Comments on the nuclear symmetry energy.

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Abstract

According to standard textbooks, the nuclear symmetry energy originates from the kinetic energy and the interaction itself. We argue that this view requires certain modifications. We ascribe the physical origin of the kinetic term to the discreteness of fermionic levels of, in principle arbitrary binary fermionic systems, and relate its mean value directly to the average level density. Physically it connects this part also to the isoscalar part of the interaction which, at least in self-bound systems like atomic nuclei, decides upon the spatial dimensions of the system. For the general case of binary fermionic systems possible external confining potentials as well as specific boundary conditions will contribute to this part. The reliability of this concept is tested using self-consistent Skyrme Hartree-Fock calculations.

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According to classic nuclear structure textbooks [1] the nuclear symmetry energy is composed of two basic ingredients: the so called kinetic and interaction parts:

$$E_{\text{sym}} = \frac{1}{2}a_{\text{sym}}T^2 = \frac{1}{2}(a_{\text{kin}} + a_{\text{int}})T^2. \tag{1}$$

This decomposition and terminology has its roots in the Fermi gas model. Within this model the strength of $a_{\text{kin}}$ can be easily evaluated to be $a_{\text{kin}} \approx 100/A$ MeV. The interaction part, on the other hand, is related to the Hartree part of a schematic isospin-isospin interaction:

$$V_{TT} = \frac{1}{2}\kappa \hat{T} \cdot \hat{T}. \tag{2}$$

The magnitude of $a_{\text{int}}$ (or alternatively interaction strength $\kappa$) can be estimated, however, only indirectly based on the estimate of $a_{\text{kin}}$ and the actual knowledge of the empirical value of the total symmetry energy strength $a_{\text{sym}}$. 
The strength of the nuclear symmetry energy consists of a repulsive volume-type \( \sim 1/A \) part which is reduced at the surface \( \sim 1/A^{4/3} \). For the purpose of this work, however, we adopt an effective volume-like symmetry energy strength \( a_{\text{sym}} \approx 150/A \text{MeV} \). This strength must be understood as the average over volume and surface contributions. It is valid for relatively light nuclei of \( A \sim 50 \div 80 \) [2]. Similar effective values are obtained from fits assuming an \( E_{\text{sym}} \sim T(T + 1) \) dependence for the total symmetry energy [3]. Let us point out, however, that none of the conclusions drawn below will depend upon the adopted strength.

An alternative way of calculating the symmetry energy is by means of the isospin cranking model [4]:

\[
\hat{H}' = \hat{H} - \omega \hat{T}.
\]  

(3)

When the nuclear hamiltonian \( \hat{H} \) can be approximated by an isospin symmetric single-particle (sp) mean-field \( h_{sp} = \sum_{\text{occ}} e_i \) the model can be straightforwardly solved analytically. It leads to the isospin parabolic energy law:

\[
E = \frac{1}{2} \varepsilon T^2
\]  

(4)

as shown in Ref. [4,5,6]. The formula (4) was formally derived for an equidistant level model characterized by a sp splitting \( \varepsilon \). Within such a model the sequence of transitions from the \( T = 0 \) ground state to \( T = 2, 4, 6, 8, \ldots \) takes place at crossing frequencies which form a simple arithmetic serie \( \varepsilon, 3\varepsilon, 5\varepsilon, \ldots \). In reality, the shell structure will affect that simple pattern leading to a sequence of nonuniformly spaced crossing frequencies determined by local shell effects. Thus for small values of the isospin strong deviations from the rule (4) may show up. However, for large values of \( T \) the uniform pattern should be recovered with \( \varepsilon \) being the measure of the mean level spacing at the Fermi energy provided that \( \varepsilon(A, T_z) \approx \varepsilon(A) \). Thus, from the perspective of the uniform isospin cranking model the ‘kinetic’ symmetry-energy term originates rather from the mean-level density than the kinetic energy. Note that, apart from the smooth mean-part, this term also carries information about the fluctuations, directly related to the local shell structure.

The mean-level spacing in nuclei can be rather easily evaluated. Including Kramers and isospin degeneracy it is equal to \( \varepsilon = 4/g(\lambda) \) where \( g(\lambda) = 6\lambda/\pi^2 \) stands for the mean density of states at the Fermi energy. The empirical value of the level density parameter \( a \), is uncertain. Typical estimates (again of an effective volume-like \( A\)-dependent type) range between \( a \approx A/10\text{MeV}^{-1} \) and \( A/8\text{MeV}^{-1} \), see [7,8,9], where the lower limit for \( a \) corresponds to the harmonic oscillator estimate [1]. Thus the contribution is:

\[
\varepsilon \approx 2\frac{\pi^2}{3a} \approx 16\frac{\pi^2}{3A} \div 20\frac{\pi^2}{3A} \approx \frac{53}{A} \div \frac{66}{A} \text{MeV}.
\]  

(5)
Let us observe that using the Fermi gas model, the estimate for $a = A/15 \text{ MeV}^{-1}$ [1] in Eq. (5) recovers exactly the kinetic part of the symmetry energy strength $a_{\text{kin}}$ discussed in the introduction. This value of the level density parameter is, however, unrealistic small.

