This is the accepted manuscript made available via CHORUS. The article has been published as:

Nuclear state densities of odd-mass heavy nuclei in the shell model Monte Carlo approach

C. Özen, Y. Alhassid, and H. Nakada

Phys. Rev. C **91**, 034329 — Published 26 March 2015

DOI: 10.1103/PhysRevC.91.034329

Nuclear state densities of odd-mass heavy nuclei in the shell model Monte Carlo approach

C. Özen[1,2], Y. Alhassid[1], and H. Nakada[3]
[1]Center for Theoretical Physics, Sloane Physics Laboratory, Yale University, New Haven, CT 06520, USA
[2]Faculty of Engineering and Natural Sciences, Kadir Has University, Istanbul 34083, Turkey
[3]Department of Physics, Graduate School of Science, Chiba University, Inage, Chiba 263-8522, Japan
(Dated: December 9, 2014)

The shell model Monte Carlo (SMMC) approach enables the microscopic calculation of nuclear state densities in model spaces that are many orders of magnitude larger than those that can be treated by conventional diagonalization techniques. However, it has been difficult to calculate accurate state densities of odd-mass heavy nuclei as a function of excitation energy. This is because of a sign problem that arises from the projection on an odd number of particles at low temperatures, making it difficult to calculate accurate ground-state energies of odd-mass nuclei in direct Monte Carlo calculations. Here we extract the ground-state energy from a one-parameter fit of the SMMC thermal energy to the thermal energy that is determined from experimental data. This enables us to calculate the state densities of the odd-even isotopes $^{149-155}$Sm and $^{143-149}$Nd as a function of excitation energy. We find close agreement with state densities extracted from experimental data. Our results demonstrate that the state densities of the odd-mass samarium and neodymium isotopes can be consistently reproduced using the same Hamiltonian of the neighboring even-mass isotopes within the configuration-interaction shell model approach.

PACS numbers: 21.60.Cs, 21.10.Ma, 21.60.Ka, 27.70.+q

I. INTRODUCTION

Reliable microscopic calculation of nuclear state densities of heavy nuclei is a challenging task because it often requires the inclusion of correlations beyond the mean-field approximation. Correlation effects can be taken into account in the context of the configuration-interaction (CI) shell model approach, but the size of the required model space in heavy nuclei is prohibitively large for direct diagonalization of the CI shell model Hamiltonian. This limitation can be overcome in part by using the shell model Monte Carlo (SMMC) method [1–5]. The SMMC method enables the calculation of statistical nuclear properties, and in particular of level densities, in very large model spaces [6–10].

Fermionic Monte Carlo methods are often hampered by the so-called sign problem, which leads to large fluctuations of observables at low temperatures [1, 2, 11, 12]. Statistical and collective properties of nuclei can be reliably calculated [6, 13] by employing a class of interactions that have a good Monte Carlo sign in the grand-canonical formulation [2, 13]. The projection on an even number of particles keeps the good sign of the interaction, allowing accurate calculations for even-even nuclei. However, the projection on an odd number of particles leads to a new sign problem, making it difficult to calculate thermal observables at low temperatures for odd-even and odd-odd nuclei. In particular, the ground-state energy of the odd-particle system cannot be extracted from direct SMMC calculations. A method that circumvents this odd-particle sign problem and enables the calculation of the ground-state energy of the odd-particle system from the imaginary-time Green's functions of the even-particle system was recently introduced in Ref. [14] and applied successfully to medium-mass nuclei. However, the application of this method to heavy nuclei is computationally intensive and requires additional development. Here we describe a practical method that allows us to determine the ground-state energy using a single-parameter fit to experimental data. We use this method to calculate the SMMC state density of odd-even rare-earth isotopes $^{149-155}$Sm and $^{143-149}$Nd with the same Hamiltonian we used to calculate the state densities of even-even rare-earth nuclei [15, 16]. We find close agreement with the state densities that are extracted from experimental data.

