Temperature dependence of volume and surface symmetry energy coefficients of nuclei

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A B S T R A C T

The thermal evolution of the energies and free energies of a set of spherical and near-spherical nuclei spanning the whole periodic table are calculated in the subtracted finite-temperature Thomas–Fermi framework with the zero-range Skyrme-type KDE0 and the finite-range modified Seyler–Blanchard interaction. The calculated energies are subjected to a global fit in the spirit of the liquid-drop model. The extracted parameters in this model reflect the temperature dependence of the volume symmetry and surface symmetry coefficients of finite nuclei, in addition to that of the volume and surface energy coefficients. The temperature dependence of the surface symmetry energy is found to be very substantial whereas that of the volume symmetry energy turns out to be comparatively mild.

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The symmetry energy coefficient a_{sym}^v of infinite nuclear matter is conventionally defined by the relation $e(X) = e(X=0) + a_{sym}^v X^2$. Here e is the energy per nucleon of the system at isospin asymmetry $X = (\rho_n - \rho_p)/(\rho_n + \rho_p)$, ρ_n and ρ_p being the neutron and proton densities, respectively of the system. For homogeneous nuclear matter, this definition works extremely well, $e(X)$ is seen to be bilinear in X for nearly all values of asymmetry [1,2]. For warm nuclear matter, the symmetry free energy coefficient f_{sym}^v is likewise obtained from $f(X,T) - f(X=0,T) = f_{sym}^v(T)X^2$, where $f(X,T)$ is the per-nucleon free energy of the matter at asymmetry X and temperature T. These asymmetry coefficients are measures of the energy or free energy release in converting asymmetric nuclear system to a symmetric one. For infinite nuclear systems at saturation density ρ_0 and temperature $T = 0$, the value of a_{sym}^v is usually taken in the range of ~ 30–34 MeV [3–5].

In the global fitting of the nuclear masses in the framework of the liquid-drop mass formula, the symmetry coefficient a_{sym} enters as a phenomenological parameter. Nuclei being finite systems, it is realized that varying density profiles of different nuclei necessitate introduction of a mass-dependent surface component in $a_{sym}(A)$ in addition to the mass-independent volume component a_{sym}^v. In the literature, two different definitions have been used for $a_{sym}(A)$. The first, hereafter referred to as I [4] is,

$$a_{sym}(A) = \frac{a_{sym}^v}{1 + \frac{a_{sym}^v}{\beta_E} A^{-1/3}} \tag{1}$$

and the second, hereafter referred to as II [6] is,

$$a_{sym}(A) = a_{sym}^v - a_{sym}^s A^{-1/3}. \tag{2}$$

In definition I, β_E is a measure of the surface symmetry energy, a_{sym}^s is the surface symmetry energy coefficient in definition II. In the limit of very large A, $(a_{sym}^v)^2/\beta_E \sim a_{sym}^s$. The phenomenological value of a_{sym}^s is taken as ~ 45 MeV [5–7] and that of a_{sym}^v/β_E is in the close range of $\sim 2.4 \pm 0.4$ [4,8,9].

It is evident that the symmetry energy coefficient has an extremely important role in describing properly the nuclear binding energies along the periodic table and in getting a broad understanding of the nuclear drip lines. It also plays a seminal role in guiding the dynamical evolution of the core collapse of a massive star and the associated explosive nucleosynthesis. A large (small) magnitude of a_{sym} inhibits (accelerates) change of protons to neutrons through electron capture [10,11]. This change in isospin asymmetry has its import in the nuclear equation of state (EOS) and thus on the dynamics of the collapse and explosive phase of a massive star. Matter in that phase is warm, it is therefore essential to know with precision the thermal dependence of the symmetry coefficients. Furthermore, in this collapse or bounce phase, the nuclear matter is inhomogeneous; it nucleates to clusters of different sizes. Knowledge about the thermal evolution of the symmetry coefficients of finite nuclei then becomes a matter of central importance.

