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Updated heat capacities of $^{161-164}$Dy nuclei

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Abstract. *This work presents the updated heat capacities of* $^{161-164}$*Dy nuclei in the nuclear temperature region from 0 to 1 MeV. The updated heat capacities are obtained within the canonical ensemble method making use of the most recent and recommended experimental nuclear level density (NLD) data together with those calculated within the back-shifted Fermi gas (BSFG) model with energy-dependent parameters. By comparing the updated heat capacities with the un-updated ones, which are obtained by using the old experimental NLD data and the BSFG with energy-independent parameters, we found that the updated and un-updated heat capacities are almost identical at low temperature, but differ from each others at high temperature. This discrepancy can be interpreted by the damping of nuclear shell structure with increasing the excitation energy. Besides, we observe that the S-shape in the updated heat capacities is much more pronounced in even-even Dy isotopes than in even-odd ones, whereas the un-updated heat capacities do not clearly exhibit this S-shape. Therefore, the updated heat capacities should provide a more convincing evidence for the signature of pairing phase transition in nuclear systems.*

Keywords: nuclear level density; back-shifted Fermi-gas model; heat capacity; $^{161-164}$Dy nuclei.
Classification numbers: 21.10.Ma; 75.40.Cx.

1. Introduction

The heat capacity of finite Fermi systems, such as nuclei, has gained many attentions because of the probable connection between its shape and the quenching of pairing correlations [1,2]. The experimental or empirical and/or heat capacity data are also crucial for testing different theoretical nuclear models including the shell-model Monte-Carlo [3] and finite-temperature Hartree-Fock-Bogoliubov [4], ect. In macroscopic systems as neutron stars, pairing correlations abruptly quench at a critical temperature T_C, resulting in a discontinuity in the heat capacity [5]. However, in finite nuclear systems, paring correlations do not quench at T_C but monotonously decrease with increasing $T > T_C$, due to the strong statistical and thermal fluctuations beyond the mean field [6]. This phenomenon might be indicated as a local change in the slope of the heat capacity curve, which is commonly referred to the S-shape of the heat capacity [2, 4, 7–10].

Practically, the heat capacity of a given nucleus is a thermodynamic quantity, which can be determined within both canonical and micro-canonical ensemble methods, providing that the experimental nuclear level density (NLD) of the nucleus, at least in some excitation energy region, is known. The micro-canonical ensemble (MCE) method seems to be incompatible with systems of a small number of particles as it quite often provides non-physical values, such as negative temperature (see e.g., Fig. 8 of Ref. [11] and Fig. 9 of Ref. [12]), when being applied to calculate thermodynamic quantities of nuclei. This never happens in the canonical ensemble (CE) method, hence it is a more judicious approach to study the thermodynamic quantities of nuclei. Nevertheless, the calculation of the heat capacity using the CE method is still imperfect because it requires to know the experimental NLD over the entire excitation energy range, namely from 0 to a few hundred of MeV. Unfortunately, the experimental NLD data are only available in the low excitation-energy region, frequently below the neutron binding energy B_n, due to the limitation of experimental technology. To overcome this drawback, one must use the theoretical NLD whenever the experimental NLD data is missing. The back-shifted Fermi gas (BSFG) NLD model, which is the most widely used phenomenological model of NLD, is often employed for this purpose [11, 13]. Fitting the BSFG formula to the experimental NLD data gives the most reliable values for its free parameters.

It is also obvious that any update in the experimental NLD data should result in a change in the values of the BSFG free parameters, thus altering the calculated heat capacity. For instance, the heat capacities of $^{93-98}$Mo isotopes have been re-investigated using the newly updated and recommended NLD data of $^{93-98}$Mo nuclei collected in 2013 [13]. It was noticed that the updated heat capacities significantly differ from those calculated using the old NLD data measured in 2003 and 2006. As a result, Ref. [13] recommended that *"to obtain the correct heat capacity and associated pairing phase transition in excited nuclei, one should use the correct NLD data and the best fitted BSFG NLD in the entire region where the experimental data are available"*.

