Complete inclusion of parity-dependent level densities in the statistical description of astrophysical reaction rates

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Abstract

Microscopic calculations show a strong parity dependence of the nuclear level density at low excitation energy of a nucleus. Previously, this dependence has either been neglected or only implemented in the initial and final channels of Hauser-Feshbach calculations. We present an indirect way to account for a full parity dependence in all steps of a reaction, including the one of the compound nucleus formed in a reaction. To illustrate the impact on astrophysical reaction rates, we present rates for neutron captures in isotopic chains of Ni and Sn. Comparing with the standard assumption of equipartition of both parities, we find noticeable differences in the energy regime of astrophysical interest caused by the parity dependence of the nuclear level density found in the compound nucleus even at sizeable excitation energies.

Key words: parity dependence, Hauser-Feshbach theory, nuclear level density, neutron capture, astrophysical reaction rates, nucleosynthesis

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1. Introduction

Nuclear reactions in systems with high level density at low and intermediate energies are commonly treated in the compound mechanism [1,2,3]. This reaction mechanism was first postulated by Bohr in his well-known independence hypothesis, stating that reactions can proceed via formation of a compound nucleus and that the decay of the compound nucleus is determined entirely by its energy, angular momentum, and parity, and not by the way it was formed [4]. This hypothesis remains valid below a projectile energy of a few tens of MeV. At higher energies, doorway states, pre-compound, and direct reactions become increasingly important. In the following, we focus on the low energy region and thus on the pure statistical picture (Hauser-Feshbach theory, e.g. [1,2]) because our ultimate goal is to propose an improved description for nuclear astrophysics. In astrophysical nuclear burning, the relevant energy in the projectile-target system does not exceed about 200 keV for neutron-induced reactions and 10–12 MeV for proton- and α-induced reactions [5]. Most astrophysically important reactions occur at even significantly lower energy.

Angular momentum conservation is included in standard Hauser-Feshbach theory and thus the Bohr hypothesis independently holds for each spin J and parity π of the compound nucleus, formed from the interaction of a projectile with a target nucleus. There are two fundamental assumptions in the derivation of this theory: 1) There are always sufficient compound-nuclear states with J^π in the relevant excitation energy range; 2) the wave func-

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tions of the compound nuclear states have random phases, so that interferences between reactions proceeding through different compound nuclear states vanish. Due to the strong energy-dependence of the nuclear level density, these assumptions are valid for most reactions (especially at intermediate energy) on stable targets studied in the laboratory. However, it was shown [5] that the level density becomes too low for the application of the Hauser-Feshbach statistical model for astrophysically important reactions involving nuclei far off stability, exhibiting small particle separation energies, or even for nuclei close to stability around closed shells [6] at the low end of astrophysically relevant energies.

For what follows it is important that in applications of the Hauser-Feshbach model one assumes that both parities are equally present in the compound nucleus at the formation energy. This presumption clearly is not valid at very low excitation energy (e.g. due to pairing effects), but there are also many indications from theory as well as some experiments that parities may not be equilibrated even at considerably large excitation energies, in some cases up to 12 MeV [7,8,9]. Similar results are found in different approaches, e.g., in combinatorial methods using single-particle energies from microscopic Hartree-Fock-Bogoliubov calculations [10] as well as in recent Shell Model Monte Carlo (SMMC) calculations [11,12]. We note, however, that very recent experimental data for ^{58}Ni and ^{90}Zr are in accord with the equal-parity assumption at excitation energies as low as 7 MeV (for ^{58}Ni in disagreement with the theoretical predictions). Nevertheless, the assumption of parity-independence of the level density is clearly doubtful for a large number of exotic nuclei in the energy range important in astrophysical environments.

In this Letter we incorporate the parity dependence of the level density into the statistical description of astrophysically capture reactions in all stages of the reaction. Parity-dependent level densities have been used before in statistical model calculations [10,9]. But these concern the distribution of initial and final states, where the first can be populated due to the finite temperature in the astrophysical environment, while the parity-dependence in the newly formed, excited compound nucleus has never been considered before. Speaking in Bohr's terms, our modification impacts the formation cross section of the compound state.

