Relativistic Mean-Field Theory and Nuclear Deformation

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Relativistic mean-field theory is used to describe ground-state deformations of nuclei. The relativistic Hartree equations are solved by expansion of the nucleon wave functions and the meson field in a harmonic-oscillator basis. Using parameters adjusted in spherical nuclei we find in axially symmetric deformed nuclei good agreement with conventional nonrelativistic calculations based on density-dependent Skyrme forces.

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In the microscopic description of nuclei the mean-field approximation plays an essential role. The conventional nonrelativistic method is based on the Hartree-Fock approximation with phenomenological effective, density-dependent interactions.[1,2] This method allows a unified quantitative description of the ground-state properties for light as well as for heavy nuclei. One of the great successes of these theories was that they were not only able to reproduce densities and binding energies in doubly magic spherical nuclei, in which the parameters of the effective interactions had been adjusted, but they also yielded the proper size of the ground-state deformations in doubly open-shell nuclei.[3]

In recent years Walecka *et al.* (for a review see Serot and Walecka[4]) showed that ground-state properties of nuclear matter, and of doubly magic nuclei, can be described in a covariant way within a mean-field approximation to a relativistic quantum-field theory of nucleons, in which the strong interactions are produced by the exchange of massive mesons. With very few adjustable parameters this model is able to reproduce the binding energy and the density of nuclear matter as well as the density profiles and the spin-orbit splitting in doubly magic spherical nuclei. So far such investigations have been restricted to spherical shapes, where rotational symmetry allows the differential equations of the model to be reduced to one radial dimension. In this Letter we study axially deformed nuclei, for which we have to deal with partial differential equations in two coordinates.

The Lagrangean density of the model has the form

$$L=\bar{\psi}[\gamma^\mu(i\partial_\mu-g_\omega\omega_\mu)-(M+g_\sigma\sigma)]\psi-\tfrac{1}{4}F^{\mu\nu}F_{\mu\nu}+\tfrac{1}{2}m_\omega^2\omega^\mu\omega_\mu+\tfrac{1}{2}\partial^\mu\sigma\partial_\mu\sigma-U(\sigma). \quad (1)$$

It contains the spinor fields $\psi(\mathbf{r})$ for the nucleons, a scalar-meson field $\sigma(\mathbf{r})$, which moves in a nonlinear potential,[5]

$$U(\sigma)=\tfrac{1}{2}m_\sigma^2\sigma^2+\tfrac{1}{3}b_2\sigma^3+\tfrac{1}{4}b_3\sigma^4, \quad (2)$$

and an isoscalar vector-meson field $\omega_\mu(\mathbf{r})$, with the field tensor $F_{\mu\nu}=\partial_\mu\omega_\nu-\partial_\nu\omega_\mu$ and the gauge $\partial^\mu\omega_\mu=0$ (in our actual calculations we also take into account the isovector ρ meson and the Coulomb field).

The variational principle gives the equations of motion, the Dirac equation for the nucleons, and Klein-Gordon equations for the mesons. In the static case, with time-reversal invariance, the spatial components of the vector-meson field ω vanish and we find

$$[-i\boldsymbol{\alpha}\cdot\nabla+g_\omega\omega_0+\beta(M+g_\sigma\sigma)]\psi_n=\epsilon_n\psi_n \quad (3)$$

and

$$(\Delta-m_\sigma^2)\sigma=+g_\sigma\rho_S+b_2\sigma^2+b_3\sigma^3, \quad (4)$$

$$(\Delta-m_\omega^2)\omega_0=-g_\omega\rho_V, \quad (5)$$

where the scalar and the vector density ρ_S and ρ_V are obtained as sums over all occupied orbitals,

$$\rho_V=\textstyle\sum_i\psi_i^\dagger\psi_i,\quad \rho_S=\sum_i\bar{\psi}_i\psi_i. \quad (6)$$

TABLE I. Parameters of the Lagrangean. The mass unit is megaelectronvolts and the coupling constants g_i and the parameters b_k are given in terms of the parameters $C_i=g_iM/m_i$ (for $i=\sigma$ and ω), $B_2=b_2/g_\sigma^3M$, and $B_3=b_3/g_\sigma^4$.