In 2003 and 2012, the Oslo group carried out experiments employing the (^{3}He,^{3}He$'$) reaction and deduced the experimental NLDs in the energy region below B_n for $^{161-162}$Dy [14] and $^{163-164}$Dy [15] nuclei. By using the BSFG model in conjunction with these measured data, they examined the thermodynamic quantities, including the heat capacity, of $^{161-164}$Dy isotopes. However, they decided to employ the energy-independent parameter version of the BSFG model, which does not account for the damping of the shell effects at high-excitation energies. Indeed, systematic works on the BSFG model have recommended the use of the BSFG version with energy-dependent parameters for the high excitation-energy region because it includes the damping of shell effects with increasing the excitation energy [16]. In addition, an additional parameter, η, was introduced in order to rescale the BSFG NLD to match the experimental average level spacings of the neutron resonance (D_0 data). These parameters are less trustworthy than those obtained from fitting the model to the specific experimental NLD data of each isotope. For example, the Oslo group calculated the global level density parameter by using a systematic equation in which the level density parameters of isobars are the same, i.e., $a = 0.21A^{0.87}$ with A being the mass number, but Fig. 2 of Ref. [16] demonstrates that the level density parameters of isobars can differ from each others up to 25%, and even more in some specific cases. In 2018, the Oslo group re-analyzed their previously conducted experiment and updated the experimental NLDs of $^{161-164}$Dy nuclei [17]. However, the heat capacities of these Dy isotopes have not yet been reexamined.

In the present work, we calculate the heat capacities of $^{161-164}$Dy nuclei using the most recent recommended NLD data in Ref. [17] in combination with the BSFG NLD model with energy-dependent parameters. The updated heat capacities will be compared with those reported in 2003 and 2012 in Refs. [14, 15].

2. Heat capacity and back-shifted Fermi gas nuclear level density formalism

Within the CE method, the heat capacity C can be derived once the partition function Z as a function of temperature T is known. Explicitly, the heat capacity is simply the first derivative of the total thermal energy $\overline{E}$ with respect to T, namely $C = \partial\overline{E}/\partial T$, where $\overline{E} = F + TS$ with F and S being the free energy and entropy. The latter can be directly calculated from the partition function Z

$$F = -T\ln Z,\ S = -\partial F/\partial T\ , \tag{1}$$

with Z being determined based on the inverse Laplace transform of the total NLD as [18]

$$Z(T) = \sum_{E_i=0}^{\infty} \rho(E_i) e^{-E_i/T} \delta E_i\ , \tag{2}$$

where $\rho(E_i)$ is the NLD at an excitation energy E_i and δE_i is the energy interval. In practice, for the low temperature below about 1.0 MeV, one can determine $Z(T)$ by summing $\rho(E_i)e^{-E_i/T}\delta E_i$ with $E_i = 0$ to about 100 MeV instead of infinity as given in Eq. (2) because $\rho(E_i)e^{-E_i/T}\delta E_i$ is negligible when $E_i \gg T$. As mentioned in the Introduction, due to the limitation of experimental NLD data, to calculate the partition function, we use the experimental data if available, otherwise the BSFG NLDs are used. Thus, Eq. (2) can be re-written as

$$Z(T) = \sum_{E_i=0}^{E_i \le E_{max}} \rho_{\rm exp}(E_i) e^{-E_i/T} \delta E_i + \sum_{E_i > E_{max}}^{E_i = 100\ {\rm MeV}} \rho_{\rm BSFG}(E_i) e^{-E_i/T} \delta E_i\ ,$$

where $\rho_{\rm exp}$ and $\rho_{\rm BSFG}$ stand, respectively, for the experimental and BSFG NLDs, whereas E_{max} is the maximum energy that the experimental NLD data are able to measure. Specifically, the values of E_{max} are 5.420, 7.100, 5.300, and 6.860 MeV for $^{161-164}$Dy, respectively.

