Quantum hadrodynamics parametrization: A least-squares fit to nuclear ground-state properties

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We study the four meson masses and coupling constants used in quantum hadrodynamics by comparing the relativistic Hartree-Fock calculation with nuclear ground-state properties. Six parameters are determined by least-squares fit to experimental ground-state properties of five spherical nuclei ^{16}O, ^{40}Ca, ^{48}Ca, ^{90}Zr, and ^{208}Pb; these properties are total binding energies, charge radii, and surface thicknesses. This work is compared with an earlier relativistic Hartree least-squares fit. We find that by including exchange terms, the best-fit meson masses are within 3% of their physical values, which is not the case if only direct terms are used. Both calculations reproduce binding energies and radii with an average error around 1%. Hartree-Fock values for the nuclear surface thickness are a substantial improvement (around 15%); however, both calculations consistently produce too small a value.

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I. INTRODUCTION

During the last decade as the energy of nuclear physics experiments has been increasing, and with new experiments proposed for future facilities such as CEBAF and the Brookhaven Relativistic Heavy Ion Collider (RHIC), there has been an increasing interest in relativistic effects in nuclear physics. Whether we look at the success of Dirac phenomenology in the nucleon-nucleus scattering process or the results of relativistic field theories in the structure problem, both suggest the importance of relativistic effects in nuclear physics. Quantum hardrodynamics (QHD), a relativistic theory of nucleons with explicit mesonic degrees of freedom, has been successfully applied to a wide range of nuclear phenomena such as nuclear matter, neutron stars, finite nuclei, and hypernuclei, as well as dynamic processes such as nucleon-nucleus and electron-nucleus scattering. For a comprehensive review of this subject, the reader is referred to a review article by Serot and Walecka [1], which also contains an extensive citation of earlier references.

In the nuclear structure problem, both relativistic Hartree (H) [2–8] and Hartree-Fock (HF) [9–12] calculations have been performed and have satisfactorily reproduced many ground-state properties, such as total binding energies, rms radii, radial charge distributions, quadrupole moments, magnetic moments, single-particle energy levels, etc. Applications include both spherical and deformed nuclei, and cover a broad mass spectrum throughout the periodic table.

When compared to the conventional nonrelativistic HF calculations, whether with the zero-range Skyrme force or a Gogny force, these relativistic calculations display two obvious advantages: First, they possess explicitly the mesonic degrees of freedom, which render the investigation of phenomena such as meson-exchange current contributions and meson retardation effects more accessible; second, in the relativistic framework, the nuclear spin-orbit forces emerge naturally out of the interplay between scalar and vector meson interactions, and have the right magnitude without introducing any extra parameters.

In relativistic QHD the nucleon, which is described as a Dirac particle, is coupled to several exchange mesons through an effective Lagrangian. The quantum numbers selected for the mesons are motivated by one-boson-exchange models [13] for nucleon-nucleon interactions; they correspond to the physical mesons ω, ρ, π, and unphysical meson σ. Since we view this as an effective Lagrangian, the parameters in the model, which are the masses and coupling constants of the mesons, need to be determined by the effectiveness of the model in reproducing nuclear properties.

One way [4, 10] is to fit the coupling constants to the infinite nuclear matter saturation values for energy and density, while holding meson masses to their physical values. However, the scalar (σ) meson has no "physical" value and only the ratio of mass to coupling constant can be determined without resorting to some data from finite nuclei.

Moreover, in relativistic HF calculations, when parameters fitted to nuclear matter saturation data are used, one finds that the binding energy of finite nuclei are too small by about 20–30%, and that deformation is not always correctly predicted in deformed nuclear calculations [12]. In temperature-dependent HF calculations the thermal response found is large compared to nonrelativistic calculations [14].

An alternative approach is to fit all these parameters directly to experimentally observable bulk properties of the nuclear ground states. In the latter approach, since there are a great deal more data to fit, one can explore the limit and the range of the application of the model,

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since the fitted parameters can be used to predict many other physical observable quantities of nuclei. In nonrelativistic HF calculations, there have been considerable efforts to improve on the parameters of the Skyrme force by using this approach [15]. In relativistic calculations, however, this type of work has been limited so far to Hartree calculations [16].

In Ref. [16] the ability of a relativistic mean-field theory to reproduce nuclear ground-state properties was investigated by an extensive fit to experimental data. Both a linear and a nonlinear model (which introduces self-interactions of the scalar meson) were investigated. The nonlinear model (eight parameters) is capable of reproducing the ground-state properties as well as the conventional Skyrme force HF calculations; however, the linear model (six parameters) is a poorer fit, and the authors of Ref. [16] conclude that an effective Lagrangian with linear coupling is not able to reproduce ground-state properties over a wide range of nuclei.

In the present paper we extend the fitting procedure to a relativistic Hartree-Fock model. The need for the extension is clear. Since we do not expect exchange contributions to be small in the case of the strong interactions found in a nucleus, there is considerable danger in limiting oneself to the Hartree approximation. Moreover, one would like to investigate the physical properties where the isovector mesons play a crucial role, such as meson-exchange currents or neutron-rich or neutron-deficient nuclei. To do so one has to include the exchange terms, since for these systems they may dominate. In the relativistic HF calculation, an important ingredient is the pion [12, 17]; by contrast the pion contribution vanishes in the Hartree calculation for spherical nuclei.

There are other unsatisfactory aspects of the least-squares fit obtained in the Hartree approximation. First, in the linear Hartree procedure, an unusually large χ^2 is obtained; the fitting also pushes the ω meson mass far above its physical value [16]. The nonlinear model reproduces the experimental data very well; however, in the self-coupling the parameter of the quartic term turns out to be negative, and for such a Lagrangian the energy spectrum is unbound from below [18]. At best, one can say that a local minimum has been found by the fitting procedure, and one hopes that the unstable regions cannot compromise the mean-field approximations.