	M	m_σ	m_ω	m_ρ	C_σ	C_ω	C_ρ	B_2	B_3
Set I	938	615.00	1008	763	18.81	16.39	12.76	0	0
Set II	938	492.25	795.36	763	19.32	15.67	12.23	−0.00246	−0.00343

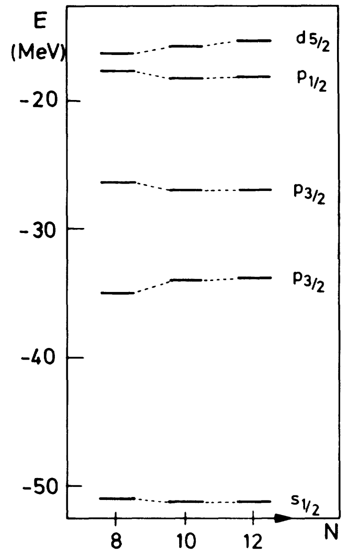

FIG. 1. The single-particle spectrum of occupied neutron orbits in ^{20}Ne for set I of force parameters and different cutoff parameters N. The oscillator constant is $\hbar\omega = 41A^{-1/3}$ for the spinors and half this value for the meson fields.

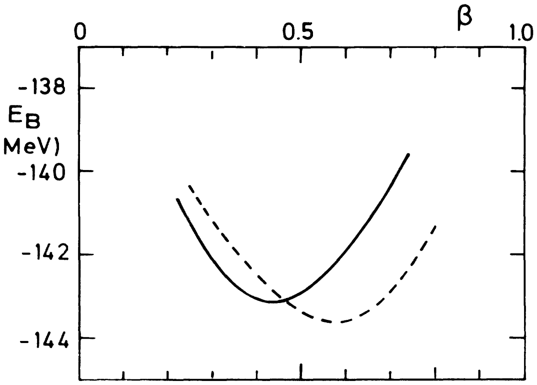

FIG. 2. The energy surface for the nucleus ^{20}Ne as a function of the deformation parameter β, which is obtained from the expectation value of the quadrupole moment of the nucleons: $\langle Q \rangle = \beta A R^2 3/4\pi$. The full line corresponds to parameter set I and the dashed line corresponds to parameter set II of Table I.

This is a set of coupled partial differential equations. In the axially symmetric case it depends on the two cylindrical variables r and z. It has to be solved under the appropriate boundary conditions for bound states. For this purpose we expand the spinors (large and small components separately) as well as the meson fields in terms of the complete set of eigenstates of a three-dimensional oscillator in cylindrical coordinates, which is well known from the literature.[3] This expansion is truncated after a fixed number of basis states N. The cutoff parameter N is chosen in such a way that convergence is achieved. It depends on the oscillator length of the basis, which is optimized in such a way that N is minimal. It turns out that $\hbar\omega = 41A^{-1/3}$ is a reasonable value. Of course, we could have chosen a deformed-harmonic-oscillator basis as in Ref. 3. Details of this method will be discussed in a separate publication.[6]

The method has been applied for the deformed nucleus ^{20}Ne. We used two well established sets of parameters for the Lagrangean which have been determined by Reinhard *et al.*[7] in spherical nuclei. They are given in Table I. Set I corresponds to the linear model, which is known to give an unrealistically large incompressibility for nuclear matter. Set II contains a nonlinear potential for the σ meson.

We study in Fig. 1 the dependence of the single-particle spectrum of occupied orbits in the nucleus ^{20}Ne on the cutoff parameter N. We find good convergence for $N=10$. Between $N=10$ and $N=12$ there are practically no differences. The corresponding deformation parameters β and binding energies E_B are for $N=8$, 10, and 12, $\beta=0.484$, 0.436, and 0.434, and $E_B/A = -7.361$, -7.155, and -7.136 MeV. We also find good convergence with this method for a spherical nu-

TABLE II. For the deformed nucleus ^{20}Ne we compare our results (for the two sets of force parameters in Table I) with density-dependent HF calculations (Skyrme II of Ref. 3) and experimental data. The results L1 and L2 are calculated with the corresponding parameters of Ref. 9. All energies in this table contain a center-of-mass correction of $-0.75\times 41\times A^{-1/3}$ MeV. Our calculations are carried out in an oscillator space of $N=10$ major shells and with an oscillator frequency $\hbar\omega = 41A^{-1/3}$.

