Study of nuclei around $Z = 28$ by large-scale shell model calculations

Y Tsunoda$^1$, T Otsuka$^{1,2,3}$, N Shimizu$^2$, M Honma$^4$ and Y Utsuno$^5$

$^1$ Department of Physics, University of Tokyo, Tokyo 113-0033, Japan
$^2$ Center for Nuclear Study, University of Tokyo, Tokyo 113-0033, Japan
$^3$ National Superconducting Cyclotron Laboratory, Michigan State University, East Lansing, Michigan, USA
$^4$ Center for Mathematical Sciences, University of Aizu, Ikki-machi, Aizu-Wakamatsu, Fukushima 965-8580, Japan
$^5$ Advanced Science Research Center, Japan Atomic Energy Agency, Tokai, Ibaraki, 319-1195, Japan

E-mail: ytsunoda@nt.phys.s.u-tokyo.ac.jp

Abstract. We study Cr and Ni isotopes by Monte Carlo shell model (MCSM) calculations in a $pfg_9d_5$ shell. In the MCSM, the wave function is represented as a linear combination of angular-momentum- and parity-projected deformed Slater determinants (MCSM bases), and we can calculate eigenstates in a large model space such as the $pfg_9d_5$ shell. We study the intrinsic shape of nuclei by using deformations of the unprojected MCSM bases. We show calculated results of Cr and Ni isotopes and a level scheme of $^{68}\text{Ni}$, and discuss the strength of the magicity of $N = 40$ in Cr and Ni isotopes and shape coexistence in $^{68}\text{Ni}$.

1. Introduction

An exotic nucleus is a nucleus whose neutron number is much larger or smaller than its proton number and shows various phenomena such as the shell evolution. An exotic nucleus has different shell structure from that of a non-exotic nucleus, which causes appearance or disappearance of magic numbers. In order to treat magic numbers 28, 50 and a submagic number 40, we use a $pfg_9d_5$ shell, which consists of the $0f_{1p}$ shell, $0g_{9/2}$ and $1d_{5/2}$ orbits, as a model space. This space is too large to perform conventional shell-model calculations and we use the Monte Carlo shell model (MCSM) [1]. We discuss the magicity of $N = 40$ in Cr ($Z = 24$) and Ni ($Z = 28$) isotopes and shape coexistence in a double-magic nucleus $^{68}\text{Ni}$.

2. Monte Carlo Shell Model

In shell-model calculations, we diagonalize the Hamiltonian matrix in the model space to obtain eigenstates. We can diagonalize the Hamiltonian matrix directly in the model space whose $m$-scheme dimension is about $10^{11}$ at most. However, the dimension reaches more than $10^{15}$ in the $pfg_9d_5$ space. Therefore, certain approximations are necessary to perform calculations in such a large model space. In the MCSM, we approximate states with linear combinations of a small number of angular-momentum-projected, parity-projected deformed Slater determinants (MCSM bases) and diagonalize the Hamiltonian matrix in a small subspace spanned by the
MCSM bases. The MCSM wave function $|\Psi_N\rangle$ is given as
\begin{equation}
|\Psi_N\rangle = \sum_{n=1}^{N} \sum_{K=-J}^{J} f_{n,K}^{(N)} P_{MK}^{J}\psi_n, 
\end{equation}
where $|\psi_n\rangle$ is a Slater determinant, $P_{MK}^{J}$ is the angular-momentum and parity projector, $c_i^\dagger$ is a creation operator, and $|\cdot\rangle$ is an inert core. The coefficients $f_{n,K}^{(N)}$ are determined by the diagonalization of the Hamiltonian in the subspace spanned by MCSM bases $P_{MK}^{J}|\psi_n\rangle$. The angular-momentum and parity projection is performed by using the numerical integration with about 50,000 mesh points. We calculate on each mesh point parallelly with a supercomputer. The coefficients $D_{lk}^{(n)}$ in the MCSM bases are determined to lower the energy eigenvalues by using the auxiliary-field Monte Carlo method and the conjugate gradient method.

