On the temperature dependence of the symmetry energy

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We perform large-scale shell model Monte Carlo (SMMC) calculations for many nuclei in the mass range $A = 56 - 65$ in the complete $pf_{3/2}d_{5/2}$ model space using an effective quadrupole-quadrupole+pairing residual interaction. Our calculations are performed at finite temperatures between $T = 0.33 - 2$ MeV. Our main focus is the temperature dependence of the symmetry energy which we determine from the energy differences between various isobaric pairs with the same pairing structure and at different temperatures. Our SMMC studies are consistent with an increase of the symmetry energy with temperature. We also investigate possible consequences for core-collapse supernovae events.

I. INTRODUCTION

Computer simulations of core collapse supernovae are currently at the forefront of research in astro-, nuclear and computational physics. As one-dimensional simulations usually fail to explode [12], the challenging question is whether core-collapse supernovae require multidimensional effects like convection, rotation or magnetic fields, or whether the microphysics input into the simulations is still insufficient or incorrect. The latter possibility involves nuclear physics ingredients like stellar electron and $\beta$-decay rates [13,14], neutrino-nucleus reactions [15,16], neutrino opacities in nuclear matter [17,18] and the nuclear equation of state (EOS) [19,20]. An essential part of the EOS is the symmetry energy which describes the energy needed to separate protons and neutrons. The special importance of the symmetry energy for the core collapse of a massive star stems from the fact that the dynamical evolution of the collapse is strongly influenced by electron captures on nuclei and free protons. These captures drive the matter in the core towards successively more neutron-rich nuclei [19,20]. The symmetry energy impacts these electron captures in two essential ways. For finite nuclei, the effectiveness of the capture depends on the magnitude of the symmetry energy $E_s$; i.e. the larger the value of $E_s$ the more difficult it is to change protons into neutrons. Furthermore, via the EOS the symmetry energy influences the amount of free protons in the core composition which in the late stage of the collapse are believed to be the dominant source for electron captures [11].

As part of global nuclear mass formulae, the symmetry energy is conventionally parametrized as $E_s = a_{\text{symm}}(N-Z)^2/A$, where $N$, $Z$, and $A$ are the neutron, charge and mass number of a nucleus. The value of the coefficient $a_{\text{symm}}$ can be determined by fit to the observed nuclear masses. For the application of the symmetry energy in core-collapse supernovae simulations, Donati et al. pointed to a possible temperature dependence of the $a_{\text{symm}}$ coefficient [18] which at the finite temperatures of the stellar collapse has been estimated to be somewhat larger than for stable nuclei ($T = 0$) hindering electron captures. The hypothesis is based on the following chain of arguments [18]. On the mean-field level correlations are successfully accounted for by using an effective mass parameter $m^* = m_\omega m_k/m$ rather than the bare nucleon mass $m$. Here, the k-mass $m_k$ simulates spatial non-localities in the Hartree-Fock potential introduced by the Pauli principle. Furthermore, the ground state mean field is found to be highly dynamical with strong coupling to surface vibrations. The non-localities associated with these surface couplings can be absorbed into the so-called $\omega$-mass $m_\omega$. This mass is found to be $m_\omega \sim 1.5 m$. However, as it is related to vibrations at low excitation energies of a few MeV, Donati et al. pointed out that $m_\omega$ should vary over the temperature range involved in the collapse phase of a supernova ($T \leq 2$ MeV). On the other hand, the typical energy scale of $m_k$ is $\approx 8$ MeV so that variations of $m_k$ with temperature are assumed to be small and unimportant during the collapse [21]. Within the Fermi gas model, the symmetry energy $E_s$ depends, via its kinetic part, on the change of the $\omega$-mass which scales like $\sim 1/m^*$. Hence, a reduction of $m_\omega$ with temperature increases the symmetry energy. Donati et al. supported their arguments by calculations of selected even-even nuclei at finite temperature using the framework of the quasiparticle random phase approximation (QRPA).

