Statistical properties of atomic structures of r-process elements

Daiji Kato[1,2*], Gediminas Gaigalas[1,3], Masaomi Tanaka[4,5]

[1]National Institute for Fusion Science, Toki 509-5292, Gifu, Japan

[2]Department of Advanced Energy Engineering Science, Kyushu University, Fukuoka 816-8580, Japan

[3]Institute of Theoretical Physics and Astronomy, Vilnius University, LT-10222 Vilnius, Lithuania

[4]Astronomical Institute, Tohoku University, Sendai, Miyagi 980-8578, Japan

[5]National Astronomical Observatory of Japan, Osawa, Mitaka, Tokyo 181-8588, Japan

Abstract

New calculations of atomic structures for r-process elements in ejecta of binary neutron star coalescence have been conducted using HULLAC and GRASP2K codes. The results are compared and used to evaluate impact of accuracy in the atomic calculations to opacities of electromagnetic emission from the ejecta. Universality and physical properties in complex open f-shell energy level structures of Nd II and Er II are investigated by coarse-graining methods. The energy level structures are well characterized in terms of statistics of the skewed normal distributions.

Keywords: neutron-star merger, r-process element, opacity of bound-bound transition, atomic structure calculation, coarse-graining, Kolmogorov-Smirnov test

1. Introduction

Gravitational waves by a binary neutron-star merger (NSM) have been detected on 2017 August 17 (GW170817 [1]) for the first time. Ejecta of the neutron-star merger are considered to be the cosmic origin of heavy elements created by the r-process, the rapid neutron-capture process that makes half of all elements heavier than iron. Radioactive decays of the synthesized r-process nuclei in the ejecta cause electromagnetic (EM) emission which is called as kilonova. The EM emission from the ejecta is delayed and dimmer if heavy r-process elements such as lanthanide and actinide (open f-shell) are abundant in the ejecta. Observed light curves of infra-red emission counterpart to GW170817 confirm the existence of some lanthanide contents in the ejecta [2]. However, atomic data for lanthanide are far too insufficient in available databases, *e.g.* NIST ASD [3], VALD [4] to make detail analysis of the EM emission. Thus, atomic structure calculations for the lanthanide elements are carried out by several research groups [5-9].

We present our atomic structure calculations for the r-process elements using two atomic codes, HULLAC [10] and GRASP2K [11], and opacities of bound-bound transitions with the calculated data. It is also demonstrated that potential usefulness of statistical analysis for extremely complex atomic structures of the lanthanide elements.

* Corresponding author's email: kato.daiji@nifs.ac.jp

2. Atomic structure calculations for opacities of bound-bound transitions

In homologous expanding gas, like points on the surface of an inflating balloon, more distant ions go away faster, i.e. velocity gradient. Because of this, line radiations from far distant ions are more red-shifted. Since the radiations are absorbed in cases that the wavelengths are red-shifted into resonance with the adjacent lines, effective opacities of bound-bound transitions in a wavelength interval becomes in proportion to densities of strong (optically thick) transitions. Lanthanide elements (open f-shell) have enormous bound-bound transitions in infra-red region giving large opacities peaking in this wavelength range. This is contrast to iron (open d-shell) which gives smaller opacities peaking in the optical range.

For the present atomic structure calculations, two different codes, HULLAC [10] and GRASP2K [11] were used. The HULLAC code, which employs a Slater-type parametric potential, is used to provide atomic data for many elements while the GRASP2K code, which enables more *ab-initio* calculations based on the multi-configuration Dirac-Hartree-Fock (MCDHF) method [12], is used to provide benchmark calculations for a few elements. In the HULLAC code calculations, the parametric potentials are optimized empirically such that the correct ground-state configuration and the lowest energies of low-lying excited-state configurations in agreement with those of NIST database are obtained. On the other hand, GRASP2K calculations are conducted by increasing the size of active space step-by-step. The GRASP2K calculation with the largest active space includes a larger number of configuration state functions than that of corresponding HULLAC calculation. Therefore, in the results of GRASP2K configuration interactions are more extensively taken into account. The Breit interaction and lowest order QED effects are included in both calculations [12].