In addition, we use the extrapolation using the energy variance [2, 3] in order to obtain more accurate energy eigenvalues. We change the number of the MCSM bases $N$ and calculate the expectation value of the energy $\langle H \rangle$ and the energy variance $\langle \Delta H^2 \rangle = \langle H^2 \rangle - \langle H \rangle^2$ of the wave function $|\Psi_N\rangle$. As $N$ increases, $\langle H \rangle$ approaches the exact energy and $\langle \Delta H^2 \rangle$ approaches zero. We fit these values by a second-order polynomial and extrapolate the energy to $\langle \Delta H^2 \rangle = 0$.

3. Effective Interaction
We calculated nuclei in the $pfgd$ shell with the effective interaction used in Ref. [4, Sec. 4]. The two-body matrix elements (TBMEs) of the interaction consist of three parts. The TBMEs of the $pf$ shell are those of the GXPFI A interaction [5] and the TBMEs of the $f_5p_9g_{9}$ shell related to the $0g_{9/2}$ orbit are those of the JUN45 interaction [6]. The GXPFI A and JUN45 interactions were determined by combining microscopically derived interactions with a minor empirical fit. The other TBMEs are from the G-matrix effective interaction [7] calculated from the chiral N3LO interaction [8]. The Coulomb interaction is not included and the isospin symmetry is conserved. We made further corrections of the single-particle energies and the monopole interaction.

4. Results
We performed the MCSM calculations of $0^+$ and $2^+$ yrast states of Cr and Ni even-even isotopes systematically and calculated many spin-parity states of $^{68}$Ni. We took 50 MCSM bases for Cr isotopes, 80 bases for Ni isotopes except $^{68}$Ni $0^+$ states, and 120 bases for $^{68}$Ni $0^+$ states. The spurious center-of-mass motion was removed by using the prescription of Gloeckner and Lawson [9]. The effective charges are taken as $(e_p, e_n) = (1.5, 0.5)e$.

Figure 1 shows the excitation energies of $2^+$ yrast states of Cr and Ni isotopes. The MCSM results reproduce the experimental values well. The excitation energies of Ni isotopes are high at $N = 40$, which suggests the magicity of $N = 40$. However, the excitation energies of Cr isotopes are low around $N = 40$ and the $N = 40$ magicity disappears. Figure 2 shows the $B(E2; 0^+_1 \rightarrow 2^+_1)$ transition probabilities of Cr and Ni isotopes. The small $B(E2)$ values of Ni isotopes and large values of Cr isotopes around $N = 40$ also indicate the $N = 40$ magicity of Ni isotopes and the missing $N = 40$ magicity of Cr isotopes. This change of the strength of $N = 40$ magicity may be caused by the change of the $N = 40$ shell gap and the $Z = 28$ magicity of Ni isotopes.

In ordinary shell-model calculations, we cannot study the nuclear deformations of $0^+$ states directly because the wave functions of $0^+$ states are spherical. In the MCSM, we can study deformations of $0^+$ states by using the MCSM bases before angular-momentum projection.
Figure 1. The excitation energies of $2^+_1$ states of Cr (left) and Ni (right) isotopes. Experimental data are taken from Ref. [10].

Figure 2. $B(E2; 0^+_1 \rightarrow 2^+_1)$ values of Cr (left) and Ni (right) isotopes. Experimental data are taken from Ref. [11].

Figure 3. Total energy surfaces of the $0^+_1, 2^+_1, 3^+_1$ states of $^{68}$Ni. The positions of the circles represent quadrupole deformations of the MCSM bases before projection. The areas of the circles represent the overlap probabilities of the bases and the resulting wave function.