In this work, however, we will concentrate on a linear model. It is important to see whether a relativistic HF calculation can bring the χ^2 down to a value comparable to the nonrelativistic result. We would also be gratified to see the meson masses, in particular the vector meson masses, emerge from the fitting procedure close to their physical values. This could establish the connection of the current model to physical one-boson-exchange models; small changes of the effective meson masses can be attributed to medium effects. Finally, the parameters obtained by the fitting procedure can be employed in other relativistic HF calculations, thus testing its predictive powers, for example, in the deformed nuclei and temperature dependent HF calculations. To make our result comparable to Ref. [16], we follow their fitting procedure; i.e., we fit the calculations for various nuclei from ^{16}O to ^{208}Pb to the following properties of nuclear ground state: total binding energy, diffraction radius, and surface thickness.

There are two different ways to solve the HF equations: One is to search directly for the numerical solutions of the differential equations (the nonspectral method). The other method is to expand the solutions in terms of a complete basis set and then, after truncating to a finite basis, perform a diagonalization. There are particular problems associated with the first method in dealing with the nonlocal nature of the exchange terms in the HF calculation; however, the second approach is, in principle, no more difficult for the HF than for the Hartree calculation [12]. We have adopted the second method. Also, from the viewpoint of computation time, the diagonalization method is much faster compared to solving the differential equations, once the basis states have been obtained and subjected to convergence tests to determine the truncation point. Since in the fitting procedure the diagonalization will have to be performed repeatedly and we need only obtain the basis states once, this method provides us with a computer code which is very efficient relative to the nonspectral approach.

The arrangement of this paper is as follows. In Sec. II we briefly review the relativistic meson-field theory and HF formalism, and in Sec. III discuss the fitting procedure. In Sec. IV we present our results for the parameters and compare them with the values from other relevant works; then we show results of more extensive calculations obtained using these parameters. Finally in Sec. V we summarize our conclusions and our outlook for further improvement of the current work.

II. MESON-FIELD THEORY AND HARTREE-FOCK APPROACH

Motivated by the relativistic one-boson-exchange description of the NN interaction [13] and Walecka model [19], we start from an effective local Lagrangian density which couples a nucleon (ψ) to four mesons with the following spin-parity and isospin quantum numbers (J^π, T):

$$\sigma(0^+,0), \quad \omega(1^-,0), \quad \pi(0^-,1), \quad \rho(1^-,1).$$

We also include electromagnetic interactions (A^μ). The Lagrangian density is written as the sum of free and interacting parts:

$$\mathcal{L} = \mathcal{L}_F + \mathcal{L}_I \,, \tag{1}$$

$$\begin{aligned}\mathcal{L}_F = {} & \bar{\psi}(i\gamma_\mu\partial^\mu - M)\psi + \frac{1}{2}(\partial_\mu\sigma\partial^\mu\sigma - m_\sigma^2\sigma^2) \\ & + \frac{1}{2}(\partial_\mu\boldsymbol{\pi}\partial^\mu\boldsymbol{\pi} - m_\pi^2\boldsymbol{\pi}^2) \\ & - \frac{1}{4}F_{\mu\nu}F^{\mu\nu} + \frac{1}{2}m_\omega^2\omega_\mu\omega^\mu - \frac{1}{4}\mathbf{G}_{\mu\nu}\mathbf{G}^{\mu\nu} \\ & + \frac{1}{2}m_\rho^2\boldsymbol{\rho}_\mu\boldsymbol{\rho}^\mu - \frac{1}{4}H_{\mu\nu}H^{\mu\nu} \,,\end{aligned} \tag{2}$$

$$\begin{aligned}\mathcal{L}_I = {} & g_\sigma\bar{\psi}\sigma\psi - g_\omega\bar{\psi}\omega^\mu\gamma_\mu\psi - \frac{f_\pi}{m_\pi}\bar{\psi}\gamma_5\gamma^\mu\boldsymbol{\tau}\psi\partial_\mu\boldsymbol{\pi} \\ & - g_\rho\bar{\psi}\boldsymbol{\rho}^\mu\boldsymbol{\tau}\gamma_\mu\psi - e\bar{\psi}\gamma^\mu\frac{1}{2}(1+\tau_3)A_\mu\psi \,,\end{aligned} \tag{3}$$

where

$$F_{\mu\nu} = \partial_\mu \omega_\nu - \partial_\nu \omega_\mu, \mathbf{G}_{\mu\nu} = \partial_\mu \boldsymbol{\rho}_\nu - \partial_\nu \boldsymbol{\rho}_\mu ,$$

$$H_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu. \tag{4}$$

There are two coupling schemes for the pion, pseudovector (PV), and pseudoscalar (PS), but there are many reasons for rejecting PS coupling. In a relativistic Hartree-Fock nuclear matter calculation Horowitz and Serot [20] found that when PS coupling is used the baryon self-energies are extremely large (about 40 times larger then their PV counterpart) at normal nuclear density, which has a drastic effect on the single-particle spectrum. The authors of Ref.[20] conclude that the HF approximation to the PS theory is inadequate for description of normal nuclear matter; they also pointed out the possibility of some sort of cancellations provided by higher order nonlinear effects; however, to include these contributions one must go beyond the Hartree-Fock approach. Before their work, Miller [9] was unable to solve the Dirac-Hartree-Fock equations for a finite nucleus when PS coupling was used. In a relativistic Hartree calculation for an odd-A deformed nucleus, where contributions from the pion are small (but not zero as is the case for spherical nuclei), we [21] also found that stable solutions can be obtained only when the PV coupling is adopted. In this work we use PV coupling for the pion.

We recognize that the PV coupling of the pion makes the Lagrangian nonrenormalizable; however, we take the view that this is an effective Lagrangian, in the sense that we use it to generate one-particle-exchange terms only. Moreover, a strict treatment of a relativistic quantum field theory would also require us to include vacuum polarization terms which are very complicated for finite nuclei and can be hardly included to all orders. The parameters in the Lagrangian will be adjusted to fit the empirical data using lowest order diagrams only, so that corrections such as vacuum polarization have already been taken into account in so far as it is possible within the framework of an effective Lagrangian. It is in this spirit that we exclude the contribution from the Dirac sea and other higher order effects.

