Parity-Projected Shell Model Monte Carlo Level Densities for \( fp \)-shell Nuclei

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We calculate parity-dependent level densities for the even-even isotopes \(^{58,62,66}\)Fe and \(^{58}\)Ni and the odd-A nuclei \(^{59}\)Ni and \(^{65}\)Fe using the Shell Model Monte Carlo method. We perform these calculations in the complete \( fp \)-\( gds \) shell-model space using a pairing+quadrupole residual interaction. We find that, due to pairing of identical nucleons, the low-energy spectrum is dominated by positive parity states. Although these pairs break at around the same excitation energy in all nuclei, the energy dependence of the ratio of negative-to-positive parity level densities depends strongly on the particular nucleus of interest. We find equilibration of both parities at noticeably lower excitation energies for the odd-A nuclei \(^{59}\)Ni and \(^{65}\)Fe than for the neighboring even-even nuclei \(^{58}\)Ni and \(^{66}\)Fe.

I. INTRODUCTION AND MOTIVATION

Nuclear level densities play an important role in theoretical estimates of nuclear reaction rates needed in various applications including astrophysical nucleosynthesis processes like the s-, r-, and rp-process. They also contribute to one of the largest uncertainties in the cross section determinations used for large-scale nucleosynthesis networks. Typically, nuclear level densities are described in these astrophysical studies by using the backshifted Fermi gas model of Gilbert and Cameron. This model extends the non-interacting Fermi gas model of Bethe by considering pairing among like nucleons via a backshift of the excitation energy \(E\). This backshift accounts for the energy required to break nucleon pairs. Furthermore, the astrophysical applications assume an empirical ansatz for the angular momentum distribution of the levels and consider equilibration of both parities at the energies of interest.

For astrophysical applications, one is often interested in the nuclear level density at rather low excitation energies. For example, the typical neutron energies in r-process nucleosynthesis reach only up to a few MeV. At such energies, nuclear structure and pairing effects strongly influence the level density and an equilibration of both parities is quite unlikely. In particular, in even-even nuclei, pairing among identical nucleons generates only positive parity states even when single-particle states of opposite parity are present. Therefore, negative parity states should be suppressed in even-even nuclei at low energies due to both pairing and the underlying single-particle structure of the mean field which groups states of the same parity, at least for nuclei with mass numbers \(A\) smaller than about 100. The parity equilibration is governed by the energy scales associated with pair-breaking and the shell gap between opposite-parity states near the Fermi surface. While the latter is typically of order 5-6 MeV for intermediate mass nuclei, the former strongly depends on the nuclear structure.

We investigate in this paper the competition of pairing and single-particle structure on the parity dependence of the level density. We perform Shell Model Monte Carlo calculations of the even-even nuclei \(^{58,62,66}\)Fe and \(^{58}\)Ni and the odd-A nuclei \(^{59}\)Ni and \(^{65}\)Fe in the complete \( fp \)-\( gds \) model space, where the single-particle states in the \( fp \) shell have negative parity, while those of the \( gds \) shell have positive parity. As we shall see, residual interactions among the protons and neutrons also influence the level density.

II. FORMALISM

The Shell Model Monte Carlo (SMMC) approach allows the determination of nuclear properties at finite temperature in unprecedentedly large model spaces, considering the important correlations among the valence nucleons. The SMMC method describes the nucleus by a canonical ensemble at temperature \(T = \beta^{-1}\) and employs a Hubbard-Stratonovich linearization of the imaginary-time many-body propagator, \(e^{-\beta H}\), to express observables as path integrals of one-body propagators in fluctuating auxiliary fields. Since Monte Carlo techniques avoid an explicit enumeration of the many-body states, they can be used in model spaces far larger than those accessible to conventional methods. The notorious sign problem that plagues Monte Carlo studies of Fermionic systems can be avoided within the SMMC by adopting a pairing+quadrupole force as residual interaction.

