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Systematics of light deformed nuclei in relativistic mean-field models

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Ground-state properties of even-even nuclei in the *s-d* shell are calculated using relativistic mean-field models of baryon-meson dynamics that include scalar meson self couplings. Axial symmetry is assumed. The systematics of intrinsic quadrupole moments are studied for a variety of parameter sets that are fitted to the same nuclear matter saturation properties. The size of the moment is strongly correlated with the nucleon effective mass M^* and the spin-orbit strength, but is only weakly affected by the compressibility or the surface energy. If parameter sets with accurate spin-orbit strengths are used, the trends for *s-d* nuclei reproduce experimental systematics and are quantitatively similar to those obtained in nonrelativistic Skyrme-Hartree-Fock calculations. The implications for quantum hadrodynamics in the mean-field (Hartree) and one-loop approximations are discussed.

I. INTRODUCTION

Relativistic approaches to nuclear physics have been widely studied in recent years. These approaches include phenomenological models, in which nucleon motion is described by a Dirac equation with large Lorentz scalar and four-vector potentials,[1] and the development of a field-theoretic framework for nuclear systems based directly on hadronic degrees of freedom (called "quantum hadrodynamics" or QHD).[2] Relativistic mean-field models have been applied to problems of nuclear structure, nuclear currents, neutron stars, and nuclear matter at finite temperature.[2]

Relativistic mean-field models can be derived as the self-consistent Hartree approximation to QHD theories based on Lagrangian densities with Dirac nucleons and Lorentz scalar and four-vector meson fields. In this approach, both the nucleon wave functions and the meson fields are determined self-consistently. The mean-field theory (MFT), or Hartree approximation, becomes exact at high density. At normal nuclear density, the MFT provides a nonperturbative starting point for calculating solutions to the full quantum field theory.

The Hartree approximation gives a reasonable description of the ground states of closed-shell nuclei when the input parameters are adjusted to reproduce empirical nuclear saturation properties. These models lead naturally to a nuclear shell structure and yield quantitatively accurate predictions for rms radii, charge densities, and neutron densities.[3,4] In addition, solutions for closed-shell ground states in the Hartree approximation provide densities for calculations of polarized proton-nucleus scattering in a relativistic framework. The predictions of spin observables, using a relativistic impulse approximation in conjunction with Hartree densities to describe the nuclear ground state, have been remarkably successful.[1]

Given the successes of the mean-field approximation, it is natural to extend the models to open-shell nuclei. In this paper, we apply relativistic mean-field models to even-even nuclei in the *s-d* shell. The extension from spherical to axially symmetric systems is simplest, and a restriction to azimuthal and reflection symmetric deformations should be reasonable for light, even-even nuclei. In the Hartree approximation, these symmetries (along with the assumption of good charge and parity for the ground state) limit the nonvanishing meson fields to the same fields that enter in spherical nuclei.[5] In particular, there are no pion fields, charged meson fields, or three-vector fields.

We start with a model Lagrangian that includes cubic and quartic scalar meson self couplings. These additional terms are consistent with renormalizability. These nonlinear couplings are often set to zero in mean-field models to minimize explicit many-body forces.[2] However, nonzero values can be used to reduce the large surface energy and compressibility that are characteristic of linear parametrizations.[6]

If the parameters in the mean-field equations are unconstrained, optimized fits of the model to properties of spherical nuclei yield *negative* quartic self-couplings.[7,8] Such parametrizations are inconsistent with a QHD derivation of the mean-field equations. In particular, the MFT assumes that the theory has a ground state; if the quartic self coupling in the Lagrangian is negative, the energy spectrum is unbounded from below.[9] Thus these mean-field models cannot be directly interpreted as approximations to a QHD theory with nonlinear scalar interactions.

We therefore propose a different interpretation: the nonlinear terms allow the density dependence of the MFT to be *phenomenologically adjusted.* We derive the mean-field equations from an MFT energy functional to which we add cubic and quartic scalar meson self couplings; these new terms simulate density dependence that could arise from corrections to the Hartree approximation. By fitting these parameters phenomenologically, we can determine the density dependence needed to reproduce experimental systematics and then use the results to test more sophisticated QHD calculations.

In Ref. 5, the relativistic Hartree equations for a model with no nonlinear meson interactions were solved for several axially symmetric nuclei using the parameter set of Horowitz and Serot.[4] The calculated quadrupole moments were somewhat smaller than those obtained in analogous nonrelativistic calculations and those derived from experimental data. The authors suggested that the differences reflected the large compressibility of the mean-field calculations. In Ref. 10, the mean-field equations were solved for ^{20}Ne for several parameter sets, including one with nonlinearities. For the nonlinear set (which had a negative quartic self coupling) taken from Ref. 8, the calculated deformation was close to that obtained in a nonrelativistic Skyrme-Hartree-Fock calculation of ^{20}Ne.

In this paper, we investigate light deformed nuclei by calculating ground-state properties of even-even nuclei throughout the *s-d* shell. We study the systematics of intrinsic quadrupole moments for a variety of parameter sets that are fitted to the same nuclear matter saturation properties. By varying the scalar meson self couplings, we can obtain sets with different compressibilities, surface energies, spin-orbit strengths, and so on. By comparing calculations with different parameter sets, we can try to isolate and identify the factors that strongly influence the deformation.

Reference 11 describes calculations of deformed (axially symmetric) nuclei in a relativistic mean-field model using a gradient iteration method on a lattice. Results are obtained for ^{12}C, ^{20}Ne, and ^{24}Mg for a variety of parameter sets. Based on these results, the authors conclude that relativistic models with parameter set fitted to the properties of spherical nuclei do not adequately describe deformed nuclei. They emphasize that their conclusion is in contrast to the situation with nonrelativistic models. *We strongly disagree with their conclusion.*

In fact, we find that relativistic models can quantitatively describe both spherical and deformed nuclei. The level of agreement between theory and experiment is similar to that obtained in nonrelativistic Skyrme-Hartree-Fock calculations. This conclusion was also reached in Ref. 10 based on results for ^{20}Ne. (Although we use a different solution method, we obtain the same results for ^{20}Ne as in Ref. 10, within the expected accuracy of the calculations.) We have extended the comparison to the entire *s-d* shell and find a remarkable correspondence between relativistic and Skyrme model predictions.

Our best descriptions of experimental systematics are obtained using models with negative quartic self couplings. These models incorporate modifications of the linear MFT which should be calculable if QHD is to provide a viable framework for describing nuclei. Improvements to the mean-field approximation include many-body corrections analogous to those in nonrelativistic frameworks (e.g., exchange or correlations), but there are also new corrections that are implied by a field-theoretic description of nuclei.