We compared calculations using two codes and available data in NIST ASD for Nd II-III and Er II-III. Agreement between HULLAC and GRASP2K results is reasonably good. However, Er II-III energy levels of HULLAC are higher than those of GRASP2K, which may be reflecting accuracy of the GRASP2K results calculated with more extended configuration interactions. The discrepancy is most significant for excited-states of Er III. For Nd II, overall agreement of our calculations with NIST data is within 30 % which is slightly better agreement than results of Autostructure code by Kasen [2]. Both HULLAC and GRASP2K give the correct ground-state and ordering of excited-state energies, except for odd-parity states of Er II. The lowest energy of $4f^{11}6s^2$ excited-state of Er II is too high comparing with that of NIST data. It may reflect difficulty in improving electron-electron correlation effects evenly between different parity states. Further investigation is ongoing.

The opacities of Nd II-III and Er II-III calculated with transition data of HULLAC and GRASP2K codes are compared. The calculations assume the Boltzmann distribution of excited-state populations with $\rho = 1 \times 10^{13}$ g cm^{-3}, $T = 5{,}000$ K or $10{,}000$ K, and $t = 1$ day after the merger. The optical depth of rapidly expanding media is in proportion to oscillator strengths multiplied by the populations for lower levels of transitions. As expected from the good agreement in the energy levels, both results of the opacities are very similar for Nd. However, significant differences are seen in the results for Er as does in the energy levels. GRASP2K calculations give larger opacities than those of HULLAC because the populations for the lower levels

of GRASP2K are larger. This discrepancy is most significant for the case of Er II and reaching to a factor of about 2 at the peak of the opacity.

3. Statistical properties of atomic structures

It is practically impossible to compare the whole open f-shell energy structures level-by-level due to uncertainty in identification of each level and quasi continuum spectra. Effective methods for evaluating such complex structures are needed for a better understanding. Coarse-graining methods are useful for understanding universal natures of complex systems and parametrization of each system. The coarse-graining methods have been applied in various fields of science including renormalization group theories [13], kinetic models of plasma turbulence [14] and molecular dynamics of complex chemical systems [15].

Figure 1 plots differential statistical-weight distributions for two excited-state configurations of Nd II binned with the finite energy interval of 0.1 eV. Results of HULLAC and GRASP2K calculations are compared with available data in NIST ASD. Although the NIST data are available only at low energies, overall profiles of the coarse-grained distributions are apparently in good agreement indicating a universal structure behind. It is noted that GRASP2K results in the figure are presented up to the ionization threshold of Nd II (10.783 eV). Based on the HULLAC results it is found that the universal structure is well depicted by the skewed normal distribution using the first three moments, i.e. mean E_{av}, variance $\sigma^2 = \langle (E - E_{\mathrm{av}})^2 \rangle$, and $\langle (E - E_{\mathrm{av}})^3 \rangle$, of the statistical-weight distribution (see Fig. 1).