There are already several successful studies of level densities using the SMMC approach. Ormand as well as Nakada and Alhassid calculated the level density for selected even-even nuclei, while Ref. extended this work to odd-A and odd-odd nuclei. Using projection techniques, Alhassid and collaborators succeeded in studying the parity dependence and the angular-momentum dependence of the level density.
for intermediate-mass nuclei. Recently, Ref. [17] explored the influence of pairing correlations and their energy dependence on nuclear level densities. All these approaches are based on the ability of the SMMC to calculate expectation values of an observable at temperature $T$ as the thermal average of a canonical ensemble (with fixed numbers of protons and neutrons). Thus for the energy excitation function, one has

$$E(\beta) = \frac{\text{Tr}[H e^{-\beta H}]}{\text{Tr}[e^{-\beta H}]} = \frac{\text{Tr}[H e^{-\beta H}]}{Z(\beta)}, \quad (1)$$

where $Z$ is the partition function, $\beta$ the inverse temperature, and $H$ the nuclear Hamiltonian. Using the parity projection operators $P_{\pm} = (1 \pm \sigma)/\sqrt{2}$, where $\sigma$ is the parity operator, one is able to calculate the ratio of the parity-projected partition function to the total partition function [13]

$$Y_{\pm}(\beta) = \frac{Z_{\pm}(\beta)}{Z(\beta)} = \frac{\text{Tr}[P_{\pm} e^{-\beta H}]}{\text{Tr}[e^{-\beta H}]} \quad (2)$$

from which one can then extract the parity-projected energy excitation functions

$$E_{\pm}(\beta) = -\frac{d\ln Y_{\pm}(\beta)}{d\beta} + E(\beta) = \frac{\text{Tr}[HP_{\pm} e^{-\beta H}]}{Z_{\pm}(\beta)} = \int \frac{dE e^{-\beta E} E \rho_{\pm}(E)}{Z_{\pm}(\beta)}, \quad (3)$$

where we have introduced the parity-projected partition functions $Z_{\pm}$ and level densities $\rho_{\pm}$.

To obtain $\rho_{\pm}$ from Eq. (4) requires an inverse Laplace transform which we treat within the saddle-point approximation:

$$\rho_{\pm}(E) = \frac{e^{\beta E \pm \ln Z_{\pm}(\beta)}}{\sqrt{-2 \pi \frac{d^2 Z_{\pm}(\beta)}{d\beta^2}}} \quad (4)$$

where $\beta = \beta(E_{\pm})$ is obtained by inverting $E_{\pm}(\beta)$. An analogous relation holds between the total level density $\rho(E)$ and the energy excitation function $E(\beta)$.

### III. RESULTS

Our SMMC calculations were performed in the complete $fp$-$gds$ model space with 50 valence orbitals for both protons and neutrons. The single-particle energies and the residual pairing-$gds$ quadrupole interaction were adopted from previous SMMC studies that successfully explored the competition of isovector pairing versus quadrupole deformation in the $A \sim 80$ mass region [18], and as a function of temperature in selected nuclei. These previous calculations clearly identified the breaking of pairs of identical nucleons in even-even nuclei around $T \approx 0.7$ MeV [20].

