Systematics of Quadrupolar Correlation Energies

M. Bender,1 G. F. Bertsch,1 and P.-H. Heenen2

1Department of Physics and Institute for Nuclear Theory Box 351560, University of Washington, Seattle, Washington 98195, USA
2Service de Physique Nucléaire Théorique, Université Libre de Bruxelles, CP 229, B-1050 Brussels, Belgium

(Received 5 October 2004; published 17 March 2005)

We calculate correlation energies associated with the quadrupole shape degrees of freedom with a view to improving the self-consistent mean-field theory of nuclear binding energies. Systematic results are presented for 605 even-even nuclei from mass number 16 to the heaviest whose mass has been measured, using the Skyrme SLy4 interaction and the generator coordinate method. Correlation energies range from 0.5 to 6.0 MeV, and their inclusion improves two qualitative deficiencies of the mean-field theory, namely, the exaggerated shell effect at neutron magic numbers and the failure of mean-field theory to describe mutually enhanced magicity. For the mass table as a whole, the quadrupolar correlations improve binding energies, separation energies, and separation energy differences by 20%-30%.

DOI: 10.1103/PhysRevLett.94.102503 PACS numbers: 21.60.Jz, 21.10.Dr

More than 3000 atomic nuclei with different combinations of proton number Z and neutron number N have been experimentally identified so far, and for about 2000 of them their masses, or, equivalently, their binding energies, have been measured [1]. This number is only a fraction (about 25%) of all the nuclei which are predicted to be bound, i.e., stable against nucleon emission. Since a large fraction of the unknown nuclei seems out of reach to be studied experimentally, an accurate theory of binding energies is needed. For example, one of the important motivations for studying nuclei far from stability is to better understand nucleosynthesis and the astrophysical environment for studying nuclei far from stability.

Among the theories of nuclear binding energy, the self-consistent mean-field theory [3] stands out as a fundamentally justified approach that is also computationally tractable over the entire mass table. Global calculations of binding energies are now available including both pairing and deformation effects in the mean field, using energy functionals of the nonrelativistic Skyrme form [4] or a relativistic mean-field model [5]. A systematic problem with such theories is an exaggeration of the increased binding at magic numbers, the shell effect. The accuracy of these pure mean-field theories is at best of 1.5–2.0 MeV rms errors in binding energies [6], much poorer than that of more phenomenological approaches such as the finite range liquid droplet model [7].

An obvious route to improve the theory is to include correlation effects. Indeed, this has already been done in a phenomenological way with good results [8,9]. Some correlation effects can be subsumed in the parametrization of the mean-field energy functional, but not all. Most obviously, the rotational correlation energy of deformed nuclei is beyond mean-field theory, which can describe only the intrinsic state of a rotational band. The requirements on a theory of correlation energies are severe. Besides being computationally tractable, it must be systematic, applicable to both spherical and deformed nuclei. One approach suggested by many-particle perturbation theory is the random phase approximation (RPA) theory of correlation energies. While it is difficult to apply RPA directly for short-ranged interactions [10], a collective treatment has recently been applied to the binding energy problem by Baroni et al. [11].

In this Letter we report on global calculations of correlation energies in another well-defined theoretical extension of the mean-field approximation [12], based on the generator coordinate method (GCM) which, contrary to RPA, is well suited to describe large-amplitude collective motion. The quadrupolar fluctuations about the mean-field solution are determined variationally by mixing configurations around the mean-field ground state. Our method includes also a projection on good angular momentum and particle number and applies to all nuclei irrespective of the shape characteristics of their ground states. It is thus systematic, which is an important criterion for constructing mass tables. It also satisfies the goal of including in the correlation energy the rotational energy of deformed states.

The technical details of our calculation are as follows. The self-consistent mean-field equations are solved using the method presented in Ref. [13]. Here the wave functions are represented on a triaxial three-dimensional spatial grid, rather than in an oscillator basis as was done in Refs. [4,5]. The effective nucleon-nucleon interaction is an energy density functional of the Skyrme form. We have used the SLy4 parameter set [14]. This set was fitted to nuclear matter properties, nuclear charge radii, as well as binding energies of doubly magic nuclei. It has recently been applied with good results to the shape coexistence of neutron-deficient Pb isotopes [15], using the same extensions of the mean-field theory as we apply here. Other Skyrme parametrizations leading to lower rms errors on masses [9] have been proposed recently. However, they are
used in conjunction with phenomenological corrections, in particular, for rotations and therefore are not appropriate for a purely microscopic theory. We included a local pairing interaction of the form used in Ref. [16], but with a reduced strength of $v_0 = -1000$ MeV fm$^3$ to compensate the explicit correlations added by the generator coordinate treatment [12].

