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Estimating the nuclear level density with the Monte Carlo shell model

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A method for making realistic estimates of the density of levels in even-even nuclei is presented making use of the Monte Carlo shell model (MCSM). The procedure follows three basic steps: (1) computation of the thermal energy with the MCSM, (2) evaluation of the partition function by integrating the thermal energy, and (3) evaluating the level density by performing the inverse Laplace transform of the partition function using maximum entropy reconstruction techniques. It is found that results obtained with schematic interactions, which do not have a sign problem in the MCSM, compare well with realistic shell-model interactions provided an important isospin dependence is accounted for. [S0556-2813(97)50210-X]

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The density of levels in nuclei plays an important role in understanding compound nuclear reactions. Two particularly important examples are the decay of the giant-dipole resonance (GDR) in hot nuclei [1], and the radiative capture of light nuclei, i.e., protons, neutrons, and alphas, in nucleosynthesis [2]. In the first case, properties of the GDR, in particular the damping width, have been studied in several nuclei for excitation energies ranging from 50 to 200 MeV, and it has been shown that the analysis of experimental data is very sensitive to the the dependence of the level density on excitation energy [3]. In contrast to the GDR studies, the particle capture probability, which determines the rate at which nucleosynthesis reactions occur, is sensitive to the level density near the particle-decay threshold: i.e., ~5–15 MeV.

In most applications where the level density is required, the Fermi-gas model estimate [4] is employed

$$\rho(E)=\frac{\sqrt{\pi}}{12a^{1/4}E^{5/4}}\exp(2\sqrt{aE}), \tag{1}$$

where E is the excitation energy, and a is the level-density parameter, which is determined by the number of single-particle states at the Fermi energy. The principal shortcoming of the Fermi gas estimate is that interactions between nucleons are ignored. Effects due to shell corrections and pairing correlations are approximated in Eq. (1) by replacing the excitation energy E by backshifted quantity $E-\Delta$ [5]. Empirically, both a and Δ exhibit a dependence on E and the number of nucleons, A, that cannot simply be estimated within the context of the Fermi gas model; a typical value for a at low-excitation energies is $a\sim A/8$.

An alternative model that explicitly includes both one- and two-body correlations is the shell model. State-of-the-art shell-model Hamiltonians, such as the universal *sd*-shell (USD) Hamiltonian of Wildenthal [6] have been very successful at describing both excitation energies and transition amplitudes for states in a wide range of nuclei ($18\leqslant A\leqslant 48$) up to excitation energies of the order 5–10 MeV. Although the shell model might appear to be the obvious method for estimating the level density at low-excitation energies, direct diagonalization of the Hamiltonian faces severe computational limitations due to the fact that the number of basis states scales as the exponential of the number of valence particles. Indeed, the large number of basis states was the motivation behind the development of the spectral distribution methods of French and others [7], which rely on the statistical properties of the elements of the Hamiltonian matrix. A central-limit theorem can be applied to describe the action of the Hamiltonian in large spaces [8]; generally reducing the problem to the calculation of the first and second moments of the Hamiltonian. In many practical applications, however, this limiting situation may not be sufficiently realized. For example, because of features of the Hamiltonian, which may be thought of as shell corrections, significant departures from ''normality'' may be observed at low-excitation energies. As a consequence, it is necessary to compute higher-order moments of the Hamiltonian or partition the shell-model space into smaller subspaces. Unfortunately, not only are these higher-order moments more difficult to evaluate, but the level density reconstructed with orthogonal Hermite polynomials may fail to be positive definite [9]. An alternative method was proposed by Pluhař and Weidenmüller [10] in which the partial level densities in the subspaces were assumed to have a form predicted by the Gaussian orthogonal ensemble (GOE), i.e., semicircular, as determined from the first and second moments of the Hamiltonian within the projected subspaces. The total level density, which in their method is guaranteed to be positive definite, is then obtained by combining the various subpartitions with the coupling between the subspaces being determined statistically from the mean off-diagonal matrix elements. This procedure also faces several limitations because of the reliance on the GOE limit for the subspaces, as well as being restricted to the first and second moments of the Hamiltonian. Consequently, in applications to more general shell-model problems, this procedure tends to lead to level densities that are somewhat broader than the exact results [11].