Clearly nuclear excitations at low energies also depend on correlations beyond those treated on the QRPA level. The model of choice for a realistic description of these correlations (e.g. pairing, 2-particle-2-hole and higher order correlations) is the nuclear shell model. Until recently, such shell model calculations for the nuclei involved in core-collapse supernovae were impractical due to the prohibitively large model spaces. This shortcoming has been overcome by modern shell model developments [19,21], where the Shell Model Monte Carlo (SMMC) technique also allows such large-scale calculations at finite temperature [22]. A first attempt to study the temperature dependence of the symmetry energy within the SMMC has been reported in [23], finding no evidence for an increase of $E_s$ with...
been made more difficult by the ‘g-extrapolation procedure’ [25] required to circumvent the notorious sign-problem in SMMC studies with realistic interactions. Furthermore, the model space considered (full \( p f \) shell) was probably too small for calculations at temperatures higher than about \( T = 1 \) MeV. We were thus motivated to perform improved SMMC studies of the temperature dependence of \( E_\alpha \). To this end, we adopted a significantly larger model space, now also including the \( g_{9/2} \) and \( d_{5/2} \) orbitals; these orbitals become important especially as \( A \) becomes larger than 65. We also adopted a schematic but still reasonable residual interaction of the pairing+quadrupole type. Such an interaction does not give rise to the sign problem [23] and allows for a determination of observables at finite temperature without employing the g-extrapolation, thus reducing the statistical uncertainties of the results.

II. SMMC CALCULATIONS OF THE SYMMETRY ENERGY

The SMMC method has been presented in great detail in [27]. The SMMC technique describes nuclear observables \( \langle A \rangle \) at finite temperature as thermal averages

\[
\langle A \rangle = \frac{\text{Tr}_A(e^{-\beta H})}{\text{Tr}e^{-\beta H}}
\]

where \( \beta = 1/T \), \( \text{Tr}_A \) denotes the many-body trace at fixed particle number \( A \) (in this case at fixed neutron and proton numbers) and \( e^{-\beta H} \) the many-body propagator. Applying the Hubbard-Stratonovich transformation, the components of \( e^{-\beta H} \) stemming from the two-body parts of the Hamiltonian (related to the residual interaction) are transformed into integrals over many one-body propagators involving fluctuating external fields. The necessary integrations are performed by Monte Carlo sampling techniques. For certain classes of residual interactions like the attractive pairing+quadrupole force employed here, the evaluation of \( \langle A \rangle \) is exact, subject only to statistical errors related to the Monte Carlo integrations.

As mentioned above, our SMMC calculations are performed within the complete \( (pf g_{9/2} d_{5/2}) \) model space. The single particle energies have been determined from a Woods-Saxon potential parametrization of \( ^{56}\text{Ni} \). As we are concerned here with a description of collective correlations at low energies, we have employed a pairing+quadrupole-quadrupole Hamiltonian

\[
H = \sum_{jmt} \epsilon(j)a_{jmt}^\dagger a_{jmt} - \frac{G}{4} \sum_{\alpha,\alpha',t} P_{jT=01,t}^\dagger(\alpha)P_{jT=01,t}^\dagger(\alpha') - \chi \sum_\mu (-1)^\mu Q_{2\mu} Q_{2-\mu}
\]

where \( Q_{2\mu} \) is the mass quadrupole moment operator given by

\[
Q_{2\mu} = \frac{1}{\sqrt{5}} \sum_{a b} \langle j_a | dV/dr Y_2 || j_b \rangle \left[ a_{a}^\dagger \times a_{b}^\dagger \right]^{2\mu}
\]

with projection \( \mu \) and \( a_{jmt}^\dagger \) (\( a_{jmt} \)) creates (destroys) a nucleon of isospin projection \( t_z \) in the orbital \( jm \), and the pairing operator \( P^\dagger \) is defined as

\[
P_{jT=01,t}^\dagger(\alpha) = (-)^j \left[ a_{\alpha,t}^\dagger \times a_{\alpha,t}^\dagger \right]^{JM=00, T=1}
\]

with \( \alpha = \{n,l,j\} \).

The one-body potential \( V \) is of the Woods-Saxon form [28]. We averaged contributions of the proton and neutron radial integrals to the quadrupole reduced matrix elements. Using the parameters \( G = 0.212 \) MeV and \( \chi = 0.0164 \) MeV\(^{-1}\)fm\(^2\), we reproduce the collective spectrum in \(^{64}\text{Ni}\) and \(^{64}\text{Ge}\). We have checked that center-of-mass contaminations are very small and do not affect our results. Our SMMC calculations have been performed with 4096 statistical samples, splitting the temperature parameter \( \beta \) into \( \beta = N_\beta \Delta \beta \) slices with \( \Delta \beta = 1/32 \) MeV\(^{-1}\) (for details see [27]).

