Even-odd staggering of pairing-force strength

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The data fits of microscopic nuclear mass formulas can be considerably improved by making the pairing force slightly stronger for an odd number of like nucleons than for an even number. Qualitatively at least, such an effect could arise from the fact that the Hartree-Fock wave function of an odd nucleus is not an eigenstate of the time-reversal operator.

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The elucidation of the r process of nucleosynthesis requires the availability of a nuclear mass table, with the experimentally inaccessible neutron-rich nuclei reliably extrapolated from the data. Recently, and for the first time, a complete mass table was derived entirely on the basis of microscopic forces, the calculation being performed within the framework of the so-called extended Thomas-Fermi plus Strutinsky integral (ETFSI) approach to nuclear structure [1–5]. This method is essentially a high-speed approximation to the Hartree-Fock (HF) method, using a Skyrme force of the form

$$
\begin{aligned}
v_{ij}=&\, t_0(1+x_0P_\sigma)\delta(\boldsymbol{r}_{ij})+t_1(1+x_1P_\sigma)\frac{1}{2\hbar^2}\{p_{ij}^2\delta(\boldsymbol{r}_{ij})+\mathrm{H.c.}\}\\
&+t_2(1+x_2P_\sigma)\frac{1}{\hbar^2}\boldsymbol{p}_{ij}\cdot\delta(\boldsymbol{r}_{ij})\boldsymbol{p}_{ij}\\
&+\frac{1}{6}t_3(1+x_3P_\sigma)\{\rho_{q_i}(\boldsymbol{r}_i)+\rho_{q_j}(\boldsymbol{r}_j)\}^\gamma\delta(\boldsymbol{r}_{ij})\\
&+\frac{i}{\hbar^2}W_0(\boldsymbol{\sigma}_\mathbf{i}+\boldsymbol{\sigma}_\mathbf{j})\cdot\boldsymbol{p}_{ij}\times\delta(\boldsymbol{r}_{ij})\boldsymbol{p}_{ij}\,,
\end{aligned}
\tag{1}
$$

where P_σ is the two-body spin-exchange operator, the index q denotes n or p, according to whether the term in question relates to neutrons or protons, respectively, and $\rho_q(\boldsymbol{r})$ denotes the density of the corresponding kind of nucleon at $\boldsymbol{r}$. The ETFSI method also takes into account pairing correlations, using a δ-function pairing force,

$$v_{\mathrm{pair}}(\boldsymbol{r}_{ij})=V_\pi\delta(\boldsymbol{r}_{ij}),\tag{2}$$

that is handled with the usual BCS treatment.

The Skyrme-force parameters and the pairing parameter V_π were determined by fitting to the mass data [4,5], although the former were subject to the constraints

$$t_2=-\frac{1}{3}t_1(5+4x_1)\tag{3a}$$

and

$$x_2=-\frac{4+5x_1}{5+4x_1}\ ,\tag{3b}$$

in order for the effective nucleon mass M_q^* to be equal to the real nucleon mass M, a condition that has been shown to improve the mass fit and the description of fission barriers (see Ref. [3]).

The overall quality of our best fit (parameter set SkSC4 in Refs. [4,5]; see also Table II below) is satisfactory, considering that there are only eight active parameters (x_2 is almost without influence on the masses). Nevertheless, a problem arises in connection with the pairing parameter V_π, since there is a tendency to overestimate even-odd mass differences (at least for nuclei with $A>80$; the opposite is the case for the relatively few nuclei with $A<80$). As already discussed in Refs. [3,4], and as can be seen below in Tables III and V, this problem becomes increasingly serious as we move to heavy nuclei. The implications for single-neutron separation energies (S_n) and β-decay energies (Q_β), both of which are of considerable importance for the r process, will be apparent. We could, of course, have reduced the errors in the even-odd mass differences simply by reducing the pairing-force strength V_π, and since these errors also con-

TABLE I. Parameters of the force SkSC11.

t_0 (MeV fm^3)	-1789.42
t_1 (MeV fm^5)	283.467
t_2 (MeV fm^5)	-283.467
t_3 (MeV fm^4)	12782.3
x_0	0.79
x_1	-0.5
x_2	-0.5
x_3	1.13871
W_0 (MeV fm^5)	124.877
γ	0.333333
V_π^+ (MeV fm^3)	-220.0
V_π^- (MeV fm^3)	-224.0

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TABLE II. Errors in the fit to the complete data set (1492 nuclei: see text). (All quantities in MeV.)

