Building Atomic Nuclei with the Dirac Equation

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The relevance of the Dirac equation for computations of nuclear structure is motivated and discussed. Quantitatively successful results for medium- and heavy-mass nuclei are described, and modern ideas of effective field theory and density functional theory are used to justify them.

I. INTRODUCTION

To understand how to build atomic nuclei with the Dirac equation, we will begin by asking some simple questions. What are the basic nuclear properties that we are trying to correlate and predict? Why use hadrons (rather than quarks and gluons) as the degrees of freedom? Why use the Dirac equation rather than the Schrödinger equation to describe the dynamics? How can we build a simple model of nuclear matter that reproduces the empirical equilibrium properties and that can be extended to calculations of medium- and heavy-mass nuclei? How does the Dirac approach predict the nuclear shell model? And how can we relate the hadronic description of nuclei to the underlying strong-interaction theory of quantum chromodynamics (QCD)?

The basic properties of nuclei provide stringent constraints on any nuclear theory. An accurate description of these properties is necessary for any useful predictions or extrapolations. We will concern ourselves primarily with bulk and single-particle nuclear properties, as listed below; a more detailed discussion can be found in Refs. [1, 2].

We certainly want to reproduce the observed shapes of nuclei: the interior density of a heavy nucleus should be relatively constant, since the nuclear forces “saturate” at the equilibrium density of nuclear matter (roughly $\rho_0 \approx 0.15 \text{fm}^{-3}$). Moreover, the nucleus should have a well-defined surface, with the density decreasing from 90% to 10% of its central value over a distance of roughly 2 fm. Finally, because of saturation, the radius $R$ of a nucleus should scale according to $R \approx A^{1/3} 1.1 \text{fm}$, where $A = N + Z$ is the total number of neutrons ($N$) plus protons ($Z$).

The total energy of the nucleus should follow the “liquid drop” formula

$$E = -a_1 A + a_2 A^{2/3} + a_3 Z^2 / A^{1/3} + a_4 (N - Z)^2 / A + \cdots ,$$

(1)

where typical values for the $a_i$ coefficients are given in Ref. [1].

The particle spectrum is determined by the qualitative features of the single-particle potential. In a nonrelativistic (Schrödinger) language, the central potential is midway between...
a harmonic oscillator and a square well; this shape determines the ordering of the levels as a function of the orbital angular momentum. (See Ref. [1], Figs. 57.1 and 57.2.) In addition, the spin-orbit potential is strong, which is instrumental in determining the major shell closures and, hence, the shell model. We will see below how these features are reproduced in a description based on the Dirac equation.

These simple nuclear features are the ones we will focus on. We expect that they can be described adequately by a single-particle equation with an effective, one-body interaction. Such an approach has many names, depending on the system being studied and on the practitioner: “shell model”, “mean-field theory”, “Kohn–Sham” density functional theory, etc. Our goal is to correlate (fit) a modest number of nuclear bulk and single-particle data and then to predict other, similar data as well as possible.

II. WHY USE HADRONS?

Well, why not? Our focus is on long-range nuclear characteristics, and all measured observables are colorless. (In fact, most of the observables relevant to us are dominated by the isoscalar part of the interaction.) Moreover, hadronic variables (baryons and mesons) are efficient, since hadrons are the particles that are observed in experiments. Colored quarks and gluons participate only in intermediate states, and such “off-shell behavior” is unobservable; by using hadrons, we expend no theoretical effort combining quarks and gluons into color singlets that can actually be observed.

So we pick the most efficient degrees of freedom by choosing hadrons. We will have to parametrize the nuclear hamiltonian anyway, since we cannot compute its true form from QCD, and hadronic variables, if combined in all forms consistent with the underlying symmetries, provide sufficient flexibility for our parametrization. We cannot guarantee that a single-particle hadronic approach will be successful in describing the observables of interest, but we want to see how well we can do.