If we believe that the nucleon is a Dirac particle and the scalar meson is a quantum degree of freedom, we are compelled to include the effects of the dynamical quantum vacuum. In particular, the zero-point energies of these particles make significant density-dependent contributions to the energy density.[2] We begin to test the validity of this new physics by including one-loop baryon and meson corrections to the Hartree approximation in calculations of deformed nuclei. We find that one-loop corrections alone do not reproduce experimental systematics.

In Sec. II, we discuss the MFT with nonlinear scalar interactions and an alternative derivation of the mean-field equations from an energy functional. We also summarize the calculation procedure. The calculated systematics of quadrupole moments and other observables in the *s-d* shell are presented in Sec. III and discussed further in Sec. IV. In Sec. V, we summarize our conclusions and discuss applications and extensions of the results.

II. MODEL AND CALCULATIONAL PROCEDURE

In this section, we discuss two different approaches to relativistic mean-field equations that include nonlinear scalar interactions. Initially we work entirely within the QHD framework, starting from a renormalizable Lagrangian and proceeding via the Hartree approximation to the mean-field equations. Some restrictions on the parameters of the theory are required. To allow for a wider class of parametrizations, we consider a more phenomenological motivation of the equations, which involves an energy functional. In this second approach, flexibility is gained in describing experimental properties of finite nuclei at the mean-field level but the direct connection with QHD is lost.

We begin with the Walecka (σ-ω) model including scalar meson self-couplings. The Lagrangian density is[2]

$$\begin{aligned}\mathcal{L}=\bar{\psi}[\gamma_\mu(i\partial^\mu-g_v V^\mu)-(M-g_s\phi)]\psi\\+\tfrac{1}{2}(\partial_\mu\phi\partial^\mu\phi-m_s^2\phi^2)-\tfrac{1}{4}(\partial_\mu V_\nu-\partial_\nu V_\mu)^2\\+\tfrac{1}{2}m_v^2 V_\mu V^\mu-V(\phi)+\delta\mathcal{L}\ ,\end{aligned}\qquad(1)$$

where

$$V(\phi)=\frac{\kappa}{3!}\phi^3+\frac{\lambda}{4!}\phi^4\ ,$$

and $\delta\mathcal{L}$ is the counterterm Lagrangian. To ensure that the theory has a ground state, $\lambda>0$.[9]

As in Ref. 5, we consider the mean-field (Hartree) approximation to this theory, in which the meson field operators are replaced by their expectation values, which are classical fields. The mean-field theory provides a nonperturbative starting point for describing the nuclear many-body system. Corrections to the self-consistent Hartree approximation (e.g., Hartree-Fock) are well defined in quantum hadrodynamics and can be investigated using quantum field theory and standard many-body techniques.

To realistically describe finite nuclei, the σ-ω model is extended to include rho mesons, pions, and photons.[2] The nuclear ground state is assumed to have good parity and well-defined charge. We further restrict our discussion to even-even nuclei, which we assume to have axial symmetry. As shown in Ref. 5, if the ground state has azimuthal and reflection symmetry, then all charged fields, three-vector fields, and pion fields vanish in the Hartree approximation. Thus, we are left with the scalar field, the time components of the vector and rho fields, and the Coulomb field. These are the same fields that are nonzero in spherical nuclei.[4,8]

The Hartree equations are derived in Ref. 4. (See Ref. 12 for a discussion of the scalar field equation with nonlinearities.) The equations for the neutral meson fields are

$$(\nabla^2 - m_s^2)\phi(r,\theta) = -g_s \sum_\alpha^{\text{occ}} \overline{U}_\alpha(\mathbf{x})U_\alpha(\mathbf{x}) + \frac{\kappa}{2}\phi^2 + \frac{\lambda}{6}\phi^3$$
$$\equiv -g_s[\rho_s(r,\theta) + \Delta\rho_s(r,\theta)] , \quad (2)$$

and

$$(\nabla^2 - m_v^2)V_0(r,\theta) = -g_v \sum_\alpha^{\text{occ}} U_\alpha^\dagger(\mathbf{x})U_\alpha(\mathbf{x})$$
$$\equiv -g_v\rho_B(r,\theta) , \quad (3)$$

where the sums run over occupied positive-energy states, and we have defined the contributions from the scalar self-couplings in Eq. (2) to be $-g_s\Delta\rho_s$. There are equations analogous to (3) for the other vector mesons (see Ref. 5). The single-particle spinors U_α satisfy a Dirac equation:

$$\{-i\boldsymbol{\alpha}\cdot\nabla + \beta[M - g_s\phi(r,\theta)] + g_v V_0(r,\theta)\}U_\alpha(\mathbf{x})$$
$$= \epsilon_\alpha U_\alpha(x) , \quad (4)$$

where we have suppressed the contributions from the rho and photon fields.

In applications of this nonlinear mean-field model, κ and λ in Eq. (2) are frequently allowed to be unconstrained. In particular, the equations are often solved for nonlinear parameter sets with $\lambda < 0$. However, when $\lambda < 0$, the preceding discussion is not applicable; *the equations cannot be derived in the mean-field approximation starting from a Lagrangian with this coupling.* The problem is that the energy spectrum is unbounded from below in such a theory.[9] In deriving the mean field approximation the theory is assumed to have a lowest energy state,[2] so it is inconsistent to allow $\lambda < 0$.

On the other hand, the best descriptions of spherical nuclei in mean-field models are achieved with nonlinear parameter sets which have negative λ. Thus, we have equations that are useful phenomenologically but which we cannot derive from a Lagrangian in the usual manner. We resolve this dilemma by interpreting the mean-field equations with nonlinear scalar terms in a different way. The motivation is that the MFT with a linear parametrization provides a reasonable description of finite nuclei, but the density dependence must be slightly altered to obtain more precise agreement with experiment. We propose interpreting nonlinear scalar interactions as a means of phenomenologically adjusting the density dependence of the MFT.

We start with the Lagrangian in Eq. (1) with $\kappa = \lambda = 0$ and construct the mean-field Hamiltonian, as described in Ref. 2. (The extension of this discussion to include additional mesons is straightforward.) By taking the expectation value of the Hamiltonian in a state specified by static meson fields and a set of occupied single-nucleon orbitals (labeled by quantum numbers α), we obtain an *energy functional* that satisfies a variational principle.[2] The mean-field ground state is obtained by minimizing the functional.

The energy functional for axially symmetric ground states is

$$E[U_\alpha,\phi,V_0] = \int d^3x \left\{ \tfrac{1}{2}\{[\nabla\phi(\mathbf{x})]^2 + m_s^2[\phi(\mathbf{x})]^2\} - \tfrac{1}{2}\{[\nabla V_0(\mathbf{x})]^2 + m_v^2[V_0(\mathbf{x})]^2\} + \sum_\alpha^{\text{occ}} U_\alpha^\dagger(\mathbf{x})\{-i\boldsymbol{\alpha}\cdot\nabla + \beta[M - g_s\phi(r,\theta)] + g_v V_0(r,\theta)\}U_\alpha(\mathbf{x}) \right\} , \quad (5)$$

subject to the constraint

$$\int d^3x\, U_\alpha^\dagger(\mathbf{x})U_\alpha(\mathbf{x}) = 1 , \quad (6)$$

for all occupied states.