In this work, a method for making realistic estimates of shell-model level densities using the Monte Carlo shell model [12] (MCSM) is presented. The power of the MCSM is that it is capable of providing *exact* results for a range of observables in model spaces where the dimensions are prohibitive for direct diagonalization. In addition, the MCSM is quite well suited to compute thermal properties, such as the energy, from which the partition function may be obtained, which then yields the level density through an inverse Laplace transform. The applicability of the MCSM to the most general of shell-model Hamiltonians, however, is lim-

ited because of the sign problem associated with the Monte Carlo weight function. One is then faced with either using an extrapolation method [13], which tends to yield larger statistical errors, or a schematic interaction that is free of the sign problem. Here, it will be shown that schematic Hamiltonians, such as a surface-delta interaction [14], possess most of the global, or collective, features exhibited by ''realistic'' Hamiltonians with one important exception: in the spectra of even-even nuclei, the higher isospin states tend to be too low in energy, thereby compressing the total level density. This improper isospin dependence can be corrected by adding the term $a\hat{T}^2$ to the schematic interaction, thus shifting the excitation energy of the higher isospin states. Unfortunately, this $\hat{T}^2$ term also has a bad sign, and cannot be computed directly. To address this problem, a simple and accurate approximation for correcting the thermal energy for the T^2 dependence in even-even nuclei is presented, and it will be shown by direct comparison that an MCSM calculation using a schematic interaction yields a reasonable estimate of the level density obtained in ''realistic'' shell-model calculations.

The procedure consists of four steps: (1) using a semirealistic schematic interaction, compute the thermal expectation value of the Hamiltonian,

$$E(\beta)=\frac{\mathrm{Tr}[\hat{H}e^{-\beta\hat{H}}]}{\mathrm{Tr}[e^{-\beta\hat{H}}]}=\frac{\sum_i E_i e^{-\beta E_i}}{\sum_i e^{-\beta E_i}}=\frac{\int dE e^{-\beta E}E\rho(E)}{\int dE e^{-\beta E}\rho(E)}, \tag{2}$$

with the MCSM; (2) correct $E(\beta)$ for the missing T^2 dependence using Eq. (9) below; (3) compute the partition function, $Z(\beta)$, via

$$\ln Z(\beta)=-\int_0^\beta d\beta' E(\beta')+\ln Z(0), \tag{3}$$

where $Z(0)$ is actually the total number of states; and (4) calculate $\rho(E)$ using maximum-entropy reconstruction techniques to perform the inverse Laplace transform of $Z(\beta)$.

The primary goal of this work is to establish the feasibility of the method for making estimates of the level density in realistic situations. To accomplish this, comparisons with exact results are necessary, and the focus of this work is the nucleus ^{24}Mg, which has four valence protons and neutrons occupying the $0d_{5/2}$, $1s_{1/2}$, and $0d_{3/2}$ valence orbitals. Because of the overall success of the USD interaction, which was explicitly developed for this model space, this interaction will be used as a benchmark for success. The schematic interaction is composed of the three single-particle energies and a two-body potential given by the surface-delta interaction (SDI) [14], which has the form

$$V(\mathbf{r}_1,\mathbf{r}_2)=-4\pi V_0\delta(\mathbf{r}_1-\mathbf{r}_2)\delta(r_1-R_0), \tag{4}$$

