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Microscopic Calculation of Nuclear Level Densities with Auxiliary-Fields Monte Carlo Method

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We have developed a microscopic method to calculate nuclear level densities in the interacting shell model using auxiliary-field Monte Carlo techniques. The method has successfully been applied to nuclei in the mass range $A \sim 50 - 70$. Shell effects and parity-dependence of the nuclear level densities are clarified by the present microscopic approach.

KEYWORDS: nuclear level densities, shell model, quantum Monte Carlo method, parity projection

I. Introduction

Level density is an important property of atomic nuclei. For example, level densities are needed to estimate neutron-capture cross sections in nucleosynthesis.[1] The (n,γ) cross sections at the temperature T are usually evaluated, if experimental data are not available, by the Hauser-Feshbach formula,

$$\sigma_{(n,\gamma)} \propto \sum_{J_i\pi_i J_f\pi_f} \int dE_f\, T^{(n)}_{J_i\pi_i}(E_i)\, T^{(\gamma)}_{J_f\pi_f}(E_f) \times \rho_{J_f\pi_f}(E_f)\, e^{-E_i/T}\,, \qquad (1)$$

where $T^{(n)}$ ($T^{(\gamma)}$) denotes the transmission coefficient of a neutron (a photon), and ρ indicates the level density, with $J_{i/f}$, $\pi_{i/f}$ and $E_{i/f}$ representing angular momenta, parities and energies of the initial and final states. The relevant energies are related to one another by $E_i = E_f + E_\gamma - S_n$, where S_n is the neutron separation energy of the final nucleus.

In many nuclei, the level densities at low excitation energies and around the neutron resonance region are well-fitted to the backshifted Bethe formula (BBF).[2] With the Lang and LeCouteur modification,[3] the BBF gives the level density at excitation energy E_x as

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

where $g = 2$ for the total level density and $g = 1$ for the parity-projected level density, and t is defined by $E_x - \Delta = at^2 - t$. Similar formula is derived for the $J\pi$-projected level density included in Eq. (1). Prediction of $\sigma_{(n,\gamma)}$ by Eq. (1) is largely affected by the single-particle level density parameter a and the backshift parameter Δ, because of the exponential variation of the level density. However, the fitted values of a and Δ are nucleus-dependent, and are difficult to be predicted with good accuracy.

It is thus desirable to calculate level densities microscopically. The interacting shell model gives a suitable framework, in which both shell effects and two-body correlations are fully taken into account. However, the size of the model space required to describe the neutron-resonance region is too large for conventional diagonalization methods, except for light nuclei. Recently we developed methods to calculate level densities within the interacting shell model,[4–6] using the shell model Monte Carlo (SMMC) approach.[7,8] This method has successfully been applied to the nuclei in the Fe to Ge region. In this paper, the present status of the SMMC approach to nuclear level densities will be shown.

II. SMMC and Level Density Calculation

In the interacting shell model, we usually assume the Hamiltonian comprised of the single-particle energies and the two-body interaction, maintaining the rotational invariance, the parity invariance and the isospin symmetry. Without loss of generality, the Hamiltonian is written as[7]

$$H = \sum_i \epsilon_i \hat{n}_i + \sum_\alpha \frac{\kappa_\alpha}{2}\hat{\rho}_\alpha^2\,. \qquad (3)$$

Here $\hat{n}_i$ denotes the number operator on the single-particle orbit i, and ϵ_i is the single-particle energy on i. $\hat{\rho}_\alpha$ represents an appropriate one-body operator (α indicating the channel), and κ_α is the coupling constant for the channel α. SMMC is a finite-temperature method. At temperature T, the canonical expectation value of an observable $\mathcal{O}$ is given by $\langle\mathcal{O}\rangle = \mathrm{Tr}(\mathcal{O}e^{-\beta H})/Z(\beta)$, where $\beta = 1/T$ and Tr indicates canonical trace for a fixed particle number. $Z(\beta) = \mathrm{Tr}\, e^{-\beta H}$ is the partition function. In the following $e^{-\beta H}$ is regarded as the evolution operator of the system for imaginary-time β. Dividing β into n time slices, we apply the Trotter decomposition to $e^{-\beta H}$,

$$e^{-\beta H} = \left(e^{-\Delta\beta H}\right)^n\,;$$
$$e^{-\Delta\beta H} = \prod_i e^{-\Delta\beta\epsilon_i\hat{n}_i} \prod_\alpha e^{-\Delta\beta\frac{\kappa_\alpha}{2}\hat{\rho}_\alpha^2} + O\left((\Delta\beta)^2\right)\,. \qquad (4)$$