From the Lagrangian (1), the Euler-Lagrange equation leads to the following equations of motion for the mesons:

$$\begin{aligned}
&(\partial_\mu \partial^\mu + m_\sigma^2)\sigma = g_\sigma \bar{\psi}\psi, \\
&(\partial_\mu \partial^\mu + m_\pi^2)\boldsymbol{\pi} = \frac{f_\pi}{m_\pi}\partial_\mu(\bar{\psi}\gamma_5\gamma^\mu \boldsymbol{\tau}\psi), \\
&\partial^\mu F_{\mu\nu} + m_\omega^2 \omega_\nu = g_\omega \bar{\psi}\gamma_\nu \psi, \\
&\partial^\mu \mathbf{G}_{\mu\nu} + m_\rho^2 \boldsymbol{\rho}_\nu = g_\rho \bar{\psi}\boldsymbol{\tau}\gamma_\nu \psi.
\end{aligned} \tag{5}$$

In this work we employ the mean-field approximation for meson fields. In that approximation the meson-field operators are replaced by their vacuum expectation values, and so these fields just behave like classical fields; in other words the quantum fluctuations are entirely neglected. Since we are interested in static solutions, the meson fields are time independent, and the nucleon-field operator can be expanded in a complete set of stationary states:

$$\begin{aligned}
\psi(x) &= \sum_\alpha [f_\alpha(\mathbf{r}) e^{-iE_\alpha t} b_\alpha + g_\alpha(\mathbf{r}) e^{iE'_\alpha t} d_\alpha^\dagger], \\
\psi^\dagger(x) &= \sum_\alpha [f_\alpha^\dagger(\mathbf{r}) e^{iE_\alpha t} b_\alpha^\dagger + g_\alpha^\dagger(\mathbf{r}) e^{-iE'_\alpha t} d_\alpha].
\end{aligned} \tag{6}$$

Here f_α and g_α together form a complete set of Dirac spinors, b_α and $b_\alpha^\dagger$ represent annihilation and creation operators for the nucleon state α, and d_α and $d_\alpha^\dagger$ are annihilation and creation operators for the corresponding antinucleon state; they satisfy the anticommutation relations for fermions. Since we do not consider the contribution from the Dirac sea, the antinucleon part in the expansion will be omitted hereafter. Now the Hamiltonian can be obtained from the Lagrangian (1) by the standard procedure and, by using the Green functions for mesons, the meson fields can be eliminated from the Hamiltonian. We obtain the following second-quantized Hamiltonian in terms of nucleon creation and annihilation operators:

$$\begin{aligned}
H = &\sum_{\alpha,\alpha'} \int f_{\alpha'}^\dagger(\mathbf{r})(-i\boldsymbol{\gamma}\cdot\boldsymbol{\nabla} + M) f_\alpha(\mathbf{r}) d^3r b_{\alpha'}^\dagger b_\alpha \\
&+ \frac{1}{2} \sum_{\alpha,\alpha',\beta,\beta'} \int f_{\alpha'}^\dagger(\mathbf{r}_1) f_{\beta'}^\dagger(\mathbf{r}_2) V(|\mathbf{r}_1 - \mathbf{r}_2|) f_\beta(\mathbf{r}_2) f_\alpha(\mathbf{r}_1) d^3r_1 d^3r_2 b_{\alpha'}^\dagger b_{\beta'}^\dagger b_\beta b_\alpha,
\end{aligned}$$

$$V(|\mathbf{r}_1 - \mathbf{r}_2|) \equiv V(r) = \sum_{i=s,v,e} V_i(r),$$

$$V_s = -g_\sigma^2 \gamma_0(1)\gamma_0(2)\frac{e^{-m_\sigma r}}{4\pi r} + g_\omega^2 \gamma_0(1)\gamma_0(2)\gamma^\mu(1)\gamma_\mu(2)\frac{e^{-m_\omega r}}{4\pi r}, \tag{7}$$

$$V_v = \boldsymbol{\tau}(1)\cdot\boldsymbol{\tau}(2)\left[\left(\frac{f_\pi}{m_\pi}\right)^2 \gamma_0(1)\gamma_5(1)\gamma^\mu(1)\gamma_0(2)\gamma_5(2)\gamma_\nu(2)\partial_\mu(1)\partial^\nu(2)\frac{e^{-m_\pi r}}{4\pi r} + g_\rho^2 \gamma_0(1)\gamma_0(2)\gamma^\mu(1)\gamma_\mu(2)\frac{e^{-m_\rho r}}{4\pi r}\right],$$

$$V_e = \frac{1}{4}[1+\tau_3(1)][1+\tau_3(2)]e^2 \gamma_0(1)\gamma_0(2)\gamma^\mu(1)\gamma_\mu(2)\frac{1}{4\pi r}.$$

Note that in this equation we have neglected retardation in the meson fields. Because of the short range nature of the nuclear force and the fact that energy transfers involved are small compared to the masses of the exchanged mesons, our HF calculation of spherical nuclei shows that even for ^{208}Pb retardation can change the total binding energy by less than 5%, while it has a still smaller effect on the single-particle spectrum [17]. Therefore we do not expect the inclusion of the retardation can have an important consequences for fitting purposes. In a spectral approach, such as the one we use in this work, the presence of the retardation in the exchange terms makes the matrix elements in the Hartree-Fock equation dependent on the single-particle spectrum which itself is redetermined at each iteration. So instead of calculating these matrix elements once and for all (as when retardation is neglected), one has to recalculate them repeatedly at each iteration until a stable solution is reached. This is prohibitively time consuming for the fitting procedure, and so in this paper the retardation is neglected.