II. CHOICE OF MODEL SPACE AND INTERACTION

In rare-earth nuclei we use the model space of Refs. [15, 16] spanned by the single-particle orbitals $0g_{7/2}$, $1d_{5/2}$, $1d_{3/2}$, $2s_{1/2}$, $0h_{11/2}$ and $1f_{7/2}$ for protons, and $0h_{11/2}$, $0h_{9/2}$, $1f_{7/2}$, $1f_{5/2}$, $2p_{3/2}$, $2p_{1/2}$, $0i_{13/2}$, and $1g_{9/2}$ for neutrons. We have chosen these orbitals by the requirement that their occupation probabilities in well-deformed nuclei be between 0.9 and 0.1. The effect of other orbitals is accounted for by the renormalization of the interaction. The bare single-particle energies in the shell-model Hamiltonian are determined so as to reproduce the Woods-Saxon single-particle energies in the spherical Hartree-Fock approximation. The effective interaction consists of monopole pairing and multipole-multipole terms [15]

$$-\sum_{\nu=p,n} g_\nu P^\dagger_\nu P_\nu - \sum_\lambda \chi_\lambda : (O_{\lambda;p} + O_{\lambda;n}) \cdot (O_{\lambda;p} + O_{\lambda;n}) : , \quad (1)$$

where the pair creation operator $P^\dagger_\nu$ and the multipole operator $O_{\lambda;\nu}$ are given by

$$P^\dagger_\nu = \sum_{nljm} (-)^{j+m+l} a^\dagger_{\alpha jm;\nu} a^\dagger_{\alpha j-m;\nu} \,, \tag{2a}$$

$$O_{\lambda;\nu} = \frac{1}{\sqrt{2\lambda+1}} \sum_{ab} \langle j_a || \frac{dV_{\rm WS}}{dr} Y_\lambda || j_b \rangle [a^\dagger_{\alpha j_a;\nu} \times \tilde{a}_{\alpha j_b;\nu}]^{(\lambda)} \tag{2b}$$

with $\tilde{a}_{jm} = (-)^{j+m} a_{j-m}$. In Eq. (1), :: denotes normal ordering and $V_{\rm WS}$ represents the Woods-Saxon potential. The pairing strengths is expressed as $g_\nu = \gamma \bar{g}_\nu$, where γ is a renormalization factor and $\bar{g}_p = 10.9/Z$, $\bar{g}_n = 10.9/N$ are parametrized to reproduce the experimental odd-even mass differences for nearby spherical nuclei in the number-projected BCS approximation [15]. The quadrupole, octupole and hexadecupole interaction terms have strengths given by $\chi_\lambda = k_\lambda \chi$ for $\lambda = 2, 3, 4$ respectively. The paprameter χ is determined self-consistently [13] and k_λ are renormalization factors accounting for core polarization effects. We use the parametrization of Ref. [16] for γ and k_2

$$\gamma = 0.72 - \frac{0.5}{(N-90)^2 + 5.3} \,, \tag{3a}$$

$$k_2 = 2.15 + 0.0025(N-87)^2 \,, \tag{3b}$$

while the other parameters are fixed at $k_3 = 1$ and $k_4 = 1$.

III. GROUND-STATE ENERGY

Because of the sign problem that originates in the projection on an odd number of particles, the thermal energy $E(\beta)$ of the odd-even samarium and neodymium isotopes can in practice be calculated only up to $\beta = 1/T \sim 4-5$ MeV^{-1}. In contrast, SMMC calculations in neighboring even-even samarium and neodymium nuclei, for which there is no sign problem, were carried out up to $\beta = 20$ MeV^{-1} [16]. Systematic errors introduced by the discretization of β [2] are corrected by calculating $E(\beta)$ for the two time slices of $\Delta\beta = 1/32$ MeV^{-1} and $\Delta\beta = 1/64$ MeV^{-1} and then performing a linear extrapolation to $\Delta\beta = 0$. For $\beta \gtrapprox 3$ MeV^{-1}, the dependence of $E(\beta)$ on $\Delta\beta$ is weaker and an average value is taken instead. The calculations for $\beta > 2$ MeV^{-1} were carried out using a stabilization method of the one-body canonical propagator for each configuration of the auxiliary fields [15].

Since our calculations of the thermal energy $E(\beta)$ for the odd-even rare-earth nuclei are limited to $\beta \sim 4-5$ MeV^{-1}, we cannot obtain a reliable estimate of the ground-state energy E_0 in direct SMMC calculations. The Green's function method of Ref. [14] was used successfully in medium-mass nuclei to circumvent the odd particle-number sign problem and extract accurate ground-state energies. However, this method becomes computationally intensive in heavy nuclei and requires additional development. Here we extract E_0 by performing a one-parameter fit of the SMMC thermal excitation energy $E_x(T) = E(T) - E_0$ to the experimental thermal energy. The latter is calculated using the thermodynamical relation $E_x(\beta) = -d\ln Z(\beta)/d\beta$, where Z is the experimental partition function in which the energy is measured relative to the ground state (see below).