The GCM has as ingredients a set of wave functions generated by constrained mean-field calculations and a Hamiltonian for calculating matrix elements among those configurations. The constraint that we use is the quadrupole operator $Q(r)$, and we minimize the function

$$E[\phi] - \lambda \int d^3r \rho(r)Q(r).$$

Here $\rho$ is the mass density and $\lambda$ is a Lagrange multiplier adjusted to get a specific value of the quadrupole moment $q = \int d^3r \rho(r)Q(r)$. The value of $q$ is positive for prolate and negative for oblate deformations. The choice of the configurations $|q\rangle$ is a computational issue that has to be carefully addressed for systematic calculations. If states are too closely spaced, there is a large redundancy as well as an excessive computational cost. We have tailored our selection of configurations for a target accuracy of 0.2 MeV in the correlation energies. In Ref. [17], it was found that this accuracy can be achieved when overlap probabilities of neighboring configurations are about 0.5 or higher, and we adopt that criterion here. We also restrict the deformations to shapes that have energies within 5 MeV of the mean-field ground state. Typically this gives $n_q = 7$–20 different configurations in our computational space [18].

There is an ambiguity in the choice of the Hamiltonian $\hat{H}$ for use with a mean-field energy functional [19]. We use the so-called mixed density for the calculation of the density-dependent term in the Skyrme Hamiltonian, as is mostly done in the literature [20]. The GCM energy is the minimum of the expression

$$\frac{\langle \Psi | \hat{H} | \Psi \rangle}{\langle \Psi | \Psi \rangle},$$

where $|\Psi\rangle$ is an arbitrary state in the basis of the $|q\rangle$. The minimization is performed by solving the corresponding discretized Hill-Wheeler equations [21]. The orientation of the intrinsic deformed states $|q\rangle$ could be considered a continuous degree of freedom to be included in the minimization, but in practice we achieve the same result by projecting the intrinsic states on angular-momentum zero when calculating matrix elements. The theoretical correlation energy is then obtained in two steps: we determine first the energy gain of an angular-momentum projected configuration $|q\rangle$ with respect to the mean-field minimum, $E_{j=0}$, and after that the additional energy gained by mixing configurations with different $q$ magnitudes, $E_{HW}$.

The needed matrix elements $\langle q'|q\rangle$ and $\langle q'|\hat{H}|q\rangle$ are calculated with the computer code described in Ref. [12]. Besides performing the rotations to calculate the matrix elements needed for angular-momentum projection, the code carries out a projection of the BCS wave function on good particle numbers $N$ and $Z$. The rotation operation is computationally very demanding, and it was necessary to find additional computational shortcuts to make the global study feasible. One important savings was the use of a topological Gaussian overlap approximation (GOA) which allows a two-point evaluation of the angular-momentum projection integrals [18,22]. The top GOA was found to be quite adequate, except for very light nuclei, where a three-point approximation was sometimes needed. Another place where we made considerable computational savings was in the calculation of off-diagonal matrix elements in the $|q\rangle$ space. In principle, an $n$-dimensional basis requires the calculation of $n(n + 1)/2$ overlaps and Hamiltonian matrix elements. These must be done explicitly for neighboring configurations, but matrix elements for more distant configurations can be estimated using another Gaussian ansatz based on a measure of the separation between the configurations [17]. A tricky point arises in the mixing of weak prolate and oblate deformations which can have very high overlaps. We deal with this problem by defining a two-dimensional metric for calculating the separation of configurations as described in Ref. [18]. With these approximations, the computational effort for the GCM minimization was reduced by 1 to 2 orders of magnitude, but still requiring on the order of $10^{17}$ floating point operations for the entire table of 605 nuclei. Results for three typical heavy nuclei are shown in Table I. The first column, $E_{def}$, gives the energy difference between the spherical and unconstrained minima in the mean-field energy. The second column, $E_{j=0}$, gives the difference between the mean-field minimum and the angular-momentum projected minimum. The third column, $E_{HW}$, gives the additional energy associated with the Hill-Wheeler mixing of deformations, and the last column, $E_{corr} = E_{j=0} + E_{HW}$, is the total correlation energy.

Our calculations include all but the lightest even-even nuclei for which the mass is known. The results presented in Fig. 1 are displayed as a function of neutron number $N$ with isotopes connected by lines. On the top panel, we show the energy difference between the SLy4 mean-field theory and experiment [23]. Here the shell effect is very prominent at neutron numbers $N = 50, 82,$ and $126$. The middle panel shows the calculated quadrupolar correla-

<table>
<thead>
<tr>
<th>Nucleus</th>
<th>$E_{def}$</th>
<th>$E_{j=0}$</th>
<th>$E_{HW}$</th>
<th>$E_{corr}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{208}$Pb</td>
<td>0.0</td>
<td>-1.7</td>
<td>0.0</td>
<td>-1.7</td>
</tr>
<tr>
<td>$^{180}$Hg</td>
<td>-3.0</td>
<td>-2.6</td>
<td>-0.5</td>
<td>-3.1</td>
</tr>
<tr>
<td>$^{170}$Hf</td>
<td>-12.2</td>
<td>-2.9</td>
<td>-0.5</td>
<td>-3.4</td>
</tr>
</tbody>
</table>
tions energies. One sees that, for most nuclei, it is between 3 and 4 MeV, irrespective of whether the nucleus is spherical or deformed. However, near doubly magic nuclei, the correlation energy is much smaller. This difference has the right sign to mitigate the too-strong shell effect of the mean-field theory. The bottom panel in Fig. 1 shows the binding energies with and without inclusion of the correlation energy. The relative overbinding at magic numbers with respect to open-shell nuclei is reduced, but there remains some residual shell effect. Since we have included only the axial quadrupolar field, there could be significant correlation energies arising from other kinds of deformation or from pairing vibrations around closed shells [11]. The rms deviation from experimental energies has been decreased from 5.3 to 4.4 MeV by quadrupolar correlations (see Table II as well for other measures of the quality of the theory).

