Towards a Hartree-Fock mass formula

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A ten-parameter Skyrme force, along with a four-parameter δ-function pairing force, have been fitted, using the Hartree-Fock-BCS method, to the masses of 1719 nuclei, both spherical and deformed, with an rms error of 0.754 MeV. The corresponding value of the symmetry coefficient J is 28.0 MeV, and that of the effective nucleon mass M^* is $1.05M$.

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I. INTRODUCTION

The r process of nucleosynthesis depends crucially on the binding energies (among other properties) of heavy nuclei that are so neutron-rich that there is no hope of being able to measure them in the laboratory (see Ref. [1] for a general review). It thus becomes of the greatest importance to be able to make reliable extrapolations of nuclear masses (and other relevant properties, such as fission barriers, deformations, nuclear radii, . . .) away from the known region, relatively close to the stability line, out towards the neutron-drip line. This means that one should have a mass formula that not only gives a good fit to the data, but also has a sound theoretical basis; generally speaking, the more microscopically grounded is a mass formula, the better one would expect its theoretical basis to be.

Until recently the masses and barriers used in all studies of the r process were calculated on the basis of one form or another of the liquid-drop model, the most sophisticated version of which is the ''finite-range droplet model'' (FRDM) [2]. Despite the great empirical success of this formula (it fits 1654 masses with an rms error of 0.669 MeV), there is still an obvious need to develop a mass formula that is more closely connected to the basic nuclear interactions. Two such approaches can reasonably, be contemplated at the present time, one being the nonrelativistic Hartree-Fock (HF) method (see Refs. [3,4] for a recent compilation of references), and the other the relativistic Hartree method, also known as the relativistic mean-field (RMF) method (see Ref. [5] for a guide to the literature on this topic). Each of these methods is characterized by a set of phenomenological parameters relating either to an effective nuclear force in the case of the HF method, or to effective bosons in the case of the RMF method; in both cases the parameters can be fitted to the mass (and possibly other) data. Not only would mass formulas based on either of these methods have a more fundamental basis, but their underlying parameter sets would permit the construction of equations of state of stellar nuclear matter that have a very direct connection with nuclear data.

Ultimately, one would wish to go to a deeper level, connecting with the two- and three-nucleon data on the one hand, and the quark model of nucleons on the other hand, but quantitative success on these lines, with the level of precision required for astrophysics, can hardly be expected in the near future. Indeed, little progress has been made even at the more modest level of the nonrelativistic HF method or of the RMF method. In neither case has the basic parameter set been fitted to the masses of more than ten or so nuclei, presumably because of the computer-time limitations that arose in the past with deformed nuclei. However, using parameter sets determined in this way, the masses (and some other properties) of more than a thousand nuclei have been calculated in both the HF [6] and RMF [5] approaches. Unfortunately, in both cases the rms errors in the resulting mass predictions for nuclei of known mass were well in excess of 2 MeV, which is unacceptable for astrophysical purposes; moreover, both sets of calculations were limited to even-even nuclei.

The result is that the most microscopically founded mass formulas of practical use are those based on the so-called ETFSI (extended Thomas-Fermi plus Strutinsky integral) method. This is a high-speed macroscopic-microscopic approximation to the HF method based on Skyrme forces (SHF method), with pairing correlations generated by a δ-function force that is treated in the usual BCS approach (with blocking). The macroscopic part consists of a purely semi-classical approximation to the SHF method, the full fourth-order extended Thomas-Fermi (ETF) method, while the second part, which is based on what is called the Strutinsky-integral (SI) form of the Strutinsky theorem, constitutes an attempt to improve this approximation perturbatively, and in particular to restore the shell corrections that are missing from the ETF part. For full details of this method see Refs. [7–11]. In the latest version of this mass formula, ETFSI-2, 1719 measured masses are fitted with an rms error of 0.709 MeV [12]. (Also to be mentioned in this context is the Thomas-Fermi mass formula of Ref. [13], which fits 1654 masses with an rms error of 0.655 MeV. However, the microscopic corrections, along with the equilibrium deformation configurations, in this mass formula are taken in their entirety from the FRDM fit [2], with the seven force parameters being fitted exclusively to the macroscopic terms, so that self-consistency is by no means assured. The ETFSI model, on the other hand, is completely self-consistent.)

As to the extent to which the ETFSI method constitutes a good approximation to the HF method, it is found that if a

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given force is run in both ETFSI and HF codes, the latter code will typically give finite-nucleus energies about 4 MeV higher than will the former code. Nevertheless, we have shown [7,8] that the two methods are essentially equivalent in the sense that when a Skyrme-type force is fitted to the same data by one method or the other they give very similar extrapolations out to the neutron-drip line: the discrepancy is less than 1 MeV for total energies and fission barriers, and less than 0.5 MeV for the neutron-separation energies S_n and beta-decay energies Q_β.

But even though it might thus seem that there is very little to be gained from constructing a HF mass formula, there are nevertheless three reasons for doing so. (i) The ETFSI method is limited, at least in its present form, to Skyrme forces for which the effective nucleon mass M^* is equal to the real mass M. Since the HF method suffers from no such limitation, an extra degree of freedom becomes available, leading to the possibility of a still better fit to the mass data. (ii) The widespread availability of HF codes makes it highly desirable that one have at one's disposal a HF effective force that has been fitted to the same mass data and with the same (or better) precision as has the best available ETFSI force (SkSC18 at the present time [12]). This need becomes even stronger when one wishes to go beyond the HF method and include RPA correlations, since here too there exist many codes constructed on an HF basis, while the ETFSI method itself has not been generalized in this respect. (iii) To calculate the equation of state of stellar nuclear matter at low temperatures, as found, for example, in decompressing neutron matter, it is necessary to include shell corrections, and the HF method will be better adapted than the ETFSI approximation to the complicated configurations that may be encountered.