The repulsive isovector term in the nuclear potential (2) can be included within the mean-field isospin cranking model. Without losing generality we can consider the one dimensional isospin cranking model [e.g. around the $x$-axis, then $\langle \hat{T}_y \rangle = \langle \hat{T}_z \rangle = 0$]. After linearisation of the interaction (2) the cranking Hamiltonian takes the following form:

$$\hat{H}^{\omega}_{\text{MF}} = \hat{h}_{\text{sp}} - (\omega - \kappa \langle \hat{T}_x \rangle) \hat{T}_x$$

with an effective isospin dependent cranking frequency. The isovector potential simply shifts the crossing frequencies from $\epsilon, 3\epsilon, 5\epsilon, \ldots$ to $\epsilon + \kappa, 3(\epsilon + \kappa), 5(\epsilon + \kappa), \ldots$ [within the equidistant level model] leading to

$$E = \frac{1}{2}(\epsilon + 2\kappa)T^2.$$  

(7)

The isovector field enters Eq. (7) with a factor of $2\kappa$, due to the restrictive treatment of the linearized interaction as a $sp$ external potential $V_T = \kappa \langle \hat{T} \rangle \hat{T}$. In this manner, the isovector term is taken into account in phenomenological potentials. Although $\kappa$ can be adjusted to yield the proper Fermi energy dependence on $T$, summing up the total energy from the occupied $sp$ energies, results in a gross overestimate of the symmetry energy. Hence, estimates of $\kappa$ based on phenomenological potentials are not very reliable. Indeed, only by means of the Strutinsky shell-correction procedure one is able to calculate the total energy. This implies, however, that the information carried out from the potential is stripped off any average trends including the mean level density and $\kappa$ in particular and only the fluctuations are transferred.

Nevertheless, the Strutinsky smooth energy can be used for crude verification of the reliability and stability of our concept. We calculated the smooth Strutinsky energies for a chain of $e-e$ $A=88$, $T_z = 0 \div 10$ nuclei. We increased the strength of the isovector potential in steps from zero to its full value. It turned out, that the level density, obtained in the calculations does not depend on $T_z$. This suggest that this method can be viewed as an independent, accurate, and simple way of calculating the mean level density at the Fermi surface.

Within the Hartree-Fock (HF) approximation, the cranking model (Eq. (3)) including an interaction $V_{TT}$ (Eq. (2)) will result in:

$$E = \frac{1}{2}(\epsilon + \kappa)T^2 + \frac{1}{2}\kappa T.$$  

(8)

Thus, the interaction (2) leads to a linear term which comes entirely from
the Fock exchange [10] or, in other words, results in $E_{\text{sym}} \sim T(T + x)$ with a $x < 1$ dependence for the symmetry energy. This form of the symmetry energy is intermediate between $E_{\text{sym}} \sim T^2$ and $E_{\text{sym}} \sim T(T + 1)$ like the formulas debated in the literature. Interestingly, the self-consistent HF or Hartree-Fock-Bogolyubov (HFB) models are believed to give a quadratic $E_{\text{sym}} \sim T^2$ type dependence although, to the best of our knowledge, this conjecture has never been discussed seriously. A dependence $\sim T(T + 1)$, on the other hand, can be deduced from the nuclear shell-model.

The interaction (2) is highly schematic as compared to the isovector part of e.g. a Skyrme type interaction. Therefore, the symmetry energy formula (8) can serve only as a guideline for further investigations which are entirely based on the Skyrme-Hartree-Fock (SHF) energy functional. Nevertheless, we will treat it literally and show that the entire concept of strictly dividing the symmetry energy into contributions from mean-level-density and interaction is very reliable and highly transparent also from the point of self-consistent fields. To investigate the isovector effects of the strong force we switched off the Coulomb interaction and assumed the equality of proton and neutron masses. The calculations presented below were done using SHF code HFODD of Ref. [11] employing various parametrisations of the Skyrme forces.