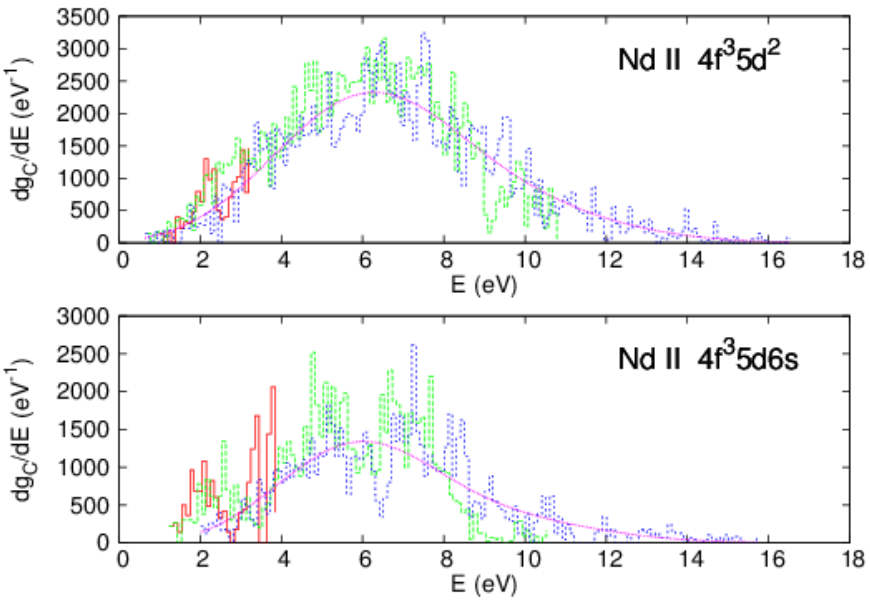

Fig. 1 Differential statistical-weight distributions of $4f^3 5d^2$ (upper) and $4f^3 5d6s$ (lower) configurations. Red color stands for NIST ASD, green GRASP2K, and blue HULLAC. The results are binned with the energy interval of 0.1 eV. Corresponding skewed normal distribution functions are plotted by purple curves.

$$\frac{dg_c}{dx} = c\left[1 - \frac{1}{2}\alpha_3\left(x - \frac{x^3}{3}\right)\right]e^{-x^2/2},$$

(1)

where $x = (E - E_{av})/\sigma$ and $\alpha_3 = \langle (E - E_{av})^3 \rangle / \sigma^3$ (referred to as skewness). The normalization constant c is determined such that the integral of the distribution function gives the total statistical-weight of the corresponding configuration. In the earlier works [16], the skewed normal distribution has already been suggested for statistical-weight distributions of the open f-shell configurations. Signs of the skewness parameters α_3 are positive for all configurations of Nd II and Er II we have studied. This implies that large angular momentum states that possess larger statistical-weights, preferably fall into the lower energy side, which is consistent with Hund's rule as long as *LS*-coupling scheme is valid. The variances of the normal distributions for Er II are larger than those of Nd II, which should be related to that electron-electron interaction energies are larger for heavier elements due to orbital shrink in a stronger nuclear attraction force. Thus, it is encouraging to parametrize complex lanthanide atomic structures in terms of the statistics of the skewed normal distribution.

In the last part of the present work, we examine statistical properties of the energy level structures for Nd II. The coarse-graining of the energy scale is somewhat ambiguous because we can choose arbitrary energy intervals. We may ask alternatively the null hypothesis as "*Statistical distributions of energy levels obtained by stochastic sampling are the skewed normal distribution*". This is, so to speak, coarse-graining of our knowledge (information) on the energy level structures. In order to judge the null hypothesis, Kolmogorov-Smirnov (KS) test [17], which is a non-parametric statistical test without binning continuous valued samples, is applied in this study. The KS test evaluates differences between the two distributions in terms of the statistic defined as,

$$D_N \equiv \sup_E |S_N(E) - P(E)|,$$

(2)

where cumulative probability distributions $S_N(E)$ and $P(E)$ are given for our problems, respectively, as,

$$S_N(E) = \frac{1}{N}\sum_{k=1}^{N} I_{[E_{\min},E]}(E_k),$$

(3)

and

$$P(E) = \frac{1}{g_c}\int_{E_{\min}}^{E} \frac{dg_c}{dx}dx.$$

(4)

$I_{[E_{\min},E]}$ is the indicator function defined as,

$$I_{[E_{\min},E]}(E_k) \equiv \begin{cases} 1, & E_k \in [E_{\min}, E] \\ 0, & E_k \notin [E_{\min}, E] \end{cases}.$$

(5)