In a HF calculation, we assume that the ground state of the nucleus with A nucleons is

$$|\Phi_g) = \prod_{\alpha=1}^{A} b_\alpha^\dagger |0). \tag{8}$$

Now we are in the position to calculate the ground-state energy of an A-nucleon system. In this work we deal with spherical nuclei only, and so a single-particle state labeled α has a characteristic j (angular momentum), m (third component of j), π (parity), t_3 (third component of isospin), and principal quantum number. Since we adopt the spectral method to solve the HF equation, each single-particle state of the system is expanded in a complete basis set; the expansion takes the form

$$f_\alpha(\mathrm{r}) = \sum_i C_i^\alpha |i\rangle \equiv \sum_n C_n^\alpha \begin{pmatrix} \frac{iG_{nj}^\pi(r)}{r}\phi_{jm}^\pi \\ \frac{-F_{nj}^\pi(r)}{r}\phi_{jm}^{-\pi} \end{pmatrix}. \tag{9}$$

In principle we can choose any complete orthogonal set for the basis functions, for example, spherical harmonic oscillator wave functions. However, in this work we would like to choose a basis which is the set of solutions of the Dirac equation with a potential as close as possible to that of the nucleus in question; we use as our expansion basis the set of self-consistent Hartree solutions for the same nucleus. This basis is easily obtained using the nonspectral method. In this way, we decrease the number of states in the expansion basis necessary to produce reasonable convergence. The size of the basis varies with the nucleus; for example, for ^{208}Pb we use ten major shells. Another merit of our basis is that our final solutions have a more realistic asymptotic behavior than those obtained using an oscillator basis; this may be crucial when our results are compared with surface features of the nucleus. One of the disadvantages is that such a basis has a partly discrete and partly continuous spectrum, and one of our earlier studies [8] showed that it is important to include continuum basis states. We therefore adopt a method of artificially discretizing the states in the continuum by confining the entire system in a large sphere (R=7–12 fm depending on the nucleus), and imposing the linear boundary condition of the MIT bag model [8, 17]. It turns out that this boundary has negligible effect on the bound states; however, it gives us a convenient way to deal with states formerly in the continuum. Of course, the completeness of the basis also requires us to include basis states from both positive and negative energy sectors.

Now inserting the expansion (9) into the Hamiltonian (7), we can calculate the ground-state energy of an A-nucleon system. Then the HF equation for a single-particle state can be obtained by performing a variation of the ground-state energy with respect to the expansion coefficient C_i with the constraint that the wave function remain normalized. The resulting (HF) equations are

$$\begin{aligned}
\sum_{i_1'} \Bigg[& \langle i|T|i_1'\rangle + \sum_{\alpha=1}^{A}\sum_{i_2 i_2'} C_{i_2}^{\alpha *}\langle i i_2|V_s|i_1' i_2'\rangle C_{i_2'}^{\alpha} + (-)^{t_3(\gamma)-1/2}\sum_{\alpha=1}^{A}\sum_{i_2 i_2'} C_{i_2}^{\alpha *}(-)^{t_3(\alpha)-1/2}\langle i i_2|V_v|i_1' i_2'\rangle C_{i_2'}^{\alpha} \\
& + [t_3(\gamma)+\tfrac{1}{2}]\sum_{\alpha=1}^{A}\sum_{i_2 i_2'} C_{i_2}^{\alpha *}[t_3(\alpha)+\tfrac{1}{2}]\langle i i_2|V_e|i_1' i_2'\rangle C_{i_2'}^{\alpha} - \delta_{t_3(\alpha),t_3(\gamma)}\sum_{\alpha=1}^{A}\sum_{i_2 i_2'} C_{i_2}^{\alpha *}\langle i i_2|V_s|i_2' i_1'\rangle C_{i_2'}^{\alpha} \\
& - \delta_{t_3(\alpha),t_3(\gamma)}\sum_{\alpha=1}^{A}\sum_{i_2 i_2'} C_{i_2}^{\alpha *}\langle i i_2|V_v|i_2' i_1'\rangle C_{i_2'}^{\alpha} - [t_3(\gamma)+\tfrac{1}{2}]\sum_{\alpha=1}^{A}\sum_{i_2 i_2'} C_{i_2}^{\alpha *}[t_3(\alpha)+\tfrac{1}{2}]\langle i i_2|V_e|i_2' i_1'\rangle C_{i_2'}^{\alpha} \\
& - 2\delta_{t_3(\gamma),-t_3(\alpha)}\sum_{\alpha=1}^{A}\sum_{i_2 i_2'} C_{i_2}^{\alpha *}\langle i i_2|V_v|i_2' i_1'\rangle C_{i_2'}^{\alpha}\Bigg] C_{i_1'}^{\gamma} \;=\; \epsilon^\gamma C_i^\gamma .
\end{aligned} \tag{10}$$

In a practical calculation, the expansion basis in (9) must be truncated after a fixed number of basis states N. Any reliable results should be independent of N, and so the number must be large enough to ensure that a satisfactory convergent solution has been reached. The convergence test we apply is detailed in Refs. [8, 12]; the reader is referred there for further information. Once the convergence test is performed, we can solve the HF equation (10) by the iteration method. Given an initial set of values for C_i, Eq. (10) is iterated until a stable solution is obtained. The criterion for a stable solution is that the energy difference between all single-particle energies during several successive iterations should be less than 10 keV. A stable solution usually can be reached after

about 15–50 iterations depending on the nucleus. The grid size for all of these calculations is 0.05 fm.

The total binding energy of a nucleus of A nucleons of mass M is

$$E = E_{\rm HF} + E_{\rm c.m.} - AM, \tag{11}$$

where $E_{\rm HF}$ is the total binding of the HF calculation and $E_{\rm c.m.}$ is a correction for the spurious center-of-mass energy; we adopt the correction from Ref. [16], $E_{\rm c.m.} = -\frac{3}{4}$ (41 MeV) $A^{-1/3}$, to ensure that our total binding is defined the same as in that reference.

In order to treat the non-closed-shell nuclei, a schematic pairing model with a constant energy gap is employed in Ref.[16]. The pairing term is assumed to have no contribution for a closed-shell nucleus. Our philosophy is that all nuclear forces should be already included in a meson-exchange mechanism. Of course, at the mean-field approximation level, no specific pairing-type force is present; however, we still prefer to do the calculations without introducing any arbitrary terms in the Hamiltonian. One would have to look beyond the mean-field approximation to investigate the effects of pairing contributions. At the nuclear matter level such an investigation has been done [22]; in this paper our intention is to seek for the parametrization of QHD in the mean-field approximation.

