

Coulomb displacement energies, energy differences and neutron skins.

A. P. Zuker^a, J. Duflo^b, S. M. Lenzi^c, G. Martínez-Pinedo^{d,e}, A. Poves^f, J. Sánchez-Solano^f

(a) IReS, Bât27, IN2P3-CNRS/Université Louis Pasteur BP 28, F-67037 Strasbourg Cedex 2, France

(b) Centre de Spectrométrie Nucléaire et de Spectrométrie de Masse (IN2P3-CNRS) 91405 Orsay Campus, France

(c) Dipartimento di Fisica and INFN, Via F. Marzolo 8, I-35131 Padova, Italy

(d) Institut for Fysik og Astronomi, Århus Universitet, DK-8000 Århus C, Denmark

(e) Department für Physik und Astronomie, Universität Basel, CH-4056 Basel, Switzerland

(f) Departamento de Física Teórica C-XI Universidad Autónoma de Madrid, E-28049, Madrid, Spain

(April 12, 2001)

A Fock space representation of the monopole part of the Coulomb potential is presented. Quantum effects show through a small orbital term in $l(l+1)$. Once it is averaged out, the classical electrostatic energy emerges as an essentially exact expression, which makes it possible to eliminate the Nolen-Schiffer anomaly, and to estimate neutron skins and the evolution of radii along yrast states of mirror nuclei. The energy differences of the latter are quantitatively reproduced by the monopole term and a schematic multipole one.

PACS numbers: 21.10.Sf, 21.10.Ft, 21.10.Gv, 21.60.Cs, 27.40.+z

The electrostatic energy of a sphere of radius R and charge Ze is easily calculated to be $E_{Cs} = 3e^2 Z^2 / 5R$ (E_{Cs} stands for “simple Coulomb energy”). It is under this guise that the Coulomb field enters the Bethe-Weizsäcker mass formula, and becomes a basic quantity in nuclear structure. Direct evidence of entirely Coulomb effects has long been available from displacement energies between mirror (or in general, analog) ground states (CDE) [1,2], and more recently from differences in yrast excitation energies in mirror pf -shell nuclei (CED) [3–7].

The CDE range from few to tens of MeV. They should be given mainly by E_{Cs} , but are underestimated by mean-field calculations: the Nolen-Schiffer (NS) anomaly [2], still an open problem.

The CED are very small (of the order of 10-100 keV). They have been semiquantitatively explained by shell model calculations using Coulomb matrix elements but there is some room for improvement.

The present letter intends to give a unified microscopic description of CDE and CED, by separating the Coulomb field into monopole and multipole components $V_C = e^2(M\omega/\hbar)^{1/2}/r = V_{Cm} + V_{CM}$ following ref. [8](DZ). The monopole V_{Cm} contains all terms quadratic in scalar products of Fermion operators $a_i^\dagger \cdot a_j$. Its diagonal part involves only proton number operators, and should be responsible for E_{Cs} , and hence for the observed CDE. The non diagonal part will not be considered here: it leads to isospin mixing, but energetically its effect is small. The multipole V_{CM} contains all non-monopole matrix elements and accounts for much of the CED.

As an introduction we examine the origin of the NS anomaly, by calculating E_{Cs} with proton radii of the form

$$R_\pi = r_0 A^{1/3} \left(1 - \nu \left(\frac{t}{A} \right)^2 - \zeta \frac{t}{A^{4/3}} \right) e^{(1.75/A)} + \mathcal{D}. \quad (1)$$

($A = N + Z$, $t = N - Z$, π , $\nu \equiv$ protons, neutrons.)

Isospin conservation is assumed, which implies that R_ν is the same as R_π for the mirror nucleus, obtained by in-

terchanging N and Z . Therefore, in Eq. (1), for $N > Z$, $\nu > 0$ represents a uniform contraction of the two fluids, while $\zeta > 0$ represents a π -contraction and a ν -dilation. Hence, a (fractional) neutron skin can be defined as

$$\Delta(\zeta) = \frac{R_\nu - R_\pi}{r_0 A^{1/3} e^{1.75/A}} = \frac{2|t|\zeta}{A^{4/3}}, \quad N > Z. \quad (2)$$

The exponential factor takes care of the increase in R_π observed in the light nuclei.

