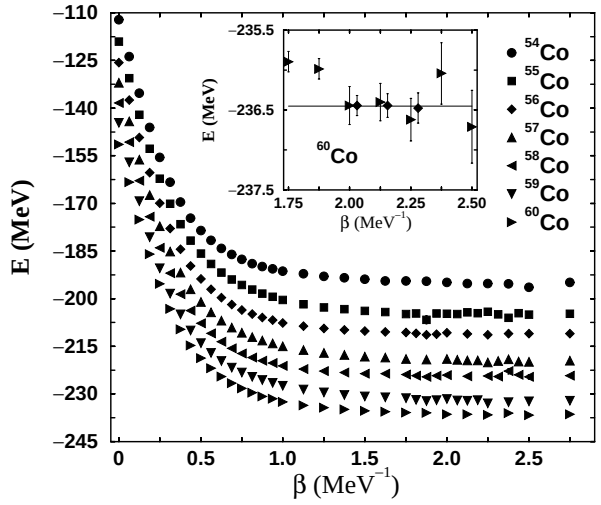

FIG. 1. The SMMC thermal energies versus β for $^{54-60}$Co (symbols). Shown on the right are the extrapolated values of the ground-state energy. Inset: the SMMC thermal energies (triangles) at large β values for ^{60}Co. The diamonds are the energies obtained by averaging the large-β results above the corresponding β.

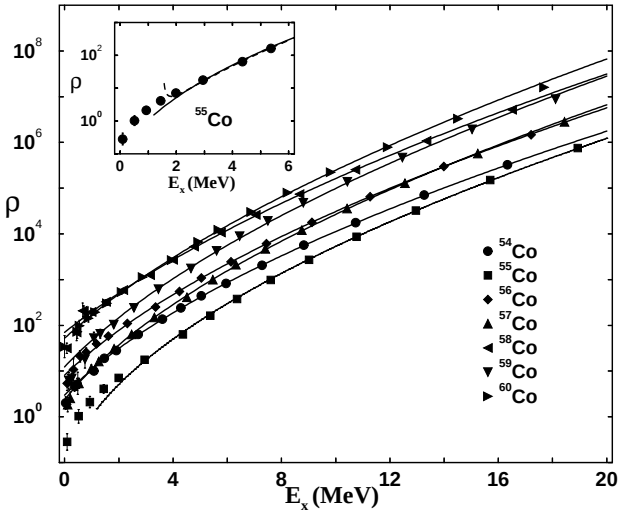

FIG. 2. The SMMC level densities of the $^{54-60}$Co isotopes. The solid lines describe a fit to the BBF (7). The inset shows the level density of ^{55}Co at low excitation energies. The circles are the SMMC results, the solid line is a fit to (7), and the dashed line is a fit to (7) but without the t term.

In calculating the level density versus excitation energy, it is important to get accurate values of the ground state energy. In Ref. [10] we used, for even-even nuclei, a two-state model (0^+ and 2^+) to obtain a two-parameter fit to the thermal energy and $\langle \boldsymbol{J}^2 \rangle$. For odd-$A$ and odd-odd nuclei this method is not useful since in general we do not know the spin of the ground state and first excited state. Moreover, these nuclei do not have a gap, and often more than two levels contribute to the thermal energy at the lowest temperatures for which Monte Carlo calculations are still possible. We estimate the ground state energy of these nuclei by taking an average of the large-β SMMC values for the thermal energy. The diamonds in the inset of Fig. 1 are such average values for ^{60}Co. We estimate the ground state energy of the odd-A and odd-odd nuclei to be reliable to about $\sim$0.3 MeV.

To calculate the level density we first find the partition function $Z_{\mathcal{A}'}$ by integrating the relation $-\partial \ln Z_{\mathcal{A}'}/\partial\beta = E_{\mathcal{A}'}$. The level density is then given by

$$\rho_{\mathcal{A}'} = (2\pi\beta^{-2}C_{\mathcal{A}'})^{-1/2} e^{S'_{\mathcal{A}}}, \tag{6}$$

in terms of the canonical entropy $S_{\mathcal{A}'} = \beta E_{\mathcal{A}'} + \ln Z_{\mathcal{A}'}$ and the heat capacity $C_{\mathcal{A}'} = -\beta^2 dE_{\mathcal{A}'}/d\beta$.

The level densities for the cobalt isotopes of Fig. 1 are shown in Fig. 2 as a function of excitation energy. These total level densities are fitted to

$$\rho(E_x) \approx g\,\frac{\sqrt{\pi}}{24}\,a^{-1/4}(E_x - \Delta + t)^{-5/4} e^{2\sqrt{a(E_x-\Delta)}}, \tag{7}$$

where t is a thermodynamic temperature defined by $E_x - \Delta = at^2 - t$ and $g = 2$. Equation (7) is a modified version of the BBF derived by Lang and Le Couteur [15]. It differs from the usual BBF by the additional "temperature" term t in the preexponential factor, and provides a better fit to the calculated level density at lower excitation energies. The solid lines in Fig. 2 are the BBF level densities (7) fitted to the SMMC level densities in the range $E_x < 20$ MeV. In general we obtain a good fit down to energies of $\sim$1 MeV or smaller. The inset shows the low energy fit for ^{55}Co. The dashed line is a fit to the BBF without t; this approximation starts to diverge around 2 MeV owing to the singularity of the preexponential factor $(E_x - \Delta)^{-5/4}$. Notice that the level density for an odd-odd cobalt (e.g., ^{54}Co) is higher than the level density of the subsequent odd-even cobalt (e.g., ^{55}Co) even though the latter has a larger mass. This is due to reduced pairing correlations in the odd-odd nucleus that lead to a smaller backshift Δ.

