On the linear term in the nuclear symmetry energy

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Abstract

The nuclear symmetry energy calculated in the RPA from the pairing plus symmetry force Hamiltonian with equidistant single-nucleon levels is for mass number \( A = 48 \) approximately proportional to \( T(T + 1.025) \), where \( T \) is the isospin quantum number. An isovector character of the pair field assumed to produce the observed odd-even mass staggering is essential for this result. The RPA contribution to the symmetry energy cannot be simulated by adding to the Hartree-Fock-Bogolyubov energy a term proportional to the isospin variance in the Bogolyubov quasiparticle vacuum, and there are significant corrections to the approximation which consist in adding half the isocranking angular velocity. The present calculation employs a smaller single-nucleon level spacing than used in a previous investigation of the model.

Key words: Symmetry energy, Wigner energy, Isobaric invariance, Isovector pairing force, Symmetry force, RPA, Hartree-Fock-Bogolyubov approximation

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The so-called symmetry energy in the semi-empirical formula for nuclear masses is quadratic in the difference \( N - Z \) between the numbers of neutrons and protons [1]. In a more general view including isobaric analogue states, this may be seen as a quadratic dependence on the isospin quantum number \( T \). Nuclei with small values of \( T \) have a larger binding energy than expected from a quadratic extrapolation from higher \( T \)-values [2]. In one parametrization of this extra binding energy, the so-called Wigner energy, a term linear in \( T \) is included in the total energy so that the symmetry energy becomes proportional to \( T(T + x) \) for some constant \( x \). The best choice of \( x \) seems to be close to 1 [3,4], possibly with a preference for a slightly larger value [5]. Other parametrizations of the Wigner energy are employed in Refs. [2] and [6].

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The origin of the Wigner energy is a debated issue [7,8,2,9,10,11,12,13,14,15,6]. For a schematic, isobarically invariant Hamiltonian, I recently showed that the Hartree-Bogolyubov energy rises quadratically in $T$, whereas the $T$-dependence of the RPA correlation energy is dominated by a term equal to half the derivative of the Hartree-Bogolyubov energy with respect to $T$. The Hartree-Bogolyubov energy and the dominant $T$-dependent term in the RPA correlation energy thus give a symmetry energy proportional to $T(T + 1)$ [16].

For the details of the theory, see Ref. [16]. The Hamiltonian is the sum of an independent-nucleon Hamiltonian with equidistant, fourfold degenerate single-nucleon levels, an isobarically invariant isovector pairing force and a symmetry force:

$$H = H_0 - G P^\dagger \cdot P + \frac{\kappa T^2}{2}, \quad H_0 = \sum_{k\sigma\tau} \epsilon_k a^\dagger_{k\sigma\tau} a_{k\sigma\tau}.$$  

Here, $P$ is a pair annihilation isovector, $T$ is the isospin, and $G$ and $\kappa$ are coupling constants. The single-nucleon energy $\epsilon_k$ takes $\Omega$ equidistant values separated by $\eta$, and $a_{k\sigma\tau}$ are single-nucleon annihilation operators. $k\sigma$ is $k$ or $\bar{k}$, where the bar denotes time reversal, and $\tau$ distinguishes neutrons from protons. Hartree-Bogolyubov optimal states are derived from a Routhian

$$R = H - \lambda A_v - \mu T_z,$$

where $A_v$ is the number of valence nucleons. The nucleon chemical potential $\lambda$ is placed midway between the lowest and the highest $\epsilon_k$, so that $\langle A_v \rangle = 2\Omega$ in the optimal state, and the isocranking angular velocity $\mu$ varied to produce a range of $\langle T_z \rangle$.

The symmetry of even $A_v/2 \pm T_z$ is imposed on the trial Bogolyubov quasiparticle vacuum. The model thus describes isobaric multiplets whose substate with $T_z = T$ belongs to a doubly even nucleus. Due to this symmetry, the $z$-coordinate of the gap isovector $\Delta = -G\langle P \rangle$ vanishes. By a suitable choice of phases, the optimal state is then an ordinary product of neutron and proton BCS states with a common real neutron and proton gap $\Delta$. For numeric convenience, $\Delta$ is kept constant with the variation of $\mu$, which results in a negligible variation of $G$.