\mathcal{D} is a phenomenological term that accounts for shell and deformation effects. It is a sum of two quartic forms $\lambda S_\pi S_\nu + \mu Q_\pi Q_\nu$ that vanish at the spin-orbit (or EI: extruder-intruder) closures at N or $Z = 6, 14, 28, 50, 82, 126$. Defining $D_\pi = (p_\pi + 1)(p_\pi + 2) + 2$, the degeneracy of the EI $_\pi$ shell (e. g., $p_\pi = 3$ for $Z = 28$ to 50), $D_{r_\pi} = p_\pi(p_\pi + 1)$, the degeneracy of the non-intruder subshells; the factors are $S_\pi = z(D_\pi - z)/D_\pi^2$ and $Q_\pi = z(D_{r_\pi} - z)/D_\pi^2$ ($z =$ number of valence protons). The parametrization is a variant of the ones in [9,10].

Fits to $R_\pi = \sqrt{5\langle r_\pi^2 \rangle / 3}$ —where $\langle r_\pi^2 \rangle$ is the measured mean square radius—for 634 nuclei (with $N \geq Z$ except two cases!) yield (r_0 and rmsd in fm)

$r_0=1.236$ $\nu=0.00$ $\zeta=0.94$ $\lambda=6.2$ $\mu=14.6$ rmsd=0.018: A good fit with a Huge Skin (HS hereafter).

$r_0=1.220$ $\nu=0.61$ $\zeta=0.00$ $\lambda=5.7$ $\mu=27.0$ rmsd=0.012: A much better fit with Zero Skin (ZS hereafter).

$r_0=1.226$ $\nu=0.45$ $\zeta=0.29$ $\lambda=5.7$ $\mu=24.0$ rmsd=0.011: An even better fit with a Minute Skin (MS hereafter).

Adding an exchange term to E_{Cs} , replacing Z^2 by $Z(Z-1)$ (conceptually better, as V_C is two-body), the main contribution to the monopole energy takes the form

$$E_{Cm} = \frac{d Z(Z-1)(1-cZ^{-h})}{\rho}, \quad d = \frac{3e^2}{5r_0} = \frac{0.864}{r_0}, \quad (3)$$

d in MeV and $\rho = (R_\pi - \mathcal{D})/r_0$: The \mathcal{D} correction can be left out for simplicity as it does not affect what follows;

the high quality fits become average ones (rmsd trebled), but still sufficient for our purpose. For the exchange term the usual choice is $h = 2/3$, while c varies appreciably [2]. Here we set $h = 1$ (explained in and after Eq. (6)). The overall factor d is fixed. *Nevertheless*, it will be allowed to vary, under the name d_f , together with c , in a fit to the 183 available CDE from reference [11]. The χ^2 values are calculated by adding 200 keV to the experimental errors, to account for uncertainties in the calculations. Obviously, consistency between R_π and E_{Cm} demands $d_f = d$. The three fits to R_π lead to:

$d=0.699$ $d_f=0.77$ $c = -0.5$ $v=0.00$ $\zeta=0.94$ $\chi^2=0.91$:
HS leads to a large overestimate of d . In other words: keeping the correct d leads to a large *underestimate* of the CDE: the NS anomaly [2,12], unresolved to this day (see however [13]).

$d=0.708$ $d_f=0.69$ $c = 1.3$ $v=0.61$ $\zeta=0.00$ $\chi^2=1.46$:
ZS leads to a small underestimate of d .

$d=0.705$ $d_f=0.71$ $c = 0.9$ $v=0.45$ $\zeta=0.29$ $\chi^2=1.20$:
MS leads to $d_f \approx d$. *The NS anomaly disappears*. Clearly, $\zeta \lesssim 0.3$ is a good guess in Eq. (2).

The NS anomaly occurs because mean field calculations *that yield good R_π* systematically overestimate R_ν : Ref. [14] contains a nice illustration of the problem. It is ironical to note that a small neutron skin was recognized as a possible solution of the anomaly—but rejected—by Nolen and Schiffer [2]. Many reasons explain why this rejection held for so long. We retain only two: neglect of the $v(t/A)^2$ term in Eq. (1), and lack of confidence in the validity of E_{Cm} . As we show next, E_{Cm} in Eq. (3) must be trusted, as it is basically an exact form of V_{Cm} .

