Isospin-projected nuclear level densities by the shell model Monte Carlo method

H. Nakada\textsuperscript{1} and Y. Alhassid\textsuperscript{2}
\textsuperscript{1}Department of Physics, Graduate School of Science, Chiba University, Inage, Chiba 263-8522, Japan
\textsuperscript{2}Center for Theoretical Physics, Yale University, New Haven, Connecticut 06520, U.S.A.

We have developed an efficient isospin projection method in the shell model Monte Carlo approach for isospin-conserving Hamiltonians. For isoscalar observables this projection method has the advantage of being exact sample by sample. The isospin projection method allows us to take into account the proper isospin dependence of the nuclear interaction, thus avoiding a sign problem that such an interaction introduces in unprojected calculations. We apply our method in the calculation of the isospin dependence of level densities in the complete $pf + g_{9/2}$ shell. We find that isospin-dependent corrections to the total level density are particularly important for $N \sim Z$ nuclei.

The level density is among the most important statistical properties of nuclei. It is required for the calculation of transition rates through Fermi's golden rule and of nuclear reaction rates through the Hauser-Feshbach theory. Applications in astrophysics include estimates of neutron and proton radiative capture rates in the $s$, $r$, and $rp$ processes [1, 2].

Most theoretical approaches to the level density are based on the Fermi gas model, i.e., Bethe’s formula \[ \rho(E_x) = \frac{\pi^{1/2}}{12} a^{-1/4} (E_x - \Delta + t)^{-5/4} \exp\left[2 \sqrt{a(E_x - \Delta)}\right], \] where $t$ represents the Lang-LeCouteur modification defined by $at^2 - t = E_x - \Delta$. The BBF describes well the experimental level densities of many nuclei if the parameters $a$ and $\Delta$ are fitted individually for each nucleus [3]. Although their global systematics have been studied extensively, these fitted parameters exhibit a significant dependence on the nucleus under consideration. Since nuclear level densities increase very rapidly with $E_x$, an accurate determination of $a$ and $\Delta$ is crucial for reliable calculations of level densities and reaction rates.

As the basic microscopic model of nuclear structure, the interacting shell model takes into account both shell effects and correlations. This model has been successful in describing the low-lying states of many nuclei and is also an attractive framework to study microscopically thermal and statistical properties of nuclei. However, the large dimensionality of the many-particle model space has limited the applicability of direct diagonalization methods of the shell model Hamiltonian in medium- and heavy-mass nuclei. This limitation has been overcome using the shell model Monte Carlo (SMMC) approach [4, 5]. While the SMMC method cannot provide a detailed spectrum of the many-particle Hamiltonian, it enables calculation of thermal and statistical properties in model spaces that are many orders of magnitude larger than those that can be treated by conventional methods.

We have developed a method [6] to calculate level densities in the SMMC approach, and applied it to nuclei in the mass range $A \sim 50 - 70$. We found good agreement with experimental data without any adjustable parameters [8, 10]. Fermionic Monte Carlo methods often suffer from the so-called sign problem, which leads to large statistical errors and a breakdown of the method at low temperatures. However, the dominating collective components of the nuclear interaction [11] usually have a good sign, and general effective interactions containing small terms that have a bad sign can be treated with the method introduced in Ref. [7]. In the calculation of level densities the sign problem was circumvented by constructing a good-sign interaction in the $pf + g_{9/2}$ shell [3] that correctly includes the dominating collective components of realistic effective interactions.

In the SMMC approach, thermal observables are averaged over all possible values of the good quantum numbers. However, many of the applications require the dependence of thermal observables on the good quantum numbers. This dependence is determined in the SMMC approach by projection methods. Parity projection was implemented in the study of the parity dependence of level densities [6, 12, 13], and a spin projection method was introduced to determine the spin distribution of nuclear levels [4]. The particle-number reprojection technique has been developed [10] to facilitate the systematic studies of level densities for a large number of nuclei.