The RPA calculation employs the standard technique of a perturbative boson expansion of products of nucleon field operators [17]. By truncating the resulting expansions of $H$ and $R$ to second order, RPA operators $\tilde{H}$ and $\tilde{R}$ are obtained. The initial symmetries of $H$ and $R$ are recovered by replacing in $\tilde{H}$ and $\tilde{R}$ truncated expansions of $A_v$ and $T$ by formal variables which obey the mutual commutation relations of the exact operators and have the same commutators with other boson operators as the truncated ones. When $\langle A_v \rangle$ and
\( \langle T_z \rangle \) are equal to eigenvalues of \( A_v \) and \( T_z \) respectively, the lowest eigenstate of the approximate Routhian thus obtained has \( A_v = \langle A_v \rangle \) and \( T = T_z = \langle T_z \rangle \). This state is also an eigenstate of the approximate Hamiltonian with an eigenvalue \( E \) that is the sum of two terms: the Hartree-Bogolyubov energy

\[
E_0 = \langle H_0 \rangle - \frac{2\Delta^2}{G} + \frac{\kappa T^2}{2}
\]

and the RPA correlation energy

\[
E_2 = \left\langle -G\Delta P^\dagger \cdot \Delta P + \frac{\kappa \Delta T^2}{2} \right\rangle + \frac{1}{2} \left( \sum \omega_{\nu} - \sum_{i<j} [b_{ij}, [\tilde{R}, b_{ij}]] \right). \tag{1}
\]

Here, \( \Delta P = P - \langle P \rangle \) and \( \Delta T = T - \langle T \rangle \), \( \omega_{\nu} \) denotes the eigenfrequencies of the boson system with Hamiltonian \( \tilde{R} \), and \( b_{ij} \) are the boson annihilation operators associated with pairs of Bogolyubov quasiparticles. \( E_0, E_2 \) and \( E = E_0 + E_2 \) are defined for any \( T = \langle T_z \rangle \) by these expressions.

In the calculation of Ref. [16], which was intended to simulate the isobaric chain with mass number \( A = 48 \), I used the Fermi gas estimate of the single-nucleon level spacing \( \eta \). As pointed out by Satula and Wyss [18] and Glowacz, Satula and Wyss [5], this gives an unrealistically large value. I have therefore repeated the calculation for two smaller values: \( \eta = 4/(6A/(c \text{ MeV})/\pi^2) \) with \( c = 8 \) and 10 [19,20,21], which gives \( \eta = 1.1 \) and 1.4 MeV respectively. Otherwise, the parameters of the present calculation are the same as in Ref. [16]: The number \( \Omega \) of equidistant, fourfold degenerate single-nucleon levels is equal to 24, the pair gap \( \Delta = 12 \text{ MeV}/\sqrt{A} = 1.7 \text{ MeV} \) [20], and the total coefficient of \( T^2/2 \) in the Hartree-Bogolyubov part of the symmetry energy \( \eta + \kappa = 2(134.4A^{-1} - 203.6A^{-4/3}) \text{ MeV} = 3.3 \text{ MeV} \) [22].

The result for the smallest single-nucleon level spacing \( \eta = 1.1 \text{ MeV} \) is shown in Fig. 1. A comparison with Fig. 1 of Ref. [16] shows that the change of \( \eta \) does not alter the situation qualitatively.\(^1\) Still, almost exactly \( E_0 - E_{0,T=0} = (\eta + \kappa)T^2/2 \). Since the pairing energy \( 2\Delta^2/G \) is essentially constant—it varies by less than .1 MeV in the range of \( T \) considered—this means that even in the presence of pairing, the ‘kinetic’ contribution to the symmetry energy, that is, the contribution from \( \langle H_0 \rangle \), is in a very good approximation equal to \( \eta T^2/2 \). This expression is easily shown to be exact for \( \Delta = 0 \).

Also like in the previous calculation, the RPA contribution to the symmetry energy \( E_2 - E_{2,T=0} \) is dominated by the frequency \( \mu \) of the normal mode associated with the direction of the isospin. This is indeed more accurately

\(^1\) Due to a computation error, \( \mu/2 - (E_2 - E_{2,T=0}) \) as shown in Fig. 1 of Ref. [16] is too large by an almost constant factor about 1.2.
true here than for larger values of $\eta$. Thus, from $T = 0$ to 4 the sum of all the other terms in $E_2$ only change by about .5 MeV for $\eta = 1.1$ MeV and about .8 MeV for $\eta = 1.4$ MeV as compared to about 1.5 MeV for the value $\eta = 2.1$ MeV given by the Fermi gas estimate. The reason for this seems obvious: With the smaller level spacing $\eta$, the isodeformation $\Delta/\eta$ is larger and the isorotation therefore more collective. This weakens the coupling between the collective and intrinsic degrees of freedom. It may be noticed that since $\Delta \propto A^{-1/2}$ and $\eta \propto A^{-1}$, the isodeformation increases with $A$. Heavier nuclei should therefore show an even more collective isorotation.