We extracted the level density parameters a and Δ for the above nuclei by fitting Eq. (7) to the SMMC level densities. The results for a and Δ versus mass number A are shown in Fig. 3. The Monte Carlo results (solid squares) are compared with the experimental data (X's) quoted in Refs. [9] and [16]. The solid lines describe the results of the empirical formulas of Refs. [17]. The calculated values of a depend smoothly on the mass, unlike some of the empirical results, and in the case of the cobalt isotopes follow the data more closely. The staggering seen in the behavior of Δ versus A is a result of pairing effects. In the empirical formulas, Δ is close to zero for odd-even nuclei, positive for even-even nuclei, and negative for odd-odd nuclei. We see that the present values of Δ follow rather closely the experimental values, and are in general in better agreement than the empirical values. The lower values of a (relative to the experimental values) for the odd-odd

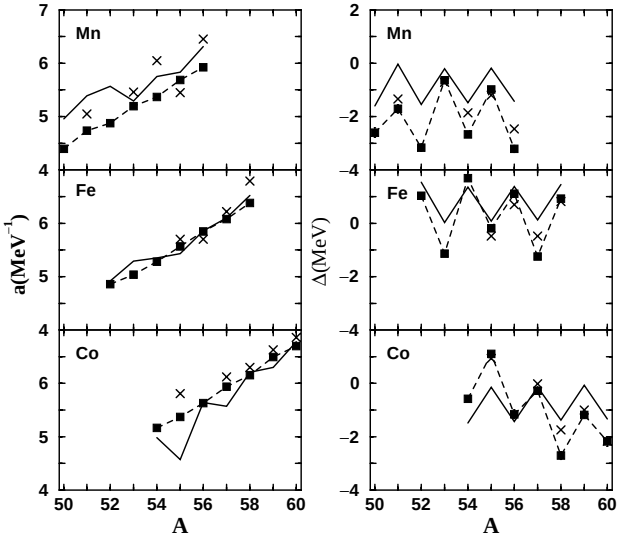

FIG. 3. The single-particle level density parameter a (left column) and the backshift parameter Δ (right column) for Mn, Fe, and Co isotopes. The solid squares (connected by dashed lines) are the results of fitting the calculated SMMC level densities to Eq. (7), while the X's are the experimental results. All the experimental values are from the compilations of [9] (assuming rigid body moment of inertia), except for ^{58}Co and ^{59}Co where the values quoted in [16] are used. The solid lines are the empirical formulas of [17].

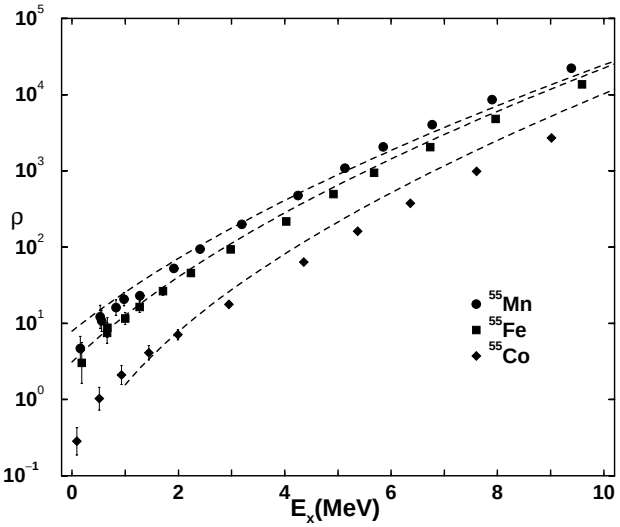

FIG. 4. The SMMC level densities of three $A = 55$ nuclei: ^{55}Mn (circles), ^{55}Fe (squares), and ^{55}Co (diamonds). The dashed lines are the experimental level densities.

manganese nuclei are compensated by corresponding lower values of Δ, and thus do not cause significant discrepancies in the level densities for $E_x \lesssim 10$ MeV.

To demonstrate how the Monte Carlo results improve over the empirical formulas we show in Fig. 4 the calculated level densities of three $A = 55$ nuclei (Mn, Fe, and Co). According to the empirical formula, $\Delta \sim 0$ for odd-A nuclei, and the values of a are similar (since A is the same). The empirical formulas therefore predict similar level densities for these nuclei. However, the SMMC level densities of these three nuclei are seen to be quite different from each other. Indeed, we find that Δ is positive for ^{55}Co, close to zero for ^{55}Fe, and negative for ^{55}Mn. The experimental level densities (dashed lines) are in good agreement with the Monte Carlo calculations, suggesting a $T_z \equiv (N - Z)/2$ dependence of the level density, which is usually ignored in empirical formulas but is clearly observed in our microscopic calculations.

In conclusion, we have described a particle-number reprojection method in the SMMC that enables the calculation of thermal properties for a series of nuclei using Monte Carlo sampling for a single nucleus. We applied the method to the calculation of level densities.

This work was supported in part by the Department of Energy Grant No. DE-FG-0291-ER-40608, and by the Ministry of Education, Science, Sports and Culture of Japan (Grants No. 08044056 and No. 11740137). Computational cycles were provided by the Cornell Theory Center, by the San Diego Supercomputer Center (using NPACI resources), and by the NERSC high performance computing facility at LBL.

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