The null hypothesis is accepted if the KS statistic D_N on average is smaller than a critical distance at a level of significance. In this study, we use the significance level of 0.05, which means that deviation of normally distributed samples over a given $P(E)$ can exceed the critical distance by chance with 5% probability. In the Fig. 2, the average values of D_N obtained by performing 1,000 tests for Nd II $4f^35d^2$ are plotted with the corresponding critical distances at the significant level of 0.05. The critical distances can be fitted by the single curve, $1.34/\sqrt{N}$. All of the averaged D_N in the figure stay below the critical distances although it is approaching to the critical distance at large N values. Thus, the null hypothesis is accepted by the present KS test for Nd II $4f^35d^2$. By increasing number of sampling N, we would acquire knowledge about more detailed energy level structures which will not completely be depicted by the skewed normal distribution resulting in the averaged D_N exceeding the critical distances.

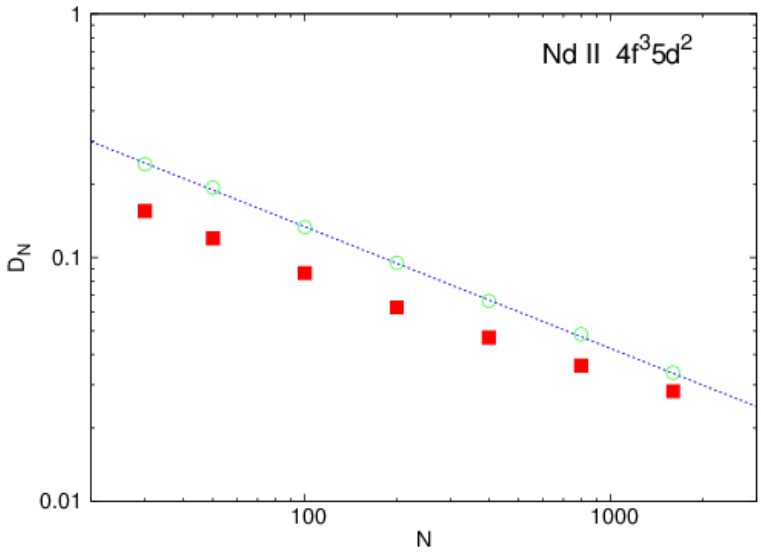

Fig. 2 KS statistic as a function of the number of sampling for $4f^35d^2$ configuration. Solid squares are D_N values averaged over 1,000 tests for each N and open circles the critical distances at the significant level of 0.05. The dotted line is the fitted critical distance curve, $1.34/\sqrt{N}$.

4. Summary and Outlook

Available atomic data (energy levels, oscillator strengths, etc) for heavy r-process elements in NSM ejecta are very limited. New calculations of the atomic data have been conducted using HULLAC and GRASP2K codes. Overall agreement in the lowest energies of configurations for Nd II-III and Er II is good. However, a significant difference remains for excited-states of Er III; GRASP2K results are in better agreement with those of NIST ASD. The lowest energy of $4f^{11}6s^2$ excited-state of Er II is too high comparing with that of NIST data. The expansion opacities of Nd II-III and Er II-III obtained with transition data calculated using HULLAC and GRASP2K are also in good agreement. The discrepancy is most significant for the case of Er II and a factor of about 2 at the peak of the opacity. Extended GRASP2K calculations,

uncertainty quantification of the atomic data, and more detailed analysis on opacities obtained with the data are ongoing focusing on Nd II-IV [18].

Coarse-graining methods are applied to elucidate the universal structure in complex energy level structures of lanthanide elements. The differential statistical-weight distributions binned with a finite energy interval are well depicted by the skewed normal distribution. Physical properties in the energy level structures can be characterized in terms of the statistics. The skewness of the distributions for Nd II and Er II shows that their energy level structures are consistent with Hund's rule. Kolmogorov-Smirnov test is applied to judge whether stochastic sampling of the energy levels leads to the heuristic skewed normal distribution. This null hypothesis is accepted for Nd II $4f^3 5d^2$ at the significant level of 0.05 as long as the number of sampling is not too large.

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