The meson fields are determined by requiring the functional to be stationary with respect to their variations; this yields (after partial integrations) the usual MFT meson field equations. In particular,

$$\frac{\delta E}{\delta\phi(\mathbf{x})} = 0 \rightarrow (\nabla^2 - m_s^2)\phi(r,\theta) = -g_s \sum_\alpha^{\text{occ}} \overline{U}_\alpha(\mathbf{x})U_\alpha(\mathbf{x}) \quad (7)$$

and

$$\frac{\delta E}{\delta V_0(\mathbf{x})} = 0 \rightarrow (\nabla^2 - m_v^2)V_0(r,\theta) = -g_v \sum_\alpha^{\text{occ}} U_\alpha^\dagger(\mathbf{x})U_\alpha(\mathbf{x}) . \quad (8)$$

The single-particle orbitals are determined similarly. The constraint Eq. (6) is imposed with a Lagrange multiplier ϵ_α which we identify with the energy eigenvalue of the Dirac equation for U_α:

$$\frac{\delta}{\delta U_\alpha^\dagger(\mathbf{x})}\left[E-\epsilon_\alpha\int d^3x' U_\alpha^\dagger(\mathbf{x}')U_\alpha(\mathbf{x}')\right]=0\rightarrow\{-i\boldsymbol{\alpha}\cdot\nabla+\beta[M-g_s\phi(r,\theta)]+g_v V_0(r,\theta)\}U_\alpha(\mathbf{x})=\epsilon_\alpha U_\alpha(\mathbf{x})\ . \quad (9)$$

The energy is minimized by solving the equations self-consistently and choosing the N and Z lowest eigenvalues to determine the occupied states.

In applying this model to nuclear matter and finite nuclei, we find that the density dependence implied by the energy functional does not totally agree with experiment: the compressibility and surface energy are too large and the spin-orbit splitting are overestimated by about 30%. There are many ways to phenomenologically alter the density dependence:

(1) We could simulate vertex corrections by giving the coupling constants a phenomenological density dependence: $g\rightarrow g(\rho)$.

(2) Medium polarization effects could be introduced by letting the masses acquire a density dependence: $m\rightarrow m(\rho)$.

(3) We could add "contact terms" of the form $a\int \overline{UU}\,VUU$, $b\int \overline{UUU}V'UUU$, etc.

(4) We could add a polynomial in ϕ.

We choose the fourth alternative and restrict ourselves to additional terms cubic and quartic in ϕ:

$$E\rightarrow E'=E+\int d^3x\left[\frac{\kappa}{3!}\phi^3+\frac{\lambda}{4!}\phi^4\right]\ . \quad (10)$$

This modification is favored for several reasons. First, it provides adequate freedom to adjust the density dependence near the saturation point. In principle, we could add ϕ^5 and higher polynomial terms, but these are not necessary to describe finite nuclei and would only introduce additional parameters. Second, in contrast to the other possibilities, Eq. (10) maintains the local coupling of mesons to baryons, producing only minimal changes in the field equations. Third, E' can still be directly derived from a renormalizable Lagrangian [Eq. (1)] for certain parameterizations ($\lambda>0$).

After the substitution $E\rightarrow E'$, the equations in the generalized mean-field model are obtained with the same prescription described above. The results are Eqs. (2)–(4). Since we are only parametrizing the density dependence in a limited domain of the functional, there is no problem with E' being unbounded below for large ϕ if $\lambda<0$. However, we must restrict the set of states over which we extremize. In practice, this means that we identify our mean-field ground state with the local minimum of E' in the regime of normal nuclear matter. We must verify at the end of the calculation that ϕ is not so large that E' is dominated by the $\lambda\phi^4/4!$ contribution.

By introducing this phenomenological density dependence we have broken the direct connection between the mean-field models and the original Lagrangian. To directly test QHD, improvements to the Hartree approximation must be calculated to see whether the phenomenological density dependence implied by successful mean-field models is predicted.

As a first step, we consider the extension of the Hartree approximation to include baryon and meson one-loop contributions.[2] These corrections are determined in nuclear matter using the renormalization conditions described in Ref. 2. The results are applied to the present calculations through a local density approximation that is described in Ref. 12. (We do not include derivative terms recently considered by Perry,[13] which may provide important corrections in finite nuceli.) The only changes to the Hartree equations are additional contributions to $\Delta\rho_s$ in the scalar field equation (2). These are

$$\{\Delta\rho_s^{\text{vac}}\}_F=-\frac{1}{\pi^2}\left[M^{*3}\log\left[\frac{M^*}{M}\right]+\tfrac{1}{3}M^3-\tfrac{3}{2}M^2M^* +3MM^{*2}-\tfrac{11}{6}M^{*3}\right]\ , \quad (11)$$

for the baryon one-loop correction and

$$\{\Delta\rho_s^{\text{vac}}\}_S=-\frac{1}{g_s}\frac{1}{64\pi^2}\left\{2(\kappa+\lambda\phi)\left[(m_s^2+\kappa\phi+\tfrac{1}{2}\lambda\phi^2)\log\left[1+\frac{(\kappa\phi+\frac{1}{2}\lambda\phi^2)}{m_s^2}\right] -(\kappa\phi+\tfrac{1}{2}\lambda\phi^2)-\frac{(\kappa\phi)^2}{2m_s^2}\right]-\phi^3\left[\frac{\kappa^2\lambda}{m_s^2}-\frac{\kappa^4}{3m_s^4}\right]\right\}\ , \quad (12)$$

for the meson one-loop correction where ϕ and $M^*\equiv M-g_s\phi$ are functions of $\mathbf{x}$.

Equations (2)–(4) are nonlinear, coupled, partial differential equations that must be solved self-consistently. Several different solution methods have been applied to this problem by different groups.[5,10,11] Here we follow Ref. 5 and expand the angular dependence of the mean fields and the source densities in a basis of Legendre polynomials. For example,

$$\phi(r,\theta)=\sum_{L=0}^{L_{\max}}\phi_L(r)P_L(\cos\theta)\ . \quad (13)$$

Only even values of L are required from symmetry considerations, and we truncate the expansion at $L = L_{\max}$. The nucleon orbitals are expanded in terms of spherical spin angle functions:[14]

$$U_\alpha(\mathbf{x}) = U_{nmt}(\mathbf{x}) = \sum_{\kappa'} \begin{pmatrix} \dfrac{iG_{n\kappa'}(r)}{r}\Phi_{\kappa' m} \\ \dfrac{-F_{n,\kappa'}(r)}{r}\Phi_{-\kappa' m} \end{pmatrix} \eta_t \;, \tag{14}$$

where η_t is an isospinor and κ' is the usual relativistic angular quantum number.[14] The allowed values of κ' are limited by the symmetries and $L_{\max}$. Note that the total angular momentum j of an individual orbital is no longer a good quantum number but m is still good. States with $\pm m$ are degenerate.