Besides collective excitations, nuclei in the mass range \( A \sim 55 - 65 \), as encountered in the early stage of the core collapse, can be strongly influenced by pairing and shell correlations due to the vicinity of the \( N = Z = 28 \) magic number. All of these modes are governed by energy scales of order \( 1 - 2 \) MeV, and hence are expected to change in the temperature range of interest. To explore the influence of the various correlations on the nuclear properties and their temperature dependence, we have performed SMMC calculations for the \( A = 56 \) and \( A = 59 \) isobars in the temperature range \( T = 0.33 - 2 \) MeV.
Fig. 1 shows the energy expectation values $E(T)$ as a function of temperature, calculated for the even-even ($^{56}$Ni, $^{56}$Fe, $^{56}$Cr) and odd-odd ($^{56}$Co, $^{56}$Mn) $A = 56$ isobars. Due to the presence of correlations, $E(T)$ exhibits strong deviations at low temperatures from the $E(T) \sim T^2$ scaling as expected from the simple Fermi gas model. The large gaps between $^{56}$Ni,$^{56}$Co and $^{56}$Fe,$^{56}$Mn are caused by the differences in pairing energy between even-even and odd-odd nuclei. The vicinity of the $N = 28$ shell gap dominates the low-temperature behavior, in particular for $^{56}$Ni and $^{56}$Co. This is more clearly visible in Fig. 2, where $E(T)$ is plotted against $(N - Z)^2$. In the conventional Bethe-Weizsäcker parametrization one has $E \sim (N - Z)^2$ in the absence of pairing and shell correlations (and without consideration of the Coulomb interaction which we also ignore). Our results suggest that the pairing correlations are approximately overcome at $T \sim 1.2$ MeV, while the shell correlations persist to somewhat higher temperatures.

Fig. 3 shows the energy $E(T)$ as a function of $(N - Z)^2$ for the $A = 59$ isobars ($^{59}$Cu, $^{59}$Ni, $^{59}$Co, $^{59}$Fe, $^{59}$Mn). As expected for odd-$A$ nuclei, the virtual absence of differences in the pairing energies results in an approximate $(N - Z)^2$ scaling, already at low temperatures. The presence of the $N = 28$ shell gap is responsible for the deviations from the $(N - Z)^2$ behavior, particularly for $^{59}$Co and $^{59}$Ni, at low temperatures.

We show in Fig. 4 the expectation value of the isoscalar mass quadrupole moment $\langle Q^2 \rangle$ as a function of temperature. The $0_f7/2$ shell closure ($N = Z = 28$) makes the nuclei $^{56}$Ni and $^{56}$Co spherical and reduces the mass quadrupole at low temperatures in this vicinity of the nuclear chart. For these two nuclei the shell correlations are overcome with increasing $T$ and $\langle Q^2 \rangle$ rises. This is different for $^{56}$Fe and $^{56}$Cr, which are quite collective in the ground state. With the breaking of the pairs (mainly of identical nucleons), caused by rising temperature, the mass quadrupole is reduced up to $T \sim 1$ MeV. Due to the presence of an unpaired proton and neutron, the change of the mass quadrupole is rather moderate in $^{56}$Mn. At higher temperatures ($T \geq 1.2$ MeV) the nuclei are approximately described by uncorrelated nucleons. The mass quadrupole increases as more nucleons are thermally promoted into the $g_{9/2}$ orbital.

In Fig. 5 we plot the $J = 0$ pairing strength between identical nucleons as a function of temperature for the set of $A = 56$ isobars. As in [24] we define the pairing strength as

$$P(J = 0) = \sum_{\alpha \geq \alpha'} M_{\alpha \alpha'}^{J=0}$$

with the pair matrix

$$M_{\alpha \alpha'}^{J=0} = \langle A_{J=0}(j_a, j_b)A_{J=0}(j_c, j_d) \rangle$$

where $\alpha = (j_a, j_b)$ and $\alpha' = (j_c, j_d)$. With increasing temperature the pairing strength decreases to the mean-field expectation value which, with our definition, is non-zero [24].

For the $N = Z$ nucleus $^{56}$Ni the proton and neutron pairing strength are identical. Due to the magicity of this nucleus, pairing is strongly reduced even in the ground state and is only slightly larger than the mean-field value at higher temperatures. The even-even nuclei $^{56}$Fe and $^{56}$Cr exhibit strong pairing among identical nucleons in the ground state. This pairing decreases rather strongly with increasing temperature. In the odd-odd nuclei ($^{56}$Co, $^{56}$Mn) the unpaired nucleons block pairing correlations. As a consequence, for example, the proton pairing strengths in these nuclei are smaller than in the neighboring nuclei $^{56}$Ni and $^{56}$Fe, despite the larger number of valence protons. In the high-$T$ (mean field) limit the proton and neutron pairing strength obviously increase with the number of valence protons and neutrons.