We demonstrate our method for ^{147}Nd. Fig. 1 shows the thermal excitation energy (left panel) and the partition function (right panel) as a function of temperature T. The SMMC results (open circles) are shown down to $T = 0.25$ MeV, below which the statistical errors become too large because of the odd particle-number sign problem. We calculated the experimental partition function (right panel, dashed line) from $Z(T) = \sum_i (2J_i+1) e^{-E_{x,i}/T}$ where $E_{x,i}$ denote the excitation energies of the experimentally known energy levels. Because of the incompleteness of the level counting data above a certain excitation energy, the experimental partition function and the corresponding average experimental thermal energy (left panel, dashed line) are realistic only for temperatures below $T \sim 0.15$ MeV. A realistic estimate of the experimental thermal energy at higher temperatures is obtained by calculating an empirical partition function

$$Z(T) = \sum_i^N (2J_i+1) e^{-E_{x,i}/T} + \int_{E_N}^\infty dE_x\, \rho(E_x) e^{-E_x/T} \,. \tag{4}$$

In Eq. (4) the discrete sum is carried out over a suitably chosen complete set of N experimental levels up to an excitation energy E_N, and the contribution of higher-lying levels is included effectively through the integral over an empirical state density $\rho(E_x)$ with a Boltzmann weight. Here we use the the back-shifted Bethe formula (BBF) [17] for the empirical state density

$$\rho_{\rm BBF}(E_x) = \frac{\sqrt{\pi}}{12} a^{-1/4} (E_x - \Delta)^{-5/4} e^{2\sqrt{a(E_x-\Delta)}} \,, \tag{5}$$

where a is the single-particle level density parameter and Δ is the backshift parameter. For these parameters we use the values in Ref. [18] determined from level counting data (at low excitation energies) and the s-wave neutron resonance data (at the neutron resonance threshold) for the given nucleus of interest. The solid lines in Fig. 1 are calculated using Eq. (4) for the empirical partition function. The number of the low-lying states N (determining E_N) are chosen such that the solid and dashed curves for the experimental partition function merge smoothly at sufficiently low temperatures. The values of a, Δ and N are tabulated in Table I for the odd-mass $^{143-149}$Nd and $^{149-155}$Sm isotopes. We determine the ground-state energy E_0 by a single-parameter fit of the SMMC thermal excitation energy (open circles) to the experimentally determined thermal excitation energy (the solid curve in

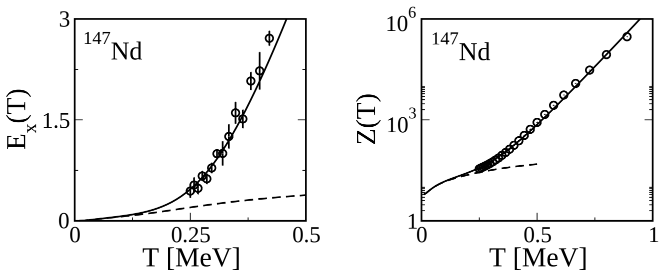

FIG. 1. Thermal excitation energy E_x (left panel) and partition function Z (right panel) versus temperature T for ^{147}Nd. The SMMC results (open circles) are compared with the results deduced directly from experimentally known levels (dashed lines), and from Eq. (4) (solid lines). The ground-state energy E_0 is obtained by a one-parameter fit of the SMMC thermal energy to the experimentally determined thermal energy as a function of temperature (solid line in the left panel).

the left panel of Fig. 1). The fit determines E_0 up to a statistical error of $\sim 0.02 - 0.03\,\mathrm{MeV}$.

We emphasize that only a single additive parameter E_0 is adjusted to fit the empirical thermal excitation energy. Nevertheless, we find close agreement of both the SMMC partition function and thermal energy with their corresponding experimental values over a range of temperatures. This is an evidence that our SMMC results are consistent with the experimental data.