If the expansions are substituted into (2)–(4), equations with different L's decouple and the problem is reduced to a system of coupled ordinary differential equations. These equations are solved by an iterative procedure similar to that described in Ref. 5. The only new feature is the addition of $\Delta\rho_s$ to the scalar field equation. This new term is expanded in Legrende polynomials numerically and, since $\Delta\rho_s$ depends on ϕ, Eq. (2) is solved iteratively.

Details concerning the filling of single-particle levels are discussed in Ref. 5. In general, both prolate and oblate self-consistent solutions for a given nucleus can be found; the energies must be compared to determine the true intrinsic ground state. However, for nuclei with close subshells, such as ^{12}C or ^{28}Si, there will also be a self-consistent *spherical* solution. The spherical solution will be preferred if it costs too much energy for single-particle levels to mix to form a prolate or oblate shape.

Self-consistent solutions with different sets of occupied single-particle levels may also be nearly degenerate. In these cases, the assumption of a sharp Fermi surface is questionable. One remedy is to include the effects of pairing correlations, which would smear the Fermi surface and remove the ambiguity. These effects are not included in the present calculations but we do not expect pairing to significantly change our results for light even-even nuclei. However, pairing in QHD must be investigated further for calculations of heavier deformed nuclei.

The accuracy of the present calculations is determined by the size of the radial mesh and the truncation of the angular basis. Convergence of the angular expansion is rapid for light nuclei. The results in Figs. 1–10 were generated using a mesh size of 0.1 fm to integrate the Dirac equations (with a fourth-order Runge-Kutta scheme) and with $L_{\max} = 4$. In selected tests with finer meshes and larger values of $L_{\max}$, quadrupole moments change by less than 1% and binding energies/particle and rms radii change by less than 0.1%.

The parameter sets used in the present investigation are characterized by the scalar meson self couplings κ and λ and by whether or not loop corrections are included in the model. The masses of the nucleon and the vector mesons and the electromagnetic coupling strength are taken from experiment: $M = 939$ MeV, $m_v = 783$ MeV, $m_\rho = 770$ MeV, and $e^2/4\pi = 1/137.036$. Once κ and λ are specified, the remaining parameters g_s, g_v, g_ρ, and m_s are determined by the requirement that the saturation properties of nuclear matter are reproduced.

We use a set of "empirical" saturation properties from Ref. 4. They are:

(1) equilibrium Fermi wave number of 1.30 fm^{-1} (this corresponds to an equilibrium density of 0.1484 fm^{-3});

(2) binding energy/nucleon at saturation of 15.75 MeV;

(3) bulk symmetry energy/nucleon of 35 MeV;

(4) rms charge radius of ^{40}Ca equal to 3.48 fm (to fix the value of m_s).

The fitting procedure is implemented using a computer code supplied by Fox.[15] As an option, one-loop baryon and/or one-loop meson vacuum corrections are included in the model as described above. Some representative parameter sets are given in Table I.

We emphasize that the parameter sets we determine for given κ and λ are not *optimally* fitted to the properties of closed shell nuclei. One could certainly "fine-tune" the other parameters to improve the systematic agreement with particular experimental quantities. However, our parameters give reasonable descriptions of spherical nuclei and provide a basis of comparison between calculations with different parameter sets. (Note also that parameter set C in Table I is similar to a nonlinear parameter set that *was* obtained as an optimal fit to properties of spherical nuclei.[8])

III. RESULTS

To compare to nonrelativistic calculations of deformed nuclei,[16,17] we use the charge quadrupole moment as a measure of the intrinsic deformation. Corresponding moments determined from experimental data are taken from Ref. 18. Comparisons to experiment must be viewed with some caution, however, since we do not project onto states of good angular momentum. Instead, we compare to absolute values for intrinsic quadrupole moments that are extracted from $B(E2)$ data us-

TABLE I. Relativistic Hartree parameter sets (no loops).

Set	g_s^2	g_v^2	g_ρ^2	m_s (MeV)	κ (MeV)	λ	M^*/M	K (MeV)
A	109.73	190.59	65.37	520.1	0	0	0.54	546.8
B	94.01	158.48	73.00	510.0	800	10	0.61	420.6
C	95.11	148.93	74.99	500.8	5000	-200	0.63	224.2
D	68.32	118.07	80.75	476.7	1500	50	0.70	342.9

ing model-dependent assumptions. (The signs are taken from static measurements). We note that the validity of the rotational model is questionable when applied to light nuclei.[19] Thus, besides the experimental uncertainties, there are theoretical uncertainties that can only be resolved with direct calculations of the $B(E2)$ values.

We have calculated ^{20}Ne using a wide variety of parameter sets with and without loop corrections. The parameters involve $-1000<\kappa<+5000$ MeV and $-200<\lambda<+200$. (Ranges of κ and λ in the QHD framework with loops included are more restricted.[15]) The results for a representative sample of parameter sets are summarized in Figs. 1–6. (The parameters are listed in Tables II and III in the Appendix.) In these figures, the linear parameter set ($\kappa=\lambda=0$) is marked by a $+$ and the dashed line indicates the charge quadrupole moment extracted from experiment data.[18]

In Fig. 1, the intrinsic charge quadrupole moment in ^{20}Ne is plotted against the nuclear matter compressibility.[20] For all parameter sets, the lowest energy solution is prolate and the predicted moment lies between 0.4 and 0.5 b. The figure reveals no apparent correlation between the compressibility and the size of the intrinsic deformation. In fact, we find parameter sets predicting the same quadrupole moment although their compressibilities differ by a factor of two.

In Fig. 2, the moment is plotted against the surface energy a_2 obtained for each parameter set by roughly fitting to a semiempirical mass formula.[21] We find no overall correlations between these quantities as well. As one might expect, the compressibility and the surface energy *are* strongly correlated. This is illustrated in Fig. 3. From Fig. 4 we find that the binding energy per nucleon (including a center-of-mass correction as in Ref. 8) is also not correlated with the quadrupole moment. This is consistent since the differences in binding energy between the various parameter sets are principally due to the differing surface energies.

If we consider the nucleon effective mass M^* in infinite nuclear matter, we find a strong correlation with the size of the deformation (see Fig. 5). (Note that all calculations with loop corrections have $M^*/M>0.7$.)