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Table 1
The parameters of the KDE0 effective interaction.

t_0 (MeV fm^3)	t_1 (MeV fm^5)	t_2 (MeV fm$^{3(1+\alpha)}$)	t_3	x_0	x_1	x_2	x_3	w_0 (MeV fm^5)	α
−2526.52	430.94	−398.38	14235.52	0.7583	−0.3087	−0.9495	1.1445	128.95	0.1676

In the low temperature domain ($T \leqslant 2$ MeV), calculations of the symmetry coefficients of atomic nuclei have been done earlier by Donati et al. [12] in a schematic model. The motion of the nucleons in a fluctuating mean-field results in a nucleon effective mass that carry signatures of nonlocality in space (the k-mass m_k) and also nonlocality in time (the energy-mass m_ω). The energy mass m_ω is seen to decrease with temperature [13,14], this brings in a decreased density of states and thus an increase in the symmetry coefficient. Calculations in this limited temperature range have further been done by Dean et al. [15] in a shell model Monte Carlo framework. It provides qualitative support to these earlier findings. The symmetry coefficients, however, are found to be much below the nominally accepted values. Evaluation of the temperature dependence of the volume and surface symmetry coefficients of nuclei have also recently been attempted by Lee and Mekjian [16] in a density functional theoretic approach. These calculations are also limited to low temperatures ($T \leqslant 3$ MeV); the approximations employed here keep the results meaningful in this small temperature domain.

Exploring the thermal evolution of the symmetry coefficients of specific atomic masses has been attempted [17] in a broader temperature range ($T \leqslant 8$ MeV) more recently. The energies and free energies of the hot nuclei are calculated in the finite-temperature Thomas–Fermi framework (FTTF) with the subtraction technique [18] with suitable choice of effective interactions. Dynamical changes in the energy-mass m_ω are taken care of. For a nucleus of mass A, the symmetry coefficient is defined as

$$a_{sym}(A, T) = \left[e_n(A, X_1, T) - e_n(A, X_2, T)\right]/\left(X_1^2 - X_2^2\right). \quad (3)$$

Here e_n's are the nuclear part of the energy per nucleon of the nuclear pair of mass A but having different charges and X_1 and X_2 are the asymmetry parameters of the nuclei. For a finite nucleus with Z protons and N neutrons, X is defined as $(N − Z)/A$. Similar to $a_{sym}(A, T)$, the symmetry free energy coefficient $f_{sym}(A, T)$ can be defined. These definitions suffer from the fact that unique values of a_{sym} or f_{sym} for a nucleus of mass A cannot be prescribed; the values depend on the choice of the isospin asymmetric nuclear pair.

The present communication is aimed to arrive at unambiguous values of the temperature dependence of the symmetry coefficients. For a set (sixty nine) of spherical and non-spherical nuclei covering almost the entire periodic table (we take $36 \leqslant A \leqslant 218$ and $14 \leqslant Z \leqslant 92$, the list of the nuclei is taken from Ref. [19]), the energies and free energies are calculated in the subtracted FTTF procedure, taking into account the dressing of the nucleon mass to energy-mass m_ω that arises from the coupling of the nucleonic motion with the surface vibrations [13,14,20]. Two effective interactions are chosen, i) the zero-range Skyrme-type interaction KDE0 [21] and ii) the finite-range modified Seyler–Blanchard (SBM) interaction. The KDE0 interaction reproduces the binding energies of many nuclei ranging from normal to exotic ones with a deviation which is much less than 0.5% for most cases. In addition, it has been extremely successful in reproducing the breathing mode energies of many nuclei, their charge radii and spin–orbit splitting. The SBM interaction also has been very successfully applied in getting properly the ground state binding energies [22], charge rms radii, giant monopole resonance energies etc. [23,24]. The SBM interaction is given by

Table 2
The parameters of the SBM effective interaction (in MeV fm units).

