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Displacement energies with the Skyrme Hartree–Fock method

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Abstract

The binding energy differences of mirror nuclei are calculated with the Skyrme Hartree–Fock method and compared to experiment. The Nolen–Schiffer anomaly can be accounted for either by dropping the Coulomb exchange term or by introducing a charge-symmetry breaking interaction. The displacement energy systematics can be quantitatively reproduced with either of these modifications. The results are important for an accurate description of the proton and neutron drip lines. The possible origins of these modifications in terms of nuclear correlations and nucleon-nucleon charge-symmetry breaking interactions are discussed.

One of the classic problems in nuclear structure physics is to understand the displacement energies of nuclei. The displacement energy is the binding energy difference between mirror nuclei (those with the same atomic number A but with the proton Z and neutron N numbers interchanged). If the nuclear force is charge symmetric, then this binding energy difference can be related to the well-understood Coulomb interaction between the protons. However, it was shown by Nolen and Schiffer [1] that there was a systematic reduction in the experimental displacement energies compared to those calculated with a charge symmetric strong interaction (the Nolen–Schiffer anomaly). There have since been many papers which have investigated the various aspects of this anomaly, and it is generally agreed that both nuclear correlations and a charge-symmetry breaking (CSB) strong interaction are important for its understanding. Previous work has focussed on the cases near the closed shell nuclei ^{16}O and ^{40}Ca [2–8]. It is the purpose of this letter to consider the properties of all measured displacement energies in the framework of the Skyrme Hartree–Fock method.

Since the implementation of the Skyrme interaction [9] by Vautherin and Brink [10], this model has proven remarkably useful and successful for nuclear Hartree–Fock calculations. It incorporates the essential physics in terms of a minimal set of parameters, e.g., an s- and p-wave expansion of an effective nucleon–nucleon interaction together with a density–dependent part which accounts for the truncation of the shell–model space to a closed-shell configuration as well as for three-body interactions. Since the interaction is phenomenological, the parameters need to be determined from experimental data.

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We start with a basic Skyrme hamiltonian which contains the central and spin-orbit potentials. The details of this interaction and the data which are used to determine its parameters are discussed in Ref. [11]. For the Coulomb interaction, one must consider the direct and exchange terms in the energy density functional. A fit of the Skyrme parameters with this normal version of the Coulomb interaction is discussed in Ref. [11] and is referred to there as the SKXce parameterization (which stands for the SKX set of parameters with the Coulomb exchange included). This interaction fits all data well with the outstanding exception of the ^{48}Ni–^{48}Ca displacement energy. This displacement energy is not measured experimentally but can be reliably extrapolated from the displacement energy systematics in the $f_{7/2}$ shell nuclei [12–14]. The recent discovery of ^{48}Ni is consistent with the mass obtained from the $f_{7/2}$ extrapolations [15]. It was found in Ref. [11] that the $A = 48$ displacement energy could be reproduced if the Coulomb exchange term is ignored in the energy density functional; this interaction is called SKX. It was suggested in Ref. [11] that the Coulomb exchange term might be cancelled by the effects of nuclear correlations which go beyond the single Slater determinant approximation.

In this letter we consider the complete set of displacement energy data in terms of the SKX model. In addition to the SKX and SKXce parameterizations mentioned above, we consider a new interaction called SKXcsb which includes charge symmetry breaking (CSB) in the *s*-wave part of the Skyrme interaction together with the usual direct and exchange Coulomb terms.

The direct Coulomb potential is obtained by folding the calculated charge distribution, $\rho_{\rm ch}(r)$, with the two-body Coulomb interaction. The exchange part of the Coulomb interaction comes from the Slater approximation [16] and is the first term of the density matrix expansion in the local density approximation [17]:

$$V_{\rm Coul,exch} = -x_c e^2 \left(\frac{3}{\pi}\right)^{1/3} \rho_{\rm ch}^{1/3}, \qquad (1)$$

where x_c is a parameter which can be used to modify its strength. This total exchange energy calculated with Eq. (1) (with $x_c = 1$) has been shown to be a good approximation to an exact calculation [18] (this will be discussed in more detail below). The charge distributions contains the center-of-mass and spin-orbit corrections [19], and there is also a small contribution to the displacement energy due to the difference between the proton and neutron masses in the kinetic energy term.