The mean-level-density $\varepsilon$ contribution can be studied simply by removing the isovector part of the Skyrme force. Then, guided by Eq. (8), the calculated HF energy is approximated by:

$$\Delta E_T^{(HF)} = E_T^{(HF)} - E_{T=0}^{(HF)} \approx \frac{1}{2} \varepsilon T^2,$$

(9)

which allows to extract $\varepsilon$ as a function of $T(=T_z)$. The results of the calculations are presented in Fig. 1. The calculations have been done for several Skyrme forces including SLy4 [12], SIII [13] and SkO [14] i.e. forces having isoscalar effective masses equal $m^*/m \approx 0.70, 0.76$ and 0.90, respectively, as well as SkP [15], SkXc [16] and MSk3 [17] i.e. forces having $m^*/m \approx 1$. The calculations were done for the even-even $A = 48, 68$ and 88 isobaric chains of nuclei from $T_z = 0$ to the vicinity of the drip line.

As anticipated, for relatively small values of $T_z$ strong variations in $\varepsilon$ are seen. However for larger values of $T_z \geq 8$ the values of $\varepsilon$ stabilize. Let us point out that the forces having effective masses considerably lower than unity have a substantially larger $\varepsilon$. However, after employing an effective mass scaling $\varepsilon \rightarrow \frac{m^*}{m}\varepsilon$ all curves are within the limits given by the estimate (5) [shaded

1 To be precise, in the following, the isovector part of the Skyrme interaction always refers to that part of the interaction that gives rise to the isovector dependence of the mean nuclear potential. Within the standard Skyrme energy density functional it is given by the isovector density dependent terms.
Fig. 1. The mean-level spacing (left hand side) calculated using only the isoscalar part of the SHF interaction for the $A = 48, 68, 88$ isobaric chains. Parametrisations used are indicated in the legend. Right hand side shows the results scaled by the isoscalar effective mass $m^*$. Shaded areas indicate the estimates given by (5). Clearly, the physical interpretation of this term as arising from the level density is evident. This observation nicely confirms the validity of our approach. Let us further observe that, with increasing $A$, all curves move towards the upper limit of (5). This, most likely, reflects the decreasing role of surface effects with increasing $A$. Indeed, more accurate estimates of the average density of states $g$, including surface effects can be done based on the semiclassical theory [18]. It can be shown that surface effects increase the density of states $g_{V+S} > g_V$ and, in turn, lower average level spacing $\varepsilon_{V+S} < \varepsilon_V$ thus giving rise to the observed trend. A detailed discussion of the $A$ dependence of the symmetry energy based on these ideas will be published elsewhere.

The dependence of $\varepsilon$ on the effective mass is directly related to the isovector
Fig. 2. The average effective strength $\kappa$ of the isovector part of various Skyrme forces. Left hand side shows the values of $\kappa$ estimated assuming $E_{\text{sym}} = (\varepsilon + \kappa)T^2/2$. Right hand side shows the values of $\kappa$ estimated assuming $E_{\text{sym}} = \varepsilon T^2/2 + \kappa T(T + 1)/2$. In both cases the values of $\varepsilon$ from the isoscalar SHF calculations have been subtracted.

part of the Skyrme interaction. A small effective mass results in a reduction of the isovector Skyrme interaction, since the overall symmetry energy must reproduce, by construction, the empirical value. This effect is seen in Fig. 2 showing the estimated values of $\kappa$ which, in this context, have the meaning of an effective strength of the isovector component of the Skyrme force. We have performed two set of calculation to extract $\kappa$. In the calculations presented in the left panel of Fig. 2, we have assumed a purely quadratic isospin dependence $\Delta E_{T}^{(HF)} = \frac{1}{2}(\varepsilon + \kappa)T^2$. The right panel, on the other hand, shows calculations that include also the linear term from Eq. (8). For both cases we have made use of the $\varepsilon$ values extracted previously (Fig. 1) from the isoscalar SHF calculations. The calculations reveal at least two striking features: (i) No major perturbations in the $\kappa(T_z)$ curves are seen for large $T_z$ pointing to a
very weak, if any, impact of the isovector fields on the average level density.

(ii) Clearly, and rather surprisingly, these calculations reveal the presence of a linear term. Indeed, the curves in the right panel of Fig. 2 show essentially no $T_z$ dependence. The only exception from this rule is the SkO force with its highly non-standard strong, repulsive isovector component of the spin-orbit force.

An interesting conjecture can be made here concerning recent very accurate self-consistent mass calculations based on Skyrme forces. [19] These calculations clearly prefer Skyrme forces of $m^*/m \sim 1$. This preference can be (partly) related to the presence of the linear term in the symmetry energy, provided, that the empirical symmetry energy has a term like $\sim T(T + x)$. Indeed, for Skyrme forces having $m^*/m < 1$ the linear term is expected to be reduced. On the other hand, there seems to be no counterpart to the $\sim \frac{1}{2}\varepsilon T$ type at the mean-field level. Such a compensating term may be calculated within the RPA theory as suggested recently by [10]. Performing RPA calculations atop of HF/HFB particularly in large-scale mass calculations is presently beyond reach. However, since the linear term describes, in fact, the isospin dispersion, and since our interpretation links the inertia parameter to the average spacing $\varepsilon$, the overall correction can easily be estimated based on Eq. (5) [scaled by the isoscalar effective mass] and the calculated isospin dispersion $\langle \Delta T^2 \rangle$.

