

Concavity for nuclear bindings

B. R. Barrett^a, B. G. Giraud^b, B. K. Jennings^c and N. P. Toberg^d

^aUniversity of Arizona, Tucson, AZ, USA

^bCEA Saclay, Gif sur Yvette, France

^cTRIUMF, Vancouver BC, Canada

^dCMS, Cambridge, UK

Abstract

Sequences of experimental ground-state energies for both odd and even A are mapped onto concave patterns cured from convexities due to pairing. These patterns yield improved estimates by interpolation or extrapolation (as appropriate) of ground-state energies for nuclei, which have not yet been measured. An example of this procedure, using the tin isotopes is given. The same patterns, completed by a list of excitation energies, give numerical estimates of thermodynamical functions, which lead to the average nucleon number $\langle \mathbf{A} \rangle(\beta, \mu)$ becoming a continuous variable at low to moderate temperatures, allowing extrapolations towards nuclear masses closer to drip lines. Estimates of the free energy and the average energy, as functions of $\langle \mathbf{A} \rangle$, provide upper and lower bounds, respectively, to ground-state energy. Finally, we discuss extensions to a two-dimensional analysis and how concavity and universality are related to the theory of the nuclear density functional.

1 Introduction

The role of concavity in nuclear structure is studied in three cases: 1.) empirical extrapolations and interpolations, 2.) nuclear thermodynamical functions, and 3.) the nuclear density functional. Our general argument follows from the well-known observation regarding N^2 and Z^2 terms, for the neutron and proton numbers, respectively, in the semi-empirical mass formula for atomic nuclei [1]. They naturally lead to a concave trend, when empirical data for nuclear ground-state (g.s.) energies are plotted for isotopic, isotonic or isobaric chains or as two-dimensional plots in N and Z . This is particularly evident, when the overall linear trend in the data, due to the fact that the binding energy (BE) per nucleon is ~ 8 MeV, is removed. We propose to smooth this trend towards concavity in the nuclear data by removing pairing effects and adding a small parabolic correction, so as to guarantee an overall positive second derivative to the plotted data. Such concave plots of the data lead to improved estimates of unknown g.s. energies by extrapolations (producing a lower bound) and interpolations (producing an upper bound). An example of this procedure is given for the tin (Sn) isotopes in Section 2.

Since concavity is also a property of several nuclear thermodynamical functions, we also extend our zero-temperature analysis to finite temperatures. In Section 3 we observe that at finite temperatures plots of the average energy $\langle \mathbf{H} \rangle$ and the free energy, $\mathbf{F} = \langle \mathbf{H} \rangle - T\mathbf{S}$, as functions of the average particle, (*i.e.*, nucleon) number $\langle \mathbf{A} \rangle$, lead to upper and lower bounds, respectively, for the energy. This allows us to put error bars on our predicted results. In Section 4 we discuss the extension of our approach to two-dimensions, *i.e.*, N and Z , and the relation of concavity with the derivation of a nuclear density functional [2]. A summary, discussion and conclusions are given in Section 5.

2 Concavity for experimental ground-state energies

We now give an example of our approach using the experimental g.s. energies for the Sn isotopes, for which considerable data is known [3–6]. The solid line in Fig. 1 shows a plot of the energies, E_A , in keV for ^{110}Sn to ^{134}Sn , in which the overall linear trend has been removed by adding $7500A + 115000$ to E_A .

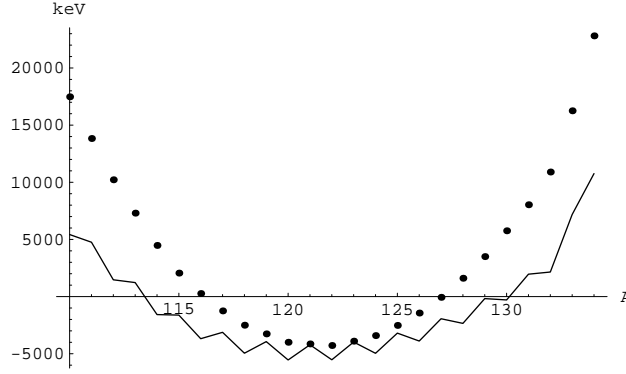


Fig. 1: Sn isotope energies: irregular line joining *raw* experimental ground-state energies $E_A + 7500A + 115000$; pairing and parabolic corrections give the nonconnected black dots.