The isospin $T$ is approximately a conserved quantum number in nuclei. Reliable treatment of the isospin dependence of the level densities could be important in $N \sim Z$ nuclei because levels with different $T$ values lie close in energy. In our SMMC studies of level densities we have used a good-sign Hamiltonian to keep the statistical errors small. While this Hamiltonian contains the dominating collective components of nuclear effective interactions, it might not describe properly the energy differences of states with different isospin values. Such...
discrepancies can be corrected by including an isospin-dependent interaction \[15, 16\]. However such an interaction has a bad Monte Carlo sign and was treated perturbatively in Refs. \[15, 16\]. Here we overcome this problem by introducing an exact isospin projection method in the SMMC approach. This \(T\)-projection enables us to determine the isospin dependence of nuclear levels and to include accurately an isospin-dependent interaction term.

We apply the method to the calculation of level densities and to determine the isospin dependence of nuclear levels and to include accurately an isospin-dependent interaction term. In the following we describe a more efficient method. We assume the nuclear Hamiltonian \(H\) at inverse temperature \(\beta\). In the HS decomposition \(e^{-\beta H} = \int D[\sigma]G_\sigma U_\sigma\), where \(G_\sigma\) is a Gaussian weight and \(U_\sigma = Te^{-\int_0^\beta d\tau h_\sigma(\tau)}\) is the propagator of the one-body Hamiltonian \(h_\sigma\) describing non-interacting nucleons moving in time-dependent auxiliary fields \(\sigma(\tau)\) (\(T\) denotes time ordering). The canonical expectation value of an observable \(O\) is then given by

\[
\langle O \rangle_{A,T} = \frac{\langle \text{Tr}_{A,T} O U_\sigma \rangle}{\text{Tr}_{A,T} U_\sigma},
\]

where \(\text{Tr}_{A,T}\) denotes a trace in the subspace of the fixed mass number \(A\) and isospin component \(T\). Since \(A = N + Z\) and \(T = (N - Z)/2\), this trace is equivalent to a trace at fixed neutron number \(N\) and proton number \(Z\). We have also used the notation \(\langle X_\sigma \rangle_W \equiv \int D[\sigma]W(\sigma)X_\sigma/\int D[\sigma]W(\sigma)\) with \(W(\sigma) = G_\sigma \text{Tr}_{A,T} U_\sigma\). Here and in the following we assume \(\text{Tr}_{A,T} U_\sigma \geq 0\) (i.e., we assume a good sign interaction and an even-even or \(N = Z\) nucleus). Otherwise the sign function \(\text{Tr}_{A,T} U_\sigma/|\text{Tr}_{A,T} U_\sigma|\) has to be included. In the Monte Carlo method we choose \(M\) samples of the field \(\sigma\) according to the weight function \(W(\sigma)\) (each sample denoted by \(\sigma_k\)), and estimate \(\langle X_\sigma \rangle_W \approx \sum_k X_{\sigma_k}/M\).

Let us consider a model space for a set of isobars (i.e., nuclei with fixed \(A\) but different values of \(T\)). Since the isospin forms a \(su(2)\) algebra, isospin projection generally requires a three-dimensional integration over the Euler angles in isospin space (in analogy with angular momentum projection). However, this integration is time consuming and in the following we describe a more efficient method. We assume the nuclear Hamiltonian \(H\) to be isospin invariant (i.e., \([H, T] = 0\)), in which case both \(T\) and \(T_z\) are good quantum numbers and the isospin multiplets (at fixed \(T\)) are degenerate with respect to \(T_z\). The subspace with fixed \(T_z\) (i.e., fixed nucleus) contains all energy eigenstates with \(T \geq |T_z|\). In the following we assume \(N \geq Z\) without loss of generality, and denote by \(T_0 = (N - Z)/2 \geq 0\) the value of \(T_z\) for a specific nucleus. If the operator \(X\) is an isoscalar, we can decompose its trace for the specific nucleus as