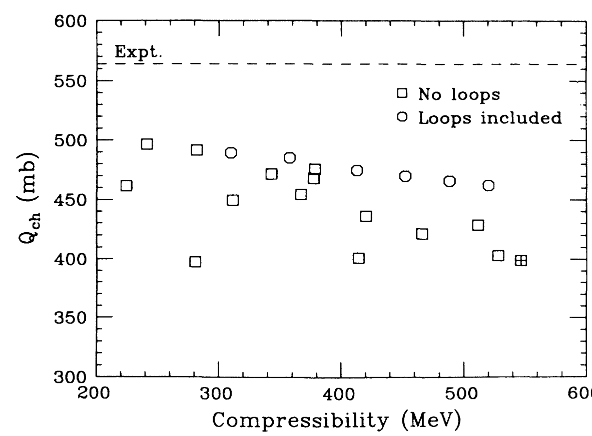

FIG. 1. Intrinsic charge quadrupole moment (mb) in ^{20}Ne vs nuclear matter compressibility (MeV) for a variety of parameter sets (described in text).

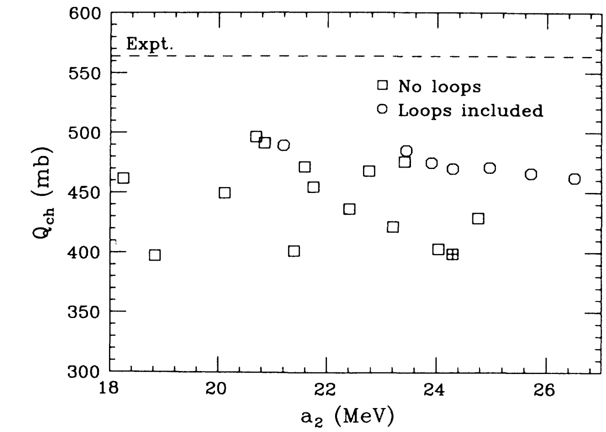

FIG. 2. Intrinsic charge quadrupole moment (mb) in ^{20}Ne vs surface energy a_2 (MeV) for the same parameter sets as Fig. 1.

The magnitude of M^* is directly related to the size of the scalar field through $M^*=M-g_s\phi$. Since the binding energy of nuclear matter depends sensitively on the cancellation of the scalar and vector fields and since we constrain the calculation to reproduce the empirical energy, the size of the vector field is indirectly determined by M^*. The spin-orbit strength depends on the sum of these fields, so a small M^* means large spin-orbit splittings.

In Fig. 6, we plot quadrupole moments against the spin-orbit strength as indicated by the energy difference predicted for the $1p_{1/2}$ and $1p_{3/2}$ levels in ^{16}O. We find a roughly linear relationship between the spin-orbit splitting and the size of the moment in ^{20}Ne. For parameter sets that predict the *same* spin-orbit splitting, the size of the moment varies slightly with the surface energy and compressibility. In particular, larger surface energies lead to smaller deformations.

Figures 1–6 indicate that if the bulk saturation properties of nuclear matter are fixed, the spin-orbit strength (which is inferred from predicted $j=l\pm\frac{1}{2}$ splittings) has the most direct influence on the size of intrinsic deformations. To further test this conclusion, the parameter

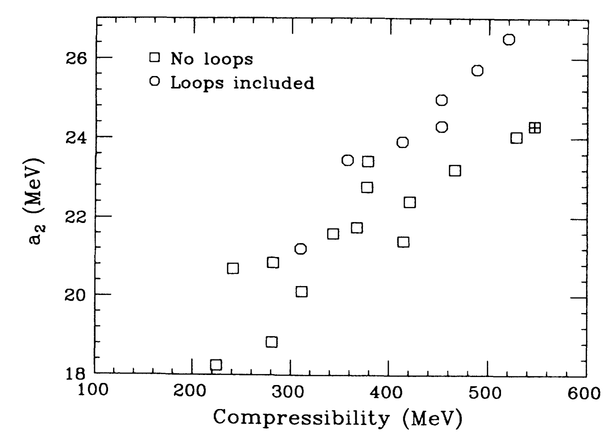

FIG. 3. Surface energy a_2 (MeV) vs nuclear matter compressibility (MeV) for the same parameter sets as Fig. 1.

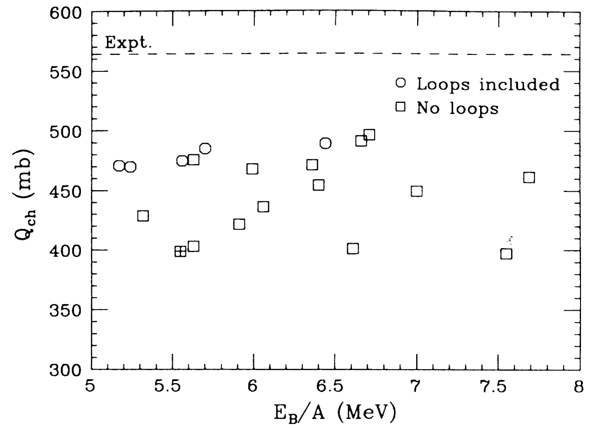

FIG. 4. Intrinsic charge quadrupole moment (mb) in ^{20}Ne vs binding energy/nucleon (MeV) for the same parameter sets as Fig. 1.

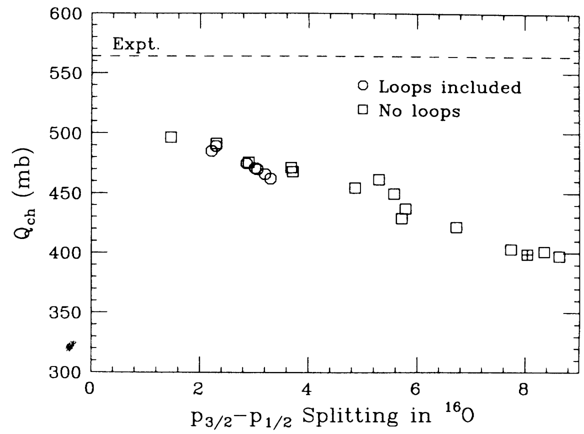

FIG. 6. Intrinsic charge quadrupole moment (mb) in ^{20}Ne vs $1p_{3/2}-1p_{1/2}$ neutron spin-orbit splitting in ^{16}O for the same parameter sets as Fig. 1.

sets detailed in Table I were selected to examine systematics in the *s-d* shell. (Set *A* is very close to the linear parameter set used in Ref. 5.) The table lists the parameters as well as the corresponding value of M^* and the compressibility in nuclear matter. If we take the splitting of the $1p_{1/2}$ and $1p_{3/2}$ neutron levels in ^{16}O as our experimental standard (≈ 6 MeV), these parameter sets have spin-orbit strengths less than, equal to, and greater than experiment (neglecting orbital rearrangement effects). Specifically, the predicted ^{16}O splittings for the four parameter sets of Table I are 8.0, 5.8, 5.3, and 3.7 MeV, respectively, for sets *A*, *B*, *C*, and *D*.