The general concave shape of the data is apparent as well as the odd-even staggering due to pairing. Next we add to each *even* nucleus energy a fixed number, for example $p(N, Z) = 1250$ keV, to suppress the increased binding due to pairing. Calculating the second differences (SDs), $E_{A+1} - 2E_A + E_{A-1}$, we find that a few of them are still slightly negative. We now make all SDs positive by adding a small, artificial, parabolic correction, $P \times (A - 122)^2$, with $P = 75$ keV. The lowest point, $A_0 = 122$, is arbitrary, because the SDs will increase by just a constant, namely twice the coefficient P of the A^2 term. Our result for the new, purely concave energies, $E'_A = E_A + 7500A + 115000 + p \times \text{Mod}[A + 1, 2] + P \times (A - 122)^2$, is illustrated by the black dots in Fig. 1.

An application of this procedure is shown in Fig. 2, in which it is assumed that the g.s. energy for ^{132}Sn is unknown. The left-hand plot shows two extrapolations and an interpolation, based on the *raw* data E_A , while the right-hand plot gives two extrapolations and the interpolation, based on the concave energies E'_A . Comparing the numerical results for both examples, one finds that in all three cases an extrapolation or interpolation from the concave energies E'_A yields a better estimate for the unknown energy, than its counterpart from the *raw* energies E_A . One also observes that for the concave energies E'_A , extrapolations *always* yield lower bounds and interpolations *always* yield upper bounds and, thereby, provide an error bar on our predictions. See Ref. [7] for the actual numerical results and more examples.

3 Concavity with thermodynamical functions

Consider the particle number operator \mathbf{A} and an usual two-body nuclear Hamiltonian $\mathbf{H} = \sum_{i=1}^A t_i + \sum_{i>j=1}^A v_{ij}$, where $A = N + Z$, t and v are the mass number, one-body kinetic energy and two-body interaction, respectively. Nuclear data tables [8,9] give precise values for a large number of lowest-lying eigenvalues E_{nA} of \mathbf{H} for many nuclei. One may, thus, reasonably estimate the grand partition function,

$$\mathcal{Z}(\mu, \beta) = \text{Tr} \exp[\beta(\mu\mathbf{A} - \mathbf{H})] = \sum_{nA} (2j_{nA} + 1) \exp[\beta(\mu A - E_{nA})], \quad (1)$$