\[
\text{Tr}_{A,T_z=T_0} X = \sum_{T \geq T_0} \text{Tr}_{A,T} X,
\]

where \(\text{Tr}_{A,T}\) represents the trace for fixed \(A\) and isospin \(T\) (not including degeneracy with respect to \(T_z\)). The trace of \(X\) for a specific isospin \(T = T_0\) is then obtained by

\[
\text{Tr}_{A,T=T_0} X = \text{Tr}_{A,T_z=T_0} X - \text{Tr}_{A,T_z=T_0+1} X.
\]

We note that \(T_z = T_0 + 1\) corresponds to a nucleus with \((N + 1)\) neutrons and \((Z - 1)\) protons. In the level density calculations we use \(X = He^{-\beta H}\) \[8\], which is an isoscalar. If \(X\) is not an isoscalar, a \(T_z\)-dependent factor is required in Eq. \(6\) and hence in Eq. \(1\).

An isospin-invariant two-body interaction can always be decomposed into a sum of squares of isoscalar one-body operators \[8\]. Therefore, the one-body Hamiltonian \(h_\sigma\) and the propagator \(U_\sigma\) in the corresponding HS representation remains isospin invariant for any configuration of the \(\sigma\) fields. Equation \(1\) then holds with \(X = OU_\sigma\) as long as \(O\) is an isoscalar observable

\[
\text{Tr}_{A,T=T_0} (OU_\sigma) = \text{Tr}_{A,T_z=T_0} (OU_\sigma) - \text{Tr}_{A,T_z=T_0+1} (OU_\sigma).
\]

Thus, \(T\) projection can be carried out for each sample by using the simpler \(T_z\) projection. Equation \(5\) guarantees that \(T\) projection is implemented exactly sample by sample. An equation analogous to Eq. \(4\) was used for angular momentum projection with the scalar operator \(X = Oe^{-\beta H}\) \[14\]. However, in contrast to the isospin projection, \(h_\sigma\) in the HS transformation is not a scalar under spatial rotations so the equation analogous to \(5\) does not hold sample by sample. We therefore expect that the present \(T\) projection method leads to statistical errors that are typically smaller than the statistical errors in the angular momentum projection of Ref. \[14\].

Based on Eq. \(5\), isospin projection can be implemented using the particle-number reprojecton technique \[10\], in which the Monte Carlo sampling is done for a reference nucleus \((N, Z)\) and thermal observables are evaluated by reprojection on a nucleus \((N', Z')\). In particular, the ratio between the \(T_z\)- and \(T_z\)-projected partition functions is given by

\[
\frac{Z_{A,T_z=T_0}(\beta)}{Z_{A,T_z=T_0}(\beta)} = 1 - \frac{\langle \text{Tr}_{A,T_z=T_0+1} U_\sigma \rangle}{\langle \text{Tr}_{A,T_z=T_0} U_\sigma \rangle}.
\]

Similarly, the expectation value of an observable \(O\) for isospin \(T = T_0\) can be calculated from
The projection on higher values of isospin is carried out according to the weight function $W(\sigma)$ for the nucleus $A, T_0$. Equation (7) (that includes reprojection on the number reprojection method of Ref. [10].

The good-sign Hamiltonian of Ref. [3], while reproducing the proper collective features at fixed isospin $T$, does not necessarily reproduce the correct isospin dependence of energy levels. This isospin dependence can be particularly important for $N \sim Z$ (i.e., $T_2 \sim 0$) nuclei, in which number of levels with $T = T_0 = (N-Z)/2$ and $T = T_0 + 1$ are comparable even close to the ground state. A simple way to account for the proper isospin dependence of the nuclear interaction is to add an appropriate function of $T^2$, $f(T^2)$, to the effective Hamiltonian. The simplest such function is $f(T^2) = \alpha T^2$ ($\alpha$ is a constant), and in the modified surface delta interaction [17]. This $T^2$ term is repulsive ($\alpha > 0$) and leads to a sign problem in the SMMC method. In Refs. [15, 16] such a $T$-dependent interaction term was treated perturbatively. However, the criterion for applicability of perturbation theory does not always hold. As we explain below, the $T$ projection method enables us to account exactly for an arbitrary function $f(T^2)$ in the Hamiltonian.