A feature of the binding systematics that has been difficult to understand in mean-field theory is “mutually enhanced magicity” [24,25], the enhancement of shell effects when both neutrons and protons are near magic numbers. This can be seen in the neutron dependences of the two-proton gap, defined as

\[ \delta_{2n}(N,Z) = E(N,Z - 2) - 2E(N,Z) + E(N,Z + 2). \]  

In the independent-particle shell model, \( \delta_{2p} \) is proportional to the difference between the Fermi energies of nuclei differing by two protons, and thus it is a measure of shell gaps. This quantity is plotted in Fig. 2 for the \( Z = 50 \) (Sn) and \( Z = 82 \) (Pb) proton gaps, with the experimental points shown by black diamonds. There is clearly a reduction of \( \delta_{2p} \) when going away from the doubly magic \(^{132}\)Sn with 82 neutrons and doubly magic \(^{208}\)Pb with 126 neutrons. Neglecting deformations, the mean-field prediction for \( \delta_{2p} \) is quite flat, as shown by the short-dashed lines on the graphs. This reflects the independence of the single-particle proton gap on the neutrons in that approximation [26]. Allowing deformations in the mean-field energies already gives a change into the right direction, as shown by the long-dashed lines. The calculation including the full quadrupole correlation energy is shown by the solid lines. Since the gain in total energy due to correlations is larger for nonmagic nuclei than for doubly magic ones, the calculation is even closer to experiment. The correlation energy thus provides a plausible explanation of mutually enhanced magicity. This conclusion is corroborated by a recent calculation of \( \delta_{2p} \) in the Sn chain using the Bohr Hamiltonian, showing also the large improvement brought by quadrupolar correlations [27].

Finally, we present the rms residuals of the theoretical and experimental energies and energy differences in Table II. In principle, the comparison should be done with readjusting the Skyrme parameters to optimize the fit for each level of the theory, but we believe the numbers shown for SLy4 without readjust will be indicative. One sees from the first two lines of the table that the residuals in the binding energy decreases by a factor of 2 when static deformations are permitted in the mean field. Further increases in accuracy are obtained by allowing the correlations that we calculated here, but the improvement is much more modest. Further improvements might be obtained by including correlation effects related to octupole deformations, pairing vibrations [11,28], or nonaxial quadrupole deformations. One of the major challenges that remains open is to identify the effect that causes the so-called Wigner energy that is responsible for the scatter of the residuals around the light \( N = Z \) nuclei in Fig. 1 and to efficiently model it.

![FIG. 1. Top panel: Difference of experimental and mean-field energies for the SLy4 interaction [4], as a function of neutron number with lines connecting isotopic chains. Middle panel: Theoretical quadrupolar correlation energies of the even-even nuclei. Note the expanded energy scale. Bottom panel: Difference of experimental and theoretical energies including the correlation energy.](image)

<table>
<thead>
<tr>
<th>Theory</th>
<th>Binding energy</th>
<th>( S_{2n} )</th>
<th>( S_{2p} )</th>
<th>( \delta_{2n} )</th>
<th>( \delta_{2p} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Spherical mf</td>
<td>11.93</td>
<td>1.64</td>
<td>1.66</td>
<td>1.23</td>
<td>1.51</td>
</tr>
<tr>
<td>Axial mf</td>
<td>5.33</td>
<td>1.07</td>
<td>0.93</td>
<td>1.17</td>
<td>1.06</td>
</tr>
<tr>
<td>( J = 0 ) proj</td>
<td>4.31</td>
<td>0.89</td>
<td>0.79</td>
<td>0.96</td>
<td>0.91</td>
</tr>
<tr>
<td>GCM HW</td>
<td>4.36</td>
<td>0.84</td>
<td>0.76</td>
<td>0.84</td>
<td>0.86</td>
</tr>
</tbody>
</table>
We thank H. Flocard and D. Lunney for stimulating conversations, and B. Sabbey for help on the calculations. This work is supported by the U.S. Department of Energy under Grant No. DE-FG02-00ER41132 and the Belgian Science Policy Office under Contract No. PAI P5-07. The computations were performed at the National Energy Research Scientific Computing Center, supported by Department of Energy under Contract No. DE-AC03-76SF00098. P. H. H. thanks the Institute for Nuclear Theory for hospitality where part of this work was carried out.


[20] We also omit some small terms that appear in the Hamiltonian formulation of the Skyrme interaction but not in the energy density functional.


[23] Since the SLy4 interaction was fitted to only magic nuclei, the other nuclei show a trend of increasing residuals with mass number. This is easily removed by a minor adjustment of parameters [6].