To validate our method, we apply it to estimate the ground-state energy of an even-even nucleus, for which the ground-state energy can be determined from large-β SMMC calculations. We expect to find similar results for E_0 in cases when the SMMC state density is in good agreement with the experimental density. As an example, we apply the method for ^{150}Sm using only the SMMC results for $T > 0.25$ MeV (comparable to the temperatures for which the SMMC thermal energy can be calculated for neighboring odd-mass nuclei with not too large errors). We find a ground-state energy of $E_0 = -255.680 \pm 0.021\,\mathrm{MeV}$ in comparison with the value of $E_0 = -255.772 \pm 0.019\,\mathrm{MeV}$ obtained by averaging the large-β values of the SMMC thermal energy. This difference of 0.092 MeV in the two values of E_0 does not lead to a significant change in the SMMC density. Similar calculations in ^{144}Nd give a difference of 0.130 MeV in the values of E_0. For ^{148}Sm and ^{148}Nd we find smaller differences of 0.02 and 0.03 MeV, respectively.

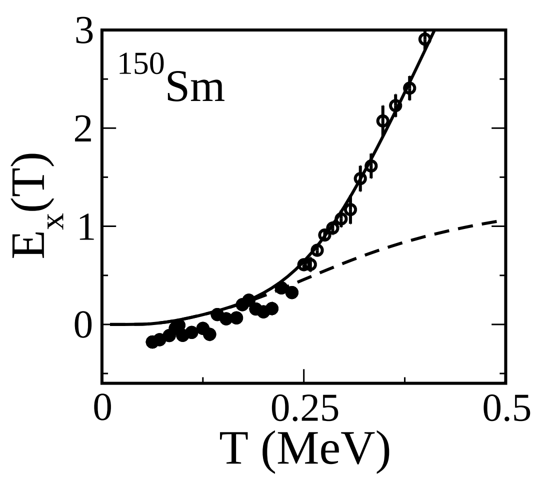

FIG. 2. The SMMC thermal excitation energy (circles) for ^{150}Sm with E_0 determined by the method used for the odd-mass nuclei (see text) is compared with the experimental results (solid and dashed lines as in Fig 1). The solid circles are large-β SMMC results that are not used in the determination of E_0.

In Fig. 2 we compare the SMMC results (open and solid circles) for the thermal excitation energy $E_x(T) = E(T) - E_0$ of ^{150}Sm (using the value of E_0 determined by the method we use for the odd nuclei) with the experimental thermal excitation energy (solid line). The solid circles are SMMC results for temperatures $T < 0.25$ MeV, which are not used in the fit to determine E_0. We observe that the SMMC results at these lower temperatures are somewhat below but still quite close to the experimental curve.

The choice of the empirical level density in Eq. (4) is not restricted to the BBF. We can also use the composite formula [19], which combines a constant temperature formula at low excitation energies with a BBF at higher excitations. The parameters of the constant temperature formula are determined from level counting data at low excitation energies, and the parameters of the BBF are then determined by requiring the continuity of the density and its first derivative at a certain matching energy. This matching energy is determined by minimizing the χ^2 deviation of the composite level density from the neutron resonance data. For the nuclei that have a matching energy solution that minimizes the above χ^2, we find that the use of either the BBF or the composite formula lead to similar results for E_0. In ^{143}Nd the ground-state energy $E_0 = -191.607 \pm 0.021$ MeV, determined using the BBF, differs from its value of $E_0 = 191.614 \pm 0.021$ MeV obtained in the composite formula approach by only $\sim 0.007\,\mathrm{MeV}$. In ^{145}Nd we find a larger difference of 0.154 MeV in the values of E_0, but the differences between the corresponding SMMC state densities are not significant. Similar calculations in ^{149}Sm give a difference of only 0.017 MeV in the corresponding values of E_0.

IV. STATE DENSITIES

The average state density is determined in the saddle-point approximation to the integral that expresses the state density as an inverse Laplace transform of the partition function. This average density is given by

$$\rho(E) \approx \frac{1}{\sqrt{2\pi T^2 C}} e^{S(E)} , \qquad (6)$$

Nucleus	a (MeV^{-1})	Δ (MeV)	N	E_N (MeV)
^{143}Nd	15.951	0.759	3	1.228
^{145}Nd	16.792	0.135	4	0.658
^{147}Nd	18.276	0.058	4	0.190
^{149}Nd	18.552	-0.644	3	0.138
^{149}Sm	19.086	-0.196	8	0.558
^{151}Sm	18.999	-0.771	8	0.168
^{153}Sm	17.848	-1.053	7	0.098
^{155}Sm	17.067	-0.834	7	0.221

TABLE I. The values of a and Δ in the BBF [see Eq. (5)] as determined from the level counting data at low excitation energies and the neutron resonance data [18], the number N of a complete set of experimentally known levels and its corresponding energy E_N used in Eq. (4) for the odd-mass $^{143-149}$Nd and $^{149-155}$Sm isotopes.

