A Relativistic Point Coupling Model for Nuclear Structure Calculations

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A relativistic point coupling model is discussed focusing on a variety of aspects. In addition to the coupling using various bilinear Dirac invariants, derivative terms are also included to simulate finite-range effects. The formalism is presented for nuclear structure calculations of ground state properties of nuclei in the Hartree and Hartree-Fock approximations. Different fitting strategies for the determination of the parameters have been applied and the quality of the fit obtainable in this model is discussed. The model is then compared more generally to other mean-field approaches both formally and in the context of applications to ground-state properties of known and superheavy nuclei. Perspectives for further extensions such as an exact treatment of the exchange terms using a higher-order Fierz transformation are discussed briefly.

1. Introduction

Relativistic mean field (RMF) models are quite successful in describing ground state properties of finite nuclei and nuclear matter properties. They describe the nucleus as a system of Dirac nucleons that interact in a relativistic covariant manner via mean meson fields (for a review see Reference 1) or via mean nucleon fields[2,3] whose explicit forms sometimes derive solely from the meson field approaches.[4] The meson fields are of finite range (FR) due to meson exchange whereas the nucleon fields are of zero range (contact interactions or point couplings PC) together with derivative terms that simulate finite interaction range to some extent.

In this work we use mean nucleon fields constructed with contact interactions (point couplings) to represent the system of interacting Dirac nucleons. We choose this approach for the following reasons: (a) possible physical constraints introduced by explicit use of the Klein-Gordon approximation to describe mean meson fields, in particular that of the (fictitious) sigma meson, are avoided and instead the effects of the various incompletely understood and higher order processes are assumed to be lumped into appropriate coupling constants and terms of the Lagrangian, as explained in Reference 2, (b) the use of point couplings allows not only (standard) relativistic Hartree calculations to be performed, but also relativistic Hartree-Fock calculations[5,6] by use of Fierz relations (up to fourth order[7]), and (c) the use of point couplings, because of their success in the Nambu-Jona-Lasino model for the low-momentum domain of QCD,[8] is perhaps the best way to test for *naturalness* of the coupling constants in the seminal Weinberg expansion[9] highlighting the role of power counting and chiral symmetry in weakening N-body forces. That is, two-nucleon forces are stronger than three-nucleon forces, which are stronger than four-nucleon forces, ..., resulting in a sequence making nuclear physics tractable. If the dimensionless coupling constants of the corresponding Lagrangian are of order 1 (*natural*) then QCD scaling and chiral symmetry apply to finite nuclei. Finally, (d), the RMF-PC model allows one to investigate its relationship to nonrelativistic point-coupling approaches like the Skyrme-Hartree-Fock (SHF) approach and the RMF-FR approach to contrast the importance and roles of the different features these models have, as well as to obtain new insights.

It is important to note here that one can also view RMF-PC as an approach that lies in between the RMF-FR approach and the nonrelativistic Skyrme-Hartree-Fock (SHF) approach which is also a well-developed self-consistent mean-field model that performs very well (for a review see Reference 10). Whereas SHF is based upon density-dependent contact interactions with extensions to gradient terms, kinetic terms, and the spin-orbit interaction, RMF-FR is based upon a coupled field theory of Dirac nucleons and effective meson fields treated at the mean-field level, where density dependence is modeled by nonlinear meson self couplings and the role of gradient terms is taken over by the finite ranges of the mesons. The kinetic and spin-orbit terms are automatically carried in both RMF models.[1] Thus, a comparison of RMF-PC and SHF addresses the differences between in-medium Dirac and Schrödinger nucleons, that is, in kinetic and spin-orbit components, whereas a comparison of RMF-PC and RMF-FR addresses the absence *vs.* presence of finite range and the different treatments of density dependence. Herein we will perform these comparisons using precisely the same fitting strategy as in recent SHF and RMF-FR adjustments[11–13] except that here we will in addition be guided by considerations of QCD scaling and chiral symmetry, that is, *naturalness*.

In this paper we will present a new fit of the parameters, the application to superheavy nuclei together with a study of the spin-orbit force, which plays an essential role in that region. For more details, see Reference 14.