In the next section we present the details of the modification. This is followed by some restricted examples for application to astrophysical neutron capture which are merely given to discuss the model and to illustrate the possible implication for astrophysics. The final section gives a summary and an outlook to future work.

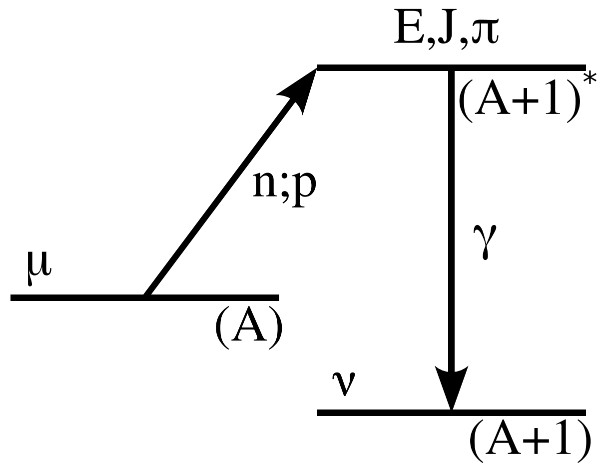

Fig. 1. Schematic sketch of the compound capture reaction. A particle (neutron or proton) is captured in the state μ in the nucleus with mass number A, exciting a state in the compound/daughter nucleus $(A+1)$ at energy E and with angular momentum and parity quantum numbers J and π, respectively. This state decays by γ emission to the state ν in the same nucleus.

2. Formalism

The Hauser-Feshbach expression for the cross section of a reaction proceeding from the target state μ with spin J_i^μ and parity π_i^μ to a final state ν with spin J_m^ν and parity π_m^ν in the residual nucleus via a compound state with excitation energy E, spin J, and parity π (see Fig. 1) is given by

$$\sigma^{\mu\nu}(E_{ij}) = \frac{\pi\hbar^2}{2M_{ij}E_{ij}} \frac{1}{(2J_i^\mu+1)(2J_j+1)} \times \sum_{J,\pi} \frac{T_j^\mu T_o^\nu}{T_{\rm tot}}, \tag{1}$$

where E_{ij}, M_{ij} are the center-of-mass energy and the reduced mass, respectively, in the initial system, while J_j is the ground state spin of the projectile. The transmission coefficients $T_j^\mu = T(E,J,\pi;E_i^\mu,J_i^\mu,\pi_i^\mu)$, $T_m^\nu = T(E,J,\pi;E_m^\nu,J_m^\nu,\pi_m^\nu)$ describe the transitions from the compound state to the initial and final state, respectively. The sum of the transmission coefficients of all possible channels are given by $T_{\rm tot}$.

As indicated, the transmission coefficients depend on the energy E and the quantum numbers for angular momentum J and parity π of the states excited in the compound nucleus. They can in principle be calculated by solving the Schrödinger equation for the appropriate degrees of freedom. Such a microscopic approach will describe simultaneously and consistently all the states in the compound nucleus including their dependence on parity. Again in principle, this microscopic Schrödinger equation can be mapped onto a complicated optical potential which depends on energy and the other quantum numbers. There have been first attempts to derive such microscopic potentials, which show indeed a strong dependence on parity [13,14]. However, these attempts are not realistic enough and are restricted to a few scattering systems. Thus in astrophysical (and other) applications of the Hauser-Feshbach model the transmission coefficients are calculated from optical potentials which are expected to give a reasonable and global account for the many nuclei needed in nucleosynthesis calculations. For our discussion it is relevant that these global optical potentials do not depend on parity and hence also a possible parity dependence of the transmission coefficients is lost. To overcome this shortcoming we propose here an indirect way. It is based on the observation, that for the average transmission coefficients, there is the relation $T \propto \langle\Gamma\rangle / D$, involving the level spacing $D = 1/\rho$ and the average level width $\langle\Gamma\rangle$ in the considered reaction channel. This linear proportionality between transmission coefficient and level density ρ leads us to define