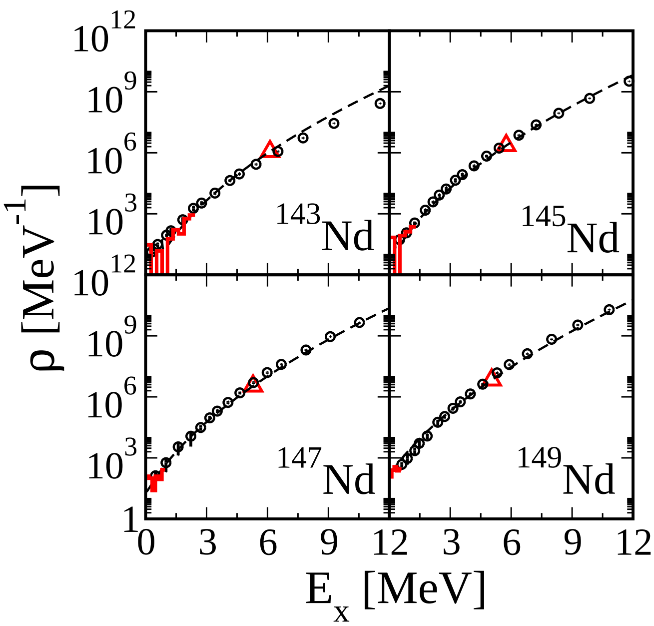

FIG. 3. (Color online). State densities of odd-mass $^{143-149}$Nd isotopes versus excitation energy E_x. The SMMC densities (open circles) are compared with experimental results. The histograms at low excitation energies are from level counting data, the triangle is the neutron resonance data and the dashed line is the BBF state density [Eq. (5)] that is extracted from the experimental data.

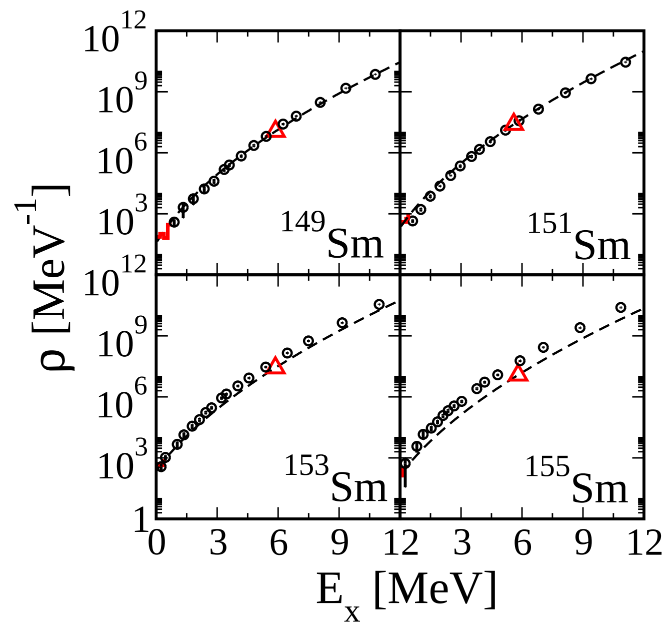

FIG. 4. (Color online). State densities of odd-mass $^{149-155}$Sm isotopes versus excitation energy E_x. Symbols and lines as in Fig. 3.

where $S(E)$ is the entropy and C is the heat capacity in the canonical ensemble. In SMMC we first calculate the thermal energy as an observable $E(\beta) = \langle H \rangle$ and then integrate the thermodynamic relation $-d\ln Z/d\beta = E(\beta)$ to find the partition function $Z(\beta)$. The entropy and the heat capacity are calculated from

$$S(E) = \ln Z + \beta E \; ; \qquad C = -\beta^2 \partial E/\partial\beta \tag{7}$$

and substituted into Eq. (6) to yield the state density.