The identification of $T$ with $\langle T_z \rangle$ provides an extension of $E_2(T)$ to negative $T$. Due to the isobaric invariance of $H$, this results in an even function. The only term in $E_2$ which is not analytic at $T = 0$ is $\mu/2$, which is replaced by $-\mu/2$ for negative $T$. It follows that $E_2 - E_{2,T=0} - \mu/2$ vanishes quadratically for $T \to 0^+$. Now, apart from a negligible correction due to the fact that $\Delta$ rather than $G$ is kept constant in the calculation, we have $\mu = dE_0/dT = (\eta + \kappa)T$. The curve in Fig. 1 is in fact well approximated by the second order polynomial $E_2 - E_{2,T=0} = (\eta + \kappa)T/2 - .033$ MeV $\times T^2$. Altogether, we thus have in a good approximation

$$E - E_{T=0} = \left( \frac{\eta + \kappa}{2} - .033 \text{ MeV} \right) T(T + x),$$

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$$E - E_{T=0} = \left( \frac{\eta + \kappa}{2} - .033 \text{ MeV} \right) T(T + x),$$
where
\[ x = \left( 1 - \frac{0.033 \text{ MeV}}{(\eta + \kappa)/2} \right)^{-1} = 1.020. \]

For \( \eta = 1.4 \text{ MeV} \), this analysis gives \( x = 1.031 \). These values are consistent with the possible indications in the data of \( x \) being slightly larger than 1 [5].

From my results in Ref. [16], Glowacz, Satula and Wyss infer \( x \approx 0.8 \) for \( T = 2 \) [5]. These authors may have calculated \( (E_2 - E_{2,T=0})T/(E_0 - E_{0,T=0}) \), which is evidently not a right way of extracting \( x \) from the energies.

Nuclear masses are extensively compared with Hartree-Fock-Bogolyubov calculations. See for example Ref. [6] and references therein. If we neglect the change of optimal state by the exchange terms in the self-consistent single-nucleon potential and pair field, the difference between the Hartree-Fock-Bogolyubov and Hartree-Bogolyubov energies, the Fock term, is in the present theory precisely the first term in Expr. (1). This is a somewhat artificial term since it is cancelled by a part of the second sum in the second term.\(^2\) In fact Eq. (1) may be recast into the form

\[ E_2 = \frac{1}{2} \left( \sum_{\nu} \omega_{\nu} - \sum_{i<j}(E_i + E_j) \right), \]

where \( E_i \) is the Bogolyubov quasiparticle energy.

Satula and Wyss seem to suggest that the RPA correlation energy may be simulated by adding \( \eta \langle \Delta T^2 \rangle /2 \) to the Hartree-Fock-Bogolyubov energy [18]. Neglecting again the change of optimal state, this amounts in the present theory to replacing \( E_2 \) by

\[ E_2^* = \left\langle -G\Delta P^+ \cdot \Delta P + \frac{(\eta + \kappa)\Delta T^2}{2} \right\rangle. \]

Since this is a modification of the Fock term, which is absent in Eq. (2), a relationship between \( E_2 \) and \( E_2^* \) is not obviously anticipated. Fig. 2 shows that in fact they depend on \( T \) very differently. In particular, \( E_2^*(T) \) is even and analytic at \( T = 0 \), so \( E_2^* - E_{2,T=0}^* \) vanishes quadratically for \( T \to 0 \). Thus \( E_2^* \) does not give the empirical cusp at \( T = 0 \) in the graph of the function \( E(T) \).