The CSB modification of the Skyrme interaction is expressed as a change to the proton–proton ('pp') and neutron–neutron ('nn') *s*-wave interactions:

$$V^{\rm pp}_{\rm Skyrme} = t_0(1-x_0)(1+x_a)\,\delta,$$

$$V^{\rm nn}_{\rm Skyrme} = t_0(1-x_0)(1-x_a)\,\delta, \qquad (2)$$

where x_a is a parameter to be determined.

The experimental data considered for the Skyrme parameter fit are those described in Ref. [11] consisting of data for doubly-magic nuclei which include 11 binding energies, 5 rms charge radii and 79 single-particle energies. These data alone determine only six of the the ten conventional Skyrme parameters (t_0, t_1, t_2, t_3, x_0 and W_0). Consideration of nuclear matter and neutron matter properties helps to constrain the remaining four (x_1, x_2, x_3 and α). SKXce contains only the usual Skyrme parameters. SKX includes the additional parameter x_c and SKXcsb contains the additional parameter x_a. The parameters are determined by minimizing the quantity $\chi^2 = \sum_i w_i^2 (d_i^{\rm exp} - d_i^{\rm th})^2/[(N_d - N_p)]$, where the sum runs over the i data points d_i. $w_i = 1/\sigma_i$ is the theoretical weight corresponding to the theoretical error σ_i, N_d is the number of data and N_p are the number of parameters. The data set is the same as that considered in Ref. [11].

The χ values for the three forms considered are 1.5 for SKXce, 0.72 for SKX, and 0.74 for SKXcsb. The larger χ value for SKXce is entirely due to the data point for the $A = 48$ displacement energy. (If the $A = 48$ displacement energy is left out of the fit [11] the χ value is 0.65.) The modification of the strength of the exchange part of SKX is such that x_c is zero within its uncertainty and for simplicity SKX is taken to have $x_c = 0$ (no Coulomb exchange). For SKXcsb, the parameter x_a is determined mainly from the $A = 48$ displacement energy and the fit gives $x_a = -0.014 \pm 0.002$. We do not regard the

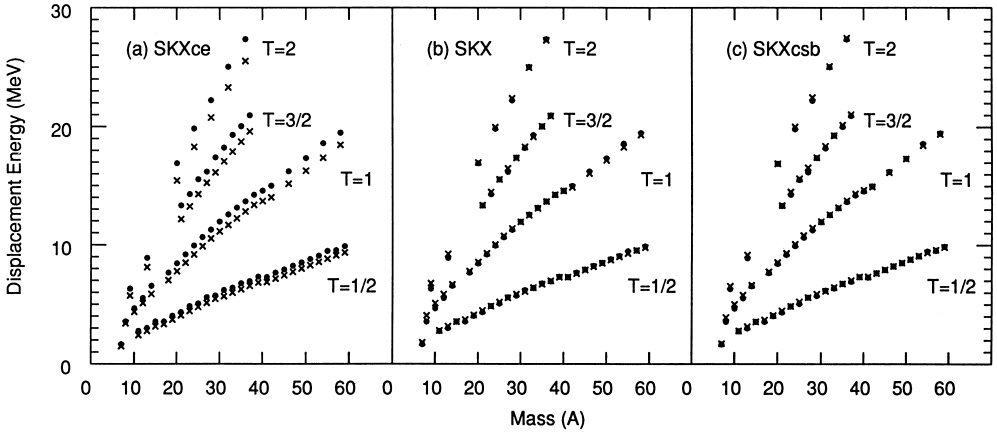

Fig. 1. Displacement energies as a function of A for SKXce (with the normal Coulomb exchange term), SKX (without the exchange term) and SKXcsb (with the exchange term and with a CSB interaction). The data are the filled circles and the calculations are the crosses.

$x_c = 0$ solution as evidence that the Coulomb exchange term itself is missing, but rather that there may be another term in the energy density functional which happens to cancell the exchange term (see below).

The results for the measured displacement energies are shown in Fig. 1 for the actual values and in Fig. 2 for the ratio and difference between the experimental and calculated values. Points are given for all cases with $A \geq 7$ where the experimental binding