In the $sp$ limit, one finds that $\langle \Delta T^2 \rangle = T$ and therefore, the interaction part of the symmetry energy follows $E^\text{int}_{\text{sym}} \sim T(T + 1)$. However, pairing correlations tend to increase $\langle \Delta T^2 \rangle$, with the largest effect in $N=Z$ nuclei, as shown in the insert of Fig. 3. Thus pairing effectively weakens the linear term leading to $E^\text{int}_{\text{sym}} \sim T(T + x)$ with $x < 1$. The impact of pairing on the value of $x$ is illustrated in Fig. 3, and defined as

$$x \equiv \frac{\langle \Delta T^2 \rangle_T - \langle \Delta T^2 \rangle_{T=0}}{T} \quad \text{where} \quad T \equiv T_z = (N - Z)/2 \quad (10)$$

The value of $x$ is calculated using the schematic, non-selfconsistent constant gap $\Delta$ BCS calculations. In the calculations the equidistant level spectrum characterized by a $sp$ splitting $\varepsilon$ was used. $2N (2Z)$ of the double degenerate levels were active in the pairing calculations, in order to take advantage of the particle-hole symmetry which in turn guarantees automatic number conservation.

As already discussed pairing has the greatest impact on $N \sim Z$ nuclei reducing the value of $x$ to $\sim 0.3$ for the $A = 88, T_z = 1$ system, see Fig. 3a. With increasing $T$, the value of $x(T)$ increases slowly to $x \rightarrow 1$. For small $T$ the actual value of $x$ changes rapidly with an increasing ratio of $\Delta/\varepsilon$ as illustrated in Fig. 3b. Since $\Delta/\varepsilon \sim A^\nu [\nu \sim 1/2 \div 2/3]$ the quenching of $x$ is expected to be more efficient in heavy $N \sim Z$ nuclei. Local shell-structure, however, may
result in oscillations of the \( \Delta/\varepsilon \) ratio and, in turn, to strong variations in \( x \).

To verify this assumption we performed self-consistent HF+BCS calculations using SLy4, SIII, SkP and MSk3 forces. The calculation scheme was similar to the one described above. First we extracted \( \varepsilon_{BCS} \) from the isoscalar Skyrme SHF+BCS calculations. Then, using these values, we extracted \( \kappa_{BCS} \). The values of \( \kappa_{BCS} \) were computed assuming \( E_{\text{sym}}^{\text{int}} \sim \kappa T(T + 1) \) and compared to corresponding values from pure SHF calculations, \( \kappa_{HF} \), see Fig. 2. The difference is shown in Fig. 4. It is always negative, and particularly large for small \( T_z \). This clearly confirms the schematic model calculations shown in Fig. 3.
Fig. 4. The difference between HF+BCS and HF values of $\kappa$. In both cases $\kappa$ has been calculated assuming $E_{\text{sym}}^{\text{int}} \sim \kappa T(T + 1)$. Note that values of $\kappa_{\text{BCS}} - \kappa_{\text{HF}}$ are always negative. This behavior shows that pairing has a similar destructive impact on the linear Skyrme related term as emerged from the simple schematic considerations shown in Fig. 3.

In conclusion, it is demonstrated that the Skyrme forces give rise to a linear term in the interaction part of $E_{\text{sym}}$ which behaves effectively similar to the schematic interaction (2), i.e. like $\sim \langle \Delta T^2 \rangle$. This term is strongly quenched in $N \sim Z$ nuclei due to $pp/nn$ pairing, which, even after including RPA correlations [10], seem to leave room for isoscalar pairing correlations in $N = Z$ nuclei. Particularly, since the data clearly indicates that the linear term of the symmetry energy in the vicinity of the $N = Z$ line is enhanced and goes like $\sim T(T + 1.25)$ [20,21]. Mass calculations with the SHF need to take into
account the fluctuations in isospin, $\sim \langle \Delta T^2 \rangle$ similar to the fluctuations in spin [17] with an inertia given by the mean level spacing at the Fermi energy. This may allow for more general Skyrme forces, not restricted to effective mass $m^* \approx m$.

In particular, the present investigation reveals that one component of the nuclear symmetry energy can directly be associated with the *mean-level density* rather than the *kinetic* energy as proposed in textbooks. Although the arguments are based on Skyrme-Hartree-Fock calculations of $A = 48, 68, \text{and} 88$ chains of nuclei, this is a general feature originating from the granularity of the fermionic single particle spectra and not related to atomic nuclei only.

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