III. WHY USE THE DIRAC EQUATION?

To motivate the Dirac equation as straightforwardly as possible, compare the particle spectrum (and fine structure) in a light atom with the spectrum in a heavy nucleus. An example of the former is given in Ref. [3], while an early example of the latter is given in Ref. [4], which is reproduced in Fig. 57.3 of Ref. [1]. The most striking result is that it is impossible to draw the atomic fine structure to scale, since the splittings are roughly 1/10,000 as large as the major-level splittings (at least for the deeply bound atomic levels). In contrast, the nuclear spectrum shows that the “fine” structure is really “gross”; the fine-structure splittings are as large as the major-level splittings to within a factor of two!

The implication is that there must be some relativistic effects that are important in nuclei (unlike light atoms), and thus it is much more natural to use the Dirac equation to describe the quasi-particle nucleon wave functions. We will now try to understand this result by building a simple model of uniform nuclear matter.
IV. A SIMPLE MODEL OF NUCLEAR MATTER

We consider a model first proposed by Walecka \[5\], which contains nucleons (ψ) and neutral (isoscalar) Lorentz scalar (φ) and vector (V\(_μ\)) mesons. This model is often referred to as “quantum hadrodynamics I” (or QHD–I, for short). The lagrangian density for this model (using the conventions of Ref. \[6\] and suppressing counterterms for simplicity) is

\[
\mathcal{L} = \bar{\psi} (i\gamma_\mu \partial^\mu - M) \psi + \frac{1}{2} (\partial_\mu \phi \partial^\mu \phi - m_s^2 \phi^2) - \frac{1}{4} (\partial_\mu V_\nu - \partial_\nu V_\mu)^2 \\
+ \frac{1}{2} m^2 V_\mu V^\mu + g_s \bar{\psi} \psi \phi - g_v V_\mu \gamma_\mu \psi .
\]  

The included degrees of freedom are the minimal ones that will allow us to understand the qualitative features of the nuclear many-body system, which is our goal. We will describe the system in terms of Dirac quasi-particles moving in classical meson mean fields, an approximation that we will elaborate on and justify later. Note that the baryon current (density) \( \bar{\psi} \gamma_\mu \psi \) is conserved.

It is important to emphasize that the Lorentz scalar and vector fields are effective fields that are introduced to parametrize the nucleon–nucleon (NN) interaction. The quanta of these fields never appear “on the mass shell” as real particles in any of the calculations discussed here. They are analogous to the phonons that describe electron–electron interactions inside a metal.

If one computes the NN interaction using one-boson exchange [purely for illustration, since the coupling constants \( g_s \) and \( g_v \) in Eq. \(2\) are large], one finds a short-range repulsion (from \( V^\mu \)) and a mid-range attraction (from \( \phi \)), which is characteristic of the NN force. Explicit pion exchange is of minor importance for our observables of interest; isoscalar, scalar and vector fields are dominant for the bulk and single-particle properties of heavy nuclei (and some multi-pion exchange is simulated by our effective fields anyway).

Consider nuclear or neutron matter at zero temperature. We can treat the mesons at the mean-field level by taking

\[
\phi \rightarrow \langle \phi \rangle \equiv \phi_0 , \quad V^\mu \rightarrow \langle V^\mu \rangle \equiv V_0 \delta^{\mu 0} ,
\]

where \( \langle V \rangle \equiv 0 \), since we assume that we are in the rest frame of the uniform matter. Note that \( \phi_0 \) and \( V_0 \) are constants.

Why should mean meson fields yield a reasonable description of the system, since QHD–I is a strong-coupling theory? Our goal is to construct an approximate energy functional of the scalar (\( \rho_s \)) and baryon (\( \rho_B \)) densities and to fit the parameters in this functional to bulk nuclear properties. The mean meson fields give us a convenient way to do this, since they satisfy the mean-field equations:

\[
\phi_0 = \frac{g_s}{m_s^2} \rho_s \equiv \frac{g_s}{m_s^2} \sum_{i}^{\text{occ}} \bar{\psi}_i \psi_i ,
\]

\[
V_0 = \frac{g_v}{m_v^2} \rho_B \equiv \frac{g_v}{m_v^2} \sum_{i}^{\text{occ}} \bar{\psi}_i \psi_i ,
\]

\[
[i\gamma_\mu \partial^\mu - g_v \gamma^0 V^0 - \frac{(M - g_s \phi_0)}{M^*}] \psi = 0 ,
\]
where “occ” signifies the occupied quasi-particle levels. (In infinite matter, we sum over states with both spin projections and with momentum \( k \leq k_F \), where \( k_F \) is the Fermi momentum.)