C_l	C_u	a	b	d	κ
348.5	829.7	0.6251	927.5	0.879	1/6

$$v_{eff}(r, p, \rho) = C_{l,u}\left[v_1(r, p) + v_2(r, \rho)\right],$$
$$v_1 = -\left(1 - p^2/b^2\right)f(\mathbf{r}_1, \mathbf{r}_2),$$
$$v_2 = d^2\left[\rho(r_1) + \rho(r_2)\right]^\kappa f(\mathbf{r}_1, \mathbf{r}_2), \quad (4)$$

with

$$f(\mathbf{r}_1, \mathbf{r}_2) = \frac{e^{-|\mathbf{r}_1 - \mathbf{r}_2|/a}}{|\mathbf{r}_1 - \mathbf{r}_2|/a}. \quad (5)$$

The strength parameters C_l for like pairs (n–n, p–p) and C_u for unlike pairs (n–p) carry information on the isospin dependence in the interaction. The densities at the sites $\mathbf{r}_1$ and $\mathbf{r}_2$ of the two interacting nucleons with momenta $\mathbf{p}_1$ and $\mathbf{p}_2$ are given by $\rho(\mathbf{r}_1)$ and $\rho(\mathbf{r}_2)$; $r = |\mathbf{r}_1 - \mathbf{r}_2|$ and $p = |\mathbf{p}_1 - \mathbf{p}_2|$. The range of the interaction is a; b and d are measures of the momentum and density dependence in the interaction and κ controls the stiffness on the nuclear EOS. The procedures for determining these parameters are given in detail in Refs. [24,25]. The parameters for KDE0 and SBM interaction are listed in Table 1 and 2, respectively. The values of the saturation density ρ_s, the volume energy, the isoscalar volume incompressibility K_∞, the volume symmetry coefficient a_{sym}^v, the symmetry incompressibility K_{sym}, the symmetry pressure L and the critical temperature T_c for these two interactions are listed in Table 3. It is worthwhile to note that the values of the symmetry coefficients a_{sym}^v, K_{sym} and L lie in the range suggested by the empirical constraints emerging out of the analyses of different recent experimental data [26–29]. The method for obtaining the density profiles of hot nuclei and their binding energies in the subtracted FTTF approach, with subsequent modification due to energy-mass with the SBM and Skyrme-type interaction has been described in some good detail in a recent article [17]; we therefore do not repeat it here. The energies and free energies of the chosen sixty nine nuclei are calculated with this prescription in a temperature grid. At a particular temperature, the energies are then fitted in the framework of the Bethe–Weizäcker mass formula

$$E(N, Z, T) = a_v(T)A + a_s(T)A^{2/3} + a_c\frac{Z^2}{A^{1/3}}$$
$$+ a_{sym}(A, T)X^2A, \quad (6)$$

$$F(N, Z, T) = f_v(T)A + f_s(T)A^{2/3} + a_c\frac{Z^2}{A^{1/3}}$$
$$+ f_{sym}(A, T)X^2A. \quad (7)$$

In Eq. (6), a_v, a_s, a_c and a_{sym} are the volume, surface, Coulomb and symmetry energy coefficients. Similarly, f_v, f_s and f_{sym} are the corresponding free energy coefficients. The Coulomb energy has an implicit temperature dependence; it does not contribute to entropy. Since they are precisely known in a calculation, we try to make a four-parameter fit with only the nuclear part of the energies and free energies,