By definition, the diagonal monopole part of V_C is ($[J] = 2J + 1$):

$$V_{Cm} = \sum_{i \leq k} \frac{z_i(z_k - \delta_{ik})}{1 + \delta_{ik}} V_{ik}, \quad V_{ik} = \frac{\sum_J V_{Cikik}[J]}{\sum_J [J]}. \quad (4)$$

The label $k \equiv plj$ stands for the quantum numbers specifying a given harmonic oscillator (ho) orbit (p is the principal quantum number). Restricting the sum to the first κ major shells containing τ orbits, V_{Cm} is brought to a sum of factorable terms by diagonalizing the matrix $\frac{1}{2}\{V_{ik}\}$ through the unitary transformation \mathcal{U} :

$$V_{Cm} = e^2 \sqrt{\frac{M\omega}{\hbar}} \sum_n \left[\mathcal{E}_n \left(\sum_k z_k \mathcal{U}_{kn} \right)^2 - \mathcal{C} \right], \quad (5)$$

where $\mathcal{C} = \sum_n z_n V_{nn}/2$ is the one-body counterterm in Eq. (4) left out of the diagonalization. By rescaling $\mathcal{E}_n = \tau E_n$, $\mathcal{U}_{kn} = (\tau)^{-1/2} U_{kn}$, the results become independent of τ . To fix ideas choose $\kappa = 8$, i. e., $\tau = 36$. We expect to extract something close to the Z^2 operator, in which case only the highest eigenvalue (E_{36}) should be non vanishing, with $U_{k36} = 1$. The diagonalization produces indeed an $E_{36} = 0.192$ that is 30 times larger than

the next and over 100 times larger than the second next. (Increasing the number of shells would only increase the number of negligible terms: Eq (5) is an *exact* representation in Fock space.) Fig. 1 shows that ($U_k \equiv U_{k36}$) is very well approximated by the form $U_p - 0.01 L^2$,

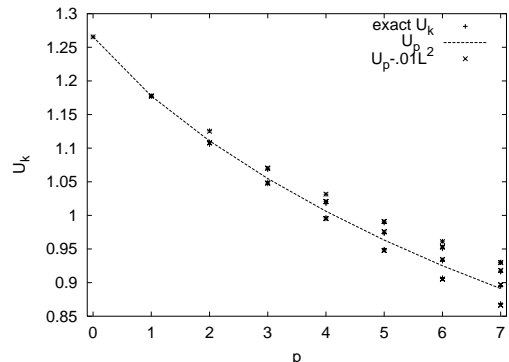


FIG. 1. Dominant factor in the DZ decomposition of V_{Cm}

where $U_p = \sum_j (2j + 1) U_k$ is the average of U_k over j -values, and $L^2 = l(l + 1) - p(p + 3)/2$ is an $l(l + 1)$ term referred to its centroid. This result is still *almost exact*. The presence of L^2 is interesting, but here we average it out, to transform the operator $\sum_p z_p U_p$ into a *c-number* by taking expectation values in Eq. (5) over ho closed shells. Introducing $b = (\hbar/M\omega)^{1/2}$, we find

$$\begin{aligned} \langle V_{Cm} \rangle &\approx \frac{e^2}{b} \left[E_{36} \langle \sum_p z_p U_p \rangle^2 - \langle \mathcal{C} \rangle \right] \\ &\approx \frac{e^2}{b} \left[E_{36} \left(\sum_p (p + 1)(p + 2) U_p \right)^2 - \langle \mathcal{C} \rangle \right] \\ &\approx \frac{e^2}{b} 0.445 (Z(Z - 1))^{(1-1/12)} (1 - 0.96/Z). \end{aligned} \quad (6)$$

The last line is a numerical fit to the previous one. $\langle \sum_p z_p U_p \rangle \approx 1.522 Z^{1-1/12} (1 - 0.48/Z)$, so $0.445 = 0.192 \times (1.522)^2$. In the exchange term: Z^{-1} is better than $Z^{-2/3}$; 0.96 is close to c in ZS and MS CDE fits. The apparently awkward 1-1/12 exponent comes out of the fit. It will be seen to be natural once we extract b from $\hbar\omega_\pi$ calculated as in [1, Eq. (2-157)], but treating separately neutrons and protons:

$$\hbar\omega_\pi = \frac{35.59(2Z)^{1/3}}{\langle r_\pi^2 \rangle} \implies \frac{e^2}{b} 0.445 = \frac{0.860 Z^{1/6}}{r_0 \rho}, \quad (7)$$

where we have used $\langle r_\pi^2 \rangle = 3r_0^2 \rho^2/5$ to bring Eq. (6) to the form of Eq. (3). The factor in $Z^{1/6} = (Z^2)^{1/12} \approx (Z(Z - 1))^{1/12}$ in $(\hbar\omega)^{1/2}$ conveniently corrects the “awkward exponent” and both equations become identical to within a 0.5% discrepancy in the d coefficient: $0.860/r_0$ in Eq. (6) *vs.* $0.864/r_0$ in Eq. (3). Therefore, E_{Cm} is essentially exact to within the averaging of L^2 . A full treatment of this term is of obvious interest.