In 1965, Gilbert and Cameron [19] introduced the BSFG model with parameters that are independent of the excitation energy. However, later microscopic studies of the NLD have indicated that the level density parameter a should depend on the excitation energy [20, 21], leading consequently to the concept of the BSFG with energy-dependent parameters. The values of free parameters in both BSFG versions can be obtained by fitting the model to the experimental data or by applying global equations derived from systematic works. The latter are preferred only once the experimental NLD data are absent. The formalism of the energy-independent parameter BSFG model was described in detail in e.g, Refs. [14, 15], therefore it will not be repeated here. We should recall that the values of free parameters of the BSFG model with energy-independent parameters, that were used to study the heat capacity of $^{161-164}$Dy nuclei in Refs. [14, 15], were determined from global equations instead of fitting to the experimental NLD data. In order to reproduce the BSFG NLD with experimental D_0 data given in RIPL-3 database [22], the authors of Refs. [14, 15] also need to scale (by introducing an additional parameter η) their BSFG NLDs by a factor of 1.19, 0.94, 0.52, and 0.56 for $^{161-164}$Dy, respectively. In the present work, we calculate the heat capacity using the BSFG model with energy-dependent parameters of the form as [19]

$$\rho_{\mathrm{BSFG}}(E) = \frac{\exp\left[2\sqrt{a(E-E_1)}\right]}{12\sqrt{2}\sigma a^{1/4}(E-E_1)^{5/4}} \ , \tag{3}$$

where a, E_1, and σ are the level density, back-shifted energy, and spin cut-off parameters, respectively. This BSFG formalism takes into account the damping of the shell effect with increasing the excitation energy, thus its level density parameter a depends on the excitation energy as follows [20]

$$a(E) = \widetilde{a}\left\{1 + \frac{\delta W}{E-E_1}[1 - e^{-\gamma(E-E_1)}]\right\} \ , \tag{4}$$

where $\widetilde{a}$ is the asymptotic level density and $\delta W\{Z,A\}$ is the shell-correction energy defined as

$$\delta W = M_{\mathrm{exp}} - M_{\mathrm{LD}} \ , \tag{5}$$

with M_{exp} and M_{LD} being the experimental and theoretical masses, respectively. Theoretical mass M_{LD} is often calculated by using the macroscopic liquid-drop formula. The damping parameter γ in Eq. (4) determines how rapidly a approaches $\widetilde{a}$. In the present work, we take the values of δW from RIPL-3 database [22], and consider $\widetilde{a}$, E_1, and γ to be free parameters, whose values are determined by fitting the BSFG NLD to the experimental NLD data given in Ref. [17] for $^{161-164}$Dy. The spin cut-off parameter σ is determined using the following equation [19]

$$\sigma^2 = 0.0888A^{2/3}\sqrt{a(E-E_1)} \ . \tag{6}$$

3. Numerical results and discussion

Figure 1 shows the experimental NLD data of $^{161-164}$Dy taken from Ref. [17] along with the fitted BSFG NLDs obtained within the present work. As can be seen, the BSFG NLDs well describe the experimental data for the excitation energy above 2 MeV for all investigated nuclei. Below 2 MeV of excitation energy, the BSFG fails to reproduce the low-energy part of the experimental NLDs. This is understandable because the BSFG model assumes that the NLD is continuous (see Eq. (3)) in the low-energy region, but the NLD data in this energy region often exhibit a characteristic step-like structure, i.e., an abrupt change in the slope of the NLD at a certain energy could be a result of the breaking of the first nucleon pair. This observed step-like structure is more pronounced in the even-even (^{162,164}Dy) than in the even-odd (^{161,163}Dy) nuclei because the latter already have an unpaired nucleon in their stable state, whereas the former must