Each factor in Eq. (4) that contains a two-body term $\hat{\rho}_\alpha^2$ can be further rewritten as, by applying the Hubbard-Stratonovich (HS) transformation,

$$e^{-\Delta\beta\frac{\kappa_\alpha}{2}\hat{\rho}_\alpha^2} = \int d\sigma_\alpha \sqrt{\frac{\beta|\kappa_\alpha|}{2\pi}}\, e^{-\Delta\beta|\kappa_\alpha|(\frac{\sigma_\alpha^2}{2} + s_\alpha\sigma_\alpha\hat{\rho}_\alpha)}$$
$$s_\alpha = \begin{cases} \pm 1 & (\text{if } \kappa_\alpha < 0) \\ \pm i & (\text{if } \kappa_\alpha > 0) \end{cases}\,, \qquad (5)$$

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where we have introduced an auxiliary field σ_α for each $\hat{\rho}_\alpha$. Combining Eqs. (4) and (5), we obtain the HS representation

$$e^{-\beta H} = \int \mathcal{D}[\sigma]\, G_\sigma U_\sigma \,. \tag{6}$$

The many-body evolution operator $e^{-\beta H}$ is now expressed in terms of a path integral over time-dependent auxiliary fields σ. In the path integral of Eq. (6), the auxiliary fields $\sigma_\alpha(\tau_m)$ at each time slice $\tau_m = m\Delta\beta$ ($m = 1, \cdots, n$) are contained. The Gaussian factor is defined by $G_\sigma = e^{-\frac{1}{2}\Delta\beta \sum_{\alpha,m} |\kappa_\alpha| \sigma_\alpha^2(\tau_m)}$, whose exponent can be regarded as a self-energy term of σ. $U_\sigma = e^{-\Delta\beta h_\sigma(\tau_n)} \ldots e^{-\Delta\beta h_\sigma(\tau_1)}$ is the evolution operator with

$$h_\sigma(\tau) = \sum_i \epsilon_i \hat{n}_i + \sum_\alpha |\kappa_\alpha| s_\alpha \sigma_\alpha(\tau) \hat{\rho}_\alpha \,, \tag{7}$$

which is a Hamiltonian for non-interacting nucleons moving in time-dependent auxiliary fields $\sigma_\alpha(\tau)$. The metric in the HS path-integral is $\mathcal{D}[\sigma] = \prod_{\alpha,m} \left[d\sigma_\alpha(\tau_m) \sqrt{\Delta\beta |\kappa_\alpha| / 2\pi} \right]$. Using Eq. (6), the HS representation of the thermal expectation of $\mathcal{O}$ is expressed as

$$\langle \mathcal{O} \rangle = \frac{\mathrm{Tr}\,(\mathcal{O} e^{-\beta H})}{\mathrm{Tr}\,(e^{-\beta H})} = \frac{\int \mathcal{D}[\sigma]\, G_\sigma \langle \mathcal{O} \rangle_\sigma \mathrm{Tr}\, U_\sigma}{\int \mathcal{D}[\sigma]\, G_\sigma \mathrm{Tr}\, U_\sigma} \,, \tag{8}$$

where $\langle \mathcal{O} \rangle_\sigma = \mathrm{Tr}\,(\mathcal{O} U_\sigma)/\mathrm{Tr}\, U_\sigma$.