\(^2\) In Ref. [16], in the third paragraph of the second column on page 289, ‘second term in the second sum’ should be as here ‘second sum in the second term’. It is understood there that if \( \Delta = 0 \), also \( G = 0 \).
The $T$-dependence of $E_2^*$ mainly reflects that of the isospin variance $\langle \Delta T^2 \rangle$. For $\Delta = 0$, we have $\langle \Delta T^2 \rangle = T$. For $\Delta > 0$, the diffuseness of the nucleon numbers makes a contribution to $\langle \Delta T^2 \rangle$ which is largest for $T = 0$. $\langle \Delta T^2 \rangle$ is an even function of $T$ and for $\Delta > 0$ analytic at $T = 0$. This results in the hyperbola-like behaviour seen in the inset of Fig. 3 of Ref. [18] and reflected in Fig. 2. For $\Delta = 0$, the first term in $E_2^*$ has a $T$-dependent part $GT/2$, which arises from blocking of the neutron-proton pairing force when nucleons are promoted from proton to neutron levels. For $\Delta > 0$, the asymptotic slope of the hyperbola gets a corresponding contribution from this term. Since $G = 0.14 \text{ MeV} \ll \eta = 3.3 \text{ MeV}$, this is small compared to the contribution of the second term. Evidently, this discussion of $E_2^*$ applies analogously to the true Fock term without the term proportional to $\eta$.

As seen from Fig. 1, the RPA contribution to the symmetry energy is in the pairing plus symmetry force model largely taken into account by adding $\mu/2$ to the self-consistent energy $E_0$. This corresponds to the approximation employed by Frauendorf and Sheikh, who added $\mu/2$ to an isocranked Hartree-Fock-Bogolyubov energy [23]. As pointed out by these authors, doing so is essentially equivalent to assigning the energy calculated for $\langle T_\alpha \rangle = T + 1/2$ or $\sqrt{T(T+1)}$ to a state with isospin $T$, where $T_\alpha$ is some isospin coordinate. In fact, if $E_0(\langle T_\alpha \rangle)$ is the calculated energy, we have $E_0\left(\sqrt{T(T+1)}\right) \approx E_0(T + 1/2) \approx E_0(T) + E_0'(T)/2 = E_0(T) + \mu/2$. Such procedures are common in ordinary cranking calculations. See references in Ref. [23]. In a context of isocranking, Satula and Wyss applied the constraint $\langle T_\alpha \rangle = \sqrt{T(T+1)}$ [24]. In the pairing plus symmetry force model, the $T$-dependence of the RPA correlation energy is seen to be taken into account by such recipes only in a crude approximation.
$E_2$ has a $T$-dependence additional to that of $\mu/2$. It is in fact this additional $T$-dependence which makes $x > 1$.

The presence of a strong isovector pair field is essential for getting $x \approx 1$. For $G = 0$ the Hartree-Fock approximation is in fact exact, and we have

$$E - E_{T=0} = \left(\eta T^2 + \kappa T (T + 1)\right)/2 = \left(\eta + \kappa\right)/2 \times T(T + x),$$

where $x = \kappa/(\eta + \kappa) = .7$ for $\eta = 1.1$ MeV. The leading contribution of the pairing force in perturbation theory $\langle -G\mathbf{P}^\dagger \cdot \mathbf{P} \rangle = G(T - 3\Omega)/2$ adds a linear term $GT/2$ to the symmetry energy, but as long as $G$ is below the threshold of pair condensation $G \approx \eta/(2 + \log(\Omega/2))$ it is much smaller than the term $\eta T/2$ required to get $x = 1$. A pair gap $\Delta$ which is comparable to the single-nucleon level spacing $\eta$ is thus necessary in order to make the quasiparticle energies and the RPA frequencies except $\mu$ so independent of $T$ that $\mu/2$ becomes the dominant term in $E_2 - E_{2,T=0}$.

In conclusion, the pairing plus symmetry force model with equidistant single-nucleon levels introduced in Ref. [16] gives in the RPA for $A = 48$ a symmetry energy proportional to $T(T + x)$, where $x \approx 1.025$. The large isovector pair field, whose strength is inferred from the observed odd-even mass staggering, is essential for this result. The RPA contribution to the symmetry energy is roughly equal to $\mu/2$, where $\mu$ is the isocranking angular velocity, but there are significant corrections to this approximation. It is in fact these corrections which make $x > 1$. The RPA contribution to the symmetry energy cannot be simulated by adding to the Hartree-Fock-Bogolyubov energy a term proportional to the isospin variance in the Bogolyubov quasiparticle vacuum.

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