III. LEAST-SQUARES FIT

One way to test the adequacy of a physical model is to evaluate the variable χ^2:

$$\chi^2 = \sum_n \left(\frac{O_n^{\rm expt} - O_n^{\rm theory}}{\Delta O_n} \right)^2 . \tag{12}$$

Here $O^{\rm expt}$ is a set of chosen observables, and $O^{\rm theory}$ are the corresponding predicted values. In experimental data analysis, the weight ΔO is the statistical error in the data. In Ref. [16] weights are determined by the expectation of the ability of the model to describe the observables in question; in this way the relative weights of their contributions are regulated. Under these circumstances the value of χ^2 is somewhat arbitrary, and one should be careful when two values are compared. To make our result comparable to that of Ref. [16], we follow their fitting procedure as far as possible: We choose the same set of physical observables and weights. The observables are the nuclear binding energy E, charge diffraction radius R, and the charge surface thickness σ. To obtain R and σ, we use the Coulomb form factor $F_C(q)$ in the form [16]

$$\begin{aligned} F_C(q) &= [F_{\rm Pr}(q)\mathcal{F}_{\rm Pr}(q) + F_{\rm Ne}(q)\mathcal{F}_{\rm Ne}(q)] \\ &\quad \times \exp[(rq)^2/A^{2/3}], \quad r = 0.51 \text{ fm} , \\ F_{\rm Pr}(q) &= 4\pi \int_0^\infty dr r^2 j_0(qr) \sum_{\alpha=1}^{Z} f_\alpha^\dagger f_\alpha , \\ F_{\rm Ne}(q) &= 4\pi \int_0^\infty dr r^2 j_0(qr) \sum_{\alpha=1}^{N} f_\alpha^\dagger f_\alpha , \\ \mathcal{F}_t(q) &= \sum_{i=1}^{4} \frac{a_{i,t}}{1 + b_{i,t} q^2}, \quad t = \text{Pr or } t = \text{Ne}. \end{aligned} \tag{13}$$

TABLE I. Expansion coefficients for proton and neutron form factors.

	$i=1$	$i=2$	$i=3$	$i=4$
$a_{i,\rm Pr}$	0.312	1.312	-0.709	0.085
$b_{i,\rm Pr}$ [fm]	0.16667	0.06658	0.02269	0.006485
$a_{i,\rm Ne}$	1	-1		
$b_{i,\rm Ne}$ [fm]	0.04833	0.05833		

Here $F_{\rm Pr}$ and $F_{\rm Ne}$ are the distributions of protons and neutrons, respectively, and $\mathcal{F}_{\rm Pr}$ and $\mathcal{F}_{\rm Ne}$ are the proton and neutron form factors; the coefficients $a_{i,t}$ and $b_{i,t}$ are given in the Table I. The remaining factor in F_C is a correction for spurious center-of-mass motion which comes from harmonic oscillator parametrization. Now the diffraction radius R is given by the first zero of the form factor:

$$R = 4.493/q^{(1)} , \quad F_C(q^{(1)}) = 0. \tag{14}$$

The surface thickness σ is determined from the suppression of the second maximum compared to the form factor of a hard sphere:

$$\sigma = \left[\frac{2}{q_m^2} \ln \left(\frac{3j_1(q_m R)}{q_m R F_C(q_m)} \right) \right]^{1/2} , \tag{15}$$

$F_C(q_m)$ is second maximum.

We select ^{16}O, ^{40}Ca, ^{48}Ca, ^{90}Zr, and ^{208}Pb for our HF fitting as established closed-shell spherical nuclei; these nuclei represent a wide range in mass number A, and we have included one pair of isotopes to represent the isotopic trend. The physical observables for these five nuclei are shown in the Table II. In Ref.[16] ^{56}Ni, ^{116}Sn and ^{124}Sn are also included, but these do not fit our criteria. Moreover, HF calculations are more complicated than Hartree calculations (the computational time of our HF codes is about 10 times longer than our Hartree calculations), and since, in the process of searching for the minimum, the HF codes will be called frequently, we need to keep the number of fitted nuclei as low as possible.

Because of these differences, the direct comparison between χ^2 of our result and that in Ref. [16] is not relevant; a more meaningful quantity perhaps is χ^2 per nucleon. The values of χ^2 from these two calculations are not as important as their predictive powers, as revealed when the best-fit parameters are used to calculate a broad spectrum of nuclei.

TABLE II. Experimental values for observables included in the fit: binding energy E_B, diffraction radius R, and surface thickness σ.

	E/A (MeV)	R (fm)	σ (fm)
^{16}O	-127.6	2.777	0.839
^{40}Ca	-342.1	3.845	0.978
^{48}Ca	-416.0	3.964	0.881
^{90}Zr	-783.9	5.040	0.957
^{208}Pb	-1636.4	6.806	0.900

In the Hartree calculation there are in principle six parameters, the masses and coupling constants for σ, ω, and ρ mesons; in the HF calculation we have two more for the π meson. Since the physical values of the pion coupling constant and mass are well established, in this work we keep these values ($f_\pi^2 = 0.9771$, $m_\pi = 138$ MeV) [12] unchanged in the fitting procedure; thus we have the same number of parameters to vary as in the Hartree calculation.

We are able to get a well-defined minimum for χ^2 which we examine as a function of the scalar meson mass. To achieve this, we choose a σ mass and vary the other five parameters of the model to find a minimum. Then we repeat the process with a new choice until the behavior of χ^2 versus the scalar mass is mapped out.

IV. RESULTS AND DISCUSSIONS

In this work we use two sets of data to determine the best fit parameters for the QHD model. In the first set the ground-state properties of ^{16}O, ^{40}Ca, ^{48}Ca and ^{90}Zr are included; the second set also includes ^{208}Pb. We try two sets of data because we would like to check whether the inclusion of heavy nuclei (represented by ^{208}Pb) changes the parameters substantially. We will see from these two case studies that we can get some insight about these parameters and even single out the contributions from individual mesons. In some applications it may be more suitable to use the parameters obtained from the first set of data, for example, when one deals with small to medium sized nuclei.

We are able to obtain a well-defined minimum of χ^2 versus the scalar mass for both sets of data. They are shown in Figs. 1 and 2. The best-fit meson parameters are shown in Table III, along with the uncorrelated error. The uncorrelated error is the allowed variation of one parameter which will keep χ^2 within one unit of its value at the minimum, while all the other parameters are held fixed.