Since h_σ is a one-body Hamiltonian, all the quantities that appear in the integrands of Eq. (8) are easily calculated for a given σ, through matrix algebra in the valence single-particle space. The canonical trace is calculated from the grand-canonical trace by applying the particle-number projection.[8] Although the dimension of the path integral in Eq. (8) is very large, the integration can be performed by the quantum Monte Carlo (QMC) methods. In the QMC methods, we assume a small but finite $\Delta\beta$. Randomly sampling the σ-fields according to the weight $W_\sigma = G_\sigma |\mathrm{Tr}\, U_\sigma|$, the thermal expectation value of $\mathcal{O}$ is evaluated by $\langle \mathcal{O} \rangle \approx \sum_\sigma \Phi_\sigma \langle \mathcal{O} \rangle_\sigma / \sum_\sigma \Phi_\sigma$, where $\langle \mathcal{O} \rangle_\sigma$ is evaluated for sampled values of the σ-fields (measurement), and $\Phi_\sigma = \mathrm{Tr}\, U_\sigma / |\mathrm{Tr}\, U_\sigma|$. The statistical error to $\langle \mathcal{O} \rangle$ can also be estimated from the variance of the measurements $\langle \mathcal{O} \rangle_\sigma$. Although Φ_σ is not necessarily positive-definite, we can make $\Phi_\sigma = 1$ in even-even nuclei for a nuclear Hamiltonian suitable to the level density calculations, as shown in Section III. For the sake of simplicity we assume $\Phi_\sigma = 1$ in the following discussions.

To calculate level densities,[4] we first compute the canonical thermal energy $E(\beta) = \langle H \rangle$ in SMMC, as a function of β. The partition function $Z(\beta)$ is then determined by a numerical integration $\ln [Z(\beta)/Z(0)] = -\int_0^\beta d\beta' E(\beta')$. Note that $Z(0) = \mathrm{Tr}\, \mathbf{1}$ is easily evaluated in finite model space. The level density $\rho(E)$ is the inverse Laplace transform of $Z(\beta)$, and its average is calculated in the saddle-point approximation,

$$\rho(E) = e^S / \sqrt{2\pi\beta^{-2} C} \,, \tag{9}$$

where $S(E) = \beta E + \ln Z$ is the canonical entropy, and $C(\beta) = -\beta^2 dE/d\beta$ is the heat capacity calculated by numerical differentiation of $E(\beta)$.

The parity projection technique in SMMC was developed in Ref.[4] Using the HS representation for $e^{-\beta H}$ and the projection operators $P_\pm = (1 \pm P)/2$ on even- and odd-parity states (P is the parity operator), the projected expectation value of $\mathcal{O}$ is represented as

$$\begin{aligned} \langle \mathcal{O} \rangle_\pm &= \frac{\mathrm{Tr}(\mathcal{O} P_\pm e^{-\beta H})}{\mathrm{Tr}(P_\pm e^{-\beta H})} \\ &= \frac{\int D[\sigma]\, W_\sigma \left[\langle \mathcal{O} \rangle_\sigma \pm \langle \mathcal{O} \rangle_{P\sigma} \zeta_P(\sigma) \right]}{\int D[\sigma] W_\sigma \left[1 \pm \zeta_P(\sigma) \right]} \,. \end{aligned} \tag{10}$$

In Eq. (10), $\zeta_P(\sigma) = \mathrm{Tr}(P U_\sigma)/\mathrm{Tr}\, U_\sigma$ and $\langle \mathcal{O} \rangle_{P\sigma} = \mathrm{Tr}(\mathcal{O} P U_\sigma)/\mathrm{Tr}(P U_\sigma)$. The operator $P U_\sigma$ can be expressed in the single-particle space as in U_σ. This allows the calculation of $\zeta_P(\sigma)$ and $\langle H \rangle_{P\sigma}$ through matrix algebra in the single-particle space. The parity-projected thermal energy $E_\pm(\beta) = \langle H \rangle_\pm$ is calculated by setting $\mathcal{O} = H$ in Eq. (10). Once we obtain $E_\pm(\beta)$, the projected densities $\rho_\pm(E)$ can be calculated via Eq. (9), as for the total level density.

The SMMC approach is computationally intensive, and it is time-consuming to implement calculations for many nuclei, if QMC samples should be varied from nucleus to nucleus. We have developed a particle-number reprojection method[6] which enables us to calculate level densities for a family of nuclei using QMC samples for a single nucleus. Let us denote the sampling nucleus by $\mathcal{A} = (Z, N)$. The partition function $Z_{\mathcal{A}'}(\beta)$ of a nucleus with $\mathcal{A}' = (Z', N')$ is evaluated in terms of its ratio to $Z_{\mathcal{A}}(\beta)$,