Let us turn to the CED in the pf shell. They are differences in expectation values of V_C for excitation energies; $\text{CED}_J = E_C^e(Z, N, J) - E_C^e(N, Z, J)$ ($Z > N$). The wavefunctions are obtained through standard shell model calculations [15,5–7] (they depend *very* little on the interaction: KB3, KB3G or FPD6). First we separate monopole and multipole pieces:

$$\text{CED}_J = \Delta \langle V_{Cm} \rangle_J + \Delta \langle V_{CM} \rangle_J \quad (8)$$

$\langle V_{Cm} \rangle_J$ is proportional to the difference of (inverse) radii between a J yrast and the ground state: $R_J^{-1} - R_0^{-1} \approx (R_J - R_0)/R_0^2$. Since R_J is very nearly the same for both members of the mirror pair (remember: the neutron skin is small), it will be proportional to the *average neutron plus proton* occupancies for the individual orbits, which we denote by $\langle m_k \rangle_J/2$, with $m_k = z_k + n_k$ (n_k is the number of neutrons). Now: to good approximation, the R_0^2 denominator is a constant over the region of interest ($A = 47\text{--}51$), furthermore, it is reasonable to assume that radii of the pf orbits depend only on l , and, finally, the $p_{1/2}$ occupancy is always negligible. Therefore, $\langle V_{Cm} \rangle_J$ can be taken to depend only on $\langle m_{p_{3/2}} \rangle_J/2$.

The multipole contribution $\Delta \langle V_{CM} \rangle_J$ is given by the expectation values of the effective Coulomb potential in the pf shell. Then

$$\text{CED}_J = a_m \langle m_{p_{3/2}} \rangle_J + \Delta \langle V_{Cpf}^{eff} \rangle_J \quad (9)$$

The value of a_m can be estimated by noting that the single particle $p_{3/2}$ state in ^{41}Sc is 200 keV below its analogue in ^{41}Ca . This number comes from two effects: a larger radius that depresses the $p_{3/2}$ orbit, and the single particle L^2 term in Fig. 1 that depresses the $f_{7/2}$ ground state orbit. The latter effect is readily found to be ≈ 150 keV by expanding $(\sum_k U_p + .01L^2)^2$ around the $A = 40$ closed shell and using the numbers in, and after Eq. (6). Then, $a_m \approx (.200 + .150)/2 = 0.175$ MeV. Note that the single particle contribution in L^2 is proportional to the *difference* of proton and neutron occupancies. It is important in $A = 41$, but typically ten times smaller than the radial effect in $A = 47\text{--}51$, so we have neglected it.

The available information on $\Delta \langle V_{Cpf}^{eff} \rangle_J$ involves only the $f_{7/2}$ matrix elements extracted from the $^{42}\text{Ti}\text{--}^{42}\text{Ca}$ pair, which yields $(7 \equiv f_{7/2}) V_{CM}^J \tau\tau\tau\tau \equiv V_{Cf_{7/2}}^{eff} = (86.9, 116.9, 10.9, -59.1)$ keV, for $J = 0, 2, 4, 6$ respectively, to be compared with the ho values $V_{Cf_{7/2}}^{ho} = (81.6, 24.6, -6.4, -11.4)$ keV. Since we are dealing with V_{CM} , the centroids $V_{\tau\tau}$ (Eq. (4)) have been removed. They are very close (304 keV for $A=42$, 308 keV for ho) *because E_{Cm} depends on conserved quantities that cannot be renormalized*. The multipole matrix elements are very different, and the data unequivocally prefer the $A = 42$ set [5,6]. The strategy adopted in these references was to use a V_{Cpf}^{eff} with $V_{Cf_{7/2}}^{eff}$, keeping V_{Cpf}^{ho} for the other matrix elements, which turned out to be almost irrelevant: the $V_{Cf_{7/2}}^{eff}$ set by itself accounts for the full V_{Cpf}^{eff} chosen in

this way. The results alternated between agreement and distortion of the observed patterns.