$$E_n(N, Z, T) = a_v(T)A + a_s(T)A^{2/3} + a_{sym}(A, T)X^2A, \quad (8)$$

$$F_n(N, Z, T) = f_v(T)A + f_s(T)A^{2/3} + f_{sym}(A, T)X^2A. \quad (9)$$
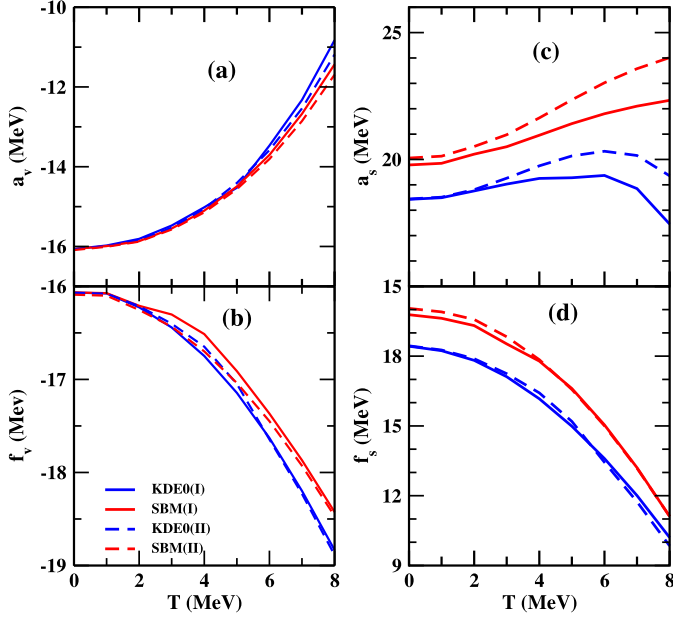
Fig. 1. (Color online.) The volume energy and volume free energy coefficients shown as a function of temperature in the left panels (a) and (b). The full and dashed lines correspond to parametrization I and II, respectively. The blue color refers to the KDE0 interaction, the red color refers to SBM. In the right panels (c) and (d), the thermal dependence of surface energy and surface free energy is shown.

Here E_n and F_n are the nuclear part of the energy and free energy of the nucleus; $a_{sym}(A, T)$ is given by Eq. (1) or Eq. (2). In a similar spirit, $f_{sym}(A, T)$ is written as

$$f_{sym}(A, T) = \frac{f_{sym}^v(T)}{1 + \frac{f_{sym}^v(T)}{\beta_F(T)} A^{-1/3}} \qquad (10)$$

or

$$f_{sym}(A, T) = f_{sym}^v(T) - f_{sym}^s(T) A^{-1/3}. \qquad (11)$$

The four-parameter set f_v, f_s, f_{sym}^v and f_{sym}^s (or β_F) has the same connotation as the set a_v, a_s, a_{sym}^v and a_{sym}^s (or β_E), except that the former set refers to free energy. The parametric values of the volume energy a_v and the volume symmetry free energy f_v are shown as a function of temperature in panels (a) and (b) of Fig. 1. At $T = 0$, a_v (or f_v) very closely reproduces the energy per nucleon of symmetric nuclear matter. At low temperatures, a_v and f_v are nearly independent of the interactions chosen, at higher temperatures, a slight dependence is observed. For a particular interaction, these values, however, do not show any significant dependence on the chosen set I or II. Both a_v and f_v are seen to change quadratically with temperature. They are very well approximated with $a_v(T) = e(T = 0) + T^2/K_1$ and $f_v(T) = f_v(T = 0) - T^2/K_2$, with $K_1 \sim 15.5$ MeV and $K_2 \sim 24.0$ MeV. It is to be noted that for infinite matter at a particular density and temperature, the energy and free energy are canonically related (the entropy $S = -(\partial F/\partial T)_\rho$, whence $K_1 = K_2$); in the present case, density is a varying profile, also $a_v(T)$ and $f_v(T)$ are obtained from a least-squares fit to the energies of a multitude of nuclei. This may explain the different values of K_1 and K_2.

In the right panels (c) and (d) of Fig. 1, the thermal evolution of surface energy and the surface free energy coefficients are shown. The surface energy (upper panel) increases slowly with temperature; with the KDE0 interaction, a slight fall at very high temperatures is, however, observed. With temperature, the surface free energy (lower panel) decreases. In the literature [30,31], different parametric forms for the dependence of surface free energy on

Table 3
Some bulk properties for infinite nuclear matter at the saturation density for the KDE0 and SBM effective interactions. The values of saturation density are in fm^{-3} and all other quantities are in MeV.