Figure 4. The level scheme of $^{68}$Ni. Experimental data are taken from Ref. [12].
Figure 3 shows the total energy surface of $^{68}$Ni obtained by the $Q$-constrained Hartree-Fock calculation [13]. There are spherical, oblate and prolate deformed three minimum points on the total energy surface. The circles on the total energy surface correspond to the MCSM bases. The quadrupole deformations of the bases are calculated before projection. The areas of the circles are proportional to the overlap probabilities of the bases and the resulting wave function. Figure 3 indicates that the $0^+_1$, $0^+_2$ and $0^+_3$ states correspond to the spherical, oblate and prolate shapes, respectively.

Figure 4 shows the level scheme of $^{68}$Ni. $^{68}$Ni is one of the interesting nuclei because its proton number 28 is a magic number and its neutron number 40 is a submagic number. Our calculated results reproduce the experimental values including non-yrast or negative-parity states, although the excitation energies are slightly overestimated. Our analysis of the deformation using the unprojected bases shows that the $0^+_1$ state is spherical, the $2^+_1$, $4^+_1$ and $6^+_1$ states are oblate deformed, and the $0^+_2$, $2^+_2$, $4^+_2$ and $6^+_2$ states are prolate deformed. There are oblate and prolate deformed rotational bands. The $8^+_1$ state is oblate deformed but has different properties from other oblate-deformed states. The excitation energies of $6^+_1$ and $8^+_1$ are close and the $B(E2; 8^+_1 \rightarrow 6^+_1)$ value is small.

5. Summary
We performed MCSM calculations of Cr and Ni isotopes in the $pf_{g9}d_{5}$ shell and studied nuclear shapes by using deformations of the unprojected MCSM bases. We showed the change of the strength of $N = 40$ magicity in Cr and Ni isotopes and three $0^+$ states in $^{68}$Ni with different shapes and close excitation energies. The calculated level scheme of $^{68}$Ni reproduces the experimental data including non-yrast or negative-parity states. These various properties were obtained from the same interaction and we are investigating other nuclei with this interaction.

Acknowledgments
We thank Prof. M. Hjorth-Jensen for providing the G-matrix effective interaction. This work has been supported by Global COE Program “the Physical Sciences Frontier” and HPCI Strategic Program field 5, MEXT, Japan. The numerical calculations were performed mainly on the K computer at the RIKEN AICS (Proposal number hp120284), the FX10 supercomputer at the University of Tokyo and the T2K Open Supercomputers at the University of Tokyo and the University of Tsukuba.

References
[1] Otsuka T, Honma M, Mizusaki T, Shimizu N and Utsumo Y 2001 Prog. Part. Nucl. Phys. 47 319
[2] Shimizu N, Utsumo Y, Mizusaki T, Otsuka T, Abe T and Honma M 2010 Phys. Rev. C 82 061305(R)
[3] Shimizu N, Utsumo Y, Mizusaki T, Honma M, Tsunoda Y and Otsuka T 2012 Phys. Rev. C 85 054301
[4] Shimizu N, Abe T, Tsunoda Y, Utsumo Y, Yoshida T, Mizusaki T, Honma M and Otsuka T 2012 Prog. Theor. Exp. Phys. 2012 01A205
[5] Honma M, Otsuka T, Brown B A and Mizusaki T 2005 Eur. Phys. J. A 25 s01 499
[6] Honma M, Otsuka T, Mizusaki T and Hjorth-Jensen M 2009 Phys. Rev. C 80 064323
[7] Hjorth-Jensen M, Kuo T T S and Osnes E 1995 Phys. Rep. 261 125
[8] Extrem D R and Machleidt R 2003 Phys. Rev. C 68 041001(R)
[9] Gloeckner D H and Lawson R D 1974 Phys. Lett. B 53 313
[10] National Nuclear Data Center, information extracted from the NuDat 2 database, http://www.nndc.bnl.gov/nudat2/
[11] Pritychenko B, Choquette J, Horoi M, Karany B and Singh B 2012 Atomic Data and Nuclear Data Tables 98 798
[12] Broda R et al. 2012 Phys. Rev. C 86 064312
[13] Ring P and Schuck P 1980 The Nuclear Many-Body Problem (New York: Springer-Verlag)