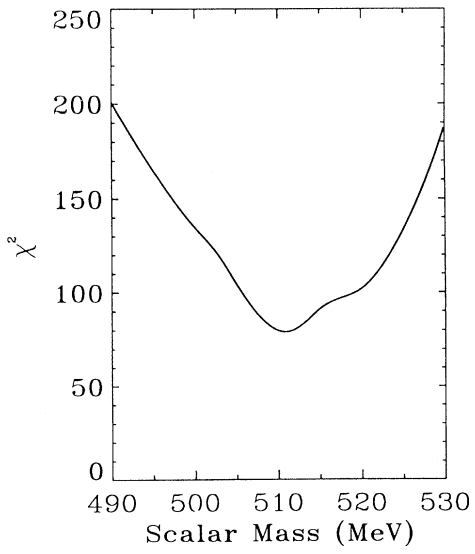

FIG. 1. The χ^2 as function of m_σ of the first set of data; the best-fit parameters which produce the minimum in the curve are given under set 1 in Table III.

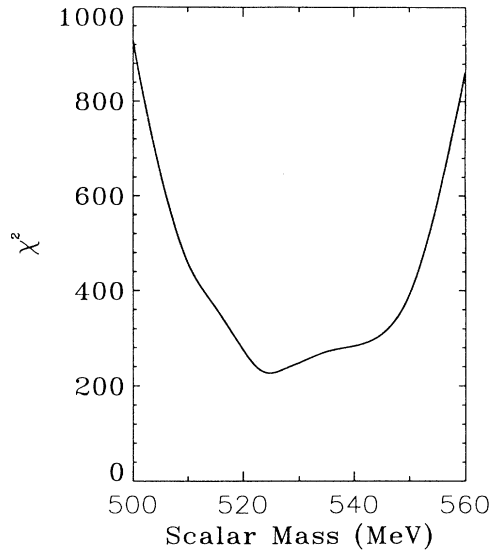

FIG. 2. The χ^2 as function of m_σ of the second set of data; the best-fit parameters which produce the minimum in the curve are given under set 2 in Table III.

From the first set of data we find that the χ^2 minimum occurs at around 80; the minimum from the second set of data is about 230. This is compared to a minimum χ^2 of more than 2000 from Hartree fitting [16]. The χ^2 per nucleon in the three cases are about 20, 46, and 250, respectively. We stress again that the more important test is to look at the predictive power of the fitted parameters, and we will use these parameters to calculate ground-state properties for a broad variety of nuclei.

Note first that the meson mass parameters from the second set of data are within 3% of their physical values, which is remarkable considering that no specifically mesonic properties are included in the data we are fitting. Also the coupling constants are close to their corresponding values in the one-boson-exchange potential (OBEP) [13]. Compared to the values obtained by Hartree fitting, we are gratified to see that including Fock terms does bring the properties of these mesons back to their physical values. The best-fit value for the vector meson mass (ω) in the Hartree fitting procedure is more than 1000 MeV [16], while the physical value is 783 MeV. Also in the Hartree fitting procedure, the ρ meson mass is not well determined by the fit, and so the authors of Ref. [16] fixed this value at 763 MeV. In the HF calculation, the ρ meson is important, because it makes large contributions in the exchange terms, while its contribution in the direct term is certainly small. Our HF fitting procedure selects a very reasonable value for the ρ meson mass.

Second, observe that the fitted parameters from the two data sets are close except for the parameters of the ρ meson. Since ρ is an isovector meson, it will play an important role in a nucleus which has a large difference in the number of protons and neutrons. The inclusion

TABLE III. Relativistic HF best-fit parameters with uncorrelated uncertainties.

	g_σ^2	g_ω^2	g_ρ^2	m_σ (MeV)	m_ω (MeV)	m_ρ (MeV)
Set 1						
Parameters	105.85	153.18	13.738	511.50	750.55	623.20
Uncorr. uncert.	±0.00058	±0.0013	±0.0012	±0.021	±0.037	±0.45
Set 2						
Parameters	108.63	148.05	13.350	525.00	760.69	752.32
Uncorr. uncert.	±0.00025	±0.0015	±0.0011	±0.029	±0.018	±0.32

of the ^{208}Pb constraints in the fitting procedure gives rise to a much more precise value for ρ meson, as is to be expected. Since ^{208}Pb has $N - Z = 44$, this gives a very strong constraint on the isovector meson ρ. For the first data set, although χ^2 per nucleon indicates a better fit, this is at the expense of a poorly determined ρ mass. Nevertheless, this set of parameters may give more satisfactory results when applied to small and medium sized nuclei.

We use the second set of parameters to calculate the ground-state properties of about 60 nuclei throughout the periodic table, and compare with the Hartree calculation of Ref. [16]. In Fig. 3 we show the binding energies from these two calculations relative to the experimental values. Basically we observe the same quality of fit to the total binding energy of the nucleus; the HF calculation exhibits an average precision about 1%. Compared to the Hartree result, the HF calculation shows slightly less binding; this may be due to the fact that we do not add a schematic pairing interaction in our calculation as is done in Ref.[16]. If we include this term, we can remove the tendency to underestimate binding, but at the expense of introducing an extra term in the Hamiltonian. We do not include ^{56}Ni and ^{116}Sn as constraints in our HF fitting procedure, although these were included in the comparable Hartree fit; even so, the HF predicted values are better than those obtained in the Hartree approximation. Generally, for non-closed-shell nuclei, a relativistic deformed nucleus calculation should be performed.

The relativistic HF and Hartree values for the charge diffraction radius compared with experimental data for these same nuclei are shown in Fig. 4. Here relativistic HF calculations are able to achieve an average precision within 1%, better than those of the Hartree calculation. The nuclei which are chosen in these calculations are believed more or less to be spherical nuclei; however, there is an evident region of deviation around mass 150 which is possible caused by deformations.