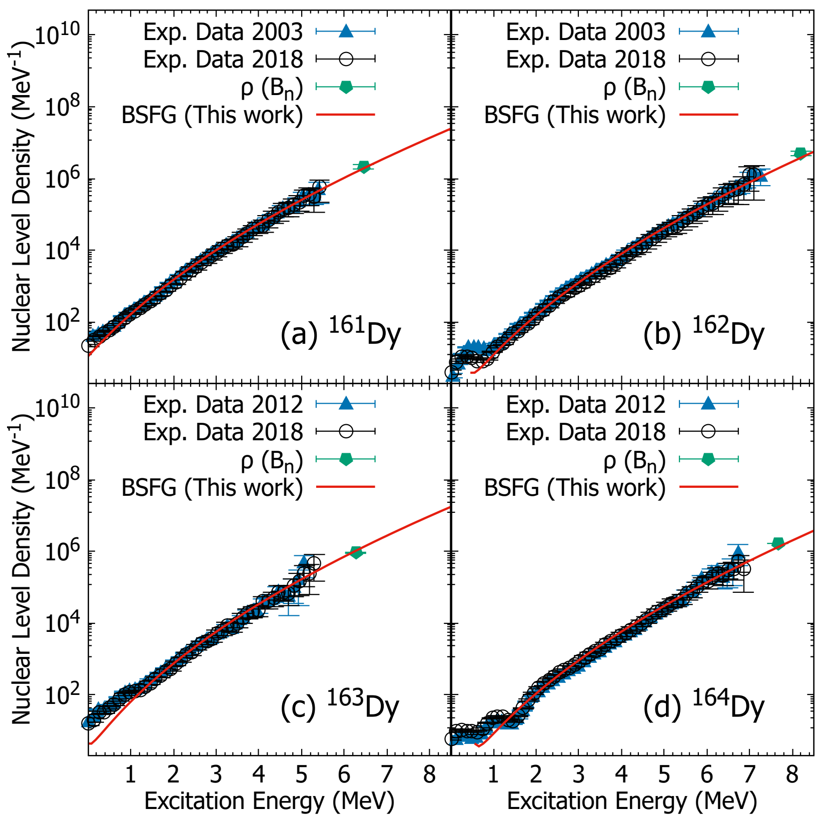

Fig. 1. Comparison between the most recent and recommended experimental NLD data of $^{161-164}$Dy given in Ref. [17] and the corresponding fitted BSFG NLDs obtained within the present work. The level densities at the neutron binding energy $\rho(B_n)$ estimated from the experimental D_0 data given in RIPL-3 database [22] are shown to evaluate the goodness of the fitting. Old experimental NLD data taken from Refs. [14, 15] are also plotted.

be excited to a specific energy in order to break the first nucleon pair. As the excitation energy increases, the breaking of consecutive nucleon pairs occurs, resulting in a high number of unpaired nucleons.The step-like structure is, thus, smoothed out and no longer observed. Figure 1 also indicates that the present BSFG well reproduces the experimental D_0 data retrieved from RIPL-3 database [22] since all the BSFG lines cross their corresponding $\rho(B_n)$ data points. The best fitted values of free parameters obtained within the present BSFG model are listed in Table 1.

Figure 2 compares the updated heat capacities of $^{161-164}$Dy calculated using the most recent and recommended experimental NLD data given in Ref. [17] and the BSFG NLDs, whose parameters values are presented in Table 1, with the un-updated ones published in Refs. [14, 15]. As stated in Sections **1** and **2**, the un-updated heat capacities are calculated using the old NLD data given in Refs. [14, 15] and the BSFG with energy-independent parameters. It is noted that the un-updated heat capacities of ^{161,163,164}Dy are directly extracted from figures presented in Refs. [14, 15], whereas the heat capacity of ^{162}Dy is calculated using the experimental NLD data

Table 1. The values of free parameters obtained by fitting the BSFG model with energy-dependent parameters to the experimental NLD data of $^{161-164}$Dy given in Ref. [17]. The values of δW and D_0 are taken from RIPL-3 database [22].

Nucleus	δW (MeV)	γ (MeV^{-1})	$\tilde{a}$ (MeV^{-1})	E_1 (MeV)	D_0 (eV)
^{161}Dy	2.76808	0.06842	15.23090	-0.53358	27.0 ± 5.0
^{162}Dy	2.46351	0.01526	16.26649	0.36851	2.4 ± 0.2
^{163}Dy	2.16632	0.11511	15.27796	-0.09472	62.0 ± 5.0
^{164}Dy	2.01707	0.05396	15.16655	0.49798	6.8 ± 0.6