$$T(E, J, \pi) = \beta(E, J, \pi)\hat{T}(E, J), \qquad (2)$$

where $\hat{T}(E, J)$ is a transmission coefficient calculated for a global, parity-independent potential (including centrifugal potential) and the parity dependence is introduced by the weighting factor ($\pi = \pm$)

$$\beta(E, J, \pi) = 2 \cdot \frac{\rho(E, J, \pi)}{\rho(E, J, +) + \rho(E, J, -)}. \qquad (3)$$

The factor 2 accounts for the proper normalization. This approach assumes that the parity dependence of the microscopic potential can be fully mapped onto the level density appearing in the standard Hauser-Feshbach equations. In the following applications we will use the same ansatz Eq. 2 also for the transmission coefficients in the final channel. As all transmission coefficients are evaluated at the same energy in Eq. 1, the β factors of the total transmission coefficient (denominator) and one of the β factors of the nominator cancel.

As mentioned above, the Hauser-Feshbach approach assumes a “sufficient” number of levels in the excited compound nucleus so that an averaged transmission coefficient T is justified and the model is applicable. For astrophysical application in the determination of astrophysical reaction rates the incident energy distribution is given by a Maxwell-Boltzmann distribution giving rise to a relevant energy window [5,3]. It has been shown that about 10 contributing levels (depending on which partial waves are dominating) within this energy window are sufficient. This basic conclusion is not affected by our treatment. However, the parity dependence may enhance or reduce the number of available relevant levels and thus the applicability limits have to be reevaluated taking into account the spins and parities of the initial states. It should be noted that we do not change the total level density but just distribute it differently between the parities.

3. Results

To explore the possible effects of our modification we have performed a series of neutron capture cross section calculations. At first we have performed conventional calculations in which we assumed parity equipartition at all energies in target, compound nucleus and residual (calculation a). Secondly we have restricted the parity dependence to the level densities of the target and residual nucleus (calculation b - these are similar to those of Mocelj *et al.* [9]). Thirdly, we used a parity-dependent level density in all three steps of the statistical treatment: the target, the compound nucleus and the residual nucleus (calculation c). Our calculations have been performed using the spin and parity dependent level densities of Hilaire and Goriely [10]. To explore how sensitive the results depend on the set of level densities adopted we have repeated our calculations using backshifted Fermi gas level densities with the parametrizations as derived by Rauscher and Thielemann [5] and the parity dependence as defined by Mocelj *et al.* [9].

In this paper we focus on (n, γ) for which the influence of the parity dependence of the level density can be discussed considering either the initial neutron capture or the final γ decay. In the following we have chosen to consider the final γ transitions which we assume to be either of parity-conserving M1 or parity-changing E1 multipolarity. The reaction scheme is shown in Fig. 1. Furthermore, we show astrophysical reaction rates which include weighted sums over thermally excited states given by a thermal Maxwell-Boltzmann distribution according to the conditions in a stellar plasma (for the relevant definitions see, e.g., Ref. [3]).

As a first example we discuss the ^{58}Ni(n,γ)^{59}Ni reaction for which experimental data are available for comparison [15].

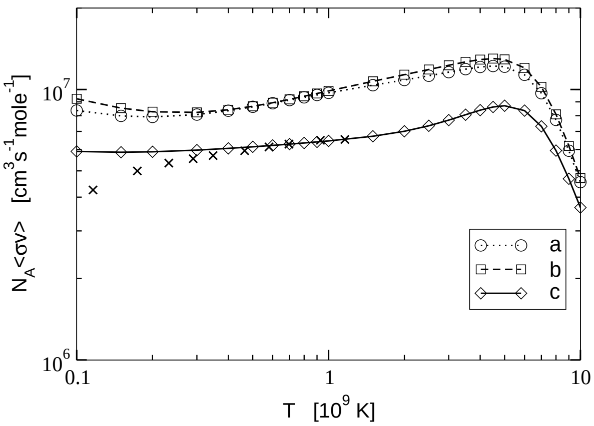

Fig. 2. Stellar reaction rate of ^{58}Ni$(n,\gamma)^{59}$Ni; crosses: recommended values from 'KADoNIS v0.2' [15], **(a)** without parity dependence, **(b)** using parity dependence for the final states, **(c)** using parity dependence for the final states *and* the compound formation using the level densities of [10]