We have shown in previous paragraphs a basic description of the structural properties of our nuclei as a function of temperature. We now turn to a calculation of the temperature dependence of the symmetry energy using our SMMC results. In the absence of pairing and shell correlations, one expects the energy expectation value of isobars, i.e. for nuclei with constant $N + Z$, to scale like $(N - Z)^2$. To minimize the differences in pairing and shell correlation energies we choose several isobaric pairs with the same pairing structure (i.e. even-even, odd-odd, odd-A) and mainly involving nuclei off the shell closure at $N = Z = 28$. Our pairs are ($^{56}$Fe, $^{56}$Cr), ($^{59}$Fe, $^{59}$Mn), ($^{59}$Cu, $^{59}$Ni), ($^{61}$Cu, $^{61}$Ga), ($^{64}$Ga, $^{64}$Cu), ($^{64}$Zn, $^{64}$Ni), ($^{65}$Cu, $^{65}$Ga), ($^{66}$Zn, $^{66}$Ni), ($^{63}$Ga, $^{63}$Cu). For each nucleus (identified by charge and neutron number) we have calculated the energy expectation value $E(T, Z, N)$ at temperatures $T = 0.33$ MeV and $1.23$ MeV. The calculations at the lower temperature, at least for even-even nuclei, resemble the ground state properties rather well. The second temperature has been chosen as a compromise such that $T$ is, on one hand, large enough compared to the energy scales of the correlations, but on the other hand, small enough not to be limited by the large, but still restricted, model space. With the abbreviations $U(T) = E(T, Z_1, N_1) - E(T, Z_2, N_2)$ and $\Delta[(N - Z)^2] = (N_1 - Z_1)^2 - (N_2 - Z_2)^2$ we define the asymmetry parameter

$$a_{\text{symm}}(T) = \frac{A}{\Delta[(N - Z)^2]}U(T).$$

At $T = 0.33$ MeV our calculation yields values for $a_{\text{symm}}$ between 7-12 MeV which is smaller than the value determined from experimental masses, $a_{\text{symm}} = 17$ MeV, indicating shortcomings in the isospin dependence of our
schematic residual interaction. To study the temperature dependence of the symmetry energy, we are interested in the relative change of \( a_{\text{symm}} \) with temperature as

\[
\delta a_{\text{symm}}(T) = \frac{a_{\text{symm}}(T) - a_{\text{symm}}(T_0)}{a_{\text{symm}}(T_0)}
\]  

(8)

where \( T_0 = 0.33 \text{ MeV} \) and \( T = 1.23 \text{ MeV} \). (Calculations at even lower temperatures than 0.33 MeV became numerically unstable in our large model space due to the relative scale of the single-particle matrix elements involved in these systems.) Fig. 7 summarizes \( \Delta U(T) = U(T) - U(T_0) \) and \( \delta a_{\text{symm}} \) for our 9 isobaric pairs. For all pairs our calculations are compatible with \( \Delta U(T) \geq 0 \), i.e. the symmetry energy increases with temperature, as predicted by Donati et al.. Upon averaging over the \( \delta a_{\text{symm}} \) for the various pairs, we find \( \delta a_{\text{symm}} = (6.2 \pm 1.8)\% \) which is approximately in agreement with the QRPA result of [18] which finds an increase of \( \sim 8\% \) of the symmetry energy between \( T = 0 \) and \( T = 1 \text{ MeV} \).

III. DISCUSSION

Our SMMC calculations are consistent with an increase of the symmetry energy with temperature, supporting the argumentation of Donati et al.. In concluding, we explore the possible consequences for the supernova collapse. As pointed out in [18] the larger symmetry energy at finite temperature will result in less electron captures and larger homologous cores, provided all other inputs are kept unchanged. However, here we like to add a word of caution. At first, we note that the recent stellar weak interaction rates [23] are based on shell model calculations performed in model spaces large enough to describe nuclear correlations and their changes with temperature properly for the temperature regime relevant for presupernova simulations [12]. These calculations described the stellar weak-interaction processes for nuclei up to mass \( A = 65 \) as they dominate the mass composition in the core of a collapsing star up to densities of order \( 10^{10} \text{ g/cm}^3 \). As the continuous electron captures drive the matter more neutron-rich during the collapse, nuclei heavier than \( A = 65 \) become important and even dominate at higher densities. For these nuclei, diagonalization shell model calculations similar to those performed in [30], are not feasible due to computational restrictions. To evaluate the relevant electron capture rates for these nuclei, a hybrid model has recently been suggested [24]. In this model the capture rates are calculated within an RPA approach with partial occupation formalism, including allowed and forbidden transitions. The partial occupation numbers represent an ‘average’ state of the parent nucleus and depend on temperature. They are calculated within our current SMMC approach at finite temperature. In the hybrid model the difference of neutron (\( \mu_n \)) and proton (\( \mu_p \)) chemical potentials are fixed by the \( Q \)-value of the capture reaction, assuming that there is no temperature dependence in the symmetry energy. The temperature dependence of the symmetry energy, however, should slightly increase the \( \mu_n - \mu_p \) difference. To study its relevance for the electron capture rates during the supernova collapse, we have calculated rates for three nuclei (\(^{72}\text{Zn} \), \(^{76}\text{Ga} \), \(^{93}\text{Kr} \)) which are atypical representatives of the heavy nuclei at densities \( \sim 10^{10} \text{ g/cm}^3 \) and a few \( 10^{11} \text{ g/cm}^3 \) \((^{93}\text{Kr} \)) [30]. The calculations have been performed for \( \mu_n - \mu_p = Q \), i.e. for no temperature dependence of the symmetry energy, and increasing the \( \mu_n - \mu_p \) difference according to the parametrized increase of the symmetry energy given in [12]. Possible final-state blocking by neutrinos have been ignored, although this effect becomes increasingly important in actual collapse simulations at densities in excess of order \( 10^{11} \text{ g/cm}^3 \).

