Total and Parity-Projected Level Densities of Iron-Region Nuclei by the Shell Model Monte Carlo Method

H. Nakada
Department of Physics, Chiba University, Inage, Chiba 263, Japan
E-mail: nakada@e.chiba-u.ac.jp

Y. Alhassid
Center for Theoretical Physics, Yale University, New Haven, CT 06520, U.S.A.
E-mail: yoram@nst.physics.yale.edu

Total and parity-projected level densities of iron-region nuclei are calculated microscopically by using Monte Carlo methods for the nuclear shell model in the complete \((pf + 0g_{9/2})\)-shell. The calculated total level density is found to be in good agreement with the experimental level density. The Monte Carlo calculations offer a significant improvement over the thermal Hartree-Fock approximation. Contrary to the Fermi gas model, it is found that the level density has a significant parity-dependence in the neutron resonance region. The systematics of the level density parameters (including shell effects) in the iron region is presented.

1 Introduction

Neutron-capture reactions play an important role in nucleosynthesis, e.g. in the \(s\) and \(r\) processes. Their rates are strongly affected by the corresponding nuclear level densities around the neutron resonance region. Most conventional calculations of the nuclear level density are based on the Fermi gas model (e.g. the Bethe formula). A phenomenological modification is often adopted where the excitation energy \(E_x\) in the Bethe formula is backshifted by \(\Delta\), giving a total level density of

\[
\rho(E_x) \approx g\frac{\sqrt{\pi}}{24} a^{-\frac{1}{2}} (E_x - \Delta)^{-\frac{3}{2}} e^{2\sqrt{a(E_x - \Delta)}}
\]

with \(g = 2\). The backshift \(\Delta\) originates in pairing correlations and shell effects, while the parameter \(a\) is determined by the single-particle level-density at the Fermi energy. By adjusting the value of \(a\) for each nucleus, Eq. (1) describes well a large volume of experimental data. However, the Fermi gas model grossly underestimates the value of \(a\), and consequently it is difficult to predict the level density to an accuracy better than an order of magnitude. Much less is known about the parity-dependence of the level density.

We have been studying the level densities of iron-region nuclei by applying the recently proposed shell model Monte Carlo (SMMC) method within the the full \(pf\)- and \(0g_{9/2}\)-shell. As a finite temperature method, it is particularly
suitable for calculations of level densities (see below). By introducing parity-projection methods for the auxiliary fields we are also able to calculate parity-projected level densities. We remark that the \((pf + 0g9/2)\) model space is sufficiently large to describe the important excitations around the neutron-resonance energies in this mass region \((E_x \sim 5 - 15 \text{ MeV})\).

2 Calculations of level densities

We adopt an isoscalar Hamiltonian of the form

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

The single-particle energies \(\epsilon_a\) are determined from a Woods-Saxon potential \(V\) plus spin-orbit interaction with the parameters quoted in Ref. The \(P^{(0,1)}\) denotes the \(T = 1\) pair-creation operator and \(O^{(\lambda,T)}\) are multipole operators with radial part of \(dV/dr\). In the present calculations we include multipole terms with \(\lambda = 2, 3\) and 4. Core polarization effects are taken into account through the use of renormalization factors \(k_\lambda\). We use \(k_2 = 2\), \(k_3 = 1.5\) and \(k_4 = 1\). The pairing strength \(g_0\) is determined from the experimental odd-even mass differences for spherical nuclei in the mass region \(A = 40 - 80\). This Hamiltonian satisfies the modified sign rule, and therefore has a good Monte Carlo sign for even-even nuclei. This enables us to perform accurate Monte Carlo calculations.

In SMMC the canonical thermal energy \(E(\beta) \equiv \langle H \rangle_\beta\) is calculated as a function of inverse temperature \(\beta\). Particle-number projection (for both protons and neutrons) is implemented exactly. The canonical partition function \(Z(\beta)\) is determined by a numerical integration of \(E(\beta), \ln[Z(\beta)/Z(0)] = - \int_0^\beta d\beta' E(\beta')\). The level density \(\rho(E)\) is then calculated in the saddle-point approximation from

\[
\rho(E) = (2\pi\beta^{-2}C)^{-1/2}e^S; \\
S(E) = \beta E + \ln Z(\beta) , \quad \beta^{-2}C(\beta) = -dE/d\beta.
\] (3)

\(C\) is the heat capacity calculated by numerical differentiation of \(E(\beta)\). To compare with experimental data, it is necessary to find \(\rho\) as a function of the excitation energy. For that purpose we determine the ground-state energy by extrapolating \(E(\beta)\) to \(\beta \to \infty\).

To calculate the parity-dependence of the level density, we have introduced parity-projection techniques in SMMC. Using the Hubbard-Stratonovich representation for \(e^{-\beta H}\) and the projection operators \(P_\pm = (1 \pm P)/2\) (\(P\) is
the space reflection operator), we can write the projected energies \( E_{\pm}(\beta) \equiv \text{Tr}(HP_{\pm}e^{-\beta H})/\text{Tr}(P_{\pm}e^{-\beta H}) \) in the form

\[
E_{\pm}(\beta) = \frac{\int D[\sigma]W(\sigma) [\langle H \rangle_{\sigma} \pm \langle HP \rangle_{\sigma}]}{\int D[\sigma]W(\sigma) [1 \pm \langle P \rangle_{\sigma}]}.
\] (4)

The integration over the auxiliary fields \( \sigma \) is performed with the usual Monte Carlo weight function \( W(\sigma) = G(\sigma)\zeta(\sigma) \), where \( G \) is a gaussian factor and \( \zeta(\sigma) = \text{Tr} \, U_{\sigma} \) is the partition function of the non-interacting propagator \( U_{\sigma} \).