In the following, we discuss various results of these calculations. Figure 1 shows the total and parity-projected SMMC level densities for $^{58,62,66}$Fe and $^{58}$Ni. We observe that, at modest excitation energies, the total level density increases with the mass number. This is expected from a Fermi gas approximation to the level density, which scales like $\rho \sim \exp\{2\sqrt{aE}\}$ with the level density parameter $a$ proportional to the mass number $A$ [1]. Interestingly, we observe an equilibration of both parities at $E \approx 11-12$ MeV in $^{58}$Fe, while equilibration occurs already around $E \approx 6$ MeV in $^{62,66}$Fe. This observation simply reflects the fact that it is energetically more costly to promote neutrons to the $gds$ shell for $^{58}$Fe, which requires neutrons to bridge the gap from the $p_{3/2}$ to the $g_{9/2}$ orbital, than for $^{62,66}$Fe. Nevertheless, it is not simply the occupation number of
the \( g_{9/2} \) orbital which matters. This quantity is shown in Fig. 2. For \(^{58}\text{Fe}\), the SMMC predicts rather little average occupation of the \( g_{9/2} \) orbital, which increases from 0.2 neutrons in the ground state to 0.3 at \( T = 1 \) MeV (corresponding to an excitation energy of about \( E \approx 6 \) MeV) to 1.0 at \( T = 2 \) MeV (\( E \approx 23 \) MeV). On the other hand, one finds an occupation number of order 1.0 in the \(^{62}\text{Fe}\) ground state, which grows to 2.1 at \( T = 2 \) MeV. For \(^{66}\text{Fe}\), the residual interaction promotes neutrons to the \( g_{9/2} \) orbital, yielding a \( g_{9/2} \) occupation number of about 3.0. The occupation grows only mildly with temperature and reaches about 3.6 at \( T = 2 \) MeV. We note that the residual interaction mainly scatters (neutron) pairs from the \( fp \) shell to the \( gds \) shell. Although these correlations are important for the nuclear structure, they do not change the parity. This is clearly seen in a comparison between \(^{62}\text{Fe}\) and \(^{66}\text{Fe}\), which shows quite a similar ratio of negative-to-positive level densities (Fig. 1), while clearly these nuclei have distinct occupation numbers of the \( g_{9/2} \) orbital (Fig. 2). While a promotion of nucleons (neutrons) is required to make negative-parity states in our model space, the strong pairing correlations also have to be overcome.

As in \([14, 20]\), we define the pairing strength as the sum over all matrix elements of the pair matrix

\[
M_{\alpha,\alpha'} = \langle A^\dagger(j_a,j_b)A(j_c,j_d) \rangle, \tag{5}
\]

with the \( J = 0 \) pair operator

\[
A^\dagger(j_a,j_b) = \frac{1}{\sqrt{1+\delta_{ab}}} \left[ a^\dagger_{j_a} \times a^\dagger_{j_b} \right]^{JM=00}, \tag{6}
\]

where \( a^\dagger_{j_a} \) creates a nucleon in the orbital \( j_a \) with angular momentum \( J_a \) \([22]\). Since only genuine pair correlations are of interest, we subtract the pure ‘mean-field’ values, i.e. those obtained without residual interaction.

As is shown in Fig. 3 the pairing strengths decrease strongly with temperature, and are reduced to about half of the ground-state values around \( T = 0.8 \) MeV (corresponding to \( E \approx 4 \) MeV). This breaking of pairs is accompanied by a peak in the specific heat (e.g. \([20]\)). We note that the proton pairing strengths are quite similar for all three iron isotopes (e.g. \([14]\)).

For \(^{62}\text{Fe}\) and \(^{66}\text{Fe}\) the ratio of negative-to-positive level densities is quite similar and equilibration is reached at excitation energies around 6 MeV; i.e., once the pairs with positive parities are sufficiently broken. This apparently requires more energy than the gap between the last occupied neutron orbital and the \( g_{9/2} \) orbital with its large degeneracy. Hence, once pairs are broken, many negative-parity states can be formed in \(^{62}\text{Fe}\) and \(^{66}\text{Fe}\). The situation is obviously different for \(^{58}\text{Fe}\) where the gaps from the last occupied proton (\( f_{7/2} \)) and neutron (\( p_{3/2} \)) orbitals to the \( g_{9/2} \) orbital are larger than 6 MeV. Thus, even at the energy at which pairs are broken, it is more likely to form positive-parity states with unpaired nucleons in the \( fp \) shell than negative-parity cross-shell states.

Ref. \([15]\) describes a model to estimate the ratio of negative-to-positive level densities on the basis of the independent particle model and a BCS treatment of pairing. It appears that this model slightly underestimates this ratio. This is due to the fact that the residual interaction mixes orbitals from adjacent shells with different parities at lower energies than obtained in the independent particle model.