We solve these equations for stationary quasi-particle states; the problem is self-consistent, since \( \rho_s = \rho_s(M^\star) \) both determines and depends on the wave functions \([5, 6]\). The nuclear/neutron matter energy function(al) then becomes

\[
E_{\text{MFT}} = \frac{g_s^2}{2m_s^2} \rho_s^2 + \frac{m_s^2}{2g_s^2} (M - M^\star)^2 + \frac{\lambda}{\pi^2} \int_0^{k_F} dt \ t^2 (t^2 + M^\star)^{1/2}, \tag{7}
\]

where the baryon density is

\[
\rho_B = \frac{\lambda k_F^3}{3\pi^2}, \tag{8}
\]

and the isospin degeneracy is \( \lambda = 2 \) for symmetric \( (N = Z) \) nuclear matter and \( \lambda = 1 \) for pure neutron matter \( (Z = 0) \). (Note that, by definition, the Coulomb force between protons is turned off.)

One can now minimize the energy density \( E \) with respect to \( \rho_B \) to find the equilibrium point, and use the empirical equilibrium point of nuclear matter \( (\text{density} = \rho_0 \approx 0.15 \text{ fm}^{-3}, \text{binding energy} = e_0 \approx 16 \text{ MeV}) \) to determine the two unknown ratios

\[
\frac{g_s^2}{m_s^2} \quad \text{and} \quad \frac{g_v^2}{m_v^2},
\]

which are expressed more conventionally (and less dimensionally) as

\[
C_s^2 \equiv \frac{g_s^2 M^2}{m_s^2} = 357.4 \quad \text{and} \quad C_v^2 \equiv \frac{g_v^2 M^2}{m_v^2} = 273.8. \tag{9}
\]

The resulting nuclear/neutron matter binding curves and the self-consistent effective mass \( M^\star \) as functions of the density are shown in Figs. 1 and 2 of Ref. \([6]\). The important features of these results are:

- Symmetric nuclear matter is a self-bound liquid with an equilibrium point as defined above. This illustrates the “saturation” of nuclear forces.

- Pure neutron matter is (generally) unbound at all densities. This reflects the positive symmetry-energy coefficient \([a_4 \text{ in Eq. } (1)]\) that enters when the number of neutrons and protons is different.\(^1\)

- The nucleon effective mass at equilibrium density is roughly \( M^\star_0 \approx 0.6M \). This shows that the scalar mean field is roughly \(-400 \text{ MeV} \) at equilibrium; the corresponding vector mean field is roughly \( 300 \text{ MeV} \), and the two fields cancel to produce the relatively small binding energy of 16 MeV. We turn now to a discussion of this point.

\(^1\) In QHD–I, this coefficient is too small. One must add a \( \rho \) meson, which couples to the difference of proton and neutron densities, to achieve an accurate result. See Ref. \([8]\).
What causes the nuclear matter saturation and the relatively small binding energy? Let’s expand \( E/\rho_B \) from Eq. (7) in powers of \( k_F \):

\[
E_{\text{MFT}}/\rho_B = M + \left[ \frac{3k_F^2}{10M} - \frac{3k_F^4}{56M^3} + \frac{k_F^6}{48M^5} - \cdots \right] + \frac{g_s^2}{2m_s^2} \rho_B - \frac{g_s^2}{2m_s^2} \rho_B
+ \frac{g_s^2 \rho_B}{m_s^2 M} \left[ \frac{3k_F^2}{10M} - \frac{36k_F^4}{175M^3} + \cdots \right] + \left( \frac{g_s^2 \rho_B}{m_s^2 M} \right)^2 \left[ \frac{3k_F^2}{10M} - \cdots \right] + \cdots
\]

The lowest-order Lorentz scalar and vector contributions (which are proportional to \( \rho_B \)) set the scale for the large mean fields. [See Eqs. (4) and (5).] This scale is consistent with chiral QCD counting rules [7, 8], but these two terms cancel almost exactly in the binding energy, leading to an anomalously small remainder. However, they add constructively in the spin-orbit interaction, leading to appropriately large spin-orbit splittings in nuclei [9, 10, 11].