The last quantity we calculate is the nuclear surface thickness as defined by Eq. (15). We consider that this quantity is not as well defined as the binding energy or charge radius, but it is useful in that it attempts to describe another nearly universal feature of nuclei, namely, the range over which the density falls off at the surface. The results are shown in Fig. 5. In this feature we would expect that relativistic HF should show a significant improvement over the Hartree calculation, and it does. Even so, the HF results are not satisfactory in comparison with what this model can achieve for the binding energy and charge radius, since the average prediction is over 10% smaller than measured. The deviation around mass 150 is even more marked in this case, again calling in question the assumption that these are spherical nuclei.

Much of the improvement of the HF over the Hartree calculation can be attributed to the contribution of the pion, which vanishes in the Hartree approximation. The presence of the pion introduces a large repulsive force, and so the scalar field σ and vector field ω need to readjust themselves to provide the proper repulsive force in the inner range and attractive force in the intermediate range of nuclear forces. Thus the masses of the σ and ω

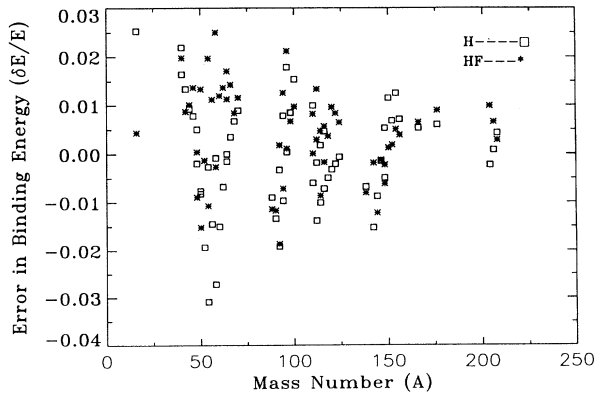

FIG. 3. The error in binding energy from relativistic HF and H calculations. Both have been calculated for a broad variety of nuclei and shown versus mass number A.

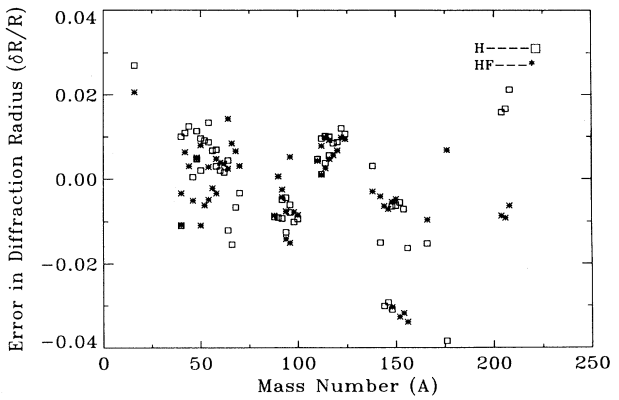

FIG. 4. The error in charge radius of relativistic HF and H calculations. The calculated nuclei are the same as those in Fig. 3.

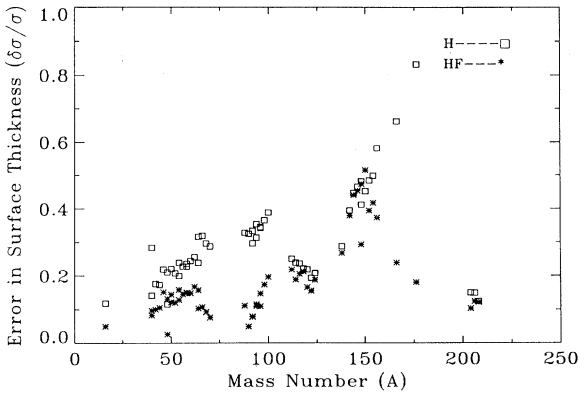

FIG. 5. The error in surface thickness of relativistic HF and H calculations. The calculated nuclei are the same as those in Fig. 3.

will change when exchange forces are included in the fit; this also leads to a different surface thickness.

Both relativistic HF and linear Hartree calculations of the surface thickness (Fig. 5) are systematically too small compared to the experimental values; i.e., both predict the nuclear surface to fall off too rapidly. We believe this suggests that in relativistic mean-field calculations as currently performed some important physics may be missing. In an earlier paper [17], we included the retardation effect of massive meson exchange in the relativistic mean-field calculation and we found that retardation provides a correction for the surface thickness in the right direction; however its contribution alone cannot account for the discrepancy. Another ingredient neglected so far in calculating the charge density is the charged meson-exchange contribution. It is possible that this contribution can have the effect of smearing the nuclear surface, and thus lead to a better description of the nuclear charge density. The need to improve the description of surface properties will remain an interesting topic for further investigation in relativistic mean-field calculations or extensions thereof.

It is instructive to look at the entire charge density distribution and at the single-particle spectrum for a representative nucleus; these are shown in Fig. 6 and Fig. 7 for ^{208}Pb. In the charge density, we do see too sharp a surface as compared to the experimental data. Also, there are more shell-related fluctuations in the interior than the experimental data suggest. This problem also exists in traditional nonrelativistic HF calculations using Skyrme forces [15, 16]. For proton single-particle energy levels, we do not see much difference between HF and linear Hartree results. As compared to experiment, it is obvious that the experimental spectrum of ^{208}Pb is more dense than the calculated spectrum. We notice that the nonrelativistic Skyrme HF calculations [16] have the same problem. The relativistic nonlinear Hartree calculation (which has two more parameters), although it is more successful for several of the properties we have examined so far, has a calculated single-particle spectrum of ^{208}Pb which is worse than our result [16].

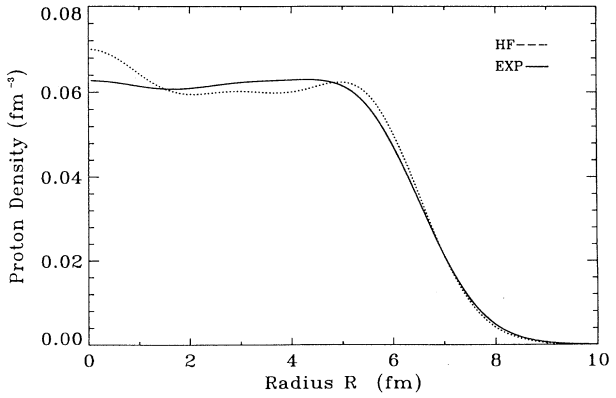

FIG. 6. The relativistic HF charge density of ^{208}Pb compared with the experimental density [23].