where $\mathbf{r}_i$ is the position vector for the ith particle and R_0 is the nuclear radius. The principal feature of the SDI is that it is basically comprised of multipole-multipole terms, with the dominant multipoles being monopole and quadrupole. Taking $R_0=3.145$ fm, $V_0=54.76$ MeV/fm^2, and evaluating the two-body matrix elements using harmonic oscillator wave functions with $\hbar\omega=13.531$ MeV, the $T=1$ USD matrix elements are reproduced by better than 500 keV. The single-particle energies are adjusted to reproduce the low-lying experimental spectra for ^{19}O and the USD shell-model spectra for ^{25}O and ^{27}O. Using fixed single-particle energies across the shell and the USD mass scaling of $(18/A)^{0.3}$ for the two-body part, the SDI Hamiltonian reproduces the USD spectra and level densities for oxygen isotopes reasonably well. On the other hand, an important component is missing, as it is not possible to reproduce the binding energies for the oxygen isotopes. This feature is generic to schematic interactions of the form multipole plus pairing, and may be ''fixed'' by adding a term dependent on the square of the isospin, $a\hat{T}^2$, as is illustrated in Fig. 1, where the binding energies for the *sd*-shell oxygen isotopes are compared for the USD interaction and the schematic Hamiltonian, with parameters $\epsilon_{d5/2}=-4.820$ MeV, $\epsilon_{s1/2}=-2.820$ MeV, $\epsilon_{d3/2}=1.530$ MeV, $V_0=54.76$ MeV/fm^2, and $a=0.546$ MeV.

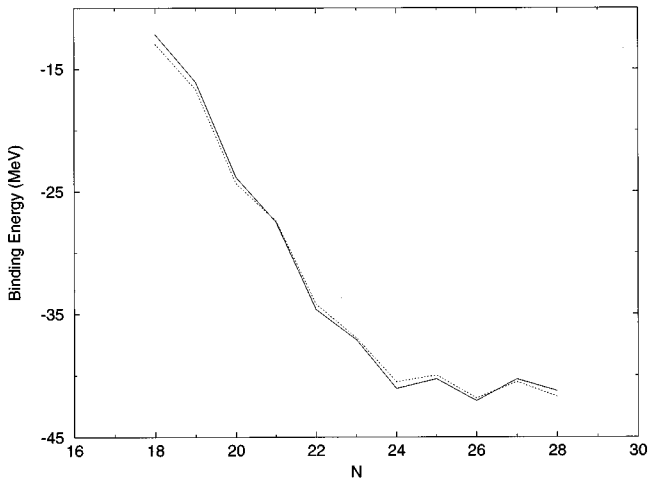

FIG. 1. Comparison of binding energies for oxygen isotopes as a function of neutron number obtained with the USD (solid line) and SDI$+0.546\hat{T}^2$ (dotted line) Hamiltonians, respectively.

From the standpoint of estimating the level density, an adequate Hamiltonian would in fact be an extension of the SDI that includes isospin-dependent components: in particular the modified surface delta interaction [15]. Because of the sign problem in the MCSM, however, it is generally not possible to treat isospin-dependent terms in the Hamiltonian. On the other hand, for a given isospin value, the SDI spectra compare well with the realistic USD results. Hence, a reasonable first-order correction may be obtained by simply shifting the higher isospin states by adding $a\hat{T}^2$ to the Hamiltonian. The magnitude of the coefficient a, however, cannot be estimated *a priori*, as it seems to differ from nucleus to nucleus and depends on the number of the protons and neutrons as well as whether the shell is more than half full. This is illustrated in Table I, where the excitation energies obtained with the SDI and USD interactions for the first $J=0^+$ states of each isospin are tabulated for ^{24}Mg and ^{32}S. Also, given in the table are the total number of states of each isospin that contribute to the total level density. Because of this unpredictable T^2 behavior, a shell-model calculation with a realistic interaction, even within a truncated model

TABLE I. Excitation energies (in MeV) for the first $J=0$ states of each isospin for the SDI and USD interactions for ^{24}Mg and ^{32}S. The number of states for each isospin contributing to the total level density is also tabulated.