$$\frac{Z_{\mathcal{A}'}(\beta)}{Z_{\mathcal{A}}(\beta)} = \frac{\mathrm{Tr}_{\mathcal{A}'} e^{-\beta H}}{\mathrm{Tr}_{\mathcal{A}} e^{-\beta H}} = \frac{\int D[\sigma] W_\sigma\, \zeta_{\mathcal{A}'}(\sigma)}{\int D[\sigma] W_\sigma} \,, \tag{11}$$

where $W_\sigma = G_\sigma \mathrm{Tr}_{\mathcal{A}} U_\sigma$ ($\mathrm{Tr}_{\mathcal{A}} U_\sigma$ is positive-definite) and $\zeta_{\mathcal{A}'}(\sigma) = \mathrm{Tr}_{\mathcal{A}'} U_\sigma / \mathrm{Tr}_{\mathcal{A}} U_\sigma$. The expectation value of an observable $\mathcal{O}$ can also be calculated by,

$$\langle \mathcal{O} \rangle_{\mathcal{A}'} = \frac{\int D[\sigma] W_\sigma \langle \mathcal{O} \rangle_{\mathcal{A}'\sigma}\, \zeta_{\mathcal{A}'}(\sigma)}{\int D[\sigma] W_\sigma\, \zeta_{\mathcal{A}'}(\sigma)} \,, \tag{12}$$

where $\langle \mathcal{O} \rangle_{\mathcal{A}'\sigma} = \mathrm{Tr}_{\mathcal{A}'}(\mathcal{O} U_\sigma)/\mathrm{Tr}_{\mathcal{A}'} U_\sigma$. The QMC sampling is done on a fixed $\mathcal{A}$, and Eq. (12) is then used to calculate observables for a family of nuclei with $\mathcal{A}'$ ($\neq \mathcal{A}$). The energy correction due to the nucleus dependence of the Hamiltonian is properly carried out.[6] This reprojection method works well as far as important samples of σ-fields are approximately the same between $\mathcal{A}$ and $\mathcal{A}'$. Although the statistical errors to level densities grow through the reprojection, this method facilitates systematic calculations.

III. Level Densities in Fe to Ge region

To compute level densities in the neutron resonance regime for $A \sim 50 - 70$ nuclei, the complete ($pf + 0g_{9/2}$) model space is adopted. We use the isoscalar Hamiltonian introduced in Ref.[4] The single-particle energies are obtained in a Woods-Saxon plus spin-orbit potential, with the parameters of Ref.[9] The two-body residual interaction consists of isovector monopole pairing and a self-consistent surface-peaked interaction.[10] Expanding the surface-peaked interaction in the multipole forms, we keep the quadrupole, octupole

and hexadecupole terms that are appropriately renormalized. The strength of the pairing interaction is determined from experimental odd-even mass differences. The Hamiltonian is uniquely determined for each nucleus by the above procedure, without adjustable parameters. It correctly includes the dominating collective components of realistic effective interactions,[11] and has a good QMC sign (*i.e.* $\Phi_\sigma = 1$) for even-even nuclei.[8] Hence this Hamiltonian is suitable to studies of the level densities.

The present Hamiltonian may not describe correctly the energy splitting due to the isospin. As far as we focus on the low energy regime up to the neutron resonance region, this problem will not be serious except for $Z = N$ nuclei. While an additional isospin-dependent interaction leads to a QMC sign problem, a perturbative way to correct the energy splitting was proposed.[12]

To describe the level density as a function of the excitation energy, the ground state energy E_0 should be evaluated accurately. For even-even nuclei, we use a two-state model (0^+ and 2^+), where E_0 and $E_x(2^+)$ are fitted to $E(\beta)$ and $\langle J^2 \rangle$ at large values of β ($\gtrsim 2.5\,\mathrm{MeV}^{-1}$).[5] For odd-$A$ and odd-odd nuclei, the thermal energy $E(\beta)$ is already close to its asymptotic value E_0 for $\beta \sim 2.5\,\mathrm{MeV}^{-1}$, because of the high degeneracy in the vicinity of the ground state. Therefore we estimate E_0 by taking an average of $E(\beta)$ for large β values.[6]

In the upper panels of **Fig. 1**, we compare the calculated total level densities with the experimental ones for ^{56}Fe, ^{60}Ni and ^{68}Zn. The experimental densities are reconstructed from the BBF (2) with experimentally determined parameters (a and Δ). It is found that the SMMC level densities reproduce the experimental data, typically within a factor of 2 for even-even nuclei,[5] in the mass range of $A \sim 50 - 70$. Level densities obtained from empirical formulae for a and Δ have been used in the astrophysics calculations so far.[14] However, there is a certain difference between the present microscopic densities and the empirical ones, and the microscopic calculations often describe the data better than the empirical formulae. For instance, empirical formulae predict similar level densities for odd-A isobars, ignoring the T_z-dependence. Yet the SMMC level densities for the $A = 55$ isobars ^{55}Mn, ^{55}Fe and ^{55}Co are quite different from one another,[6] in fairly good agreement with experiments.