and the negative of the grand potential

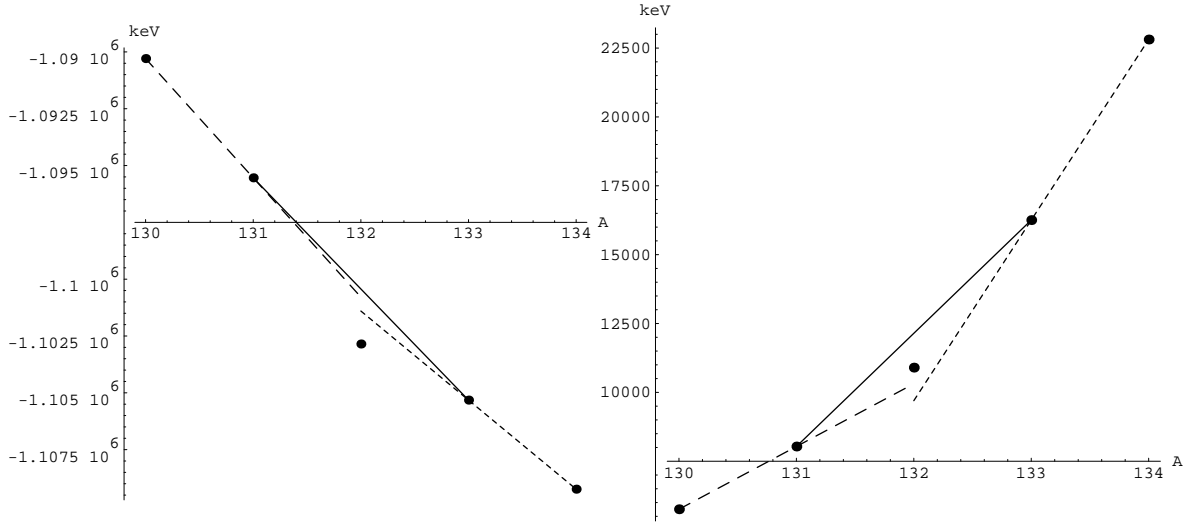


Fig. 2: Left, raw energies: full line, interpolation from ^{131}Sn and ^{133}Sn ; long dashes, extrapolation from ^{130}Sn and ^{131}Sn ; short dashes, extrapolation from ^{134}Sn and ^{133}Sn . Dots represent the experimental energies E_A . Right: same inter- and extrapolations, concave data.

$$-\Omega(\mu, \beta) = \langle (\mu \mathbf{A} - \mathbf{H}) \rangle + T \mathbf{S} = \beta^{-1} \ln \mathcal{Z} = \beta^{-1} \ln \left\{ \sum_{nA} (2j_{nA} + 1) \exp [\beta (\mu A - E_{nA})] \right\}, \quad (2)$$

provided that i) the temperature, $T = \beta^{-1}$, is low enough to allow a truncation of the spectrum to include only those states provided by the tables and ii) the chemical potential, μ , selects mainly those nuclei in which we are interested. We use $-\Omega$, because it is known to be a concave function of T and μ .

From Eqs. (1) and (2) and the derivatives of $-\Omega$ with respect to μ and T , we can determine $\langle \mathbf{A} \rangle$, the entropy \mathbf{S} , $\langle \mathbf{H} \rangle$, and, consequently, the free energy $\mathbf{F} = \langle \mathbf{H} \rangle - T \mathbf{S}$. Our goals are:

1. To determine $\langle \mathbf{H} \rangle$ and $\langle \mathbf{A} \rangle$ as a function of μ for a given finite temperature T .
2. To obtain $\langle \mathbf{H} \rangle$ as a function of $\langle \mathbf{A} \rangle$ by eliminating μ between these two quantities. Note that A is discrete but $\langle \mathbf{A} \rangle$ can be treated as a continuous variable at an appropriate temperature. From the definition of the free energy, it follows that \mathbf{F} is also a continuous function of $\langle \mathbf{A} \rangle$. In addition, it is straightforward to prove that \mathbf{F} is a concave function of $\langle \mathbf{A} \rangle$.
3. To determine a sufficient temperature T , at which $\langle \mathbf{A} \rangle$ can be treated as a continuous variable and $\langle \mathbf{H} \rangle$ is a concave function of $\langle \mathbf{A} \rangle$.
4. To utilize $\langle \mathbf{H} \rangle$ and \mathbf{F} to set error bars on our predicted, extrapolated g.s. energies.

Figure 3 gives a plot of the particle number fluctuation for the Sn isotopes for two values of T , *i.e.*, $T = 60$ and 150 keV. Our criterion, for $\langle \mathbf{A} \rangle$ to be continuous, is that the particle number fluctuation be at least 0.5 or larger, which is seen to be true for $T = 150$ keV but not for $T = 60$ keV. We also find that for $T \sim 150$ keV $\langle \mathbf{H} \rangle$ becomes a concave function of $\langle \mathbf{A} \rangle$. As seen in Fig. 4, $\langle \mathbf{H} \rangle$ approaches the physical g.s. energy from above and the free energy \mathbf{F} approaches it from below, in the limit of $T \rightarrow 0$. Thus, at a given temperature T , $\langle \mathbf{H} \rangle$ and \mathbf{F} provide upper and lower bounds, respectively, on the physical