	^{24}Mg		^{32}S		
T	USD	SDI	USD	SDI	# States
0	0.000	0.000	0.000	0.000	166,320
1	12.872	9.351	7.312	4.735	332,640
2	15.425	7.903	12.060	6.434	237,600
3	33.923	22.528	33.468	22.268	83,160
4	46.040	26.251	45.404	26.328	11,880

space, for a single angular momentum for a few isospins is necessary to determine a reasonable estimate for a. For ^{24}Mg, the improper isospin dependence is corrected on average with $a=1.507$. On the other hand, to illustrate that the SDI interaction gives a good representation of the low-lying collective behavior for ^{24}Mg, the excitation energies of the lowest few $T=0$ states are compared with the USD values in Table II.

Using the Monte Carlo shell model (MCSM) techniques described in Ref. [12], the expectation values of observables such as the Hamiltonian, $\hat{T}^2$, etc., were evaluated for the SDI interaction as a function of the inverse temperature, β, in the range $0\leqslant\beta\leqslant 1$ MeV^{-1} in increments of $\Delta\beta=1/80$ MeV^{-1}. In order to ensure sufficient accuracy, 2000 Monte Carlo samples were taken for each β value, and multiple time slices were used in all MCSM calculations with $\beta\geqslant 0.0375$ MeV^{-1}, with the maximum number of 40 being used at $\beta=1$ MeV^{-1}. Typical Monte Carlo uncertainties for the energy observable ranged from 10 keV for small values of β to about 120 keV for $\beta\sim 1$ MeV^{-1}.

With $E(\beta)$, the partition function is obtained via Eq. (3), and the level density is then given by the inverse Laplace transform of $Z(\beta)$. Although a saddle-point approximation may be employed, giving $\rho(E)=e^{\beta E+\ln Z}/\sqrt{-2\pi\partial E/\partial\beta}$, this method tends to be somewhat unstable at low-excitation energies due to difficulties associated with computing the derivative in the denominator. An alternative method is to evaluate the inverse transform using maximum-entropy (MaxEnt) reconstruction techniques [16]. The starting point is to bin $\rho(E)$ into N_R bins of equal width ΔE, namely

$$\rho(E)=\sum_i^{N_R} f_i\{\theta[E-(E_i-\Delta/2)]-\theta[E-(E_i+\Delta/2)]\}\,, \tag{5}$$

TABLE II. Comparison between the USD and SDI excitation energies (in MeV) for the lowest few $T=0$ states in ^{24}Mg. Shown are the first ten states as predicted by the USD interaction, and then the lowest $J=7$ and 8 states.

J	USD	SDI	J	USD	SDI
0	0.000	0.000	0	7.561	6.778
2	1.509	1.973	1	7.764	7.253
2	4.122	4.146	5	7.883	8.281
4	4.378	4.845	6	8.263	8.460
3	5.097	5.326	7	12.283	12.596
4	5.934	5.314	8	12.088	10.974

where f_i is the number of levels contained within the ith bin. With this level density, the reconstructed partition function is then

$$Z_R(\beta)=\sum_i^{N_R}\frac{2f_i}{\beta}e^{-\beta E_i}\sinh(\beta\Delta E/2)\,. \tag{6}$$

The goal of MaxEnt is to find the set of values $\{f_i\}$ that maximize the extended entropy functional $\alpha S-\chi^2/2$, where

$$\chi^2=\sum_j^{N}\frac{[Z(\beta_j)-Z_R(\beta_j)]^2}{\sigma_j^2} \tag{7}$$

quantifies how well the reconstruction reproduces the N calculated values of the $Z(\beta_j)$ (note $N_R\leqslant N$) and the information entropy, S, is given by

$$S=\sum_i^{N_R}[f_i-D_i-f_i\ln(f_i/D_i)]\,. \tag{8}$$

In the MaxEnt method, it is necessary to specify a default model $\{D_i\}$, which may be used to characterize any prior information known about the problem at hand. In this case, it is well known that within a finite model space, the level density exhibits a Gaussian character [17], which may be used to define the default model. For finite-space, shell-model calculations, the total number of states is known and the first and second moments of the level density may be obtained from $E(\beta=0)$ and $dE(\beta)/d\beta|_{\beta=0}$, respectively. The reconstructed $\{f_i\}$ also depend on α, which governs the relative weight between the default model and chi-square. Here, α was chosen so that $\chi^2\sim N$. Finally, the uncertainty in the f_i values may be obtained in a manner similar to least-squares fitting from the curvature matrix $\partial^2(\alpha S-\chi^2/2)\partial f_i\partial f_j$.