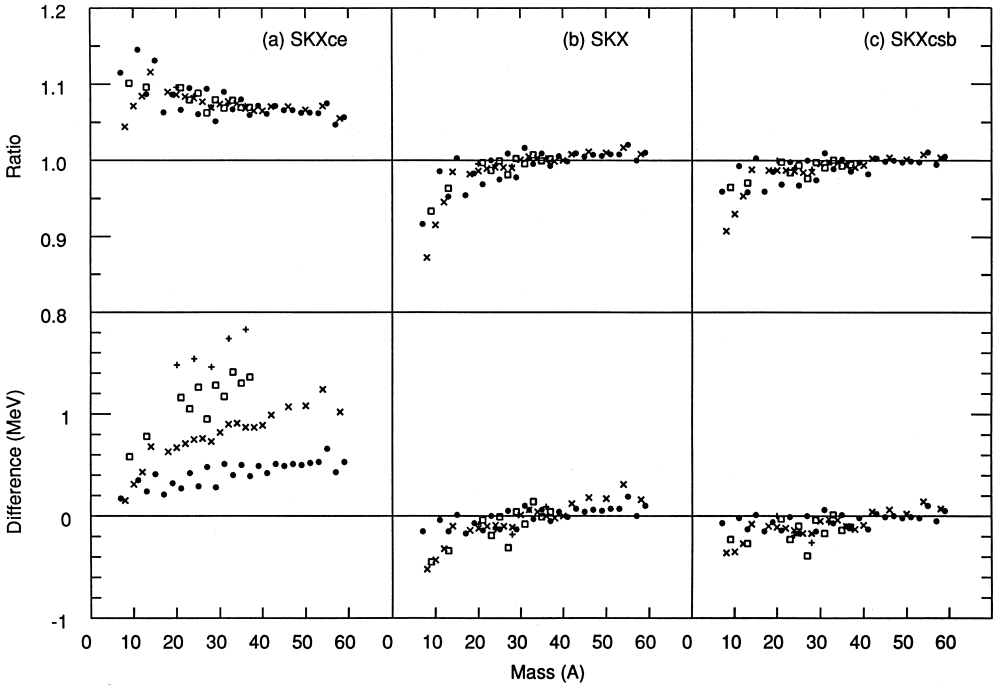

Fig. 2. Top: the ratio experiment/theory for the points in Fig. 1; Bottom: the difference experiment–theory. The symbols are filled circles for $T = 1/2$, squares for $T = 1$, crosses for $T = 3/2$ and plusses for $T = 2$.

energies are known. (The few cases where the the binding energy of the proton-rich nucleus is measured but the ground state is unbound to proton decay are not included since the continuum, which is not treated here, might be important.) The theoretical displacement energy is the difference between the total Hartree–Fock binding energies of the mirror nuclei. The displacement energies obtained in this way automatically takes into account the core-polarization of the core nucleons by the valence nucleons [6] (the Auerbach–Kahana–Weneser [20] effect). All calculations are constrained to be spherical, and the shell-model orbitals are filled in integer steps in the order in which they occur in the mass-dependent potential.

The results of Fig. 1 are remarkable. It shows it is possible to reproduce the quantitative details of the displacement energies within the Skyrme HF framework. One observes a kink in the systematics (both experiment and theory) associated with the change in shell structure at $A = 16$ and $A = 40$. When the displacement energies are converted to the *b*-coefficient of the isobaric mass multiplet equation by dividing the displacement energy by $|2T_z|$, the results lie on a universal curve (see, for example, Ref. [14]); however, we use the displacement energy representation in Fig. 1 in order to separate the data.

For the SKXce comparison in Fig. 1a, one observes the systematic deviation between experiment and theory associated with the Nolen–Schiffer anomaly. For the heaviest nuclei the ratio in Fig. 2a goes to a constant value of about 1.06. It is well known [1] that the displacement energies are sensitive to the rms charge radii, and it is important to note that the SKX interactions reproduce the experimental charge radii of ^{16}O, ^{40}Ca and ^{48}Ca to better than one percent (see Fig. 10 of Ref. [11]). These calculations do not take into account the increase in the radius due to deformation, but as observed in Fig. 10 of Ref. [11] the experimental increase relative to SKX theory in the rms charge radii for the nuclei between the closed shells is at most about 3% and is more typically 1%. The displacement energies are also sensitive to the rms radius of the valence orbits, and the SKX type interactions give radii for the $d_{5/2}$ orbit in ^{17}O and the $f_{7/2}$ orbit in ^{41}Ca which are within 2% of those deduced from the magnetic electron scattering form factors [7].

The experimental displacement energies are much better reproduced by the SKX (b) and SKXcsb (c) fits. The agreement between experiment and theory for SKX and SKXcsb are nearly identical, but the differences in Fig. 2 are slightly flatter with SKXcsb. Although the physical origin of the SKX and SKXcsb corrections are completely different, they are both short-ranged additions to the energy density functional. (We note that some mean-field calculations such as those in the relativistic approach leave out the Coulomb exchange by default.)