2. The Model

2.1. The Lagrangian. The elementary building blocks of the point-coupling vertices are two-fermion terms of the general type

$$(\bar{\psi}\mathcal{O}_\tau\Gamma\psi), \quad \mathcal{O}_\tau \in \{1, \tau_i\}, \quad \Gamma \in \{1, \gamma_\mu, \gamma_5, \gamma_5\gamma_\mu, \sigma_{\mu\nu}\} \qquad (1)$$

with ψ the nucleon field, τ_i the isospin matrices and Γ one of the 4×4 Dirac matrices. There thus is a total of 10 such building blocks characterized by their transformation character in isospin and in spacetime.

The interactions are then obtained as products of such expressions to a given order. The products are coupled, of course, to a total isoscalar-scalar term. By "order" we mean the number of such terms in a product, so that a second-order term corresponds to a four-fermion coupling, and so on. In second order only the ten elementary currents squared and contracted to scalars may contribute, but at higher orders there is a proliferation of terms because of the various possible intermediate couplings.

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In analogy to the nonrelativistic Skyrme-force models, one goes one step beyond zero range and complements the point-coupling model by derivative terms in the Lagrangian, as e.g. $\partial_\nu \bar{\psi}\vec{\tau}_i \Gamma_j^\mu \psi$. The derivative is understood to act on both $\bar{\psi}$ and ψ.

In the present work we consider the following four-fermion vertices: isoscalar-scalar, $(\bar{\psi}\psi)^2$ corresponding to the σ-field, isoscalar-vector, $(\bar{\psi}\gamma_\mu\psi)(\bar{\psi}\gamma^\mu\psi)$ corresponding to the ω-field, and isovector-vector, $(\bar{\psi}\vec{\tau}\gamma_\mu\psi)\cdot(\bar{\psi}\vec{\tau}\gamma^\mu\psi)$, corresponding to the ρ-field, together with their corresponding gradient couplings $\partial_\nu(\ldots)\partial^\nu(\ldots)$.

These constitute a complete set of second-order scalar and vector currents whose coupling strengths in the corresponding Lagrangian we wish to test for naturalness. We neglect all tensor couplings in the present work because they have had little effect in corresponding RMF-FR calculations.[1] Finally, the pseudoscalar channel (π-meson) is not included here because it does not contribute at the Hartree level.

Given the vast number of possible higher-order terms we begin with those that have already been demonstrated to be of use in the existing calculations with the RMF-FR and RMF-PC approaches. These are the familiar nonlinear terms in the scalar coupling, $(\bar{\psi}\psi)^3$ and $(\bar{\psi}\psi)^4$, as well as a nonlinear vector term $[(\bar{\psi}\gamma_\mu\psi)(\bar{\psi}\gamma^\mu\psi)]^2$ as used in some RMF-FR[15] and RMF-PC[2] models. Finally, of course, the electromagnetic field and the free Lagrangian of the nucleon field must be included.

Combining all of these terms, we obtain the Lagrangian of the point-coupling model as