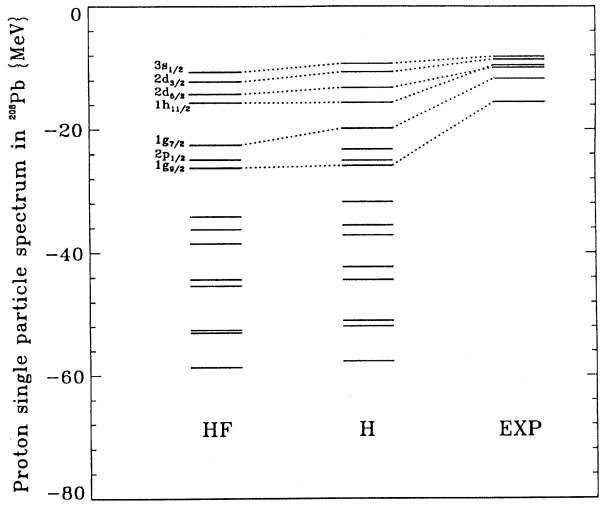

FIG. 7. Relativistic HF and H proton single-particle spectra for ^{208}Pb compared with the experimental values [24].

V. CONCLUSIONS

We have studied the QHD parametrization by using a relativistic HF calculation and fitting to known nuclear properties. The nucleon, which is described by a Dirac particle, is coupled to a scalar (σ), a vector (ω), an isovector vector (ρ), an isovector pseudoscalar (π), and a photon (γ) through a local Lagrangian. We treat this Lagrangian as an effective model Lagrangian, with free parameters being the coupling constants and masses of the exchanged mesons. We search for the best set of parameters by a least-squares fit to nuclear ground-state properties. Specifically, we fit the binding energies, charge radii, and surface thicknesses of five spherical nuclei ^{16}O, ^{40}Ca, ^{48}Ca, ^{90}Zr, and ^{208}Pb. We use these parameters to calculate the same quantities for a wide variety of nuclei to check the predictive value of the model.

This work follows an earlier study [16] in which a relativistic Hartree calculation was fitted to similar data. In that study, both linear and nonlinear (with σ field self-coupling terms) models were explored, and while it was found that the nonlinear relativistic Hartree model

is comparable to the successful nonrelativistic HF calculations using the Skyrme force, the linear model proved to be a poorer fit. Thus the authors of Ref. [16] conclude that an effective Lagrangian with only linear couplings is not able to reproduce the nuclear ground-state properties over a wide range of nuclei.

Since the real counterpart of the Skyrme HF calculation would be a relativistic HF calculation, we had hoped to show that the nonlinear terms, which are also present in the Skyrme Hamiltonian in the form of density-dependent interactions, would no longer be necessary. Whereas in the linear model the vector meson (ω) mass is far away from the physical mass, we find that by including the exchange terms but still using the linear model, we obtain a minimum with all meson masses close to their physical masses. The best-fit mass parameters are within 3% of their physical masses. Some small deviation from free values is to be expected due to the medium effects in the nucleus. But this is still remarkable in the sense that these relativistic models, although based on the boson-exchange principle, do not introduce the properties of the mesons explicitly, but only in terms of the quantum numbers to be carried. Yet, using only physical data from finite nuclei, we find masses and coupling constants which are close to those used in the OBEP [13]. This should strengthen the connection between the QHD and the OBEP model of nucleon-nucleon interactions.

With the same number of parameters (we fix the pion parameters), we find that the relativistic HF is superior to the relativistic Hartree when we use the best-fit set of parameters to study the binding energy, radius, and skin thickness of a wide variety of nuclei. We conclude that the relativistic linear HF model, by properly including the exchange terms, is capable of reproducing those nuclear ground-state properties quite satisfactorily.

While it is true that we fix the pion parameters in the fitting procedure, we find no substantial improvement from allowing them to vary after the fact. We have not tried a full simultaneous eight-parameter fit for reasons of economy, but exploratory calculations show that the four masses and four coupling constants used could not be significantly changed without destroying the agreement with the basic properties of finite nuclei.

Some features of both relativistic HF and Hartree calculations seem to indicate that some physics is missing in the current model. The surface thickness is still too small and there is too much structure in the interior charge density. Retardation effects [17] can help reduce the discrepancy, but these are not large enough. So far the charged meson-field contributions have not been taken into account in the total charge distribution; these will be included later.

We may also compare the relativistic HF with the nonlinear Hartree calculation. The nonlinear model has certain advantages, especially in the match to values of the surface thickness. However, one is aware of the fact that there are two more free parameters; this brings the total close to that of the Skryme parametrization in the nonrelativistic HF. Moreover, in the nonlinear model, the best-fit parameters assign a negative value to the quartic self-coupling constant. For such a Lagrangian the energy spectrum is unbounded below [18]; i.e., there is no true minimum energy.

It will be interesting to investigate a nonlinear HF model, but we would be reluctant to sacrifice the feature of our present model that the meson masses are close to their physical masses. It is not clear that the elusive σ meson with its self-coupling should be taken seriously as a body to be exchanged in the sense of HF calculations. More likely it represents a set of terms which relieve us of the need to calculate higher order contributions in the real meson fields or possible gluon contributions. Nevertheless, one would like the quartic term to be positive.

To go beyond HF including possible two-particle two-hole components is reasonable and seems to be indicated, for example, by $(e, e'p)$ studies which appear to find protons in states which would be unoccupied in the perfect Fermi sea. One component of this type, namely, pairing correlations, was included in the Hartree calculation [16] by adding a pairing energy term to the Hamiltonian and including a mandatory correlation in the wave function in the form of a smeared Fermi surface defined by an invariable gap parameter. This is a small effect but apparently necessary for nuclei in the pf shell and beyond. One would like to see the need for pairing to come more naturally out of nuclear forces.

ACKNOWLEDGMENTS

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