The quadrupole moment systematics in the *s-d* shell are shown in Fig. 7. Sets *B*, *C*, and *D* each qualitatively reproduce the experimental pattern of deformations including the alternations between prolate and oblate deformation. As we observed with ^{20}Ne, the size of the deformation is larger for weaker spin-orbit strengths and, for equal spin-orbit strengths, the deformations are slightly larger for sets which predict smaller surface energies. If the splitting is too large, nuclei with closed subshells such as ^{28}Si and ^{12}C are found to have spherical intrinsic ground states. (This means that the self-consistent spherical solution has lower energy than any prolate or oblate solution.) This is the case for set *A*. The systematics for calculations including loop corrections, which have $M^*/M \gtrsim 0.7$, are quantitatively similar to those obtained with set *D*.

Figure 8 shows that if the experimental ^{16}O splitting is achieved (sets *B* and *C*), the systematics are very similar to those obtained from nonrelativistic Skyrme-Hartree-Fock calculations. The experimental systematics are quantitatively reproduced although the predicted magnitude of the deformations are generally smaller than experiment (but similar to the Skyrme II predictions). Sets *B* and *C* predict similar moments even though the compressibilities and surface energies for these sets are very different (see Table I).

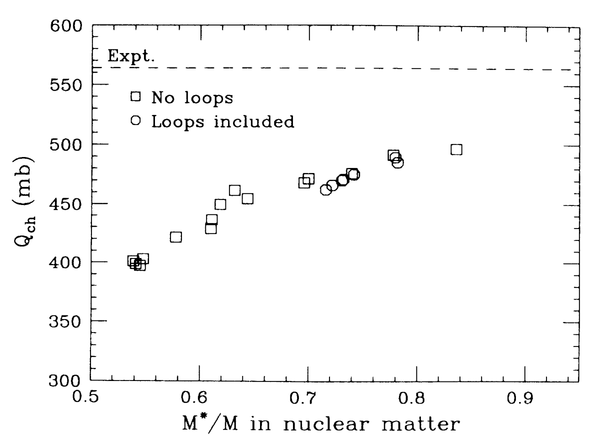

FIG. 5. Intrinsic charge quadrupole moment (mb) in ^{20}Ne vs effective mass M^*/M in nuclear matter for the same parameter sets as Fig. 1.

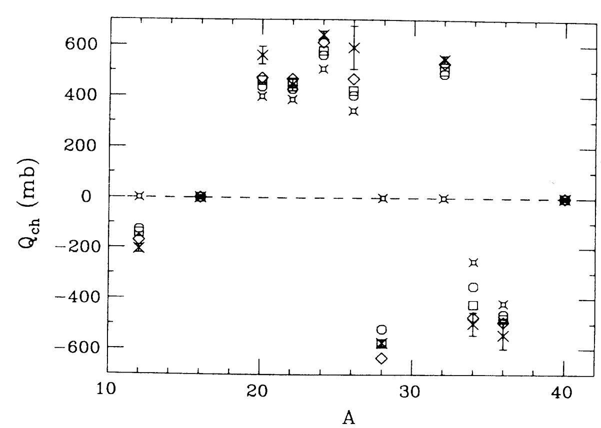

FIG. 7. Intrinsic charge quadrupole moment (mb) in even-even *s-d* nuclei for the relativistic Hartree parameter sets *A* (¤), *B* (○), *C* (□), and *D* (◇) from Table I. Moments derived from experimental measurements (×) are taken from Ref. 18.

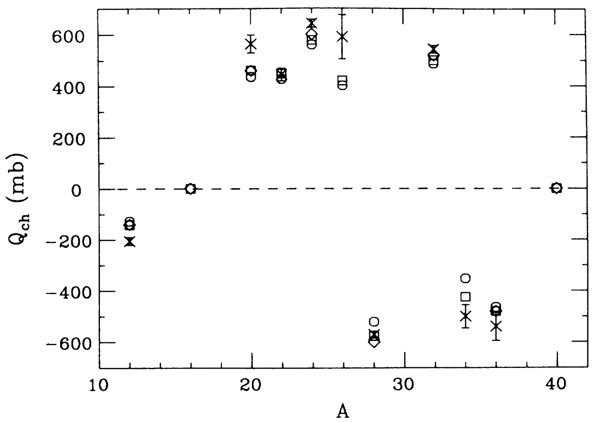

FIG. 8. Intrinsic charge quadrupole moment (mb) in even-even s-d nuclei for parameter sets B (○) and C (□) from Table I and a nonrelativistic Hartree-Fock calculation with the Skyrme II interaction (◇) from Ref. 16. Moments derived from experimental measurements (×) are taken from Ref. 18.

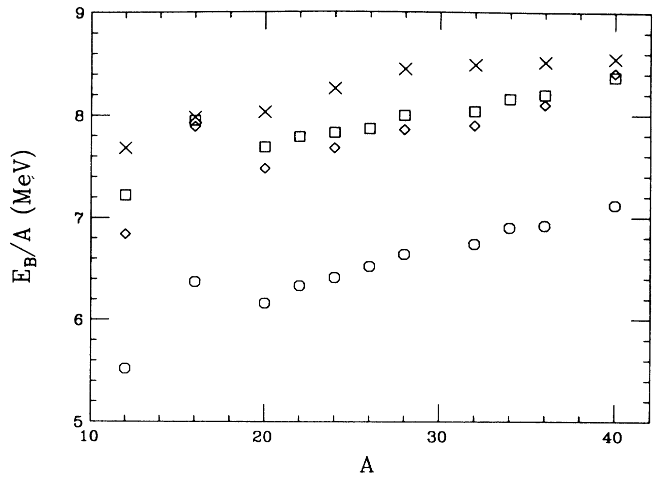

FIG. 10. Binding energy/particle in even-even s-d nuclei for parameter sets B (○) and C (□) from Table I and a nonrelativistic Hartree-Fock calculation with the Skyrme II interaction (◇) from Ref. 16 compared with experimental data (×) from Ref. 17.

If we examine the rms charge radii for sets B and C, we find quantitative agreement with the Skyrme predictions and experimental data (see Fig. 9). The differences between these sets are emphasized in Fig. 10, which shows the systematics of the binding energies per nucleon. (Note that these binding energies do not include a correction from projecting out a $J = 0$ ground state from the intrinsic state; such a correction would tend to narrow the discrepancy between theory and experiment.) The large surface energy of set B leads to significant underbinding while set C and the Skyrme interaction make similar predictions.