Actually, the limitation of the ETFSI method to an effective mass of $M^*=M$ was not a gross defect, since it is known that to have the correct single-particle (s.p.) level density in the vicinity of the Fermi surface one must have M^*/M equal to, or slightly larger than, 1.0 [14–16], and without the correct s.p. level density it is impossible to fit the masses of open-shell nuclei, even if a fit to the masses of doubly magic nuclei is possible. On the other hand, all nuclear-matter calculations with forces that are realistic in the sense that they fit the two- and three-nucleon data indicate that at the equilibrium density $M^*/M \simeq 0.7$ [17,18]. Rough experimental confirmation that M^* is considerably smaller than M first came from measurements of the deepest s.p. states in light nuclei [19] (for a theoretical discussion see, for example, Refs. [20–22]). More precise empirical information comes from analyses of the giant isoscalar quadrupole and isovector dipole resonances. From the former one finds [23] a value of around $0.8M$ for the nuclear-matter isoscalar effective mass M_s^*, defined in Eq. (9a) below, while from the latter one finds [24] a value of around $0.7M$ for the nuclear-matter isovector effective mass M_v^*, defined in Eq. (9b) below.

However, there is no contradiction between these two values of M^*/M (i.e., 0.7–0.8 on the one hand, 1.0–1.1 on the other), since Bernard and Giai [25] have shown that one can obtain reasonable s.p. level densities in finite nuclei with realistic values of M^*/M, i.e., of 0.7–0.8, provided one takes into account the coupling between s.p. excitation modes and surface-vibration RPA modes. Since the good agreement with measured s.p. level densities found in Refs. [14–16] was obtained without making these corrections it must be supposed that the resulting error is being compensated by the higher value of M^*/M, i.e., $M^*/M \simeq 1.0$, which may thus be regarded as a semiempirical value that permits considerable phenomenological success with straightforward HF, or other mean-field calculations, without any of the complications of Ref. [25]. It is in this way, in fact, that the ETFSI mass formulas [11,12] have achieved their high level of precision. Nevertheless, by releasing the constraint of M^*/M being exactly equal to unity one may hope for further improvement in the quality of the fit.

Actually, nearly all of the many HF forces that have been constructed impose the constraint of a realistic value for M^*/M, i.e., 0.7–0.8, but that this choice is incompatible with correct masses of open-shell nuclei is well illustrated by the force SLy4: see Figs. 1–4 of Ref. [4]. It seems, in fact, that the only HF forces that adopt the semiempirical value of $M^*/M \simeq 1.0$ are SkP [26] and the forces T1–6 [27], but they have been fitted to only a very small number of nuclei, and so cannot serve as the basis of a mass formula. The object of the present paper is to rectify this situation by making a HF fit of a Skyrme-type force to essentially all the measured masses, with the effective nucleon mass M^*/M being taken as a free fitting parameter. While this latter feature is essential for a good fit to the masses, and will lead to improved fission barriers [27,28], it should not be forgotten that there are several applications in which it is essential to impose at the outset the realistic value of 0.7–0.8 for M^*/M, e.g., for the calculation of giant multipole resonances.

In Sec. II we summarize the required SHF formalism, and discuss our treatment of pairing. In this same section we also explain our fitting strategy, which involves two distinct phases. The first of these phases is limited to spherical nuclei, and is described in Sec. III, while the second phase, involving both spherical and deformed nuclei, is described in Sec. IV.

II. THE SHF-BCS METHOD

The Skyrme forces that we consider have the usual form

$$v_{ij}=t_0(1+x_0P_\sigma)\,\delta(\mathbf{r}_{ij})+t_1(1+x_1P_\sigma)\frac{1}{2\hbar^2}\{p_{ij}^2\delta(\mathbf{r}_{ij})+\text{H.c.}\}$$
$$+t_2(1+x_2P_\sigma)\frac{1}{\hbar^2}\mathbf{p}_{ij}\cdot\delta(\mathbf{r}_{ij})\mathbf{p}_{ij}+\frac{1}{6}t_3(1+x_3P_\sigma)$$
$$\times\rho^\gamma\delta(\mathbf{r}_{ij})+\frac{i}{\hbar^2}W_0(\boldsymbol{\sigma}_i+\boldsymbol{\sigma}_j)\cdot\mathbf{p}_{ij}\times\delta(\mathbf{r}_{ij})\mathbf{p}_{ij}, \qquad (1)$$

where P_σ is the two-body spin-exchange operator. The total energy $E_{\rm HF}$ corresponding to this force is, in a standard notation [20],

$$E_{\mathrm{HF}}=\int \mathcal{E}(\mathbf{r})d^3\mathbf{r}=\int \mathcal{E}^{\mathrm{nuc}}(\mathbf{r})d^3\mathbf{r}+\int \mathcal{E}^{\mathrm{Coul}}(\mathbf{r})d^3\mathbf{r}, \tag{2}$$