As was mentioned above, the SDI interaction exhibits a bad isospin dependence that can be corrected by adding the term $a\hat{T}^2$ to the Hamiltonian. Unfortunately, this additional term has a bad sign in the MCSM and cannot be evaluated directly. The extrapolation method of Ref. [13] could be used, but at a significant computational cost and larger statistical errors. Instead, for even-even nuclei, where the low-lying states are unaffected by the additional term, a perturbative approach may be more useful. Towards this end, $a\hat{T}^2$ is added to the SDI Hamiltonian, and the energy is evaluated by expanding the $a\hat{T}^2$ terms in the exponential in Eq. (2) to first order in β. Unfortunately, a further limitation is imposed due to computational limitations that make it impractical to evaluate the expectation value of n-body operators in the MCSM beyond $n=2$. Given these considerations, the first-order correction to the energy is estimated as

$$E_{\rm corr}=\beta a\frac{\partial\langle\hat{T}^2\rangle}{\partial\beta}+a\langle\hat{T}^2\rangle\,. \tag{9}$$

In comparison with exact results, Eq. (9) works quite well, although it tends to ''over correct'' by approximately 10%. This over correction, which may be due to the neglected $(\hat{T}^2)^2$ terms in the expansion, can be damped by multiplying $E_{\rm corr}$ by the factor $e^{-\beta a\langle\hat{T}^2\rangle}$. For illustrative purposes, both $E(\beta)$ and $\ln Z(\beta)$ are shown in Fig. 2 for ^{20}Ne using the SDI interaction with and without the iosospin correction factor. In

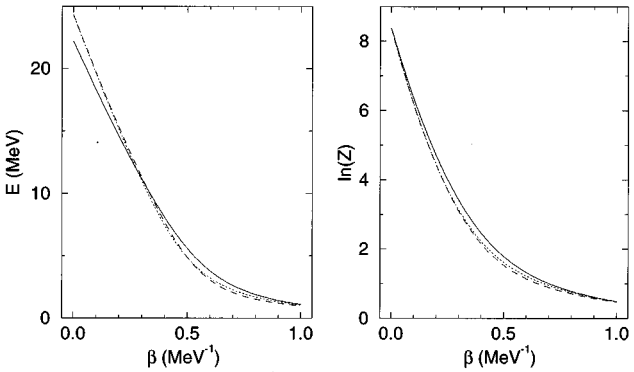

FIG. 2. Plot of the energy, $E(\beta)$, and partition function, $Z(\beta)$ for ^{20}Ne, as a function of β for the SDI and SDI$+a\hat{T}^2$ Hamiltonians. The solid and dashed lines represent the SDI and SDI $+a\hat{T}^2$ results obtained from the exact eigenvalues, while the dotted line shows the SDI results corrected via Eq. (9).

the figure, the solid and dashed lines represent $E(\beta)$ and $Z(\beta)$ obtained by using the exact eigenvalues of a shell-model diagonalization for the SDI and SDI$+a\hat{T}^2$ Hamiltonians, respectively. The dotted line represents the results obtained by adding $E_{\rm corr}$ to the SDI results. From the figure, it is seen that the corrected values very accurately reproduce both the energy and partition function of the SDI$+a\hat{T}^2$ Hamiltonian.