It is important to notice the different behavior of the vector and scalar interaction terms in Eq. (10). Whereas the vector interaction enters at only linear order in \( \rho_B \), the scalar interaction enters at all orders; moreover, the leading scalar term at every order in \( \rho_B \) looks exactly the same, and they all add constructively. These terms are precisely what one gets by shifting the nucleon mass in the nonrelativistic kinetic energy term \( 3k_F^2/10M \) from \( M \to M^* \approx M - g_s^2 \rho_B/m_s^2 \). These additional, repulsive, velocity-dependent interactions reduce the strength of the lowest-order, attractive scalar contribution and are crucial for establishing the location of the equilibrium point of nuclear matter. Thus the different behavior of the vector and scalar interactions leads to large relativistic interaction effects in the nuclear matter energy density. In contrast, the relativistic corrections to the kinetic energy (the nonleading terms in the first pair of square brackets) are indeed small; this is not where the important “relativity” is.

V. MEAN-FIELD THEORY FOR NUCLEI

We now compute the bulk and single-particle properties of atomic nuclei using essentially the same simple lagrangian discussed above. Our treatment follows that of Ref. [10], which is more than twenty years old, but which is still sufficient to illustrate the important points. We will discuss modifications and more modern treatments later.

The basic idea is to allow the mean meson fields to be spatially dependent, and we will consider only spherically symmetric nuclei for simplicity. We again look for stationary quasi-nucleon states, and so the mean-field equations become [6]

\[
\nabla^2 \phi_0(r) - m_s^2 \phi_0(r) = -g_s \rho_s(r) , \tag{11}
\]

\[
\nabla^2 V_0(r) - m_v^2 V_0(r) = -g_v \rho_v(r) , \tag{12}
\]

\[
\{-i \alpha \cdot \nabla + g_v V_0(r) + \beta [M - g_s \phi_0(r)] \} \psi_\alpha(x) = \epsilon_\alpha \psi_\alpha(x) . \tag{13}
\]

These are coupled, nonlinear, differential equations that must be solved self-consistently. They are sometimes called Dirac–Hartree equations [6, 12] but are more accurately described as Kohn–Sham equations [13], as we discuss in more detail below.
As one might expect, an accurate description of nuclear properties is not possible using only nucleons and isoscalar mesons. One must extend the model to include at least the Coulomb interaction between protons and an isovector $\rho$ meson that allows for a more realistic description of the nuclear symmetry energy. (See Refs. \[10, 12\] for details.) The augmented model now contains four adjustable parameters:

$$g_s, \quad g_v, \quad g_{\rho}, \quad m_s.$$ (The heavy meson masses are fixed at some “large” mass scale that is roughly equal to the nucleon mass $M$.) The couplings are fitted to the equilibrium point of symmetric nuclear matter and to the nuclear matter symmetry energy; the length scale, which is determined by $m_s$, is set by fixing this parameter to reproduce the rms charge radius of a doubly magic nucleus, such as $^{40}$Ca.

Many nuclear structure calculations have been carried out within this relativistic mean-field theory (RMFT) framework. (See, for example, Refs. \[10, 12\] or the extensive list of references in Ref. \[6\].) One finds that the bulk properties of nuclei are well reproduced even in this relatively simple mean-field theory. Moreover, the single-particle spectrum reveals the well-known nuclear shell structure; this comes for free, since the parameters are fitted to the bulk properties of nuclear matter (and one nuclear length scale).