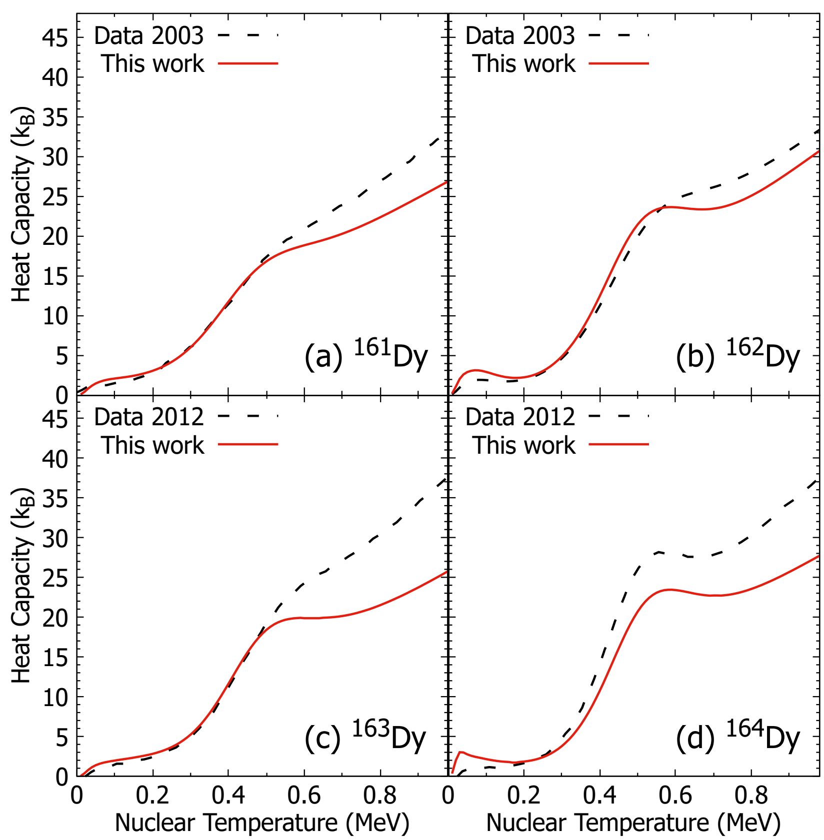

Fig. 2. Comparison between the updated heat capacities determined within the present work with the un-updated ones presented in Refs. [14, 15]. The un-updated heat capacity of ^{162}Dy was not presented in any figure of Ref. [14], so we have to re-calculate it (please see text for more detail).

and the BSFG with energy-independent parameter given in Ref. [14]. It can be seen in Fig. 2 that the updated and un-updated heat capacities are almost the same in the temperature regions below 0.5 MeV for $^{161-163}$Dy and 0.3 MeV for ^{164}Dy. This result is expectable since the experimental NLD data in the low-energy region are often obtained by counting the number of discrete levels in the experimental level scheme at low energy. For instance, one can see in Fig. 1 that the experimental NLD data in the low-energy region are almost identical for all the 2003, 2012, and 2018 datasets. The difference between the updated and un-updated heat capacities is observed at higher temperatures. Specifically, the updated heat capacities of four investigated nuclei are smaller and less steep than the un-updated ones. This discrepancy comes from the differences between the BSFG NLDs used. It is clear to see in Fig. 3 that the BSFG NLDs used to calculate