Although they have the same neutron number, the isotones \(^{58}\text{Fe}\) and \(^{58}\text{Ni}\) differ in their single-particle structure, and this shows in their level densities. The fact that \(^{58}\text{Fe}\) has four neutrons in the \( p_{3/2} \) orbital, compared to two in the case of \(^{58}\text{Ni}\), allows for a larger amount of negative-parity states at low energies in \(^{58}\text{Fe}\), since these states are generated by configurations with one and three neutrons in the \( gds \)-orbitals for \(^{58}\text{Fe}\) but with only one neutron for \(^{58}\text{Ni}\). As a consequence, the parity unbalance in the level density persists to higher excitation energies in \(^{58}\text{Fe}\) than in \(^{58}\text{Ni}\). At modest excitation energies, this difference can be approximately accounted for...
by a constant energy shift of about 3 MeV, simulating the shell gap in $^{58}$Ni.

While the structure of even-even nuclei is strongly dominated by pairing at low excitation energies, thus leading to the dominance of positive-parity over negative-parity states, the situation is different for odd-$A$ nuclei. In this case, the unpaired nucleon is not hindered by pairing and can, depending on the single-particle structure, occupy negative-parity states ($fp$ shell) or positive-parity states ($gds$ shell). To investigate the differences between even-even and odd-$A$ nuclei, we also calculated the SMMC level densities for $^{59}$Ni and $^{65}$Fe. For $^{59}$Ni, the unpaired neutron occupies a $p_{3/2}$ orbital. Despite the fact that this neutron is not hindered by pairing, it will nevertheless, at low excitations energy, mainly occupy orbitals in the $fp$ shell; consequently, negative-parity states dominate the $^{59}$Ni level density at low excitation energies. This is indeed born out of our SMMC calculation (Fig. 4), which yields a balance between negative- and positive-parity level densities at excitation energies around 13 MeV. Comparing with $^{58}$Ni (Fig. 1), where the equilibration energy is about 16 MeV, we see that neutron pairing, e.g., the residual interaction, indeed has a significant effect in the equilibration of positive and negative parities.

The neutron single-particle structure of $^{65}$Fe corresponds to a single hole in the $fp$ shell. Thus, low-energy excitations can be achieved by either changing the hole structure in the $fp$ shell or by promoting the neutron to the $g_{9/2}$ orbital, which, however, has the opposite (positive) parity to the ground state. As a consequence, one expects equal distribution of negative- and positive-parity level densities already at low excitation energies. This is indeed observed in our SMMC calculations (Fig. 4), where we find the same level densities for both parities down to $E_x \approx 1.5$ MeV, corresponding to the lowest temperature for which we have been able to perform SMMC calculations in the odd-$A$ systems. (An odd-$A$ sign problem occurs even in the presence of good sign interactions [8].)

**IV. CONCLUSIONS**

In summary, we calculated parity-projected level densities for several even-even and odd-$A$ $fp$-shell nuclei using the Shell Model Monte Carlo approach. For even-even nuclei, we confirm that the low-energy spectrum is dominated by pairing among nucleons, resulting in a dominance of the positive-parity level density. Although the pairs break at excitation energies of a few MeV, the contribution of negative-parity states depends strongly on the single-particle structure of the nuclei. If the Fermi energies of protons and neutrons are relatively well separated from orbitals with the opposite parity, an equal distribution between parities in the level densities is achieved at higher excitation energies than for nuclei with Fermi energies close to the oscillator shell closure. As examples for this difference, we presented parity-projected level densities for $^{58}$Fe, $^{58}$Ni, and $^{66}$Fe. The same general trend can be observed for odd-$A$ nuclei ($^{59}$Ni and $^{65}$Fe). However, as these nuclei have an unpaired neutron, the balance between negative- and positive-parity level densities is achieved at somewhat lower excitation energies than in the neighboring even-even nuclei.

The SMMC approach has again been proven to be a powerful tool to microscopically study nuclear level densities. In the future, it will be used to explore the angular-momentum dependence of the level density. First steps towards this goal have been presented in [10, 21].

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[22] There is a misprint in [14, 20]. As in the present work, the plotted pairing strengths are the sum over the matrix elements of the pair matrix $M$, not the sum over its eigenvalues.