where

$$\begin{aligned}\mathcal{E}^{\mathrm{nuc}}(\mathbf{r})=&\frac{1}{4}t_0\{(2+x_0)\rho^2-(2x_0+1)(\rho_p^2+\rho_n^2)\}+\frac{1}{8}\{t_1(2+x_1)+t_2(2+x_2)\}\tau\rho+\frac{1}{8}\{t_2(2x_2+1)-t_1(2x_1+1)\}\\ &\times(\tau_p\rho_p+\tau_n\rho_n)+\frac{1}{32}\{3t_1(2+x_1)-t_2(2+x_2)\}(\boldsymbol{\nabla}\rho)^2\\ &-\frac{1}{32}\{3t_1(2x_1+1)+t_2(2x_2+1)\}\{(\boldsymbol{\nabla}\rho_p)^2+(\boldsymbol{\nabla}\rho_n)^2\}+\frac{1}{24}t_3\rho^{\gamma}\{(2+x_3)\rho^2-(2x_3+1)(\rho_p^2+\rho_n^2)\}\\ &+\frac{1}{2}W_0\{\mathbf{J}\cdot\boldsymbol{\nabla}\rho+\mathbf{J}_p\cdot\boldsymbol{\nabla}\rho_p+\mathbf{J}_n\cdot\boldsymbol{\nabla}\rho_n\}-\frac{1}{16}(t_1x_1+t_2x_2)J^2+\frac{1}{16}(t_1-t_2)(J_p^2+J_n^2)\end{aligned} \tag{3a}$$

(note particularly that we retain the terms in J^2 and J_q^2), while for the Coulomb term we have, making the Slater approximation in the exchange part,

$$\mathcal{E}^{\mathrm{Coul}}=\frac{e^2}{2}\rho_p(\mathbf{r})\int\frac{\rho_p(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}d^3\mathbf{r}'-\frac{3e^2}{4}\left(\frac{3}{\pi}\right)^{1/3}\rho_p^{4/3}. \tag{3b}$$

Minimizing E_{HF} with respect to arbitrary variations in the s.p. wave functions $\phi_{i,q}$, where i labels all quantum numbers, and q denotes n (neutrons) or p (protons), leads to the HF equation

$$\left\{-\boldsymbol{\nabla}\cdot\frac{\hbar^2}{2M_q^*(\mathbf{r})}\boldsymbol{\nabla}+U_q(\mathbf{r})+V_q^{\mathrm{Coul}}(\mathbf{r})-i\mathbf{W}_q(\mathbf{r})\cdot\boldsymbol{\nabla}\times\boldsymbol{\sigma}\right\}\phi_{i,q}=\epsilon_{i,q}\phi_{i,q}, \tag{4}$$

where the nuclear part of the central s.p. field, $U_q(\mathbf{r})$, the Coulomb field $V_q^{\mathrm{Coul}}(\mathbf{r})$, and the spin-orbit s.p. field $\mathbf{W}_q(\mathbf{r})$ are as follows:

$$\begin{aligned}U_q(\mathbf{r})=&\frac{1}{2}t_0\{(2+x_0)\rho-(2x_0+1)\rho_q\}+\frac{1}{8}\{t_1(2+x_1)+t_2(2+x_2)\}\tau+\frac{1}{8}\{t_2(2x_2+1)-t_1(2x_1+1)\}\tau_q\\ &+\frac{1}{16}\{t_2(2+x_2)-3t_1(2+x_1)\}\nabla^2\rho+\frac{1}{16}\{3t_1(2x_1+1)+t_2(2x_2+1)\}\nabla^2\rho_q+\frac{1}{24}t_3[(2+x_3)(2+\gamma)\rho^{\gamma+1}\\ &-(2x_3+1)\{2\rho^{\gamma}\rho_q+\gamma\rho^{\gamma-1}(\rho_p^2+\rho_n^2)\}]-\frac{1}{2}W_0\boldsymbol{\nabla}\cdot(\mathbf{J}+\mathbf{J}_q),\end{aligned} \tag{5}$$

$$V_q^{\mathrm{Coul}}(\mathbf{r})=e^2\int\frac{\rho_p(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}d^3\mathbf{r}'-e^2\left(\frac{3}{\pi}\right)^{1/3}\rho_p^{1/3}, \tag{6}$$

and

$$\mathbf{W}_q(\mathbf{r})=\frac{1}{2}W_0\boldsymbol{\nabla}(\rho+\rho_q)+\frac{1}{8}(t_1-t_2)\mathbf{J_q}-\frac{1}{8}(t_1x_1+t_2x_2)\mathbf{J}. \tag{7}$$

As for the effective-mass term, we have

$$\begin{aligned}\frac{\hbar^2}{2M_q^*(\mathbf{r})}=&\frac{\hbar^2}{2M}+\frac{1}{8}\{t_1(2+x_1)+t_2(2+x_2)\}\rho(\mathbf{r})\\ &+\frac{1}{8}\{t_2(2x_2+1)-t_1(2x_1+1)\}\rho_q(\mathbf{r}).\end{aligned} \tag{8}$$

The effective mass so defined is a function of the local density and neutron/proton ratio, but if we set $\rho_n=\rho_p=\frac{1}{2}\rho_0$, where ρ_0 is the equilibrium density of symmetric nuclear matter, we obtain the nuclear-matter isoscalar effective mass, M_s^*, according to

$$\frac{\hbar^2}{2M_s^*}=\frac{\hbar^2}{2M}+\frac{1}{16}\{3t_1+t_2(5+4x_2)\}\rho_0. \tag{9a}$$