As there is no justification in accepting an enormous renormalization for the $f_{7/2}$ orbits and leave the rest of the interaction unchanged, we shall attempt a more general treatment, by exploring the possibility of writing an effective interaction solely in terms of $V_{Cf_{7/2}}^{eff}$ —properly renormalized to give a plausible account of the full V_{Cpf}^{eff} . First we check that the program can be enacted for the ho set. We try

$$\Delta \langle V_{Cpf}^{ho} \rangle_J = b \Delta \langle V_{Cf_{7/2}}^{ho} \rangle_J + a \langle m_{p_{3/2}} \rangle_J : \quad (10)$$

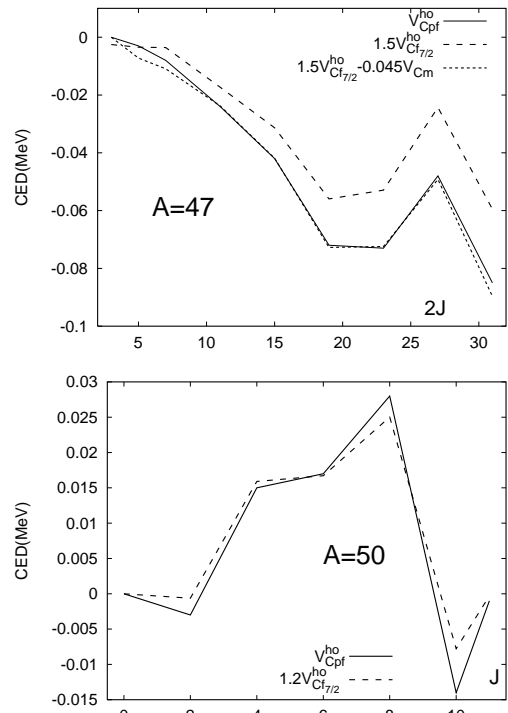


FIG. 2. Calculated CED normalizations

Eq. (10) is only a *numerical recipe*, but it works well, as seen in Fig. 2, representative of the quality of the adjustment in the four cases (parameters in Tab I). Next, assume that the prescription applies to the renormalized case and try to *invent* an effective interaction consistent with the data and *respecting the condition that the a_m parameter in Eq. (9) be a constant that should be determined carefully*. There is no room for invention here.

TABLE I. Adopted parameters in Eq. (10) and Eq. (11)

A	b	a	b_M	a_M	a_m
47	1.5	-0.045	0.75	-0.080	0.150
49	1.5	0.000	0.75	0.000	0.150
50	1.2	0.000	0.60	0.000	0.150
51	1.6	-0.030	0.80	-0.054	0.150