| Force	ρ_s	a_v	K_∞	K_{sym}	a_{sym}^v	L	T_c
KDE0	0.161	−16.1	229	−144	33	45.2	14.7
SBM	0.154	−16.1	238	−101	31	59.8	14.9
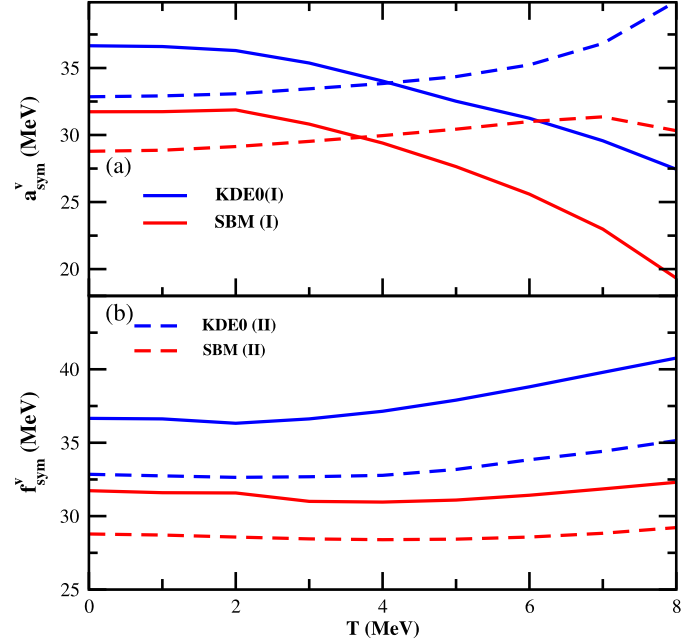
Fig. 2. (Color online.) The volume symmetry energy and the volume symmetry free energy coefficients plotted as a function of temperature. The lines and the colors have the same meaning as in Fig. 1.

temperature have been used. We find that the form of the type $f_s = f_s(T = 0)[(T_c^2 - T^2)/(T_c^2 + T^2)]^\alpha$ used in Ref. [31] gives a reasonably good fit with our calculated values for both the interactions using both the parameter set I and II with $\alpha \sim 0.95$.

In Fig. 2, the evolution of the volume symmetry energy a_{sym}^v and the volume symmetry free energy f_{sym}^v coefficients with temperature are displayed in panels (a) and (b), respectively. The behavior of a_{sym}^v depends on how $a_{sym}(A)$ is defined. In definition I, it falls with temperature, in definition II, it shows a slow increase. The nature of the fall of a_{sym}^v (in I) or its increase (in II) is nearly the same for both the interactions. The coefficient f_{sym}^v, however, shows nearly no dependence on temperature for both the interactions and in both definitions.

In the left panels of Fig. 3, the thermal dependence of the coefficients β_E and β_F as used in Eqs. (1) and (10) in the definition I of $a_{sym}(A)$ and $f_{sym}(A)$ is shown. At $T = 0$, the value of β_E or β_F is 12.1 and 13.9 MeV for the SBM and KDE0 interactions, respectively; they compare well with the value of ~ 13 MeV obtained from analyses of the 'experimental' symmetry energies of isobaric nuclei [9]. With temperature, β_E decreases for both the interactions; β_F shows a nominal increase. We have, however, noticed that both a_{sym}^v/β_E and f_{sym}^v/β_F are nearly temperature independent, lying in the range of $\sim 2.64 \pm 0.01$.