To determine the proper isospin dependence in the Hamiltonian, we extract from experimental data the excitation energy $E_x(T)$ of the lowest level for each isospin value $T$. When not directly measured, the experimental values of $E_x(T)$ can be obtained from the measured masses of the corresponding isobars, together with estimates of the Coulomb energy differences among them. For the latter we use $E_C(A, Z) - E_C(A, Z - 1) = \frac{3}{8}(2Z - 1)e^2/R_C$ with $R_C = 1.24A^{1/3}$ fm. We then shift the calculated value of $E(T)$ (the lowest energy of isospin $T$), by $\delta E(T) = E(T_0) + E_x(T) - E(T)$ (for $T > T_0$), so as to reproduce the experimental value of $E_x(T)$. This shift defines the function $f(T^2)$ in the effective Hamiltonian. The modified $T$-projected level densities are then determined by shifting the excitation energy at each $T$ by $\delta E(T)$.

We first apply the isospin projection method to the nucleus $^{58}\text{Cu}$. The effective interaction consists of $T = 1$ pairing interaction and surface-peaked multipole-multipole interaction terms (quadrupole, octupole and hexadecupole) as in Ref. [3]. Since $^{58}\text{Cu}$ is an $N = Z$ (i.e., $T_0 = 0$) odd-odd nucleus, its $T = 1$ levels have analog levels in its neighboring even-even nuclei with $T_2 = \pm 1$. The lowest $T = 0$ and $T = 1$ levels can be quite close because of the pairing energy. The experimentally observed ground state of $^{58}\text{Cu}$ has $T = 0$, while the lowest $T = 1$ state is close to it with an excitation energy of $E_x(T = 1) = 0.203$ MeV. However, for the good-sign Hamiltonian of Ref. [3], we find $E(T = 1)$ to be well below $E(T = 0)$. The energy $E(T = 1)$, describing the ground state of the even-even nucleus with $T_2 = 1$, is determined directly from $(H)_{A,T_2 = 1} = \langle \text{Tr}_{A,T_2 = 1}(H U_\sigma)/\text{Tr}_{A,T_2 = 1}(U_\sigma) \rangle_W$ at low temperatures (as in Ref. [9]), while $E(T = 0)$ is determined from Eq. (7) with $T_0 = 0$ and $O = H$. All other energies $E(T)$ (for $T > 1$) are determined from $\langle H \rangle_{A,T_2 = T}$, similarly to $E(T = 1)$. Once we determine the energies $E(T)$, we adjust their differences to match the experimental values of $E_x(T)$.

In Fig. [1] we present the $T$- and $\pi$-projected level densities of $^{58}\text{Cu}$ with the corrected values of $E_x(T)$. An empirical BBF for the $T$-projected level densities (including the Lang-LeConteure modification [4]) is given by

$$\rho_T(E_x) = g(2T + 1)^{5/2} \alpha^{-3/4}(E_x - \Delta + t)^{-7/4} \times \exp\left[2\sqrt{\alpha(E_x - \Delta)}\right], \quad (9)$$
where \( g = 1 \) for a \( T\pi \)-projected density and \( g = 2 \) when parity is not projected. The projected SMMC level densities can be well fitted to Eq. (9) if we use \( T\pi \)-dependent values for \( a \) and \( \Delta \). The correction to \( E(T) \) is described by a shift of the corresponding \( \Delta \), but does not affect \( a \).