It has been assumed in nucleosynthesis calculations that even- and odd-parity levels have equal densities. While few data are available regarding the parity-dependence of level densities, our microscopic SMMC calculations show significant parity-dependence in the $A \lesssim 60$ region, as viewed in the lower panels of Fig. 1. This parity-dependence originates in the subshell structure in this mass region, *i.e.* the energy gap between the pf and $g_{9/2}$ orbits,[5] and has been well described by a simple model[15] which assumes random filling of the valence orbits under the subshell structure and the pairing correlations. It will be important to see how the parity dependence influences predictions of $\sigma_{(n,\gamma)}$ by Eq. (1), and thereby the nucleosynthesis calculations.

The SMMC level densities can be well-fitted to the BBF (2). Thus the parameters a and Δ can be extracted from the

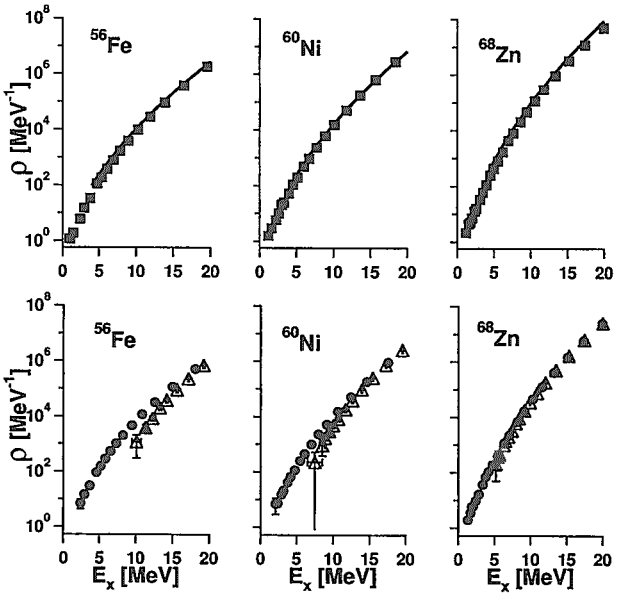

Fig. 1 Upper panels: SMMC (solid squares) and experimental (solid lines) total level densities. The experimental BBF parameters are taken from Refs.[13] (for ^{56}Fe and ^{60}Ni) and [2] (for ^{68}Zn). Lower panels: SMMC even-parity (solid circles) and odd-parity (open triangles) level densities.

microscopically calculated level densities by a χ^2 fitting. The extracted values for the Mn, Fe and Co nuclei obtained with the particle-number reprojection method are shown in **Fig. 2**. In comparison, experimental data (when available) and the empirical parameters[14] are also presented. The SMMC values of Δ are in good agreement with the experimental ones. The staggering in Δ is a result of pairing correlations. In the empirical formula, $\Delta \sim 0$ for odd-A nuclei, is positive for even-even nuclei, and is negative for odd-odd nuclei. This is not always the case in our microscopic calculations and in the experimental data. The SMMC values of a are found to depend smoothly on A, unlike some of the empirical results, and in the case of the Co isotopes follow the data more closely.

Figure 3 shows systematics of the parameters a and Δ obtained from the SMMC level densities, in the Fe to Ge region. We here restrict ourselves to even-even nuclei, in order to view clearly effects other than the pairing. Direct results without the number reprojection are presented. Comparing the calculated a values with the empirical ones,[14] we find a notable difference at $A \sim 70$. For the backshift Δ, there seems to be enhancement at the magic number Z or $N = 28$ in the SMMC results, which was not obtained in the empirical formulae. Parity-projected level densities can also be fitted by the BBF (2) with $g = 1$, but with parity-specific parameters $a_\pm$ and $\Delta_\pm$. Significant parity-dependence in the parameters is found for the $A \lesssim 60$ nuclei, where $\Delta_- > \Delta_+$ and $a_- > a_+$.