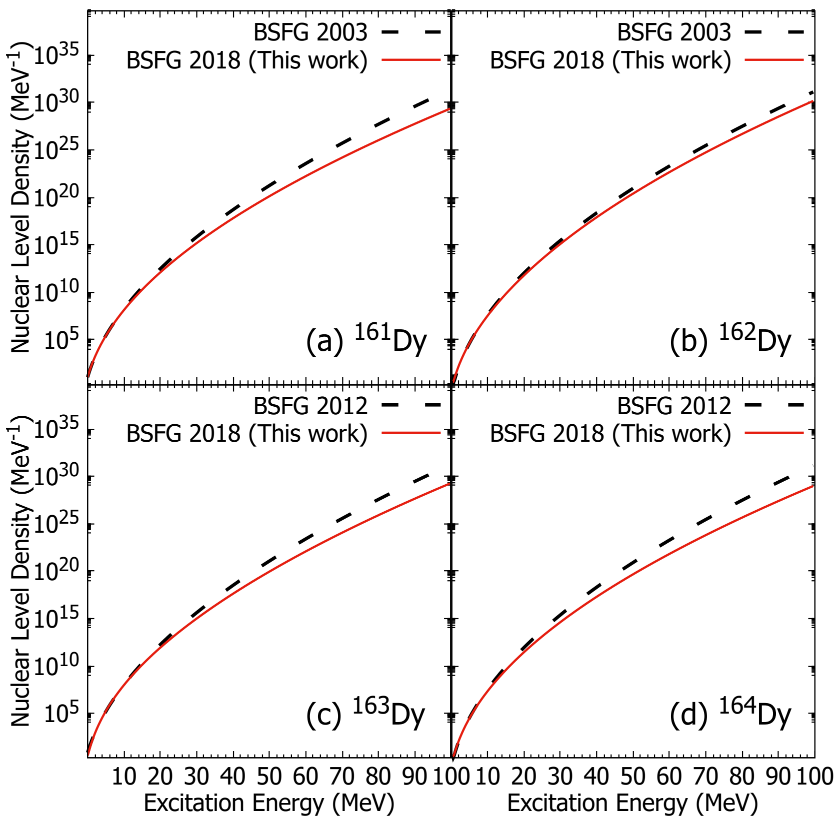

Fig. 3. Comparison between the BSFG NLDs in the excitation-energy region from 0 to 100 MeV used to calculate the updated and un-updated heat capacities in Fig. 2.

the updated heat capacities (denoted as BSFG 2018) are lower than those used to determine the un-updated heat capacities (denoted as BSFG 2003 and BSFG 2012) in the high-energy region, while they are practically the same in the low-energy region. The discrepancy between the BSFG 2003 and BSFG 2018 NLDs of ^{162}Dy (Fig. 3b) is smallest, which results in the small difference between the updated and un-updated heat capacities of this nucleus (Fig. 2b). For the remaining Dy isotopes, the differences between the BSFG 2018 and 2003/2012 NLDs are significant (Figs. 3a, c, and d), leading to a large discrepancy between their updated and un-updated heat capacities (Figs. 2a, c, and d). It is worthwhile to recall that the BSFG NLDs, which are used to compute the updated heat capacities, take into account the damping of the shell effect with increasing the excitation energy (see e.g., Eq. (4)). This damping is not included in the BSFG NLDs that are used to calculate the un-updated heat capacities. Therefore, the difference between the updated and un-updated heat capacities in the high-temperature region can be interpreted by the damping of nuclear shell structure. To explicitly understand the influence of nuclear shell effect on the heat capacity, we show in Fig. 4 the heat capacities of ^{161}Dy obtained by using different values of shell correction δW within a range of 0 to 10 MeV. This figure clearly indicates that the shell correction can significantly alter the shape of the calculated heat capacities, which consequently lead to different physical interpretations of the associated pairing phase transition. Thus, one should use NLD models that take into account the nuclear shell effect to accurately study the nuclear heat capacity.

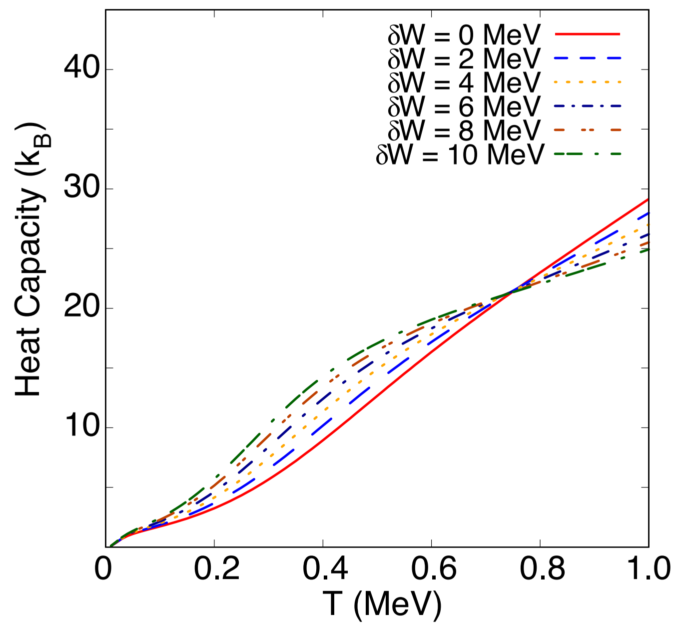

Fig. 4. The BSFG heat capacities of ^{161}Dy obtained by using different shell corrections δW.