Fig. 2 shows the rate for this reaction as a function of temperature. One observes basically no difference between calculations a) and b); i.e. the consideration of a parity dependence in the level densities of the target and residual nucleus has no effect in this case. This is in agreement with the findings of Mocelj *et al.* [9] and is mainly caused by the fact that both calculations use the experimentally known spectrum at low energies. However, considering the parity dependence of the level density in the compound nucleus (calculation c) reduces the rate by about 30% which is a non-negligible effect. The origin of this reduction becomes clear when one inspects Fig. 3 which shows the ratio of parity-projected level densities for ^{58,59}Ni defined as $\rho_\pi = \rho(E,\pi) = \sum_J \rho(E,J,\pi)$. We have summed over all spins as different values in J have qualitatively the same dependence in the ratio ρ_-/ρ_+ plotted in Fig. 3. For the (n,γ) reaction on ^{58}Ni the γ transitions in the compound nucleus ^{59}Ni are dominated by E1 multipolarity at the relevant energies. At these energies above the neutron threshold negative-parity states dominate the spectrum of ^{59}Ni due to the negative parity of the unpaired neu-

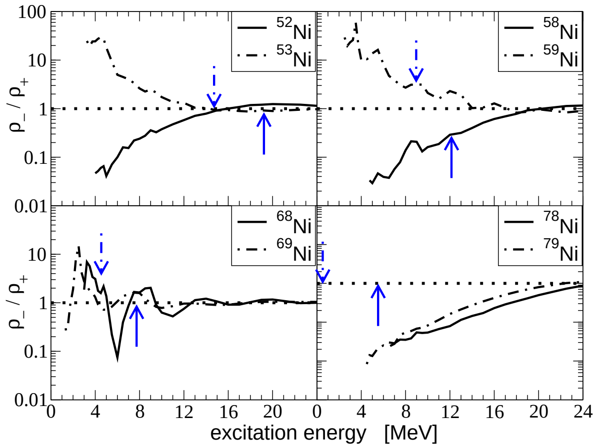

Fig. 3. Ratios ρ_-/ρ_+ of several nickel nuclides; the parity distribution is from Hilaire *et al.* [10] - we used $\rho(E,\pi) = \sum_J \rho(E,J,\pi)$ here; the arrows mark the neutron separation energy of the corresponding nickel isotope.

tron occupying single particle states in the pf shell. Thus initial states for E1 transitions into these states must have positive parity and at stellar conditions they have to reside just above the neutron threshold energy ($S_n = 9$ MeV in ^{59}Ni). At such modest excitation energies the nuclear models predict still a dominance of negative parity over positive parity states in the level density. As we use the same *total* level density in all calculations a), b), and c), the ratio $\rho_-/\rho_+ > 1$ at the relevant energies yields a reduction of the dominant E1 transitions compared to a calculation which assumes parity equipartition, i.e. $\rho_-/\rho_+ = 1$. We note that this reduction gets smaller with increasing temperature as then higher excitation energies, at which the ρ_-/ρ_+ gets closer to unity, contribute more to the stellar reaction rate.

For M1 transitions the effect is opposite as these require negative-parity initial states for this reaction. These are enhanced compared to the parity-equipartition assumption and hence the contribution of the M1 transitions relatively increase. This, however, has not much effect on the total cross section which is dominated by E1 transitions.

It is also satisfying that our calculation yields a slightly better agreement with the empirical data from the KADoNIS compilation when parity-dependent level densities are incorporated into the statistical model (see Fig. 2).