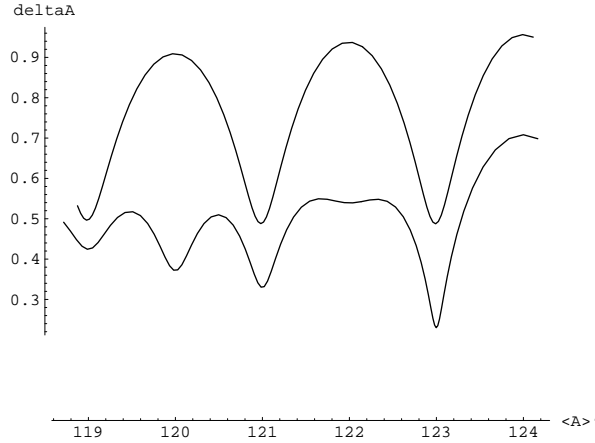


Fig. 3: Particle number fluctuation. Upper (lower) curve, $T = 150$ (60) keV.

g.s. energy for a given value of T . These bounds allow us to place error bars on our predicted values of unknown g.s. energies, as we extrapolate $\langle \mathbf{H} \rangle$ as a function of $\langle \mathbf{A} \rangle$ towards the drip lines. From Fig. 4 we observe that for the Sn isotopes and $T \sim 150$ keV we obtain an error bar of ~ 500 keV between the energy and the free energy. Note that in Fig. 4 we have used the concavity tuned energies E'_{nA} ; consequently, the primes on all quantities.

4 Two-dimensional analysis and the nuclear density functional

What we have done in Sections 2 and 3 for one-dimensional studies in N or Z can be extended in a similar manner to a two-dimensional analysis in terms of N and Z . Again one can calculate SDs in the N , Z , A and $N - Z$ directions and make an A -dependent pairing correction [10] plus a small parabolic term.

Rather than make a systematic study in two-dimensions in this paper, we would prefer to discuss the relation of concavity with the derivation of a nuclear density functional. Recall that, given an arbitrary many-body density matrix \mathcal{M} in Fock space, the density functional follows from the definition [11],

$$\mathcal{F}[\rho_p, \rho_n] = \text{Inf}_{\mathcal{M} \rightarrow \rho_p, \rho_n} \text{Tr } \mathbf{H} \mathcal{M}. \quad (3)$$

Here the symbol, $\mathcal{M} \rightarrow \rho_n, \rho_p$, means that a minimization of the energy is performed upon density matrices having the same neutron and proton profiles ρ_n, ρ_p . A nucleus is identified by the integrals, $N = \int d\vec{r} \rho_n(\vec{r})$ and $Z = \int d\vec{r} \rho_p(\vec{r})$, and a later minimization is performed with respect to the profiles ρ_n, ρ_p under such identification constraints,

$$E_{ZN} = \text{Inf}_{\rho_n \rightarrow N, \rho_p \rightarrow Z} \mathcal{F}[\rho_n, \rho_p]. \quad (4)$$

The functional \mathcal{F} should be universal, in the nuclear physics sense. Namely, it should not depend on N and Z . (In atomic and molecular physics, universality of the density functional has a different meaning; it refers to arbitrary external potentials.) While BCS and Hartree-Bogoliubov calculations allow a distinction between even and odd particle numbers, universality in density profile space does not allow such a separate treatment. Observe, furthermore, that, because of the fact that there are many convexities

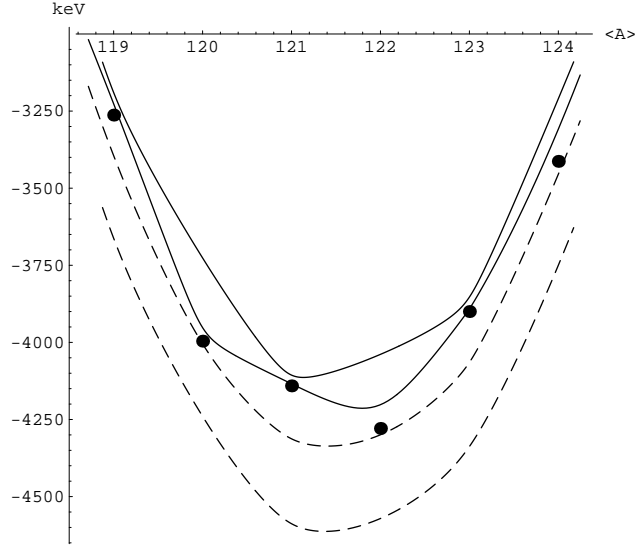


Fig. 4: Energy $\langle \mathbf{H} \rangle'$ (full curves) and free energy \mathbf{F}' (dashed ones) as functions of $\langle \mathbf{A} \rangle'$, calculated from concavity tuned energies E'_{nA} . Dots represent tuned, ground-state energies, $E'_{0A} \equiv E'_A$, already used in Fig. 1 and the rhs part of Fig. 2. Upper full and lower dashed curves, $T = 150$ keV. Lower full and upper dashed curves, $T = 60$ keV. Notice how the full curves turn out to be concave.