The temperature-dependent surface symmetry coefficients a_{sym}^s and f_{sym}^s as used in Eqs. (2) and (11) in the definition II are shown in the right panels of Fig. 3. At $T = 0$, a_{sym}^s is 44.8 MeV and 39.2 MeV for the KDE0 and SBM interactions, respectively, close to the phenomenological value of ~ 45 MeV [6]. With temperature, for both the interactions, a_{sym}^s increases sharply showing
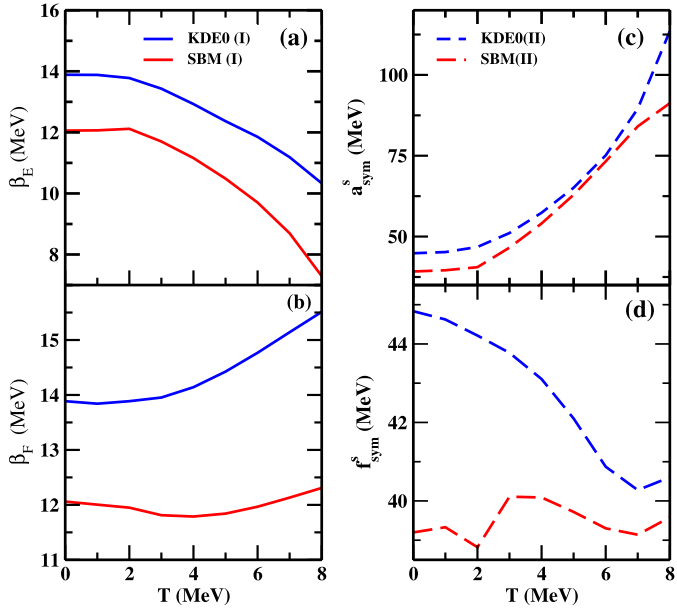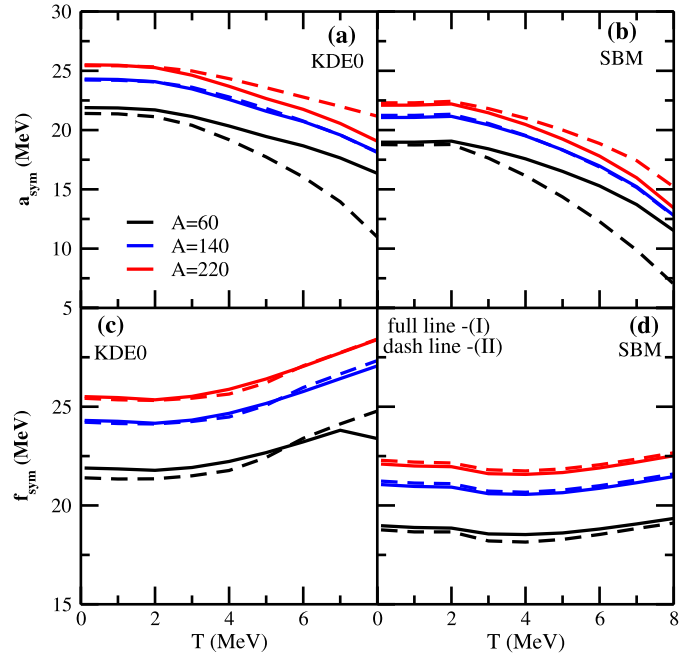
Fig. 3. (Color online.) The thermal dependence of the coefficients β_E and β_F (from parametrization I) is displayed in panels (a) and (b). The thermal evolution of the surface symmetry coefficients a_{sym}^s and f_{sym}^s (from parametrization II) is shown in the right panels (c) and (d). The blue and red lines in both the left and right panels refer to calculations with the KDE0 and SBM interactions, respectively.
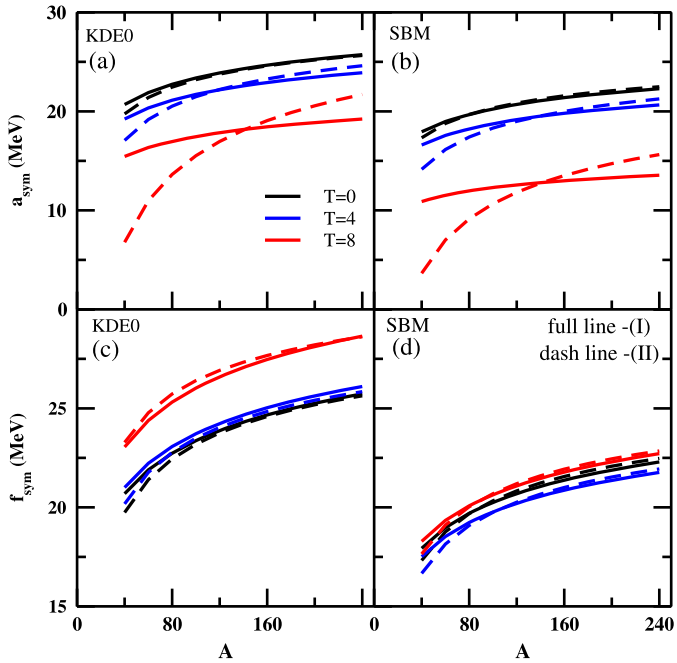
Fig. 4. (Color online.) The symmetry coefficients $a_{sym}(A)$ and $f_{sym}(A)$ shown as a function of mass number for three temperatures. The full and dashed lines refer to parametrization I and II. The black, blue and red lines correspond to $T = 0$, 4, and 8 MeV, respectively.

the growing importance of the surface term in $a_{sym}(A)$. The surface free energy coefficient f_{sym}^s, however, displays a slow decrease with temperature for the KDE0 interaction. As for the SBM interaction, f_{sym}^s is nearly temperature-independent.