Fig. 4 shows the neutron capture rates for the chain of nickel isotopes as obtained with full parity treatment (calculation c) relative to the standard treatment without parity dependence (calculation a). To understand the results one has to consider that the importance of parity-dependent level densities in the statistical calculation of stellar reaction rates depends on several ingredients: 1) the energy dependence of the ratio ρ_-/ρ_+, 2) the excitation energy of the neutron threshold in the compound, 3) the competition of parity-changing (E1) vs. parity-conserving (M1) γ transitions.

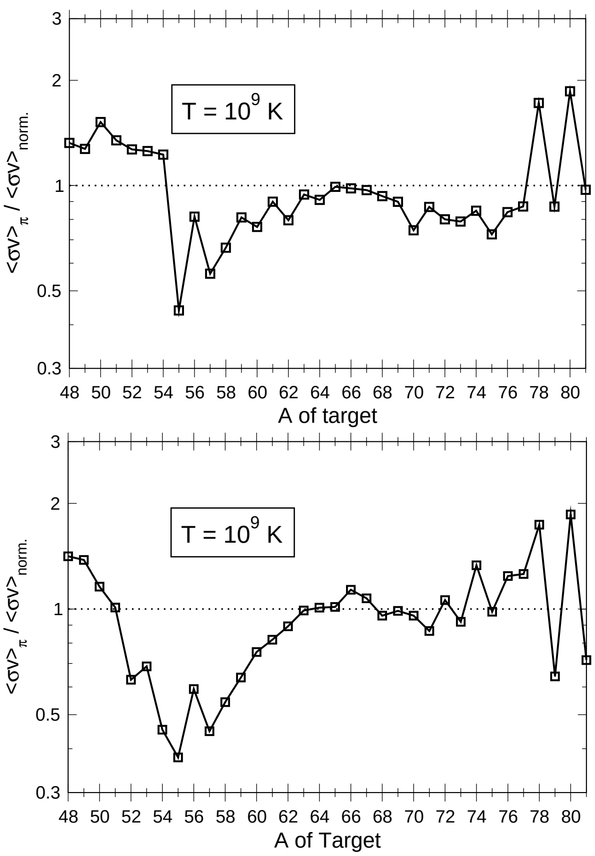

Fig. 4. Ratios of the stellar neutron capture rates of Ni isotopes with parity influence in target, compound, and residual to the stellar rate without any parity influence - the upper graph was made by using the level densities from [10] and the lower graph by using the parity distribution from [9] combined with a level density from [5]. The ratios are shown for a temperature $T = 1$ GK of the stellar plasma.

The ratio ρ_-/ρ_+ is shown in Fig. 3 for several nickel isotopes. Obviously positive parity states dominate the low-energy spectrum for even-even nuclei, while negative parity-states are more abundant at low energies for odd-A nuclei. With increasing energy the ratio ρ_-/ρ_+ tends to unity. However, the energy at which parity equipartition is reached depends on nuclear structure, i.e. it is basically determined by the energy difference of the Fermi energy to the nearest level with different parity and the occupation of the levels. Thus, the equipartition is achieved at increasingly higher energies from ^{48}Ni to ^{56}Ni, where the $f_{7/2}$ and $d_{3/2}$ orbitals matter. By adding more neutrons it becomes energetically easier to excite those to the $g_{9/2}$ level to make levels of opposite parity. As the energy difference to this level decreases with increasing neutron number states with opposite parity (compared to the ground state parity) can be reached at lower energies [1] . However, only the excitation of an odd number of nucleons from or into the next oscillator shell changes the parity of the state. This leads to an oscillatory behavior in the ρ_-/ρ_+ ratios at energies already below the neutron thresholds (indicated by arrows in Fig. 3). For ^{68}Ni with the neutron number $N = 40$ the pf shell is completely occupied in the independent particle model. Hence parity-changing transitions appear at quite low energies in the nickel isotopes around ^{68}Ni. Moving to even larger neutron numbers, and thus closer to potential r-process nuclei around ^{78}Ni, nickel isotopes have mainly positive parity states at low energies as orbitals in the gds shell have positive parity. We note further that equipartition is reached at somewhat higher energies (about 3 MeV) in even-even nuclei than in odd-A nuclei due to pairing.