in the pattern of *raw* energies, there *exist many cases* where, for instance, three nuclei, A_1, A_2, A_3 , are such that $N_2 = (N_1 + N_3)/2$ and $Z_2 = (Z_1 + Z_3)/2$ and $(E_1 + E_3)/2 < E_2$. Then, in a search for E_2 , the mixture density matrix, $\mathcal{M}_{mix} = (|A_1\rangle\langle A_1| + |A_3\rangle\langle A_3|)/2$, provides the correct average particle numbers N_2, Z_2 , but an absurd energy, lower than E_2 . This effect can also be understood from the right-hand side of Fig. 2, where the interpolated value from the concave-corrected data *must always* be an upper bound, *i.e.*, must be above the physical g.s. energy for a given value of A . This is not necessarily true for the *raw* data, although it happens to be so in the left-hand side of Fig. 2. Therefore, we conclude that concavity is a *mandatory condition* for the *universality* of \mathcal{F} .

5 Summary, discussion and conclusions

We have demonstrated how a list of g.s. energies for a sequence of isotopes can be turned into a concave pattern. This involves simple manipulations; for instance, an explicit term, accounting for pairing in even nuclei, can be subtracted from the bindings. This unifies the treatment of odd and even nuclei, a notoriously difficult problem. If needed, a small quadratic correction can also be added to guarantee concavity at all points along the sequence.

Similar arguments leading to concavity clearly hold for isotones as well, and, furthermore, for any other sequence of neighboring nuclei in any direction across the nuclear table. Once this empirical tuning has been implemented, linear (or more general) extra- and interpolations of the concave pattern can provide surprisingly accurate and robust estimates of, or bounds for, binding energies. These tuning terms, which are added to induce concavity, are, of course, subtracted *in fine* (see Ref. [7] for details).

We then defined a more ambitious extra- and interpolation scheme, involving thermodynamical functions from a grand canonical ensemble, because such functions may have rigorous concavity properties. Theorems are, indeed, available to prove such properties. For instance, the free energy is a concave

function of the average particle number and is also a decreasing function of the temperature. We also discovered that the average energy at nonzero temperature turns out, in general, to be a concave function of the average particle number, depending upon the temperature.

For every given, finite temperature, we found that the average energy and the free energy, as functions of the average particle number, give upper and lower bounds, respectively, for the concave envelope of the g.s. energies. When the temperature vanishes, both bounds converge to the exact results. At this vanishing temperature, however, the analyticity of such thermodynamical functions is lost, because their limit is only piecewise continuous. It is, therefore, necessary to retain a minimum temperature, if one wants to obtain practical extrapolations for the prediction of exotic nuclei. A minimum amount of particle number fluctuation is necessary to validate the conversion of particle number, an initially discrete quantity, into a continuous variable. We implemented numerical estimates of several thermodynamical functions at moderate temperatures, a few hundred keV at most. This yields a “band”, enclosing g.s. energies between the average energy and the free energy. The width of the band defines an error bar, which can be trusted, when extrapolations are made. We can make the strong conclusion that the combination of concavity and extrapolations of thermodynamical functions gives a systematic set of upper and lower bounds for the prediction of g.s. energies.

Our last, and perhaps most important result, is the connection between concavity and the universality of the density functional. In a two-dimensional analysis, we argued that the nuclear Hamiltonian *must* be concave in terms of the proton and neutron number operators, so as to guarantee obtaining consistent energy minima everywhere in density space. Based on numerical studies, we estimate that this concavity correction can be made minimal if counterterms for pairing are also added.

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