In general, the updated heat capacities reveal the same physical information as the un-updated ones, that is, all investigated Dy isotopes exhibit an *S*-shaped heat capacity and this *S*-shape is more pronounced in even-even than odd-even isotopes. For a better visualization, we re-plot the heat capacities that are already given in Fig. 2 with a different arrangement in Fig. 5.

One can easily see in Fig. 5 that the *S*-shapes in the updated heat capacities of even-even ^{162,164}Dy are more pronounced than those of odd-even ^{161,163}Dy (Fig. 5b), while *S*-shapes in the un-updated heat capacities of ^{162}Dy and ^{163}Dy are almost the same (Fig. 5a). The fact that the even-even nuclei, which contain strong pairing correlation, always exhibit stronger *S*-shape than odd-even and odd-odd ones, which include weaker pairing correlation, the *S*-shape predicted by the updated heat capacities should reflect the more reliable physics than that predicted by the un-updated heat capacities. In other words, we can consider the updated heat capacities a more confident proof for predicting the pairing phase transition in finite systems.

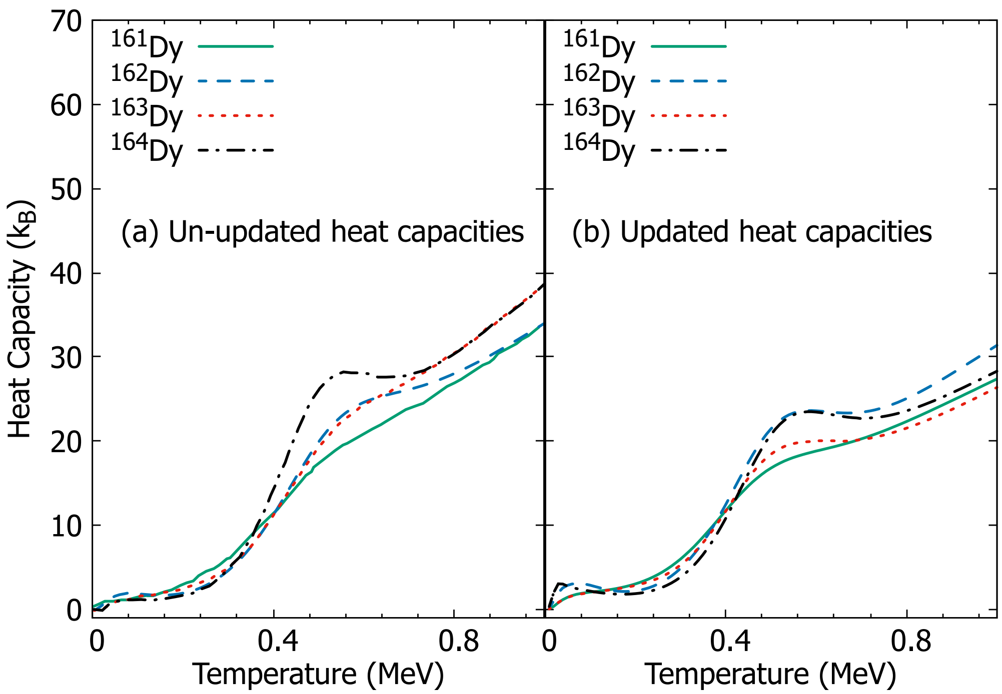

Fig. 5. Comparison of the updated and un-updated heat capacities of $^{161-164}$Dy isotopes.

4. Conclusions

In the present work, the heat capacities of $^{161-164}$Dy have been determined using the most recent and recommended experimental NLD data together with the theoretical NLDs obtained within the BSFG model with energy-dependent parameters. The obtained results, called the updated heat capacities, have been compared with the un-updated heat capacities determined previously using the old experimental NLD data and the BSFG model with energy-independent parameters. It is shown that the updated and un-updated heat capacities are almost the same in the low-temperature region ($T \lesssim 0.4$ MeV). In the high-temperature region, the updated heat capacities are smaller and less steep than the un-updated ones. This can be explained by the damping of the shell effect in nucleus with increasing the excitation energy, which is employed in the BSFG with energy-dependent parameters. In general, the updated heat capacities confirm and provide more convincing evidences on the physical information that the *S*-shape in the heat capacity of even-even nuclei is more pronounced than that of even-odd or odd-odd ones.

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Conflict of interest

The authors have no conflict of interest to declare.

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