Fig. 3 also shows the neutron separation energies [16] which obviously decrease with increasing neutron number along an isotope chain. The odd-even staggering is due to pairing.

Usually E1 transitions, which are modelled by a Lorentzian centred around the giant dipole resonance in our approach [2], dominate over M1 transitions, which are described by the single-particle model which makes the M1 strength energy independent [2]. However, if the capture occurs at energies significantly below the giant dipole resonance, E1 transitions are strongly suppressed relative to M1 transitions in this model and the latter can dominate. This can occur in very neutron-rich isotopes with very low neutron thresholds.

For the nickel isotopes with largest proton excess we calculate an enhancement in the stellar rates if the parity dependence of the level densities is considered (Fig. 4). For these nuclei the neutron thresholds are quite high and, due to the excitation of an odd number of nucleons from the ds shell, there is an enhancement of states in the compound with oppo-

[1] The protons do not play an important role for determining the parity at low energies since nickel is a closed shell nucleus for protons.

site parity to the ground state. This yields a slight increase in the rate. The larger effect stems from the fact that for these nuclei low-energy states are experimentally not known and have to be modelled. These states, however, are likely to have the same parity as the ground state (positive for even-even and negative for odd-A proton-rich isotopes). Considering this fact increases the rate compared to calculations which assume parity equipartition also at low excitation energies.

For the isotopes $^{55-62}$Ni we observe a reduction of the rate, if parity dependence is considered. The origin is the same as discussed above for the case of ^{58}Ni, as E1 transitions are reduced as $\rho_+/\rho_- < 1$ ($\rho_-/\rho_+ < 1$) at the energies just above the neutron threshold for odd-A (even-even) isotopes.

For the isotopes $^{63-72}$Ni the neutron thresholds are located at energies where the ratio of parity-dependend level densities is rather close to unity, but still shows some oscillatory behavior. As a consequence the rates are slightly enhanced or reduced depending on the fact whether the ratio is just above or below unity at the energies above the neutron threshold.

For the most neutron-rich Ni isotopes, states with the same parity as the ground state dominate the spectrum at energies around the neutron threshold. This leads to a reduction of the rate if E1 transitions dominate. However, for the capture on the nickel isotopes ^{78}Ni and ^{80}Ni the thresholds are so low (0.52 MeV and 0.17 MeV, respectively) that M1 transitions contribute more in our model than E1 captures; hence the rate is increased compared to the case where parity equipartition is assumed. Due to pairing the neutron threshold in ^{80}Ni is at 3.7 MeV and E1 capture dominates. We note that these nuclei are close to the r-process path. Hence our discussion clearly shows that the effect of parity-dependend level densities on the neutron capture rate is quite sensitive to the neutron separation energies and the competition of M1 and E1 transitions which are both not sufficiently well known yet. We also note that the low density of states makes the use of a statistical model for the very neutron-rich isotopes questionable. Furthermore direct neutron captures should contribute to the rates for these nuclei. Here the parity dependence of the optical potential should be incorporated into the models and possible effects studied.

We have repeated our calculation of neutron captures on the nickel isotopes using the parity distribution of Mocelj *et al.* [9] combined with the back-shifted Fermi gas model of Rauscher *et al.* [5]. As is shown in the lower graph of Fig. 4 the effects are quite similar to those obtained with the Hilaire and Goriely level densities [10].