IV. DISCUSSION

In Ref. 5, the bulk compressibility and surface energy of nuclear matter in relativistic mean-field models were suggested as important factors in determining equilibrium deformations in open-shell nuclei. Figures 1–3 show that the compressibility and the surface energy are correlated with each other but neither is strongly correlated with the size of the quadrupole moment. If parameter sets with equal values of M^* are compared, smaller surface energies lead to slightly larger deformations; however, this effect is minor compared to the M^* dependence. These conclusions are confirmed by the comparison of systematics in the s-d shell (Figs. 7 and 8).

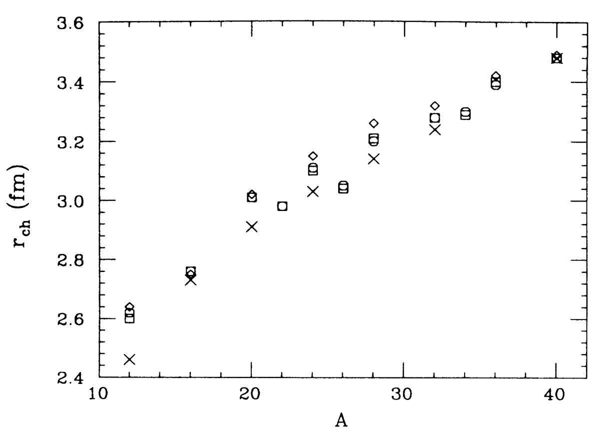

FIG. 9. rms charge radii in even-even s-d nuclei for parameter sets B (○) and C (□) from Table I and a nonrelativistic Hartree-Fock calculation with the Skyrme II interaction (◇) from Ref. 16 compared with experimental data (×) from Ref. 17.

In contrast, the quadrupole deformations are very sensitive to the spin-orbit force. The importance of the spin-orbit interaction can be simply understood from the mixing of spherical basis states in the expansion of Eq. (14) for single-particle levels near the Fermi surface (tightly bound single-particle levels remain essentially spherical). For example, consider ^{20}Ne as initially being a spherical ^{16}O core to which four $d_{5/2}$ valence nucleons are added. The single-particle levels will not have definite angular momentum j if the system is deformed; self-consistency will mix spherical-basis states with other angular quantum numbers (e.g., $d_{3/2}$ and $s_{1/2}$) into the valence levels so the valence wave functions will develop these additional components [these correspond to different κ' terms in Eq. (14)]. The degree of mixing will depend critically on the spin-orbit strength; for example, a strong spin-orbit force will inhibit the mixing of $d_{3/2}$ and $d_{5/2}$ components. The result is smaller deformations for open subshell nuclei and the possibility that a spherical intrinsic ground state is the lowest energy solution for closed subshell nuclei.

In particular, the linear parameter set A leads to spherical self-consistent ground states for ^{12}C, ^{28}Si, and ^{32}S and the smallest deformations among the parameter sets of Table I for the other s-d shell nuclei. Note that the differences in energy between spherical and deformed solutions for set A are small; for example, there is a self-consistent prolate solution for ^{32}S only 0.25 MeV/nucleon less bound than the spherical solution. Furthermore, the reduced spin-orbit force in set B or C is sufficient to lower the energy of the prolate solution below that of the spherical solution. Thus the quadrupole systematics provide a *sensitive* experimental test of mean-field models. We conclude that the failure of the linear parameter set reflects the limitations of the Hartree approximation but does not indicate gross discrepancies with experiment. We do not interpret this failure as strong evidence for nonzero κ and λ in QHD Lagrangians (see, for example, the discussion below of Brueckner-Hartree-Fock).

Figure 7 shows that experimental systematics for intrinsic quadrupole moments are reproduced by increasing M^*/M slightly over the value obtained in the mean-field theory with $\kappa=\lambda=0$ (from 0.54 to 0.6–0.65). This is achieved in our mean-field models by incorporating scalar self couplings (see Table I); these nonlinear terms provide a simple way of altering the density dependence of the mean-field energy functional. Consequently, they can *simulate* physics which has been left out of the Hartree approximation. To directly test QHD, improvements to the Hartree approximation must be calculated to see whether they predict the phenomenological density dependence implied by mean-field models that successfully describe experiment.

As a first step in this program, we have considered one-loop corrections to the MFT. (One loop corrections are discussed in detail by Fox.[15]) If we focus on quadrupole deformations, predictions of models including loop corrections are reasonable (the systematics are similar to those of set D in Fig. 7). However, the spin-orbit splitting of single-particle levels becomes quite small. If we require that mean-field parameter sets reproduce the experimentally observed spin-orbit splittings in light nuclei, the nucleon effective mass is typically 0.6–0.65M. This range is also consistent with Dirac phenomenology. However, with loop corrections included, the effective mass is greater than 0.7 M, and the surface energy is large.[15] Thus, one-loop corrections alone are not the answer.[22]

More promising is the inclusion of exchange and correlation corrections to the Hartree approximation. Brueckner-Hartree-Fock calculations in nuclear matter have larger M^* and lower compressibility than the linear MFT.[23] Thus, we can speculate that calculations in finite nuclei using an effective G-matrix from relativistic BHF calculations in nuclear matter may reproduce experimental systematics for light nuclei without explicit nonlinear couplings.

If one wishes to work solely at the mean-field level with a "best fit" parameter set, the set described in Ref. 8 (which is similar to set C from Table I) is probably close to optimal for describing properties of both spherical and (light) deformed nuclei. This includes reproducing experimental binding energies, rms radii, and quadrupole deformations. Ground-state calculations with this parameter set can provide suitable nuclear densities and orbitals as input to many additional calculations, such as electron and proton scattering, which can further test the mean-field model.

However, the applications of this mean-field model are necessarily limited. The presence of a negative quartic meson self coupling ($\lambda<0$) indicates that the model cannot follow from a Lagrangian in the mean-field approximation; a theory defined by such a parameter set does not have a ground state.[9] This was the motivation for introducing the energy functional in Sec. II. The consequence is that extrapolations of the model away from the density region of normal nuclear matter are, at best, questionable. Systematic improvement of this approach based on an underlying Lagrangian and techniques of quantum field theory is limited. These restrictions were recognized by the authors of Ref. 8, who caution that their nonlinear parameter set might only be applicable for ground state calculations.

A potential problem with the mean-field parametrizations is that the coupling constant for the ρ meson must be quite large to generate a symmetry energy of 35 MeV in nuclear matter. The rho couplings from Table I are at least twice as large as typical values from one-boson exchange potential (OBEP) fits to scattering data. This might be troubling if we calculate quantities which are sensitive to g_ρ. We note, however, that the quadrupole moments of light nuclei are not very sensitive. For example, if we calculate ^{22}Ne using parameter set B and then recalculate with g_ρ set to zero, the intrinsic quadrupole moment changes by about 1%.