$$
\begin{aligned}
\mathcal{L} &= \mathcal{L}^{\rm free} + \mathcal{L}^{\rm 4f} + \mathcal{L}^{\rm hot} + \mathcal{L}^{\rm der} + \mathcal{L}^{\rm em}, \\
\mathcal{L}^{\rm free} &= \bar{\psi}(\mathrm{i}\gamma_\mu\partial^\mu - m)\psi, \\
\mathcal{L}^{\rm 4f} &= -\frac{1}{2}\alpha_{\rm S}(\bar{\psi}\psi)(\bar{\psi}\psi) - \frac{1}{2}\alpha_{\rm V}(\bar{\psi}\gamma_\mu\psi)(\bar{\psi}\gamma^\mu\psi) \\
&\quad -\frac{1}{2}\alpha_{\rm TV}(\bar{\psi}\vec{\tau}\gamma_\mu\psi)\cdot(\bar{\psi}\vec{\tau}\gamma^\mu\psi), \\
\mathcal{L}^{\rm hot} &= -\frac{1}{3}\beta_{\rm S}(\bar{\psi}\psi)^3 - \frac{1}{4}\gamma_{\rm S}(\bar{\psi}\psi)^4 - \frac{1}{4}\gamma_{\rm V}[(\bar{\psi}\gamma_\mu\psi)(\bar{\psi}\gamma^\mu\psi)]^2, \\
\mathcal{L}^{\rm der} &= -\frac{1}{2}\delta_{\rm S}(\partial_\nu\bar{\psi}\psi)(\partial^\nu\bar{\psi}\psi) - \frac{1}{2}\delta_{\rm V}(\partial_\nu\bar{\psi}\gamma_\mu\psi)(\partial^\nu\bar{\psi}\gamma^\mu\psi) \\
&\quad -\frac{1}{2}\delta_{\rm TV}(\partial_\nu\bar{\psi}\vec{\tau}\gamma_\mu\psi)\cdot(\partial^\nu\bar{\psi}\vec{\tau}\gamma^\mu\psi), \\
\mathcal{L}^{\rm em} &= -eA_\mu\bar{\psi}[(1-\tau_3)/2]\gamma^\mu\psi - \frac{1}{4}F_{\mu\nu}F^{\mu\nu}. \qquad (2)
\end{aligned}
$$

Note that we use the nuclear physics convention for the isospin where the neutron is associated with $\tau_3 = +1$ and the proton $\tau_3 = -1$.

As it stands this Lagrangian contains the nine coupling constants $\alpha_{\rm S}$, $\alpha_{\rm V}$, $\alpha_{\rm TV}$, $\beta_{\rm S}$, $\gamma_{\rm S}$, $\gamma_{\rm V}$, $\delta_{\rm S}$, $\delta_{\rm V}$, and $\delta_{\rm TV}$. The subscripts indicate the symmetry of the coupling: "S" stands for scalar, "V" for vector, and "T" for isovector, while the symbols refer to the additional distinctions: α refers to four-fermion terms, δ to derivative couplings, and β and γ to third- and fourth order terms, respectively.

The model thus contains one or two free parameters more than analogous RMF-FR models. This happens because most RMF-FR models make the tacit assumption that the masses in the ω- and ρ-field can be frozen at the experimental values of the really existing mesons. The assumption is justified to the extent that the actual fits to observables are not overly sensitive to these masses. In the RMF-PC model, however, experience will still have to show whether the derivative-term coefficients can be eliminated in a similar way, so that for the present work all parameters are regarded as adjustable.

Similar to the RMF-FR approach, we consider the RMF-PC approach as an effective Lagrangian for nuclear mean-field calculations at the Hartree level without anti-nucleon states (no-sea approximation), and include pairing and center-of-mass corrections in the standard way.[16,17]

2.2. Coupling Constants. In addition to the older parametrization PC-LA[2] that was based on a relatively small set of data and partly relied on naturalness of the parameters to restrict their freedom, we also fitted a new parameter set for the version of the model given in eq 2. The parameters are fitted in the same way as NL-Z2.[18] The set of nine coupling constants emerging from the fitting procedure with the lowest value of χ^2 is called PC-F1, and its performance is compared to that of NL-Z2 in Figure 1.

Comparing the average errors between PC-F1 and NL-Z2, we see slightly different trends. NL-Z2 is superior with respect to binding energies and surface thicknesses. It does, however, perform less brilliantly concerning radii. The total χ^2 of NL-Z2 is 132.7 which is 34% larger than that for PC-F1. The overall performance of the point-coupling thus seems to be a bit better, although the difference is not dramatic.

Since we know that spin-orbit coupling is crucial for superheavy elements,[18] we show in Figure 2 the relative errors for a selection of spin-orbit splittings in ^{16}O, ^{132}Sn, and ^{208}Pb. We have taken care to choose splittings which can be deduced reliably from spectra of neighbouring odd nuclei.[19] All RMF forces, except for PC-LA, perform very well. We see now that the well fitted point coupling model PC-F1 does as well as finite range RMF. The ability to describe the spin-orbit force correctly is thus a feature of the relativistic approach. The force PC-LA falls clearly below the others. The poor performance is related to the too weak fields at large densities. The example demonstrates that one needs a sufficiently large set of observables to pin down the nuclear mean field sufficiently well.