Also, setting $\rho_q=0, \rho=\rho_0$ leads to the nuclear-matter isovector effective mass, given by

$$\frac{\hbar^2}{2M_v^*}=\frac{\hbar^2}{2M}+\frac{1}{8}\{t_1(2+x_1)+t_2(2+x_2)\}\rho_0. \tag{9b}$$

Pairing correlations are taken into account in the BCS approximation (with blocking), using a δ-function pairing force,

$$v_{\text{pair}}(\boldsymbol{r}_{ij})=V_{\pi q}\delta(\boldsymbol{r}_{ij}). \tag{10}$$

We shall always allow the pairing-strength parameter $V_{\pi q}$ to be different for neutrons and protons, but without further generalization there is a tendency to overestimate even-odd mass differences, with serious implications for both the S_n and Q_β, especially in the case of heavy nuclei (see Sec. 4 of Ref. [9]). We could, of course, have reduced the errors in the even-odd mass differences simply by taking a weaker pairing force, and since these errors also contribute to the overall error of the mass fit it might be expected that the latter would improve at the same time. This is not so, since 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 mass fit and optimizing the fit to the even-odd differences may be in conflict if we limit ourselves to the simple parametrization (10) of the pairing force.

A way around this problem [29] is to allow $V_{\pi q}$ to be slightly stronger for an odd number of nucleons ($V_{\pi q}^-$) than for an even number ($V_{\pi q}^+$), i.e., the pairing force between neutrons, for example, depends on whether N is even or odd. As noted in Ref. [29], this ‘‘staggered pairing’’ device can indeed lead to improved fits, but its *ad hoc* character might be found to be rather unsatisfactory. However, the very concept of a pairing force is highly phenomenological, and in deriving it from more realistic forces the Pauli principle could conceivably give rise to staggering effects of this sort: the strength of the pairing force itself could be subject to ‘‘blocking’’ by an odd nucleon. Moreover, the HF wave function of an odd nucleus is not an eigenstate of the time-reversal operator [20], and in projecting out from it a state of good time-reversal properties the total energy will be lowered. 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. In our own calculations further compensation may be required by the fact that our HF codes do not treat odd-A and odd-odd nuclei completely self-consistently, since we suppose that the unpaired nucleons do not perturb the field generated by the even-even core.

Note that we do not use the Lipkin-Nogami variant of the BCS method, because in the ETFSI calculations we found better mass fits with the conventional form of the method. A possible reason for this is discussed in Sec. 4 of Ref. [9].

Computational details. As explained below, we use both spherical and deformed HF-BCS codes. These are written in terms of an expansion of the s.p. functions in a harmonic-oscillator basis. In the summation over s.p. states in the BCS calculation we include all continuum states up to an energy of $1\hbar\omega$, where $\hbar\omega$ is the oscillator strength. In calculating the Coulomb energy we fold over the finite size of the proton, assuming the charge to be Gauss-distributed with an rms radius of 0.8 fm. A correction is made for the spurious center-of-mass motion, using the method of Butler *et al.* [30].

In our deformed code we also subtract out from the total computed energy the spurious rotational energy

$$E_{\text{rot}}=\frac{\hbar^2}{2\mathcal{I}}\langle\hat{J}^2\rangle, \tag{11}$$

where $\hat{J}^2$ represents the usual angular-momentum operator, and $\mathcal{I}$ is the moment of inertia. For this latter quantity we write

$$\mathcal{I}=b\{(1-a)\mathcal{I}_{\text{crank}}+a\mathcal{I}_{\text{rigid}}\}, \tag{12}$$

where $\mathcal{I}_{\text{crank}}$ is the cranking-model [31] value of the moment of inertia with pairing correlations included [32], and $\mathcal{I}_{\text{rigid}}$ is the rigid-rotor value. The coefficients a and b are determined by fitting to experimental moments of inertia: see Tables 1 and 10 of Ref. [9]. We take the value $a=0.25$ for all nuclei, while $b=1$ for even-even nuclei, 1.2 for odd-A nuclei and 1.4 for odd-odd nuclei (see Sec. 5 of Ref. [9], where the best value of a for the ETFSI model was found to be 0.20).

Fitting strategy. Even though the computer-time considerations that led to HF mass fits being limited in the past to only a very small number of nuclei are no longer applicable, the fact remains that most nuclei are deformed, and a mass fit entails that every nucleus that is included in the fit has to be calculated many times over. Thus making a direct fit with a deformed HF code to all of the more than 1700 measured masses would impose a very serious strain on one's computer facilities if one varied all 14 force parameters. Some simplifications have to be made, and in particular we adopt the strategy of dividing the fit into two distinct phases.

In the first phase (Sec. III) the fit is limited to the 400 or so spherical, or quasispherical, known nuclei, which can be computed with a much more rapid spherical HF code. The force resulting from this fit, while not final, is used to tie down once and for all (for the purposes of the present paper) the nuclear-matter parameters a_v (the energy per nucleon at equilibrium in symmetric nuclear matter), ρ_0 [the corresponding density, or equivalently the Fermi momentum k_F, given by $((3\pi^2/2)\rho_0)^{1/3}$], J (the symmetry coefficient), and the effective masses M_s^* and M_v^*. In the second phase (Sec. IV) we fit to essentially all nuclei, including deformed nuclei, but the parameter search is constrained by imposing the values of the nuclear-matter parameters a_v, k_F, J, M_s^*, and M_v^* determined in the first phase.