IV. Summary and Future Prospect

We have developed a novel microscopic method to calculate nuclear level densities, using the shell model Monte

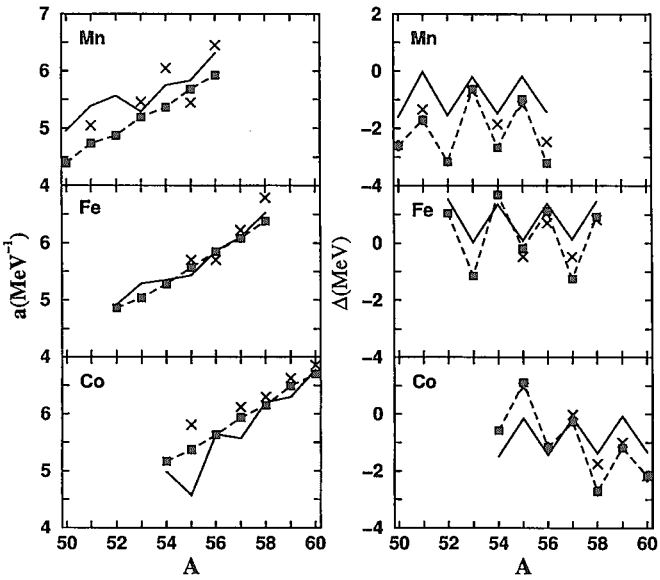

Fig. 2 The BBF parameters a and Δ for Mn, Fe and Co isotopes. The squares (connected by dashed lines) are extracted from the SMMC level densities, while the crosses are the experimental results taken from Refs.[2] and [16] (for ^{58,59}Co). The solid lines show the empirical values of Ref.[14] Taken from Ref.[6]

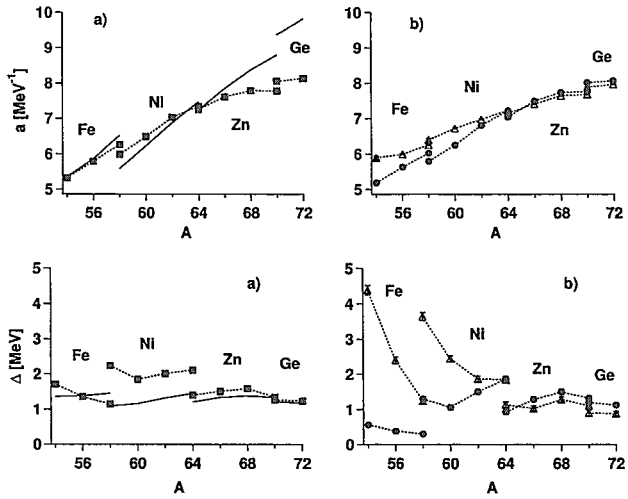

Fig. 3 BBF parameters a and Δ extracted from the SMMC level densities, for even-even $A = 50 - 70$ nuclei. Upper left: a for the total level densities (squares), compared with the empirical values of Ref.[14] (solid lines). Upper right: a_+ (circles) and a_- (triangles) of the even- and odd-parity level densities. Lower left: Δ for the total level densities (squares), together with the empirical values (solid lines). Lower right: Δ_+ (circles) and Δ_- (triangles) for the parity-projected densities.

Carlo approach. Our calculated total level densities in the $A \sim 50 - 70$ mass region are in good agreement with the available experimental data. This method provides us with a promising tool to investigate nuclear level densities from a microscopic standpoint.

Relevant to the level density calculations, the parity projection and the particle-number reprojection methods are exploited within SMMC. The former enables us to compute parity-projected level densities, and the latter facilitates systematic studies of level densities. Shell effects have been observed in the systematics. We clarify the parity dependence of the level densities in the $A \lesssim 60$ region, which originates in the subshell structure. It would be interesting to determine whether the parity dependence of level densities affects the nucleosynthesis calculations.

Extensive application of the present methods to the heavier nuclei, where the quadrupole deformation should be taken into consideration, is under way. An exact method of the isospin projection is also being developed.[17] We can then study isospin dependence of the level densities, and obtain more reliable level densities for $Z = N$ nuclei than the perturbative method.[12]

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