A comparison with calculations in Ref. [16] may now be in order. In both calculations, the surface symmetry coefficient seems to be more sensitive to temperature compared to the volume symmetry coefficient. However, in Ref. [16], in the limited temperature

Fig. 5. (Color online.) The thermal dependence of the symmetry coefficients of nuclei shown for three mass number. The full and dashed lines refer to parametrization I and II. The black, blue and red lines correspond to $A = 60$, 140 and 220, respectively.

range they explore, the temperature dependence of the surface coefficients seem to be more pronounced than those seen in the present calculation. There are subtle differences too, the lack of self-consistency of the density profiles used in [16] along with the low-temperature, high-density approximations involved may be the reason behind these differences.

In Fig. 4, the mass dependence of the $a_{sym}(A)$ and $f_{sym}(A)$ is shown at three temperatures, $T = 0$, 4 and 8 MeV. Panels (a) and (b) in the figure display $a_{sym}(A)$ for KDE0 and SBM interactions, respectively; panels (c) and (d) display $f_{sym}(A)$. The full lines correspond to definition I for the symmetry coefficients, the dashed lines do the same for definition II. The general findings are: for a particular mass number, $a_{sym}(A)$ decreases with temperature, $f_{sym}(A)$ increases. At fixed temperature, $a_{sym}(A)$ and $f_{sym}(A)$ increase with A; this follows from the definitions. The values of $f_{sym}(A)$ seem to depend little on the parametrization I or II; similar is the case for $a_{sym}(A)$ except at very high temperature.

For the fixed values of nuclear masses, the temperature dependence of $a_{sym}(A)$ and $f_{sym}(A)$ are exhibited in Fig. 5. The masses chosen are $A = 60$, 140 and 220. Panels (a) and (b) in this figure display $a_{sym}(A)$ for KDE0 and SBM interactions, respectively; panels (c) and (d) do the same for $f_{sym}(A)$. The black lines pertain to $A = 60$, the blue lines to $A = 140$ and the red lines correspond to $A = 220$. The general findings in Fig. 4 that $a_{sym}(A)$ falls and $f_{sym}(A)$ shows a very slow increase with temperature is reinforced from this figure. For the SBM interaction, a near constancy of $f_{sym}(A)$ with a slight dip in the middle of the temperature range is seen. This was also occasionally observed earlier [23] with a different definition of $f_{sym}(A)$ − in the spirit of Eq. (3). It is also observed that for a chosen interaction, both parametrization I and II yield nearly the same value of the symmetry coefficients except for $A = 60$ at higher temperatures.

To summarize, in a liquid-drop-model-inspired fit of the total energies and free energies of a system of nuclei evaluated in a subtraction-implemented finite temperature Thomas–Fermi framework, the temperature dependence of the symmetry energy

coefficients of nuclei have been evaluated in this communication. Two different energy density functionals, one with the zero-range Skyrme-type KDE0 and the other with a finite-range SBM interaction have been employed for this purpose. The general behavior of the temperature dependence of the symmetry coefficients seems to be nearly independent of the energy functional used. For cold systems, the calculated volume and surface symmetry energy coefficients lie within the constraints set from analyses of different experimental data. With temperature, the symmetry free energy coefficients show a weak change. A strong temperature dependence of a_{sym}^v is however observed, the temperature dependence of a_{sym}^s is even stronger; this results in a rapid fall in $a_{sym}(A)$ of the atomic nucleus as the temperature rises. The calculations, in addition throw light on the thermal mapping of the volume and surface energies which are in excellent qualitative agreement with those in common usage.

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