However, while this reduces the number of independent parameters that have to be searched from 14 to nine, the amount of computer time required for this second and final phase would still be excessive if we did not adopt further simplifying procedures. The essential step is to define for each nucleus a deformation energy

$$E_{\text{def}}=E_{\text{sph}}-E_{\text{eq}}, \tag{13}$$

where E_{eq} is the energy at the equilibrium deformation and E_{sph} the energy in the spherical configuration, both calculated with the deformed code. Now E_{def} as defined by this equation is much less sensitive to the exact values of the Skyrme-force parameters than either of the two absolute energies on the right-hand side, a fact which makes the construction of a HF mass formula a feasible proposition if the fits of the second phase are made according to the following three-step reiterative procedure.

(1) With the force resulting from the limited spherical-nucleus fit of the first phase (Sec. III), or with the one emerging from the complete fit of step (3) below, we make a full (unconstrained) deformed HF calculation of the energy E_{eq} of each of the more than 1700 nuclei in our data set. This calculation is performed just once for each nucleus: there is no question of data fitting with the much slower deformed code.

(2) With the same force that went into step (1) we use the deformed HF code to calculate the energy E_{sph} of each nucleus of our data set when a spherical configuration is imposed. The deformation energy E_{def} defined by Eq. (13) can now be calculated for the current force, and all measured masses renormalized to their ''equivalent spherical-configuration'' values. The rms error of the current force is calculated with the spherical code by comparing the masses it gives with the *renormalized* experimental masses.

(3) Using next the spherical code, the force is refitted to the masses of *all* nuclei in our data set, renormalized as described in step (2); this fit is constrained to keep the same nuclear-matter parameters a_v, k_F, J, M_s^*, and M_v^* as determined in phase (1). We stress that this is the only point at which a fit is made, and it is always the spherical code that is used: the use of the deformed code is limited to the calculation of the E_{def}. Making the fit with the spherical code is meaningful only because of the relative insensitivity of E_{def} to small changes in the force parameters. However, because E_{def} will change slightly over the course of this refit the new force it gives rise to is fed back into step (1), and a new iteration cycle begins.

The process can be halted on completion of step (2) during any iteration cycle, since we will then have a complete set of masses calculated self-consistently with a given force. However, for an optimal fit it will be necessary to reiterate until there is sufficient convergence of the rms error emerging from step (2).

III. PRELIMINARY CALCULATIONS ON SPHERICAL NUCLEI

All of the fits (MSk1-5) described in this section were made to 416 spherical, or quasispherical, nuclei, the criterion being that the deformation energy E_{def} [see Eq. (13)] given by the ETFSI-1 table [11] does not exceed 0.30 MeV. Even in these quasispherical fits we renormalize the experimental masses by these values of E_{def}, as explained in Sec. II. All the mass data used in this paper come from the 1995 Audi-Wapstra compilation [33].

Our fitting procedure works as follows. Of the ten Skyrme parameters, x_1 and γ take the same fixed values throughout, -0.5 and 0.333 333, respectively, these values having been found to give optimal fits in rough preliminary tests (actually, the mass fits are rather insensitive to x_1, but only because we have retained in the expression for the total energy E_{HF} the terms in J^2 and J_q^2). Of the remaining eight parameters, x_0, t_2, and W_0 are fitted automatically to the mass data, using the CERN routine MINSQ. The five degrees of freedom that remain are handled in terms of the nuclear-matter parameters a_v, k_F, J (the symmetry coefficient), and the effective masses M_s^* and M_v^* defined above; the expressions for a_v, k_F, and J are given in Ref. [34] by Eqs. (2.12), (2.15), and (2.20), respectively. Also, we always impose the constraint $M_s^*=M_v^*\equiv M^*$, preliminary tests having shown that there is no advantage to doing otherwise (it then follows that $x_2=-0.5$ in all cases). The four remaining degrees of freedom, corresponding to a_v, k_F, J, and M^*/M, are adjusted manually.

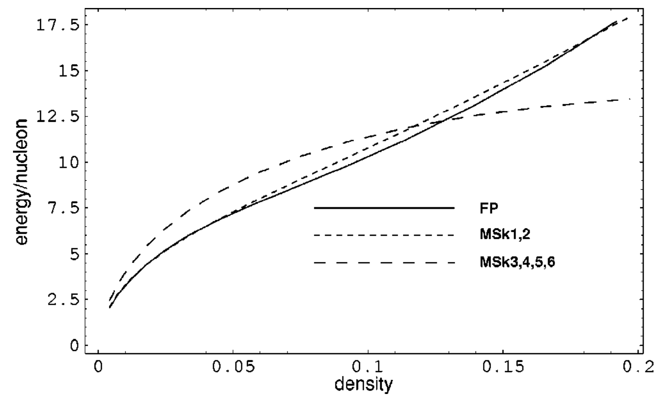

FIG. 1. Energy per nucleon (MeV) of neutron matter as a function of density (nucleons fm^{-3}) for the forces of this paper, and for the calculations of Ref. [18].

Of these degrees of freedom, all of which relate to nuclear matter, we take for k_F the fixed value of 1.326 fm^{-1} ($\rho_0=0.1575\ \mathrm{fm}^{-3}$), this value always giving an optimal mass fit and, at the same time, an rms charge radius of ^{208}Pb that is in close agreement with the experimental value of 5.50 fm [35]. We also varied M^*/M systematically, and found that the best fit was consistently given by the value 1.05, in accordance with the findings of Refs. [14–16], while the ''realistic'' value of 0.7–0.8 led to fits that were unacceptably bad.