Both \( U_{\sigma} \) and \( P \) can be represented by matrices in the single-particle space. \( E_{\pm}(\beta) \) are then calculated through matrix algebra in this single-particle space, similarly to the calculation of \( E(\beta) \). Once we find \( E_{\pm}(\beta) \), the calculation of the projected densities \( \rho_{\pm}(E) \) is analogous to that of the total level density.

3 Results

3.1 \(^{56}\text{Fe}\)

Results for total level density in \(^{56}\text{Fe}\) are presented in the left panel of Fig. 1 as a function of \( E_x \). The SMMC results are the solid squares and include statistical errors (often the errors are too small to be visible). Although it is difficult to measure the total level density directly, it can be reconstructed from a few parameters that are determined experimentally. The solid line in Fig. 1 shows this experimental level density as determined from charged particle spectra. Our SMMC result is in good agreement with the experimental results. We have observed similar agreement (to within a factor of two) for other nuclei in the iron region. Consequently, accurate level densities can be calculated in the present approach. In particular, we extract the level density parameters \( a \) and \( \Delta \) via a fit of our microscopically calculated level densities to Eq. (1). Using the energy range \( 4.5 \text{ MeV} < E_x < 20 \text{ MeV} \), we obtain \( a = 5.780 \pm 0.055 \text{ MeV}^{-1} \) and \( \Delta = 1.560 \pm 0.161 \text{ MeV} \) for \(^{56}\text{Fe}\). In Fig. 1 we also compare our SMMC results with those of the thermal Hartree-Fock approximation (HFA) (dashed line). The kink observed in the HFA level density around \( E_x \sim 9 \text{ MeV} \) is a signature of a shape phase transition, but it is washed out in the SMMC due to strong two-body correlations.

The Fermi gas model predicts equal positive- and negative-parity level densities at all energies. However, this is unrealistic in the neutron resonance regime of iron-region nuclei where the excitation energy is comparable to the energy gap among major shells (i.e. the gap between the \( pf \) and \( g_{9/2} \) shells). The SMMC parity-projected level densities of \(^{56}\text{Fe}\) are shown in the right panel of Fig. 1. They are well fitted to Eq. (1) with \( q = 1 \), but with parity-specific parameters \( a_{\pm} \) and \( \Delta_{\pm} \). We find \( a_+ = 5.611 \pm 0.073 \text{ MeV}^{-1} \), \( \Delta_+ = \)
Figure 1: Level densities of $^{56}$Fe. Left: Total level densities in SMMC (solid squares) and in the HFA (dashed line). The solid line is the experimental level density. Right: positive-parity (circles) and negative-parity (triangles) level densities in SMMC.

$0.550 \pm 0.196$ MeV and $a_- = 6.209 \pm 0.625$ MeV$^{-1}$, $\Delta_- = 3.172 \pm 1.637$ MeV. Since negative-parity states in $^{56}$Fe are possible only when $g_{9/2}$ is populated, $\rho_-$ is lower than $\rho_+$ at low energies. Thus the backshift $\Delta_-$ is larger than $\Delta_+$. On the other hand, at high excitation energies positive- and negative-parity level densities are approximately equal, resulting in $a_- > a_+$.

### 3.2 Systematics and shell effects

We discuss now the nucleus-dependence of the level density parameters $a$ and $\Delta$ for even-even nuclei in the $50 < A < 70$ region: $^{54-58}$Fe, $^{58-64}$Ni and $^{64-68}$Zn. Among them $^{54}$Fe and the Ni isotopes have $f_{7/2}$-subshell closure for protons and/or neutrons ($Z$ or $N = 28$). Fig. 2 shows the calculated values of $a$. It is interesting to see whether shell effects (at $Z$ or $N = 28$) can be observed in the level density parameters. We have found enhancement of the backshift parameter $\Delta$ at $Z$ or $N = 28$. However, no strong shell effects are observed in the single-particle level density parameter $a$ and it increases smoothly as a function of $A$. For the parity-projected level densities we find that $a_-$ increases as a function of $A$ more moderately than $a_+$. This is because more excitations to the $g_{9/2}$ orbits become possible (for fixed $E_x$) as $A$ increases. It would be interesting to investigate how the parity-dependence affects the neutron-capture reaction rates.
Figure 2: The single-particle level density parameter $a$ as a function of $A$, for the total (left) and parity-projected (right) level densities. Points corresponding to isotopes with a given $Z$ are connected by dashed lines. In the right panel, values of $a_+$ are shown by circles and values of $a_-$ by triangles.

4 Conclusion

We have used the auxiliary fields Monte Carlo method to calculate the level density of iron-region nuclei in the complete $(pf + 0g_{9/2})$-shell, and found good agreement with experimental results. The introduction of a parity-projection technique in the SMMC allows us to study the parity-dependence of the level density parameters. The systematics of these parameters have been presented.

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