Force	E/A (MeV)	$R^p_{\rm char}$ (fm)	$R^n_{\rm rms}$	Q^p (b)	Q^n	β
I	−7.72	2.85	2.72	0.38	0.37	0.44
II	−7.75	3.04	2.91	0.48	0.46	0.58
Skyrme II	−7.48	3.02	···	0.46	···	0.55
Expt.	−8.03	2.91	···	0.54 ± 0.03	···	0.65 ± 0.04
L1	−8.14	2.70	2.60	0.32	0.32	0.40
L2	−7.55	2.86	2.80	0.37	0.36	0.46

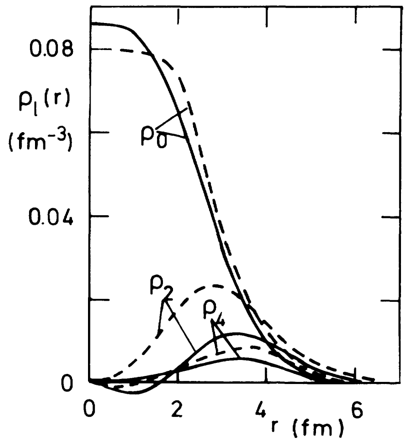

FIG. 3. The transition densities ρ_L for the charge distribution as a function of the radius r (calculated with the force II). The dashed lines correspond to the Skyrme-II-force calculation of Ref. 3.

cleus ^{16}O, where we get the binding energies -7.385, -7.395, and -7.389 MeV.

In Fig. 2 we show the "energy surfaces" for the two sets of parameters in ^{20}Ne. It is obtained by a constrained relativistic Hartree calculation with the quadratic constraining operator[8] $(Q-\langle Q\rangle)^2$. Q is the mass quadrupole operator for the nucleons $Q=r^2Y_{20}$ used as the time component of an external vector field. For both sets we have a well pronounced prolate minimum. In the nonlinear model it lies at a deformation of $\beta=0.58$, which is close to the value obtained by conventional Hartree-Fock (HF) calculations with Skyrme forces given in Table II.

In order to study the deformation of the nucleus ^{20}Ne in more detail, we have calculated the deformed charge density $\bar{\rho}$ by folding the point density ρ_v of Eq. (6) for protons with a Gaussian form factor $[\exp(-r^2/0.46)]$ and decomposed this "intrinsic" density $\bar{\rho}$ in terms of spherical harmonics,

$$\bar{\rho}(r)=\sum_L \rho_L(r) Y_{L0}(\theta,\phi). \quad (7)$$

The transition densities $\rho_L(r)$ for quadrupole and hexadecouple deformations are given in Fig. 3. They are in qualitative agreement with the corresponding quantities calculated in the Skyrme model.[3]

In conclusion, we present here a method to carry out relativistic mean-field calculations for axially deformed nuclei. Its validity is checked by the study of the convergence with the cutoff parameter N. We find that within this relativistic description we can reproduce nuclear deformations by using parameter sets adjusted to spherical doubly magic nuclei. In particular, we find that the precise value of the deformation depends somewhat on the set of parameters used in the calculations. The nonlinear model of Boguta and Bodmer[5] gives better agreement with the experimental nuclear deformation of ^{20}Ne. For the application of this theory to heavy deformed nuclei, pairing correlations are crucial. Investigations along this line are in progress.[10]

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Note added.— After finishing these calculations we received a paper by Suk-Joon Lee *et al.* (Ref. 9), which treats the same problem using a different technique —varying the Lagrangean (1) on a discrete mesh in configuration space. This group concluded that the parameters fitted to describe spherical nuclei and infinite nuclear matter fail to reproduce nuclear deformations. We could not reproduce their results. Subsequently, the authors of Ref. 9 published an erratum [Phys. Rev. Lett. **59**, 1171(E) (1987)]. Now their corrected results are in reasonable agreement with our calculations and with experiment.

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