The differences between experiment and theory for SKX and SKXcsb shown in Fig. 2 have an rms value of about 100 keV for large A. The deviation with experiment becomes worse for light nuclei, and this is generally related to the breakdown of the mean-field approximation when the number of particles becomes small. Part of the deviation from the mean-field is due to the small differences between the Slater approximation of Eq. (1) and the exact exchange energy [18] as well as the ''pairing'' part of the Coulomb interaction which can be treated by shell-model configuration mixing [13,21,22]. In addition, some of the deviation for the lightest nuclei is related to the fact that the SKX single-particle energies are not in perfect agreement with experiment [11] – a defect which is emphasized for the low- and loosely bound (halo) nature of some single-particle states in light nuclei. This halo aspect can be taken into account on a case by case basis by adjusting the potential to reproduce individual separation energies for light nuclei, as in the Woods–Saxon approach of Ref. [23] (which also does not include the Coulomb exchange term).

Thus we have shown that the experimental displacement energies can be reproduced if the Coulomb exchange part of the Hartree–Fock potential is ignored (SKX). They can be equally well reproduced by keeping the Coulomb exchange and introducing a one parameter CSB interaction (SKXcsb). The relative importance of these two mechanisms must be decided on some other basis. A correct description of the displacement energies within the mean field approximation is obviously important for understanding the position of the proton drip lines. $A = 99$, $T = 1/2$ is the heaviest case for which the proton-rich nucleus is expected to be bound. The calculated displacement energies for $A = 99$ are -13.54 MeV

(SKXce), −14.03 MeV MeV (SKX) and −14.15 MeV (SKXcsb). The introduction of the extra terms in the Skyrme hamiltonian which are needed for the displacement energies also has an influence on the neutron drip line; for example the binding energies of ^{176}Sn are −1158.0 MeV (SKXce), −1149.0 MeV (SKX) and −1148.4 MeV (SKXcsb).

We now discuss how the SKXcsb interaction can be compared with CSB nucleon-nucleon (NN) scattering data. Analysis of the NN scattering data together with a model for the NN interaction gives [24,25] $\Delta a_{\rm CSB} = a_{\rm pp} - a_{\rm nn} = 1.5 \pm 0.5$ fm for the difference in the 'pp' and 'nn' scattering lengths. Modern NN potentials such as the AV18 [26] and CDbonn99 [27] are designed to reproduce this difference. It is not easy to interpret the CSB contribution to the displacement energies directly in terms of a CSB NN potential due the short-range nuclear correlations and their dependence on the strong NN potential. Probably the most realistic way to do this is to consider the CSB contribution to the displacement energies obtained with the variational Monte Carlo approach for $A = 7$ [28] and the BHF approach for $A = 15$ and $A = 17$ [27]. For example, the CSB displacement energy for the $A = 17$, $d_{5/2}$ state is 92 keV with AV18 [27] to be compared with 355 keV with SKXcsb. From these comparisons we find that the effect of the empirical CSB interaction obtained for SKXcsb is a factor of 3–4 larger than expected from AV18 or CDbonn99. Thus we conclude that either there is a significant NNN or many-body CSB contribution whose origin is unknown, or that a major part of the displacement energy anomaly is due to nuclear correlations. Possible many-body CSB effects at the quark levels have recently been examined [29].

Next we discuss the Coulomb exchange term. As mentioned above the Slater approximation of Eq. (1) which is commonly used in HF calculations gives a total exchange energy which is in good agreement with exact calculations [18]. However, it may not be so precise for the exchange energy associated with the displacement energy for a nucleon near the Fermi surface. For example, an exact calculation for the exchange contribution to the displacement energy for the $f_{7/2}$ orbit in $A = 41$ gives −0.26 to −0.30 MeV [2,7] to be compared with the SKXce result of −0.44 MeV. Thus there is about a 30% reduction in the Slater approximation to the exchange corrections at this basic level.

The effect of nuclear correlations have been considered for the displacement energies near ^{16}O and ^{40}Ca [3,4,6–8,27]. These type of corrections are due to configuration mixing in the shell-model basis which go beyond the single Slater determinant (closed-shell) HF assumption. The leading order terms involve 2p–2h admixtures in the ground state but the full effect may require 4p–4h and higher. The correlations have recently been discussed in the general HF framework by Bulgac and Shaginyan [30] in terms of a surface-vibration contribution to the Coulomb correlation energy. They suggest that this type of correlation can almost exactly cancel the Coulomb exchange energy. We note that the form of the energy density functional to be associated with the correlations does not have to be the same as that of the Coulomb exchange in Eq. (1), but empirically there appears to be no need to introduce another type of term.