	SkSC4	SkSC11
$\sigma_{\mathrm{rms}}(M)$	0.736	0.715
$\bar{\epsilon}(M)$	-0.061	0.082
$\sigma_{\mathrm{rms}}(S_n)$	0.524	0.439
$\sigma_{\mathrm{rms}}(Q_\beta)$	0.683	0.642

tribute to the overall rms error of the mass fit it might be expected that the latter would improve at the same time. This is not so, as we discuss in Sec. 4 of Ref. [3]: the point is that the pairing force not only generates even-odd fluctuations but also contributes a much smoother (though shell-dependent) term to the total energy. Thus optimizing the overall fit and optimizing the fit to the even-odd mass differences are in conflict as far as V_π is concerned. This is the case, we find, not only for a pairing force of the above form (2), but also for more general density-dependent forces [6]; for simplicity we shall limit the discussion to the former kind.

We have verified that the problem persists if we replace the blocking variant of the BCS method that we have used in our published fits [3] by the standard form of the theory (see, for example, Ref. [7]). As for the Lipkin-Nogami method (see, for example, Ref. [8]), we have already shown [3] that it leads to worse global fits, and therefore do not pursue this method here.

We find that the pairing problem exists also in the HF method, and in particular does not go away on reiterating to self-consistency (calculating the shell corrections in the ETFSI method involves just one iteration of HF). The reason why this problem does not seem to have been encountered in previous HF calculations is simply that most take $M_q^* < M$, and thus can have no pretence to fitting the masses of open-shell nuclei.

Thus we believe that this problem of the pairing strength will be encountered in any mass formula that is at least as microscopically based as is the ETFSI method. However, it does not arise in more phenomenological mass formulas such as the finite-range droplet model (FRDM) [9], where the pairing is treated in such a way that it influences only the even-odd mass differences, without generating any additional contribution to the mass that varies smoothly between closed shells.

What is required is an extra degree of freedom, allowing the even-odd mass differences to be adjusted without affecting the slowly varying background. The only way that we have found to achieve this is by the brute-force device of allowing the pairing strength to be stronger for an odd number of nucleons than for an even number, i.e., the pairing force between neutrons, for example, depends on whether the neutron number N is even or odd. The purpose of the present note is to describe this approach to the pairing-force problem.

TABLE III. rms errors in the fit to the fourth-order even-odd mass differences $\Delta_{e\text{-}o}^{(4)}$ of several isotope chains, with rms errors of S_n shown in parentheses. (All quantities in MeV.)

Z	SkSC4	SkSC11
30	0.585 (0.671)	0.617 (0.700)
50	0.185 (0.205)	0.083 (0.140)
62	0.193 (0.408)	0.201 (0.366)
70	0.438 (0.497)	0.225 (0.396)
82	0.334 (0.335)	0.253 (0.249)
90	0.395 (0.484)	0.087 (0.294)
96	0.711 (0.705)	0.217 (0.255)
100	0.655 (0.582)	0.169 (.215)

TABLE IV. rms errors in the fit to the fourth-order even-odd mass differences $\Delta_{e\text{-}o}^{(4)}$ of several isotone chains. (All quantities in MeV.)

N	SkSC4	SkSC11
30	0.728	0.754
50	0.112	0.154
70	0.512	0.541
82	0.216	0.158
92	0.099	0.120
112	0.088	0.221
126	0.161	0.092
144	0.091	0.120

With the new pairing degree of freedom we refit to the same mass data as were used for the determination of our previous best parameter set, SkSC4 [4,5], i.e., to the 1492 nuclei with $A \geqslant 36$ given in the 1988 data compilation [10]. The resulting new parameter set, labeled SkSC11, is shown in Table I. The Skyrme parameters are identical to those of SkSC4, but there are now two pairing parameters, V_π^+ for nucleons of which there is an even number, and V_π^- for nucleons of which there is an odd number. The unique value of V_π in set SkSC4 was -220 MeV, and we see that this remains unchanged here when the corresponding number of nucleons is even. The only difference with respect to set SkSC4 thus lies in the pairing strength for nucleons of which there is an odd number, and even here the change is minimal, the increase in the attraction being less than 2%. Actually, we studied the possibility of allowing the two pairing parameters $V_\pi^\pm$ to be different for neutrons and protons, but the improvement in the fit was insignificant, certainly not enough to justify the introduction of two new parameters. We also tried refitting the Skyrme parameters in the presence of the new pairing force, but no change resulted.