Do the results of Figs. 7–10 prove that relativistic mean-field models can accurately describe deformed nuclei? Since we have only compared calculated intrinsic properties to corresponding quantities extracted from experiment, we should be somewhat cautious in assessing the level of the agreement. Certainly, calculations that go beyond the present treatment to directly predict $B(E2)$ values will permit a more definitive evaluation. Furthermore, we have used values of the quadrupole moments extracted from $B(E2)$ values, as in Ref. 24, and these are usually smaller than those taken from static measurements.[24] Thus, the comparison to experiment ultimately may be worse than indicated in Fig. 8.

On the other hand, the reproduction of the systematic pattern of deformations in the s-d shell is a nontrivial result (it has been considered one of the triumphs of the Skyrme model[17]) and the present quantitative agreement is impressive. Furthermore, the agreement with the nonrelativistic Skyrme interactions is independent of the precise experimental numbers. In fact, the mean-field models considered in this paper might be viewed as relativistic analogs of the nonrelativistic Skyrme model. We note that the Skyrme interactions have been clearly successful in reproducing moments in heavy deformed nuclei; this will be an important test of relativistic mean-field models.

V. SUMMARY

In this paper, we calculate the ground-state properties of even-even nuclei in the s-d shell using relativistic mean-field models of baryon-meson dynamics. We derive the mean-field equations for finite nuclei from an

TABLE II. Relativistic Hartree parameter sets (no loops).

g_s^2	g_v^2	g_ρ^2	m_s (MeV)	κ (MeV)	λ	M^*/M	K (MeV)	Q_{ch} (mb)
109.73	190.59	65.37	520.1	0	0	0.54	546.8	399
108.13	187.15	66.27	519.1	100	0	0.55	528.3	403
101.53	173.73	69.56	514.4	500	0	0.58	466.1	421
84.70	143.00	76.18	497.8	1500	0	0.66	367.1	454
94.01	158.48	73.00	510.0	800	10	0.61	420.6	436
68.32	118.07	80.75	476.7	1500	50	0.70	342.9	471
67.26	118.99	80.59	477.6	500	100	0.70	377.3	468
45.22	80.19	86.65	428.7	2500	100	0.78	281.9	491
27.96	52.44	90.33	368.6	2500	200	0.84	240.9	496
89.95	158.47	73.00	510.0	−1000	100	0.61	511.7	429
52.90	98.65	83.92	455.3	−500	200	0.74	378.3	476
114.93	191.15	65.23	518.9	2000	−100	0.54	414.2	401
95.45	154.93	73.75	505.3	3000	−100	0.62	311.4	450
117.82	188.66	65.88	516.1	4000	−200	0.55	280.7	397
95.11	148.93	74.99	500.8	5000	−200	0.63	224.2	461

energy functional that includes cubic and quartic scalar meson self couplings with coupling constants κ and λ, respectively. For positive λ, the functional and the equations can be directly derived in the self-consistent mean-field (Hartree) approximation to a QHD Lagrangian field theory. In this work, we allow a wider class of parametrizations by interpreting nonlinear scalar interactions as a means of phenomenologically adjusting the density dependence of the energy functional. In particular, we allow $\lambda < 0$.

We examine the systematics of intrinsic quadrupole deformations for a wide variety of parameter sets fitted to the same nuclear matter saturation properties. We conclude that the size of the moment is strongly correlated with the nucleon effective mass M^* and the spin-orbit strength but is only weakly affected by the compressibility or the surface energy. This correlation can be simply understood in terms of the mixing of single-particle levels with different j, as dictated by the spin-orbit strength.

We find that successful descriptions of spherical nuclei in relativistic mean-field models (which include accurate spin-orbit splittings) can be extended to describe the observed systematics of light deformed nuclei *without changing the parameters.* Furthermore, the mean-field systematics are in quantitative agreement with results from nonrelativistic Skyrme-Hartree-Fock calculations.

However, to achieve this agreement in a mean-field model, scalar meson self couplings (or some other means of altering the density dependence) must be included. The MFT with a linear parameter set ($\kappa=\lambda=0$) fails to predict any deformation for closed subshell nuclei (e.g., ^{28}Si), primarily because of overly large spin-orbit splittings (M^* is too small). By allowing nonzero κ and λ, we can reproduce empirical nuclear matter saturation with increased values of M^*. We find that the observed systematics of quadrupole deformations is reproduced by models in which $M^* \gtrsim 0.6\,M$. The best descriptions of experimental binding energies, rms radii, and quadrupole deformations are achieved in models with $\lambda < 0$.

It remains to be seen whether the phenomenological density dependence implied by mean-field models with negative λ arises within the QHD framework from improvements to the mean-field approximation. In this paper, we investigate one-loop corrections for a variety of allowed κ and λ, including $\kappa=\lambda=0$. One-loop corrections increase M^* to $\gtrsim 0.7\,M$, resulting in adequate quadrupole systematics but very small spin-orbit splittings. In addition, the surface energy is quite large.[15] Thus, one-loop corrections alone are not the answer. (The potential application of relativistic Brueckner-Hartree-Fock calculations of nuclear matter[23] to finite nuclei is more promising.)

There are numerous applications of the present investigation and many directions in which it can be extended. These include:

TABLE III. Relativistic Hartree parameter sets (loops included).

g_s^2	g_v^2	g_ρ^2	m_s (MeV)	κ (MeV)	λ	M^*/M	K (MeV)	Q_{ch} (mb)
54.04	102.58	83.30	457.3	0	0	0.73	452.5	470
55.11	106.55	82.67	460.3	−500	1	0.72	488.3	466
53.21	101.97	83.40	455.2	−100	10	0.73	455.2	471
55.90	109.38	82.21	463.6	−1000	10	0.72	520.1	462
51.74	97.00	84.17	451.1	500	10	0.74	413.0	475
40.34	78.19	86.93	422.0	500	100	0.78	357.6	485
44.19	79.86	86.70	426.5	2500	10	0.78	309.8	489

(1) Using the deformed nuclear densities and orbitals to generate electron-scattering form factors and spin observables for proton scattering.

(2) Projecting states of good angular momentum from deformed intrinsic ground states. Direct calculations of transition rates among the extracted states are needed to clarify the relationship between intrinsic quantities and physical observables.

(3) Applying the calculational techniques to heavier nuclei like the rare earths.

(4) Allowing for ground states without axial symmetry. These will contain three-vector fields for the vector mesons (and a pion field), but the same calculational techniques can be applied. This extension also permits the direct calculation of odd-A nuclei.

(5) Incorporating pairing correlations in the relativistic approach. These are important in nonrelativistic descriptions of certain deformed nuclei such as ^{58}Ni as well as heavier nuclei.[25]

Work on these topics is in progress.

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APPENDIX: MEAN-FIELD PARAMETER SETS

The parameter sets used in Figs. 1 – 6 are listed in Tables II and III. The entries correspond to those of Table I, except that the charge quadrupole moment of ^{20}Ne in mb is given in the final column.

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