As for the symmetry coefficient J, we constrain it to conform to some of the known properties of neutron matter. Now the solid line (FP) in Fig. 1 shows as a function of density the energy per nucleon of pure neutron matter, as calculated by Friedman and Pandharipande [18] for the realistic force $\mathrm{v}_{14}+\mathrm{TNI}$, containing two- and three-nucleon terms. More recent realistic calculations of neutron matter [36–38] give similar results up to nuclear densities; higher densities do not concern us here. We find that the best fit to the curve FP is obtained if we impose on the mass fits the constraint $J=30$ MeV (forces MSk1 and 2), while lower values of J lead to softer neutron-matter curves, with a non-physical collapse occurring below nuclear-matter densities for $J<28$ MeV. On the other hand, the quality of the mass fits improves if we take lower values of J, although it starts to deteriorate again somewhere between 28 and 27 MeV. We

TABLE I. Parameters of the forces developed in this paper.

	MSk1	MSk2	MSk3	MSk4	MSk5	MSk6
t_0 (MeV fm^3)	−1813.03	−1830.67	−1810.32	−1827.96	−1827.96	−1827.96
t_1 (MeV fm^5)	274.828	260.301	269.092	254.129	254.326	258.483
t_2 (MeV fm^5)	−274.828	−293.742	−269.092	−287.569	−287.766	−291.924
t_3 (MeV fm$^{3(1+\gamma)}$)	13050.1	13442.1	13027.5	13419.5	13419.5	13419.5
x_0	0.365395	0.356875	0.631485	0.610360	0.605152	0.576591
x_1	−0.5	−0.5	−0.5	−0.5	−0.5	−0.5
x_2	−0.5	−0.5	−0.5	−0.5	−0.5	−0.5
x_3	0.449882	0.409759	0.903680	0.835063	0.827182	0.783956
W_0 (MeV fm^5)	116.708	116.663	116.871	115.943	115.932	118.807
γ	0.333333	0.333333	0.333333	0.333333	0.333333	0.333333
$V_{\pi n}^+$ (MeV fm^3)	−220.0	−220.0	−220.0	−220.0	−220.0	−227.0
$V_{\pi p}^+$ (MeV fm^3)	−224.0	−224.0	−228.0	−228.0	−228.0	−242.0
$V_{\pi n}^-$ (MeV fm^3)	−220.0	−220.0	−220.0	−220.0	−224.0	−236.0
$V_{\pi p}^-$ (MeV fm^3)	−224.0	−224.0	−228.0	−228.0	−232.0	−251.0

adopt therefore the value $J=28$ MeV, this giving the best mass fit consistent with the known stability of neutron matter (forces MSk3–6). (It is not clear whether the exact minimum in the rms error occurs after or before collapse, but the changes in the rms error in this region, i.e., between 27 and 28 MeV, are quite insignificant, being of the order of 0.005 MeV.) While we see that the fit to the FP curve of Fig. 1 is not as good for $J=28$ MeV as for 30 MeV, we note that even at subnuclear densities the neutron-energy curves of Refs. [36–38] do not agree exactly with the FP curve and there is a sufficient margin of uncertainty to make it difficult to exclude $J=28$ MeV on this basis. Moreover, both Refs. [36] and [37] calculate the symmetry energy of nuclear matter as a function of density for various realistic forces, and we find that their results are compatible with all values of J lying in the range 27 to 30 MeV. (In Ref. [39] it was stated that the relative positions of the neutron and proton s.p. spectra are very sensitive to J, but we find that once a large number of masses have been fitted, as in the present calculations, this is no longer the case, and that it is impossible to distinguish between different values of J on this basis.)

Our preferred value of J, 28 MeV, is to be compared with the value of 32.73 MeV found in the most recent droplet-model fit, the FRDM [2]. (An almost identical value of J, 32.65 MeV, emerges from the zeroth-order Thomas-Fermi calculation of Ref. [13], but this evaluation is not independent of the FRDM value, since the shell corrections and equilibrium deformation configurations, which themselves are J dependent, are taken directly from the FRDM. Self-consistency then requires that the same value of J be found in the purely macroscopic fit: had a significantly different value of J been found this would simply have indicated a failure of self-consistency in the adopted procedure.) The value of 28 MeV was also found with the ETFSI fits of Ref. [40], in which all nuclear masses were fitted, not just the 400 or so spherical or quasispherical nuclei. The present calculation confirms that the ETFSI result was not simply a quirk of the semi-classical approximation, or possibly of the somewhat restricted parametrization of the density distributions that was adopted in the ETFSI model. In a separate calculation [40] we tried to force higher values of J by including an extra t_3 term in the Skyrme force, but to no avail. We are thus led to believe that the value of 28 MeV for J is quite robust, within the framework of Skyrme-type forces.

It is, of course, important to understand the contradiction with the FRDM result, and Ref. [40] suggests one way in which the FRDM could lead to a spuriously high value of J. At the same time, since Skyrme-type forces are not the last word in effective forces, there is an obvious need for parallel studies with finite-range (Gogny-type) forces and also in RMF theory before drawing any definitive conclusions concerning the real value of J. However, such mass fits would have to be as extensive as those we have performed here with Skyrme-type forces, and thus would make even heavier demands on computer time. In any case, we stress that our objective here is to build a mass formula, not determine the value of J, but as long as we are using Skyrme forces as the basis of our mass formula, we have no option but to take the value of J as being close to 28 MeV.