Shown in Fig. 3 are the reconstructed level densities obtained for ^{24}Mg using the SDI (top) and SDI$+1.507\hat{T}^2$ (bottom) Hamiltonians, respectively. For the reconstruction, $E(\beta)$ was normalized relative to the ground state value, which was evaluated to be $-76.844(200)$ MeV by performing MCSM calculations for $1.75\leqslant\beta\leqslant2.25$ MeV^{-1} and extrapolating for $\beta\rightarrow\infty$. The histogram in both panels represents the exact level density for ^{24}Mg using the USD Hamiltonian, and was obtained by direct diagonalization and placing the 28503 ($J_z=0$) eigenvalues into 1 MeV bins while including the $2J+1$ degeneracy. Because of the near Gaussian structure of the level density, $\rho(E)$ is only plotted up to 45 MeV, which is slightly larger than the centroid of the USD level density ($\sim$42 MeV). From the top panel, it is clear that the level density obtained from the SDI Hamiltonian alone is much too compressed (centroid at $\sim$36 MeV), and overpredicts the $\rho(E)$ by nearly a factor of two for $E\leqslant20$ MeV. On the other hand, the corrected level density represents a considerable improvement (centroid $\sim$40 MeV), and gives a reasonable representation of the USD level density for excitation energies $\leqslant20$ MeV.

At this point, it is important to note an important limitation in using the shell model to estimate the nuclear level density. Because of the fact that all calculations are by necessity limited to a finite model space, the shell-model level density will always have a Gaussian character, and at some point will always underestimate the true level density because of the presence of states representing excitations outside of the model space. For the most part, the shell model is best suited to describe states at lower-excitation energies.

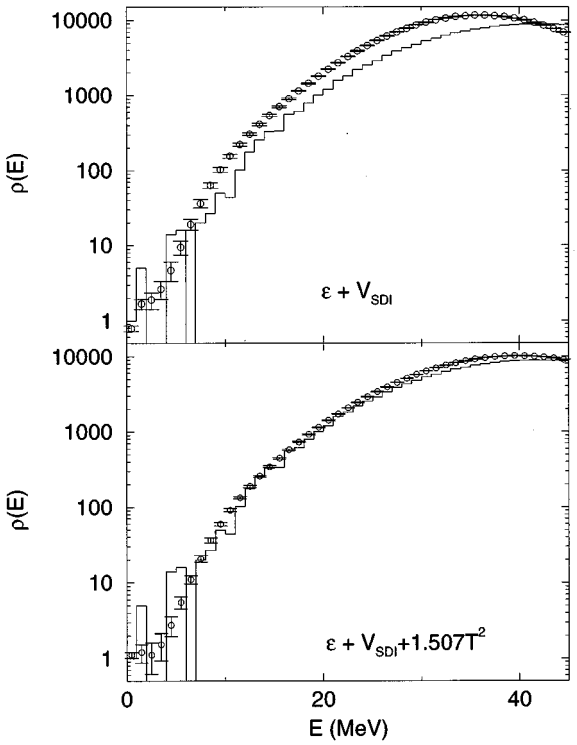

FIG. 3. Reconstructed level densities obtained for ^{24}Mg using the SDI (top panel) and the SDI$+1.507\hat{T}^2$ (bottom panel) Hamiltonians, respectively. The histogram in both panels represents the ^{24}Mg level density obtained with the USD interaction.

Hence, it is not realistic to expect that the shell model could provide an estimate of the level density for excitation energies around 40–50 MeV. In the case of a single major oscillator shell, such as the sd shell used here, the results are comparable to experimental data for $E\leqslant10$ MeV. On the other hand, by enlarging the model space to include more configurations, say another major oscillator shell such as the fp shell, the method presented here can be used to make estimates for the level density up to excitation energies of the order 15–20 MeV. In this case, however, it will also be necessary to account for states of differing parity, as well as spurious excitations of the center of mass.

To conclude, the procedure outlined here can successfully describe the level density of a realistic nuclear system, and plans are currently underway to compute level densities for ^{22}Mg, ^{26}Si, ^{30}S, and ^{34}Ar, which are needed to make estimates of (α,γ) reaction rates of astrophysical interest [18]. In addition, the method will also be applied to ^{162}Dy and ^{172}Yb where experimental data [19] for $\rho(E)$ exists for excitation energies up to the neutron separation energy. In these nuclei, since the protons and neutrons occupy different major shells, the problems associated with the higher isospin states pointed out here are most likely to be mitigated.

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