The three well performing models all have very similar spin-orbit potentials whereas PC-LA has one 10% stronger which is shifted a little bit to larger radii. This difference yields the observed mismatch in the spin-orbit splittings.

2.3. Superheavy Elements. The upper panel of Figure 3 shows the relative errors in binding energies for the heaviest even-even nuclei with known experimental masses (compare

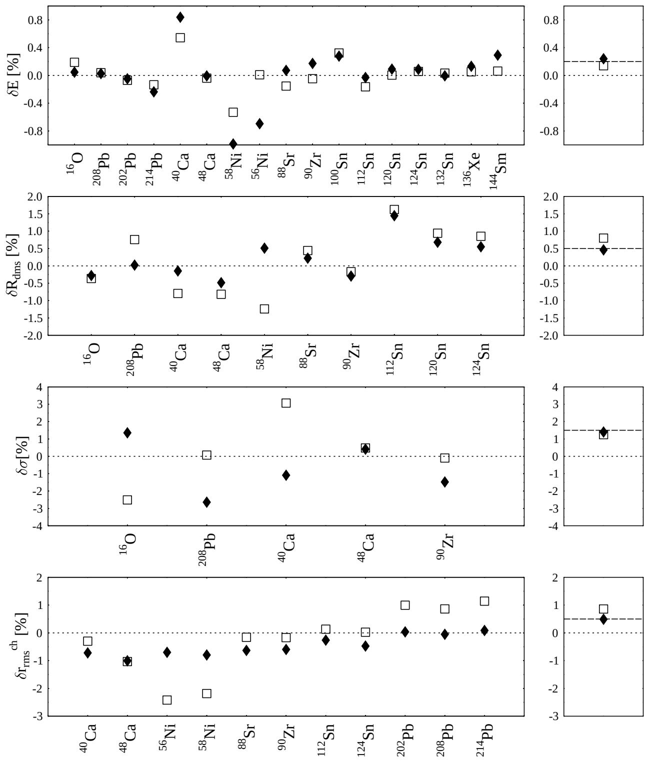

Figure 1. Errors in percent for the observables binding energy, diffraction radius, surface thickness, and rms charge radius for PC-F1 (filled diamonds) and NL-Z2 (open squares) are seen on the left. The right panels show the absolute mean errors for the corresponding observables, where the dashed lines indicate the chosen relative errors ΔO in the fitting procedure.

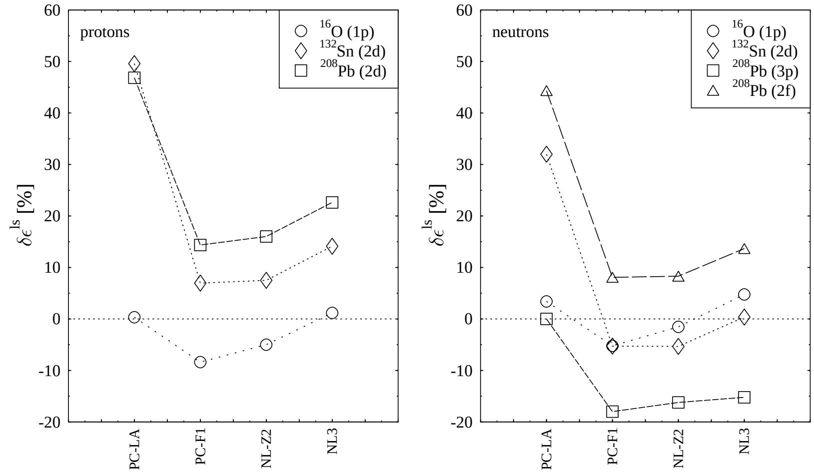

Figure 2. The percentage error in *ls*-splittings for protons (left) and for neutrons (right). The experimental errors are smaller than the size of the symbols used in these figures. The lines serve to guide the eye.