Referring to Tables I and II, we present these different features in terms of four different fits, MSK1–4, that we have made with different fixed values of J and M^*: for the first two $J=30$ MeV, and for the second two 28 MeV, with MSk1 and MSk3 each having $M^*/M=1.00$, while MSk2 and MSk4 each have $M^*/M=1.05$. In each case we have fitted the parameters x_0, t_2, and W_0 automatically to the mass data, as always, while varying a_v and the pairing parameters manually, the latter with the constraint of no staggering, so that there are just two pairing parameters. It will be seen from Table III that $J=28$ MeV gives a better fit than 30 MeV, while 1.05 is a better value than 1.00 for M^*/M.

Taking next the values of J and M^*/M found for the best of these four forces, MSk4, we introduce the degree of freedom corresponding to staggered pairing, and refit the 416 masses, varying a_v, x_0, t_2, W_0, and all four pairing parameters. In this way we arrive at the force MSk5; it will be seen from Table III that the staggered-pairing feature has led to a significant reduction in the rms errors of the absolute masses,

TABLE II. Nuclear-matter parameters of the forces of Table I (see text).

	MSk1	MSk2	MSk3	MSk4	MSk5	MSk6
a_v (MeV)	-15.83	-15.83	-15.79	-15.79	-15.79	-15.79
ρ_0 (fm^{-3})	0.1575	0.1575	0.1575	0.1575	0.1575	0.1575
J (MeV)	30.0	30.0	28.0	28.0	28.0	28.0
M_s^*/M	1.00	1.05	1.00	1.05	1.05	1.05
M_v^*/M	1.00	1.05	1.00	1.05	1.05	1.05
K_v (MeV)	233.7	231.6	233.2	231.5	231.1	231.1
G_0	-0.1828	-0.2585	-0.004121	-0.06958	-0.07017	-0.0826
G_0'	0.2515	0.2275	0.2667	0.2448	0.2442	0.2318
$\rho_{\mathrm{frmg}}/\rho_0$	1.3	1.3	1.6	1.5	1.5	1.4

of the S_n, and of the Q_β. This is our final fit to the masses of the 416 spherical or quasispherical nuclei, and phase 1 of the project outlined in Sec. II is now complete. (Table III also shows the precision with which we reproduce the charge radius of ^{208}Pb; a comparable agreement for other nuclei is found.)

Further comments on force properties listed in Table II. Even though the nuclear-matter incompressibility K_v [see Eq. (2.16) of Ref. [34])] is not a fitted quantity, line 6 of Table II shows that all our forces developed so far are in excellent agreement with the experimental value of 231 ± 5 MeV extracted from breathing-mode measurements [41]. However, our calculation should not be regarded as an independent determination of K_v, since it has been shown [39] that with a suitable generalization of the Skyrme force (t_4 term) it is possible to change K_v, along with the breathing-mode energies, while maintaining the fit to masses (at least to those of doubly magic nuclei). Rather, the agreement we find here could be taken as an indication that the simple form of Skyrme force 1 is adequate for our present purposes, and that generalizations are not necessary.

Lines 7 and 8 show the Landau G_0 and G_0' parameters of our forces, as defined in Ref. [42]. Our values of G_0 are in reasonable agreement with the experimental value of approximately zero [43], but there is in all cases a serious disagreement with the experimental value of 1.80 for G_0' [43]. In principle, we could have fitted G_0' by adjusting x_1, a degree of freedom that has not yet been exploited, but the mass fits would then have deteriorated drastically, and the good agreement with experiment found for G_0 destroyed. In any case, we do satisfy the condition $G_0' > -1$, necessary for the stability of symmetric nuclear matter against a spin-isospin flip [44].

Line 9 indicates the density ρ_{frmg}, expressed in terms of the equilibrium density of symmetric nuclear matter ρ_0, at which neutron matter flips over into a ferromagnetic state that has no energy minimum and would collapse indefinitely [45]. It will be seen that for all our forces this happens only at densities significantly higher than nuclear-matter densities, for which the nonrelativistic Skyrme-form force is expected to be invalid anyway.

IV. INCLUSION OF DEFORMED NUCLEI, AND FINAL FIT

We expand our data set now to include all nuclei with $A \geqslant 36$ for which measured masses are given in the 1995 compilation [33], with the exception of nuclei for which $N = Z, Z \pm 1$, since they are subject to Wigner-term anomalies (see, for example, Refs. [46–52]). These anomalies are highly conspicuous in the ETFSI-1 mass table [11], manifesting themselves as an underbinding with respect to experiment of about 2 MeV for such nuclei; they cannot be removed without leaving the HF-BCS framework (see also the

TABLE III. Errors in the data fit of the forces of Table I. The first line gives the number of nuclei fitted. $\sigma(M)$, $\sigma(S_n)$, and $\sigma(Q_\beta)$ denote the rms errors in the fit to the absolute masses, the neutron-separation energies, and the beta-decay energies, respectively, while the ϵ quantities refer to the corresponding mean errors. The last line gives the calculated rms charge radius R_{ch} of ^{208}Pb (in fm^{-1}), to be compared with the experimental value of 5.50 fm^{-1}. All quantities (except for the first and last lines) are in MeV.