We show the results in Fig. 7 as a function of the electron chemical potential \( \mu_e \) in the environment, calculated at five points along a typical collapse trajectory made available to us by [30]. Note that \( \mu_e \) scales with the density as \( \sim \rho^{1/3} \). At the lowest density point (\( \rho \approx 10^{10} \text{ g/cm}^3 \)), the electron chemical potential \( \mu_e \) is of the same order as the \( Q \)-value for \(^{72}\text{Zn} \) (a representative nucleus at these conditions), making the capture rate sensitive to a change in \( \mu_n - \mu_p \) difference. We find that the capture rate is decreased by a factor of order 3, if the difference increases as suggested by [18]. \(^{76}\text{Ga} \), another nucleus present in the matter composition at these conditions, has a smaller \( Q \)-value. Hence, the effect of an increase in \( \mu_n - \mu_p \) does affect the rate significantly less. This shows the importance which an increase of the symmetry energy with temperature in the capture rates rests on the competition between the growth of the electron chemical potential and the typical \( Q \)-values of the nuclei in the matter composition along the collapse trajectory. At about \( 10^{11} \text{ g/cm}^3 \), \( \mu_e \) is of order 20 MeV, while typical \( Q \)-values are of order 10 MeV. Thus, an effective change in the \( Q \)-value by about 10% has only little effect on the capture rate. This can be seen in Fig. 7 where the effect of a temperature-dependent increase in the \( \mu_n - \mu_p \) difference becomes less relevant with increasing density. This suggests that the proposed temperature dependence of the symmetry energy decreases the capture rate on nuclei during a small period of the collapse. The absolute changes, even during this period, appear to be rather mild so that one does not expect significant changes for the collapse trajectory.

In conclusion, we performed SMMC calculations in an \( 0f_{1p-1p}0g_{9/2}1d_{5/2} \) model space using an effective pairing+quadrupole Hamiltonian. We found that the symmetry energy increases as a function of temperature by about
6% on average. When applying this symmetry change to electron captures occurring along a typical core-collapse mass trajectory, we found marginal differences in the calculated rates.

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FIG. 1. Energy expectation value $E = \langle H \rangle$ as a function of temperature $T$ for selected $A = 56$ isobars.
FIG. 2. Energy expectation value $E(T)$ as a function of neutron excess calculated at different temperatures for selected $A=56$ isobars.
FIG. 3. Energy expectation value $E(T)$ as a function of neutron excess calculated at different temperatures for selected $A = 59$ isobars.
FIG. 4. Expectation value of the isovector mass quadrupole $\langle Q^2 \rangle$ as a function of temperature for selected $A = 56$ isobars.
FIG. 5. Isovector proton (full circles) and neutron (squares) pairing strength $P(J = 0)$ as a function of temperature for selected $A = 56$ isobars.
FIG. 6. $\Delta U(T)$ (upper panel) and $\delta_{\text{symm}}$ (lower panel) for the pairs of isobars specified in the text and identified by the quantity $\Delta(N-Z)^2/A$. The single large error bar comes from taking energy differences between odd-A nuclei. Generally odd-A systems possess a larger statistical error for a given number of samples than their even-even or odd-A counterparts.
FIG. 7. Dependence of the electron capture rates ($\lambda$) on the $\mu_n - \mu_p$ difference for five relevant chemical potentials ($\mu_e$) along the collapse trajectory. Filled points represent the rates for temperature-independent $\mu_n - \mu_p$ differences, and non-filled points represent the rates for the temperature-dependent differences.