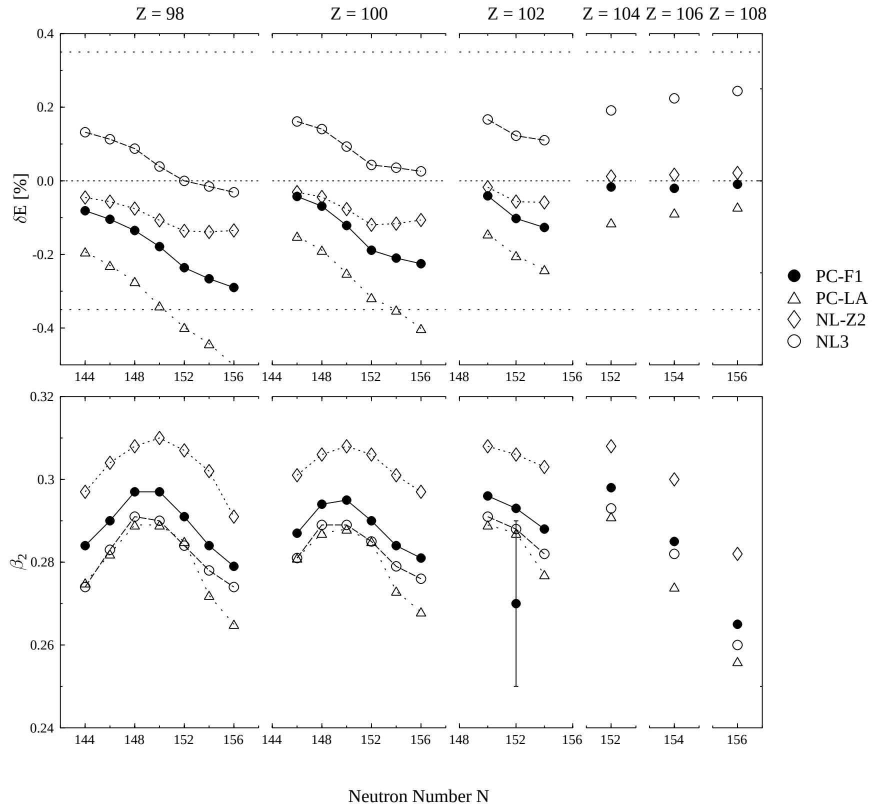

Figure 3. Deviation in % of the calculated energies from the experimental values (upper figure) and ground-state deformations (lower figure) in axially deformed and reflection symmetric calculations. The errors for the binding energies are smaller than the size of the symbols used in this figure. The symbol with error bars indicates the measured ground-state deformation together with its uncertainty of ^{254}No (Ref. 22, 23).

with a similar figure in Reference 20). The lower panel delivers as complementing information the ground-state deformations expressed in terms of the dimensionless quadrupole deformation β_2. The calculations were performed allowing axially symmetric deformation assuming reflection-symmetric shapes. The agreement is remarkable. All forces (with some exceptions for PC-LA) produce only small deviations which stay well within the given error band. This is a gratifying surprise because we are here 40–50 mass units above the largest nucleus included in the fit. It is to be noted that most SHF forces do not perform so well and have general tendency to underbinding for superheavy nuclei.[20] There are also (small but) systematic differences between the RMF models. NL3[21] generally overbinds a little while NL-Z2 and PC-F1 tend to underbind. All forces show yet unresolved isovector trends. The increase of the binding energy with increasing neutron number is too small. These trends are already apparent for known nuclei (details for PC-F1 not shown in this paper). The reasons for all these trends are not yet understood. Finally, mind the kinks visible for the $Z = 98$ and $Z = 100$ isotopes at neutron number $N = 152$ which hint at a small (deformed) shell closure there.