Extensions of this simple model have been made to “fine-tune” the results. In the 1980’s, numerous authors added terms involving nonlinear interactions of the scalar field:

$$L' = - \frac{1}{3!} \kappa \phi^3 - \frac{1}{4!} \lambda \phi^4,$$ (14)

and in the 1990’s, various practitioners added vector self-couplings, like

$$L'' = + \frac{1}{4!} \zeta g_4(V_\mu V^\mu)^2,$$ (15)

as well as other nonlinear and gradient-coupling terms, some motivated by the ideas of effective field theory; see the discussion below. (Many calculations in these extended models are cited in Ref. \[6\]. For an alternative approach that uses only nucleons in a lagrangian that contains numerous powers of fermion fields, see Ref. \[14\] and references therein.)

These additional nonlinearities can be interpreted in terms of many-body nuclear forces, and they introduce additional density dependence into the nuclear energy functional, which allows it to more accurately reproduce the true energy functional. The new parameters are fitted either to additional nuclear matter properties, or to other theoretical calculations of nuclear matter (based on the Schrödinger equation), or to a selected set of data from finite nuclei. The basic conclusion from these extended calculations is that the successful qualitative features predicted by the original simple models persist, but the quantitative accuracy increased by nearly two orders of magnitude over a period of twenty years. For a comparison of the accuracy of results obtained with different collections of parameters, see, for example, Refs. \[7, 8\]. For some recent state-of-the-art predictions of this approach (that is, calculations of nuclei that are not included in the fitting procedures), see Ref. \[15\].

But it still remains for us to understand at a deeper level why these simple relativistic mean-field calculations can do such an excellent job of reproducing certain nuclear observables. For this, we must study . . .
VI. MODERN DEVELOPMENTS

The discussion in this section is a synopsis of the formalism presented in Refs. [6, 7, 13, 17], which is based on the ideas of modern effective field theory (EFT) and density functional theory (DFT). The interpretation of the earlier, successful results using EFT/DFT puts them on a firm theoretical basis.

First of all, we interpret QHD as a nonrenormalizable EFT. This means that it contains known long-range interactions that are constrained by the underlying QCD symmetries, plus a complete (but non-redundant) set of generic short-range interactions, i.e., “contact” and “gradient” terms. The borderline between short and long ranges is characterized by the breakdown scale \( \Lambda \) of the EFT; empirically, we find that \( \Lambda \approx 600 \text{ MeV} \) for QHD [8].

If we ignore strangeness, then only nucleons and pions are “real” (stable) particles. The other field quanta are always virtual and just let us parametrize the NN interaction. As in any lagrangian theory, there are different ways to choose the generalized coordinates (fields), but some coordinates may be more efficient than others [8, 14].

The QHD EFT lagrangian explicitly exhibits the symmetries of QCD: The global, chiral \( SU(2)_L \times SU(2)_R \) symmetry is nonlinear, approximate, and spontaneously broken [6]. The remaining global, isovector subgroup \( SU(2)_V \) is realized linearly. It is straightforward (but usually tedious) to include electromagnetic interactions through the familiar local \( U(1) \) gauge symmetry [7].

The basic strategy for using the QHD lagrangian has been developed over the last several years [6, 7, 16]. First, assign an index \( \nu \) to each term in the lagrangian:

\[
\nu = d + n/2 + b ,
\]

where \( d \) is the number of derivatives (not counting those that act on nucleon fields), \( n \) is the number of nucleon fields, and \( b \) is the number of non-Goldstone bosons.

Now organize the lagrangian in powers of \( \nu \) and truncate. This gives an expansion in inverse powers of a heavy mass scale \( \Lambda \approx M \), which has been shown to be reliable in calculations of medium- and heavy-mass nuclei [8]. Practically speaking, in the nuclear many-body problem, this expansion is in powers of \( k_F/M \), where \( k_F \) is the Fermi momentum at equilibrium nuclear density (\( k_F/M \approx 1/3 \)).

Use the truncated lagrangian to construct an energy functional, which is to be interpreted within the DFT framework: We approximate the functional using factorized densities or fields, which produces a mean-field form of the functional. Expand it as a power series in density and momentum (by counting powers of \( \nu \) and fit the remaining parameters to a restricted set of experimental data [8]. These data typically include nuclear binding energies, prominent features of the nuclear electromagnetic charge form factors, and single-particle energy splittings for the least-bound orbitals [7]. Define a set of Kohn–Sham (KS) single-particle orbitals that satisfy differential equations obtained by extremizing the energy functional with respect to the densities and fields. This procedure guarantees that all of the source terms in these equations are local. The KS orbitals are tailored to the generation of the ground-state density, and they include short-range and correlation effects adequately, if the mean-field energy functional is a good approximation to the true energy functional [17].