The total level density is obtained by summing over the \( T\pi \)-projected level densities (after taking into account the shifts \( \delta E(T) \)). The corresponding total level density for \( ^{58}\text{Cu} \) is shown in Fig. 2 (solid squares). For comparison we also show the total level density obtained by a direct SMMC calculation (i.e., without \( T \) projection) for the in- 
...
of the total level density for the higher energy regime. For this nucleus the perturbative method gives almost the same level density as the unperturbed density.

While the isospin-dependent corrections are important in $T_z = 0$ nuclei (and possibly in some $|T_z| = 1$ odd-odd nuclei), we have confirmed that these corrections are insignificant for $|T_z| > 0$ nuclei (at least up to $E_x \sim 20$ MeV). Since levels with $T > T_0$ ($T_0 \geq 1$) are well separated in energy from the $T = T_0$ levels already with the good-sign Hamiltonian, the density of all $T > T_0$ levels is less than half the density of the $T = T_0$ levels.

In summary, we have developed an efficient isospin projection method for an isospin-conserving Hamiltonian in the SMMC approach and applied it to nuclei in the complete $pf + g_{9/2}$ shell. This isospin projection is exact sample by sample and thus leads to statistical errors that are typically smaller than the statistical errors in a corresponding spin projection method. We have used this projection method to take into account the proper isospin dependence of the nuclear interaction, avoiding a sign problem that occurs when such an isospin-dependent interaction is included in unprojected calculations. For $N = Z$ nuclei, we find that this isospin dependence can lead to significant corrections to the total level density.

This work is supported in part by the U.S. DOE grant No. DE-FG-0291-ER-40608 and as Grant-in-Aid for Scientific Research (C), No. 19540262, by the MEXT, Japan. Computations were carried out on the PC cluster Helios and IBM SP3 in JAERI, and on CP-PACS at the Center for Computational Physics at the University of Tsukuba.

[1] E. M. Burbidge, G. R. Burbidge, W. A. Fowler and F. Hoyle, Rev. Mod. Phys. 29, 547 (1957).
[2] T. Rauscher, F.-K. Thielemann and K.-L. Kratz, Phys. Rev. C 56, 1613 (1997).
[3] H. A. Bethe, Phys. Rev. 50, 332 (1936).
[4] J. M. B. Lang and K. J. LeCouteur, Proc. Phys. Soc. (London) A 67, 585 (1954).
[5] W. Dilig, W. Schantl, H. Vonach and M. Uhl, Nucl. Phys. A 217, 269 (1973).
[6] G. H. Lang, C. W. Johnson, S. E. Koonin and W. E. Ormand, Phys. Rev. C 48 (1993) 1518.
[7] Y. Alhassid, D. J. Dean, S. E. Koonin, G. Lang, and W. E. Ormand, Phys. Rev. Lett. 72, 613 (1994).
[8] H. Nakada and Y. Alhassid, Phys. Rev. Lett. 79, 2939 (1997).
[9] H. Nakada and Y. Alhassid, Phys. Lett. B 436, 231 (1998).
[10] Y. Alhassid, S. Liu and H. Nakada, Phys. Rev. Lett. 83, 4265 (1999).
[11] M. Dufour and A. P. Zuker, Phys. Rev. C 54, 1641 (1996).
[12] Y. Alhassid, G. F. Bertsch, S. Liu and H. Nakada, Phys. Rev. Lett. 84, 4313 (2000).
[13] C. Özen, K. Langanke, G. Martinez-Pinedo, and D. J. Dean, Phys. Rev. C 75, 064307 (2007).
[14] Y. Alhassid, S. Liu and H. Nakada, Phys. Rev. Lett. 99, 162504 (2007).
[15] W. E. Ormand, Phys. Rev. C 56, R 1678 (1997).
[16] K. Langanke, Phys. Lett. B 438, 235 (1998).
[17] P. J. Brussaard and P. W. M. Glaudemans, Shell Model Applications in Nuclear Spectroscopy (North-Holland, Amsterdam, 1977).