Finally we have performed a series of calculations for the neutron capture on the tin isotopes (Fig. 5). Again E1 transitions dominate and for the same reasons as explained in details above (e.g. for the case of ^{58}Ni) the consideration of parity-projected level densities lead to a reduction of the rates. For the tin isotopes $^{120-130}$Sn the neutron intruder state $h_{11/2}$, with the opposite parity to the other orbitals in the *gds* shell, plays a special role which has no equivalent for the nickel isotopes. It leads to a rather fast parity equilibration in the level densities which reaches ratios ρ_-/ρ_+ close to unity at energies around the neutron thresholds [10]. As a consequence the rates for neutron captures on the mid-shell tin isotopes change only mildly if a parity dependence of the level densities is considered. For the heavier tin isotopes, the $N = 82$ neutron shell gap at ^{132}Sn and the fact that the two lowest single particle orbitals beyond $N = 82$ ($f_{7/2}, p_{3/2}$) have the same parity as the $h_{11/2}$ intruder level have the effect that the equipartition of parities is reached at larger excitation energies than the respective neutron thresholds for tin isotopes beyond ^{132}Sn. For similar reasons as for the case of ^{58}Ni, the capture rate is reduced for these tin isotopes. The odd-even dependence in the rates are caused by the pairing effects in the neutron threshold energies. For the even heavier tin isotopes the neutron intruder state $i_{13/2}$, with opposite parity to $h_{11/2}, f_{7/2}, p_{3/2}$ becomes important resulting in a fast parity equipartition of the level densities. As a consequence the capture rates do not change much, if parity-dependent level densities are used.

4. Conclusion

We have presented a simple method in the framework of the statistical Hauser-Feshbach theory to account for a full parity dependence including non-uniformly distributed parities in the nuclear level density of the compound nucleus. This goes beyond previous work which only accounted for parity-dependent level densities in the initial and final channels but not in the compound step of the reaction. We applied our method to capture reactions on Ni and Sn nuclei, using a parity dependence in all steps of the compound nucleus reaction. We conclude that this treatment can have a noticeable

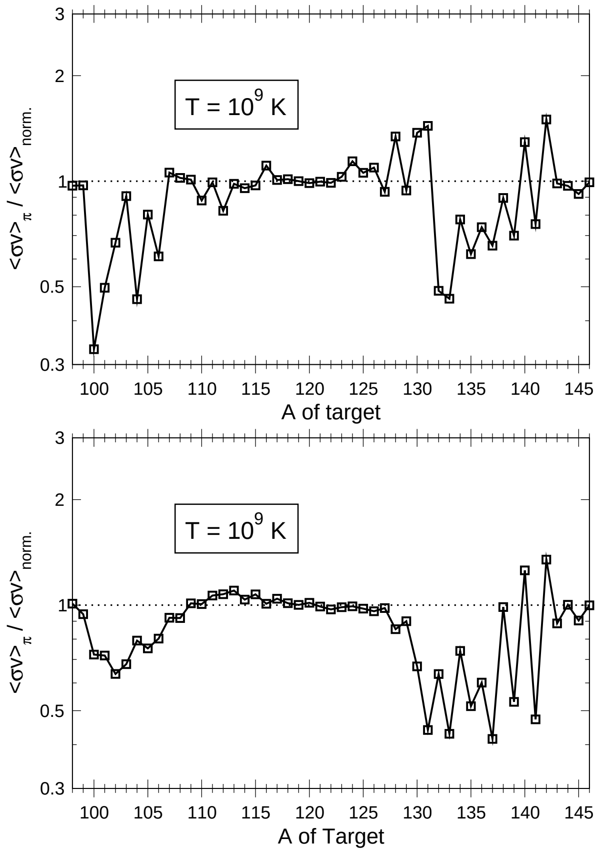

Fig. 5. Ratios of the stellar neutron capture rates of Sn isotopes with parity influence in target, compound, and residual to the stellar rate without any parity influence - the upper graph was made by using the level densities from [10] and the lower graph by using the parity distribution from [9] combined with a level density from [5]. The ratios are shown for a temperature $T = 1$ GK of the stellar plasma.

effect on astrophysical reaction rates for nuclei far from stability. In principle, our approach can also be extended to include a spin dependence or a more general dependence on the level density of the compound nucleus. This will be the focus of future work.

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