The SMMC state densities for the odd-mass neodymium and samarium isotopes are shown by open circles in Fig. 3 and Fig. 4, respectively. We compare these SMMC densities with the level counting data (histograms) and with the neutron resonance data (triangles). We also show the empirical BBF level densities (dashed lines). For the neodymium nuclei (Fig. 3), we find excellent agreement of the SMMC results (open circles) with the experimental state densities (both level counting and neutron resonance data) and the BBF state densities (dashed lines). For the samarium nuclei (Fig. 4), a similarly good agreement is observed for ^{149}Sm and ^{151}Sm. We also find overall good agreement for ^{153}Sm and ^{155}Sm, although we observe some discrepancies between the SMMC and the experimental state densities at the neutron resonance energy. Since the neutron resonance data point is used to determine the parameters of the BBF state densities, similar discrepancies are observed between the SMMC and the BBF state densities for ^{153}Sm and ^{155}Sm.

V. CONCLUSION

We have carried out SMMC calculations for the odd-mass rare-earth isotopes $^{149-155}$Sm and $^{143-149}$Nd. The sign problem that originates in the projection on an odd number of particles makes it difficult to calculate directly the ground-state energy. We circumvent this problem in practice by carrying out a one-parameter fit of the SMMC thermal excitation energy to the experimental thermal excitation energy as determined from level counting data at low excitation energies and the neutron resonance data at the neutron separation energy. We then calculate the SMMC state densities of the odd-even samarium and neodymium isotopes as a function of excitation energy and find them to be in good agreement with state densities extracted from available experimental data. Thus, the state densities of the odd-mass samarium and neodymium isotopes are consistently reproduced using the same configuration-interaction shell model Hamiltonian that successfully reproduced the state densities of the neighboring even-mass isotopes.

ACKNOWLEDGEMENTS

This work is supported in part by the Turkish Science and Research Council (TÜBİTAK) grant No. ARDEB-1001-110R004, by the U.S. DOE grant No. DE-FG-0291-ER-40608 and as Grant-in-Aid for Scientific Research (C) No. 25400245 by the JSPS, Japan. Computational cycles were provided by the NERSC high performance computing facility at LBL and by the facilities of the Yale University Faculty of Arts and Sciences High Performance Computing Center.

[1] C. W. Johnson, S. E. Koonin, G. H. Lang and W. E. Ormand, Phys. Rev. Lett. **69**, 3157 (1992).

[2] G. H. Lang, C. W. Johnson, S. E. Koonin and W. E. Ormand, Phys. Rev. C **48**, 1518 (1993).

[3] Y. Alhassid, D. J. Dean, S. E. Koonin, G. Lang, and W. E. Ormand, Phys. Rev. Lett. **72**, 613 (1994).

[4] S. E. Koonin, D. J. Dean, K. Langanke, Phys. Rep. **278**, 1 (1997).

[5] Y. Alhassid, Int. J. Mod. Phys. B **15**, 1447 (2001).

[6] H. Nakada and Y. Alhassid, Phys. Rev. Lett. **79**, 2939 (1997).

[7] W. E. Ormand, Phys. Rev. **C56**, R1678 (1997).

[8] Y. Alhassid, S. Liu, and H Nakada, Phys. Rev. Lett. **83**, 4265 (1999).

[9] Y. Alhassid, S. Liu, and H Nakada, Phys. Rev. Lett. **99**, 162504(2007).

[10] C. Özen, K. Langanke, G. Martinez-Pinedo, and D. J. Dean, Phys. Rev. C **75**, 064307 (2007).

[11] S.R. White, D.J. Scalapino, R.L. Sugar, E.Y. Loh, J.E. Gubernatis, and R.T. Scalettar, Phys. Rev. B **40**, 506 (1989).

[12] W. Von der Linden, Phys. Rep. **220**, 53 (1992).

[13] Y. Alhassid, G. F. Bertsch, D. J. Dean, and S. E. Koonin, Phys. Rev. Lett. **77**, 1444 (1996).

[14] A. Mukherjee and Y. Alhassid, Phys. Rev. Lett. **109**, 032503 (2012).

[15] Y. Alhassid, L. Fang and H. Nakada, Phys. Rev. Lett. **101**, 082501 (2008).

[16] C. Özen, Y. Alhassid, H Nakada, Phys. Rev. Lett. **110**, 042502 (2013).

[17] W. Dilg, W. Schantl, H. Vonach, M. Uhl, Nucl. Phys. A **217**, 269 (1973).

[18] C. Özen and Y. Alhassid, to be published.

[19] A. Gilbert and A.G.W. Cameron, Can. J. Phys. **43**, 1446 (1965).