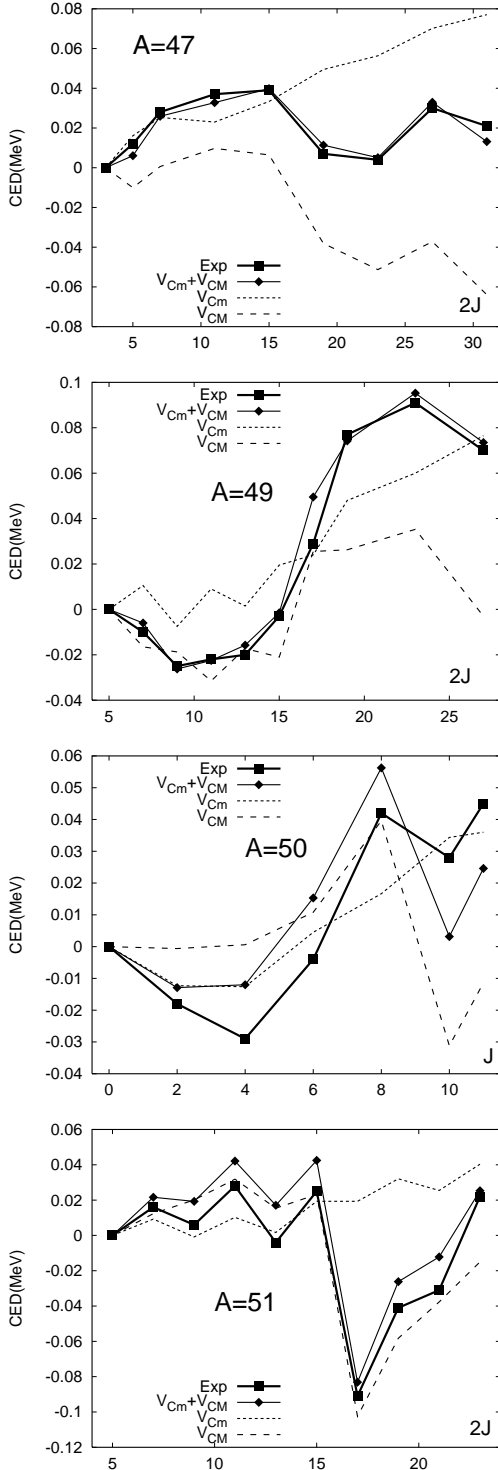


FIG. 3. Experimental [4–7] and calculated CED for the pairs ^{47}Cr - ^{47}V , ^{49}Mn - ^{49}Cr , ^{50}Fe - ^{50}Cr , and ^{51}Fe - ^{51}Mn .

Let us write

$$\begin{aligned} \text{CED}_J &\equiv V_{Cm} + V_{CM} \\ &= a_m \langle m_{p_{3/2}} \rangle_J + b_M \Delta \langle V_{Cf_{7/2}}^{eff} \rangle_J + a_M \langle m_{p_{3/2}} \rangle_J \end{aligned} \quad (11)$$

For $A \approx 50$, a_m —estimated at $A = 41$ —must be reduced

by a factor $(41/50)^{2/3} \approx 0.88$ to account for the R_0^2 denominator (after Eq. (9)). Therefore, we set $a_m = 0.15$. Now choose $b_M = b/2$, $a_M = 1.8a$. Eq. (11) with these parameters (Tab I) yields CED that in Fig. 3 are seen to agree well, even very well, with experiment. The mild exception is $A = 50$, discussed in detail in Ref. [7], which contains a heuristic introduction to our CED results.

The monopole V_{Cm} and multipole V_{CM} contributions, shown separately in Fig.3, indicate that the latter reproduces only roughly the experimental patterns: The addition of V_{Cm} is indispensable to bring quantitative agreement. It is especially worth noting that the strong signature effect in the $A = 49$ band is erased in the CED by the out-of-phase V_{Cm} and V_{CM} . Conversely, the signature staggering is enhanced in $A = 51$.

The monopole contribution provides valuable information about the evolution of yrast radii. As a consequence, the use—and even the validity—of the schematic multipole term (the “invention”) must be assessed by the focus it brings to the monopole one, which *must* be present in a form very close to that in Eq. (9).

To conclude: once the NS anomaly is resolved, the Coulomb field fulfills the—long held—hope of providing information about radii not directly measured. The L^2 terms offers intriguing prospects. A complete analysis of V_{Cm} , including non-diagonal contributions, is in order to estimate isospin impurities. The renormalization of V_{CM} remains an open problem.

This work owes much to a stay of AZ at the UAM, made possible by a scholarship of the BBVA foundation.

-
- [1] A. Bohr and B. Mottelson, *Nuclear Structure* vol I (Benjamin, Reading, 1964).
 - [2] J. A. Nolen and J. P. Schiffer, *Ann. Rev. Nuc. Sci.* **19**, 471 (1969)
 - [3] J.A. Sheikh, P. Van Isacker, D.D. Warner and J.A.Cameron, *Phys. Lett.* **B 252**, 314 (1990).
 - [4] C. O’Leary *et al.*, *Phys. Rev. Lett.* **79**, 4349 (1997).
 - [5] M.A. Bentley *et al.*, *Phys. Lett.* **B 437**, 243 (1998).
 - [6] M.A. Bentley *et al.*, *Phys. Rev. C* **62**, 051303(R) (2000).
 - [7] S. M. Lenzi *et al.*, submitted to PRL.
 - [8] M. Dufour and A. P. Zuker, *Phys. Rev. C* **54**, 1641 (1996).
 - [9] J. Duflo, *Nucl. Phys.* **A576**, 29 (1994).
 - [10] J. Duflo and A. P. Zuker, *Phys. Rev. C* **59**, R2347 (1999).
 - [11] G. Audi and A.H. Wapstra, *Nucl. Phys.* **A595**, 409 (1995).
 - [12] N. Auerbach, *Phys. Rep.* **98**, 273 (1983).
 - [13] A. Bulgac and R. Shaginyan, *Phys. Lett.* **B 469**, 1 (1999), S. A. Fayans and D. Sawischa, *nucl-th/0009034*.
 - [14] J. Bartel, M. B. Johnson, M. K. Singham and W. Stocker, *Phys. Lett.* **B 296**, 5 (1992).
 - [15] E. Caurier, ANTOINE code, Strasbourg (1989-2001).