	MSk1	MSk2	MSk3	MSk4	MSk5	MSk6
Number	416	416	416	416	416	1719
$\sigma(M)$	0.848	0.816	0.784	0.730	0.709	0.754
$\epsilon(M)$	-0.048	-0.054	0.028	-0.063	-0.030	-0.042
$\sigma(S_n)$	0.559	0.558	0.549	0.556	0.501	0.434
$\epsilon(S_n)$	-0.019	-0.010	-0.027	-0.013	-0.010	0.025
$\sigma(Q_\beta)$	0.753	0.742	0.729	0.735	0.674	0.564
$\epsilon(Q_\beta)$	-0.0526	-0.0712	-0.0768	-0.0783	-0.0811	0.053
$R_{\mathrm{ch}}(^{208}\mathrm{Pb})$	5.500	5.503	5.499	5.502	5.502	5.503

discussion in Ref. [10]). We are left then with a total of 1719 masses in our data set, which is identical to the one taken in the ETFSI-2 fit [12] (the deformation parameters given by this latter are taken as the starting values in our deformed HF calculations).

This data set is fitted by the reiteration of the three-step scheme outlined in Sec. II, an essential feature of which is that the fit of step 3 is always made under the constraint of keeping the same nuclear-matter parameters a_v, k_F, J, and M^*/M as found for the force MSk5 in the spherical-nucleus fits of Sec. III. We are thus left with varying just x_0, t_2, and W_0, which is done automatically, and the pairing parameters, which is done manually. (x_1 and γ are left unchanged from the values used in Sec. III.)

Three complete iteration cycles brought us from force MSk5 to force MSk6, for which the rms error for the 1719 nuclei of our data set is 0.754 MeV (Table III). It seems that further improvement is impossible as long as we keep the constraints emerging from Sec. III, i.e., maintain the same nuclear-matter parameters a_v, k_F, J, and M^*/M as found for the best spherical-nucleus fit MSk5. Exploiting these degrees of freedom, along with those associated with x_1 and γ, could lead to some further reduction in the rms error of the fit.

We see from Table II that the nonfitted nuclear-matter properties of force MSk6, i.e., K_v, G_0, G_0', and ρ_{frmg}, are very similar to those of force MSk5. Indeed, the most striking difference between our final force MSk6 and the best spherical-nucleus fit MSk5 is that the introduction of deformed nuclei into the fit has led to a much stronger pairing force (Table I). Presumably, the specific function of this enhanced pairing is to give an increased attraction midshell (where the deformed nuclei are situated), relative to nuclei nearer to shell closure. In any case, we see that a pairing force that is optimal for spherical nuclei will be suboptimal for deformed nuclei, and *vice versa*. It must be stressed that staggering is an absolutely essential feature of the pairing term in MSk6, since otherwise the even-odd mass differences would be unacceptably large.

V. CONCLUSIONS

We have fitted a ten-parameter Skyrme force, along with a four-parameter δ-function pairing force, to 1719 nuclear masses, using the HF-BCS method. With just seven of the 14 parameters being freely varied in the fit to the complete data set, the rms error of our final force, MSk6, is 0.754 MeV, but this could probably be improved a little if we relaxed the constraint of imposing on our fits the values of the nuclear-matter parameters a_v, k_F, J, M_s^*, and M_v^* that optimized the fit to spherical nuclei (force MSk5); attention should be paid in particular to the effective masses. We could likewise investigate the degrees of freedom associated with x_1 and γ, although for the first of these we have to ensure that the phase transition to a ferromagnetic state does not occur at too low a density [45], while for the second we would not want to destroy the excellent agreement with experiment that we already have for the incompressibility K_v. However, whether or not we eventually improve on the recent ETFSI-2 fit to the identical set of mass data [12], for which the rms error was 0.709 MeV, we see from Table III that the rms errors in the S_n and Q_β, quantities of greater importance for the r process than the absolute masses themselves, are already slightly smaller for MSk6 than for ETFSI-2, for which the corresponding values are 0.455 and 0.577 MeV. In any case, we have demonstrated that constructing a HF mass formula is now a practical proposition.

The nuclear matter corresponding to force MSk6 has the following parameters: $a_v = -15.79$ MeV, $\rho = 0.1575\ \mathrm{fm}^{-3}$ ($k_F = 1.326\ \mathrm{fm}^{-1}$), $M^*/M = 1.05$, and $J = 28$ MeV. Our value for the last of these parameters, the nuclear-matter symmetry coefficient, was obtained under the constraint that neutron matter must not collapse at nuclear or subnuclear densities, and agrees with the value extracted from ETFSI-model fits to the mass data [40]. We conclude that the value $J = 28$ MeV is quite robust, within the framework of Skyrme-type forces.

While the force MSk6 presented here is, with its effective-mass parameter $M^*/M \simeq 1.0$, well adapted to the HF calculation not only of nuclear masses but presumably also of fission barriers, it should not be forgotten that there are applications for which forces having a realistic value of M^*/M (0.7–0.8), such as those of will still be essential, e.g., the calculation of the giant dipole resonance. However, the mass fits obtained with such forces are considerably inferior to what we have found here: with the same data set of 416 nuclei as we took in Sec. III the best fit we could find had an rms error of 1.141 MeV, which is to be compared with 0.709 MeV for force MSk5.

Note added in proof. We have now realized this project, varying essentially *all* the force parameters. The rms error of this new force, MSk7, is 0.702 MeV for the same data set of 1719 nuclei to which we fitted the force MSk6 of the present paper. A complete mass table, HFBCS-1, corresponding to this force is being submitted for publication, and is available on the web at http://www-astro.ulb.ac.be

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