\footnote{Time derivatives acting on nucleon fields will generally bring down factors of the nucleon mass or energy, which are not small compared to \( \Lambda \).}
The mean-field energy functional constructed above omits some long-range contributions, which are generally nonlocal and nonanalytic functions of the densities. These contributions can be added systematically, by computing loop integrals using the well-known rules of EFT [18]. The effect of these loop contributions on the energy functional of atomic nuclei is an important topic for future study.

VII. SUMMARY

The most important points in the preceding discussion can be summarized as follows:

- The Dirac equation provides an economical and natural way to describe bulk nuclear properties and the nucleon single-particle spectrum, with the correct spin-orbit force (that is, the nuclear shell model) arising automatically.

- Kinematical relativistic effects are small in nuclei, but dynamical relativistic effects from the interactions are important.

- Modern QHD EFT’s incorporate the basic symmetries of QCD.

- The mean-field approach to heavy nuclei is really DFT, implemented through KS quasi-particle orbitals. The tested validity and accuracy of our truncation procedure for both fitted and predicted results shows that we really know something about the energy functional for cold nuclear matter near equilibrium density!

- The energy functional can be extended beyond the mean-field parametrization using well-defined rules of EFT to compute the long-range contributions of loop integrals. This has been done recently [18].

- The QHD/EFT/DFT/KS formalism provides a true representation of QCD in the low-energy nuclear domain.

The basic message of this talk is: the Dirac equation is relevant for nuclear-structure physics, even though you might not expect it to be. Our quantitative successes justify its usage, but the modern theoretical ideas of EFT and DFT explain why it works.

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[1] A. L. Fetter and J. D. Walecka, Quantum Theory of Many-Particle Systems (McGraw–Hill, N.Y., 1971), chs. 11 and 15.
[2] J. D. Walecka, Theoretical Nuclear and Subnuclear Physics (Oxford U. Press, N.Y., 1995), part I.
[3] J. D. Bjorken and S. D. Drell, Relativistic Quantum Mechanics (McGraw–Hill, N.Y., 1964, 1998), fig. 4–2.
[4] M. G. Mayer and J. H. D. Jensen, Elementary Theory of Nuclear Shell Structure (Wiley, N.Y., 1955), p. 58.
[5] J. D. Walecka, Ann. of Phys. 83, 491 (1974).
[6] B. D. Serot and J. D. Walecka, Int. J. Mod. Phys. E 6, 515 (1997).
[7] R. J. Furnstahl, B. D. Serot, and H.-B. Tang, Nucl. Phys. A615, 441 (1997); A640, 505(E) (1998).
[8] R. J. Furnstahl and B. D. Serot, Nucl. Phys. A671, 447 (2000).
[9] W. H. Furry, Phys. Rev. 50, 784 (1936).
[10] C. J. Horowitz and B. D. Serot, Nucl. Phys. A368, 503 (1981).
[11] R. J. Furnstahl, J. J. Rusnak, and B. D. Serot, Nucl Phys. A632, 607 (1998).
[12] B. D. Serot and J. D. Walecka, Adv. Nucl. Phys. 16, 1 (1986).
[13] R. J. Furnstahl and B. D. Serot, Comments Nucl. Part. Phys. 2, A23 (2000).
[14] J. J. Rusnak and R. J. Furnstahl, Nucl. Phys. A627, 495 (1997).
[15] M. A. Huertas, Phys. Rev. C 66, 024318 (2002).
[16] R. J. Furnstahl, B. D. Serot, and H.-B. Tang, Nucl. Phys. A598, 539 (1996).
[17] W. Kohn, Rev. Mod. Phys. 71, 1253 (1999).
[18] Y. Hu, Ph.D. thesis, Indiana University (2000), unpublished.