All forces predict strong prolate ground-state deformations for these superheavy nuclei ($\beta_2 \approx 0.26$–0.31). The trends look similar for all forces. The largest deformations appear at $N = 148$ and/or $N = 150$. But there are systematic differences in detail: NL-Z2 has always larger ground-state deformations than the other forces, while PC-F1, PC-LA, and NL3 show much similar deformations. The difference is probably related to the surface energy: NL-Z2 has a lower surface energy than NL3. The symbol with error bars at $Z/N = 102/152$ in Figure 3 corresponds to the measured ground-state deformation of ^{254}No (Ref. 22, 23). This deformation is overestimated by all forces, PC-LA and NL3 stay within the error bars, though. The error ranges from 6 to 13% which is still acceptable.

The prediction of new magic shell closures in superheavy elements varies amongst the mean field models.[24] For protons one has a competition between $Z = 114$, 120, and 126. For neutrons one finds $N = 172$ and 184. The finite-range RMF models agree in predicting a doubly magic $^{292}120_{172}$. Precisely the same result emerges from PC-F1. This doubly magic nucleus is thus a common feature of relativistic models. For the density profile of $^{292}120_{172}$, we observe a central depression in accordance with other mean-field approaches.[18,25,26]

In deformed calculations done in the way as described in Reference 20, we obtain, again in agreement with other relativistic models, deformed shell closures at $Z = 104$ for the protons and $N = 162$ for the neutrons. The nuclei in that region of the nuclear chart have deformations with $\beta_2 \approx 0.2$–0.3. Thus also in the deformed case, these different types of RMF models agree well concerning their predictions of shell structure for superheavy elements.

3. Summary and Prospects

In summary one may thus conclude that the use of relativistic point-coupling models produces results of similar quality as the finite-range ones, even regarding the surface properties, with differences, of course, noticeable in the details. It should be noted that larger differences appear in quantities not discussed here, such as the density distributions. While this does not lead to new conclusions for superheavy nuclei at this moment, this model opens the way to valuable new insights for two reasons:

(1) It can be expanded to include a full treatment of exchange terms. In recent work[7] we have shown that it is possible to generalize the Fierz transformation to higher-order terms, allowing the reformulation of the exchange contributions in terms of densities and currents. Although the expressions arising in this way are quite complicated, their numerical evaluation should be straightforward.

(2) The examination of naturalness of the coupling constants may be a helpful way to make fits more unique. Following Manohar and Georgi[27] we can scale a generic Lagrangian term of the physical series as

$$\mathcal{L} \sim -c_{lmn} \left[\frac{\overline{\psi}\psi}{f_\pi^2 \Lambda}\right]^l \left[\frac{\vec{\pi}}{f_\pi}\right]^m \left[\frac{\partial^\mu, m_\pi}{\Lambda}\right]^n f_\pi^2 \Lambda^2 , \qquad (3)$$

where ψ and $\vec{\pi}$ are nucleon and pion fields, respectively, f_π and m_π are the pion decay constant, 92.5 MeV, and pion mass, 139.6 MeV, respectively, $\Lambda = 770$ MeV is the ρ meson mass, and (∂^μ, m_π) signifies either a derivative or a power of the pion mass. Dirac matrices and isospin operators (we use $\vec{t}$ here rather than $\vec{\tau}$) have been ignored. Chiral symmetry demands[28] $\Delta = l + n - 2 \geq 0$, such that the series contains only *positive* powers of $(1/\Lambda)$. If the theory is *natural*,[27,29] the Lagrangian should lead to dimensionless coefficients c_{lmn} of order unity. Thus, all information on scales ultimately resides in the c_{lmn}. If they are natural, QCD scaling works.

The nine QCD-scaled coupling constants of the parameter set used in this paper turn out to be all natural. So far as we are aware, this is the *first complete set of natural QCD-scaled coupling constants*, with order up to Λ^{-2}, that has been obtained with unconstrained least-squares parameter adjustment to measured ground-state observables.

The main problem with this type of effective field theory has been the unambiguous extraction of the coupling constants, where changing one affects the contributions from all the others, making it difficult to judge the physical appropriateness of the corresponding interaction terms of the Lagrangian. The naturalness of the coupling constants, however, appears to provide an additional physical constraint that substantially reduces these ambiguities. Furthermore, this physical constraint derives from low-momentum QCD scaling and chiral symmetry.

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