Despite the minimal difference between the old parameter set SkSC4 and the new set SkSC11, we see from Tables II–V

TABLE V. rms errors in the fit to the Q_β values of several β-decay chains. (All quantities in MeV.)

A	SkSC4	SkSC11
80	0.525	0.653
81	0.803	0.774
131	0.309	0.273
132	0.308	0.270
154	0.533	0.524
155	0.410	0.403
200	0.619	0.572
201	0.693	0.634
220	0.502	0.220
221	0.535	0.439
234	0.868	0.209
235	0.560	0.310

TABLE VI. Errors in the fit to the odd-odd nuclei of Table II. (All quantities in MeV.)

	SkSC4	SkSC11
$\sigma_{\rm rms}(M_{o\text{-}o})$	0.749	0.697
$\bar{\epsilon}(M_{o\text{-}o})$	-0.125	0.166

that there is a significant improvement in the fit to the data. Table II shows the global fit for all 1492 mass-data points, with the first line representing the rms error of the fit to the absolute masses, and the second the mean error of the same fit (the change in this latter quantity is not an improvement at all but simply reflects the increased mean attraction of the new force). The last two lines of Table II, respectively, show the rms errors in the fits to the S_n and Q_β; the improvement in the former quantity is particularly gratifying, that in the second somewhat less so.

In order to see how these improvements are distributed over the nuclear chart we show in Tables III and IV, respectively, the rms error in the fourth-order even-odd mass difference $\Delta^{(4)}_{e\text{-}o}$ [11] for several typical isotope and isotone chains; the former table also gives, in parentheses, the rms error in S_n for the particular isotope chain. We see that the pairing problem with the original force SkSC4 was worst for the high-Z isotope chains, and that it is these chains that show the most improvement with the modified pairing. Elsewhere the new force never makes the fit significantly worse, and often improves it. It will be seen that for both the $Z=30$ and $N=30$ chains the fit is rather poor with both the old and new forces; in both cases we are dealing with nuclei for which $A<80$. In Table V we show the rms error in the Q_β values for several β-decay chains. Here too the advantages of the new force are greatest in this respect for heavy nuclei, while, as before, there are no cases where the use of the new force is seriously disadvantageous.

Despite this empirical success of our device of making the pairing strength depend on the number parity, its *ad hoc* character might be found to be rather unsatisfactory, but it should not be forgotten that the very concept of a pairing force is highly phenomenological, and that in formally deriving it from more realistic forces the Pauli principle could conceivably give rise to such effects: the pairing force itself could be subject to "blocking" by an odd nucleon. Moreover, it should be realized that the HF wave function of an odd nucleus is not an eigenstate of the time-reversal operator [12], and that in projecting out from it a state of good time-reversal properties the total energy will be lowered (this would also happen in the shell correction of the ETFSI calculation). Thus the extra pairing attraction that we give to odd nuclei could be regarded, at least qualitatively, as compensating for our failure to make this projection.

Moreover, with the pairing attraction being greater for an odd number of nucleons there will be an extra enhancement of the binding in odd-odd nuclei. Thus we shall be simulating in some way the residual attraction between the last odd neutron and the last odd proton that is known to exist (see, for example, Refs. [11,13]), but which we have hitherto neglected in the ETFSI approach. Table VI, showing the fits to just the odd-odd nuclei, is instructive in this respect. Comparing the first column of this table with the first column of Table II shows that with force SkSC4 the odd-odd nuclei are fitted less well on average than the other nuclei, and that in particular they are more underbound. Comparing then the second columns of these two tables shows that with the new force the odd-odd nuclei are actually fitted better than the others (they are also seen to be more overbound than the others, which means that our equivalent residual attraction between the last odd neutron and the last odd proton is too strong).

We have shown that the pairing properties of the ETFSI mass formula can be improved considerably by making the pairing strength depend on whether the number of nucleons involved is even or odd. This new degree of freedom has a certain measure of physical sense, and is not entirely *ad hoc* in character. The value of this device is not limited to the ETFSI method, and could be expected to improve the quality of a direct HF approach to the mass formula.

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