In summary, we have provided two possible extensions of the conventional Skyrme Hartree–Fock hamiltonian which are necessary for reproducing nuclear displacement energies; SKX where the Coulomb exchange term is absent, and SKXcsb where a CSB potential is added. Both of these methods (or any combination of them) are able to quantitatively reproduce the experimental displacement energies. These modifications are essential for an accurate account of the proton and neutron drip lines.

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References

[1] J.A. Nolen, J.P. Schiffer, Ann. Rev. Nucl. Sci. 19 (1969) 471.
[2] J.W. Negele, Nucl. Phys. A 165 (1971) 305.
[3] H. Sato, Nucl. Phys. A 296 (1976) 378.
[4] A. Poves, A.L. Cedillo, J.G.M. Gomez, Nucl. Phys. A 293

(1977) 397; J.G.M. Gomez, A. Poves, Z. Phys. A 284 (1978) 183; A. Barroso, Nucl. Phys. A 281 (1977) 267.
[5] S. Shlomo, Rep. Prog. Phys. 41 (1978) 957.
[6] N. Auerbach, Phys. Rep. 98 (1983) 273.
[7] T. Suzuki, H. Sagawa, A. Arima, Nucl. Phys. A 536 (1992) 141.
[8] H. Sagawa, N. van Giai, T. Suzuki, Phys. Lett. B 353 (1995) 7; T. Suzuki, H. Sagawa, N. Van Giai, Phys. Rev. C 47 (1993) R1360.
[9] T.H.R. Skyrme, Phil. Mag. 1 (1956) 1043; Nucl. Phys. 9 (1959) 615; 635 (1959).
[10] D. Vautherin, D.M. Brink, Phys. Rev. C 5 (1972) 626.
[11] B.A. Brown, Phys. Rev. C 58 (1998) 220.
[12] B.A. Brown, Phys. Rev. C 43, R 1513 (1991); C 44, 924 (1991).
[13] B.J. Cole, Phys. Rev. C 54 (1996) 1240; Phys. Rev. C 58 (1998) 2831.
[14] W.E. Ormand, Phys. Rev. C 53 (1996) 214; Phys. Rev. C 55 (1997) 2407.
[15] B. Blank et al., Phys. Rev. Lett. 84 (2000) 1116.
[16] J.C. Slater, Phys. Rev. 81 (1951) 85.
[17] J.W. Negele, D. Vautherin, Phys. Rev. C 5 (1972) 1472.
[18] C. Titin-Schnaider, P. Quentin, Phys. Lett. 49B (1974) 397.
[19] B.A. Brown, S.E. Massen, P.E. Hodgson, Phys. Lett. 85B (1979) 167; J. Phys. G 5 (1979) 1655.
[20] E.H. Auerbach, S. Kahana, J. Weneser, Phys. Rev. Lett. 23 (1969) 1253.
[21] W.E. Ormand, B.A. Brown, Nucl. Phys. A 440 (1985) 274; Nucl. Phys. A 491 (1989) 1.
[22] B.A. Brown, R. Sherr, Nucl. Phys. A 322 (1979) 61.
[23] R. Sherr, G. Bertsch, Phys. Rev. C 32 (1985) 1809.
[24] G.A. Miller, B.M.K. Nefkens, I. Slaus, Phys. Rep. 194 (1990) 1.
[25] G.Q. Li, R. Machleidt, Phys. Rev. C 58 (1998) 3153.
[26] R.B. Wiringa, V.G.J. Stoks, R. Schiavilla, Phys. Rev. C 49 (1995) 2950.
[27] C. Harzer, H. Muther, R. Machleidt, Phys. Lett. B 459 (1999) 1.
[28] B.S. Pudliner, V.R. Pandharipande, J. Carlson, S.C. Pieper, R.B. Wiringa, Phys. Rev. C 56 (1997) 1720.
[29] K. Tsushima, K. Saito, A.W. Thomas, Phys. Lett. B 465 (1999) 36; C.J. Horowitz, J. Piekarewicz, Los Alamos preprint nucl-th/0002005.
[30] A. Bulgac, V.R. Shaginyan, Nucl. Phys. A 601 (1996) 103; Phys. Lett. B 469 (1999) 1; Eur. Phys. J. A 5 (1999) 247.