Mapping exchange in relativistic Hartree-Fock

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We show that formally for the standard ansatz relativistic point-coupling mean-field (RMF-PC) model a lagrangian density $L$ is not equivalent in Hartree and Hartree-Fock approximations. The equivalency can be achieved only if we use a “complete” ansatz at the cost of introducing new parameters in the model. An approximate treatment of the exchange terms from standard RMF-PC indicates that these effects cannot be easily, if at all, absorbed by a Dirac-Hartree approximation.

Key words: relativistic Hartree-Fock, relativistic mean-field model, finite nuclei
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1 Introduction

Relativistic mean-field models, which describe the nucleus as a system of Dirac nucleons that interact with each other by exchanging mean meson fields, have been successful in describing nuclear matter and ground state properties of finite nuclei [1–8]. Applications include the calculation of deformed nuclei [8,10–12], odd nuclei [8], nuclei at the driplines [13], the potential energy surfaces of heavy nuclei [8], and the prediction of superheavies [9,8,14]. Another variant is the point-coupling model [18,15,17]. The difference between this model and the Walecka model is the replacement of the mesonic potentials of the Walecka model by explicitly density-dependent potentials. Nikolaus, Hoch,
and Madland [17] used the Hartree form of this model to calculate some observables of finite nuclei and nuclear matter. They obtained similar predictive power as the Walecka model, but used different weights and observables from Ref. [1] to obtain their parameter set. In Ref. [18], Rusnak and Furnstahl have shown the profitability of applying the concepts of effective field theory to the point-coupling model. A more recent discussion about the point-coupling model can be found in Ref. [15, 16]. It consists of a careful way to obtain a new parameter set for the point-coupling model which is likely to correspond to the optimal minimum by combining different methods for the $\chi^2$ minimization. This parameter set was applied to a wide area in nuclear theory, from spherical finite nuclei, axially deformed nuclei, superheavy elements, potential energy surfaces, nuclear matter, neutron matter, up to exotic nuclei. It could be shown that point-coupling models can deliver a predictive power for finite nuclei comparable to models employing meson exchange. On the other hand, especially concerning isovector properties, the point-coupling model suffers from the same unresolved systematic deviations.

From the success of the RMF (Walecka and point-coupling) models, we suppose that the exchange effect is already absorbed effectively in the coupling constants of the model due to the fitting procedure, but some calculations which take into account the exchange explicitly by using the linear Walecka model have shown that this does not seem to be the case [19, 20]. Understanding this situation seems necessary and interesting. Unfortunately, due to the finite range of the mesons and the mesonic nonlinearity of the RMF model, it is difficult to expand this model in the above direction. This problem does not appear if we use the point-coupling model [17], because in this model the linear and nonlinear terms are explicitly density dependent. Therefore in this paper, we choose the point-coupling model for a first study of the role of the exchange effects.

We would like to stress that we regard this work as a model study. The aim is to check the principle effects of exchange terms as compared to an effective Hartree theory. This is done for the two-body point-coupling terms of the standard RMF model. Higher order couplings are treated without exchange and the pseudoscalar (pionic) channel is omitted for the time being.

In the following, we will use the phrase strict Hartree for an ansatz that is taken from the start in the Hartree approximation. We will use Hartree-Fock for a model in which the exchange terms are treated explicitly. If this model can be transformed into a form consisting of local currents and densities only (no matter how complicated they are), we will call the result of this rewriting an effective Hartree theory. Mapping formally this general form onto a Dirac-like structure leads to the Dirac-Hartree theory.
2 The formulation of Hartree-Fock Point-Coupling Model

2.1 Basic one-particle operators and densities

We begin by defining the basic Dirac & isovector matrices $\Gamma_j$. There are two sets

$$
\Gamma_j \in \begin{cases} 
H = \{1, \gamma_\mu, \gamma_\mu \vec{\tau}\} \\
HF = H \cup \{\vec{\tau}, \sigma_{\mu\nu}, \sigma_{\mu\nu} \vec{\tau}, \gamma_5, \gamma_5 \vec{\tau}, \gamma_5 \gamma_\mu, \gamma_5 \gamma_\mu \vec{\tau}\}
\end{cases}
$$

The “Hartree” set $H$ covers the currents initially given in the RMF-PC Lagrangian. The “Hartree-Fock” set $HF$ covers all conceivable Dirac matrices as they are produced by the Fierz transformation [28]. The currents are defined as:

$$
\hat{J}_j = \hat{\bar{\psi}} \Gamma_j \hat{\psi}, \quad \hat{A}_{j\mu} = \partial_\mu \hat{J}_j, \quad \hat{B}_{j\mu} = \hat{\bar{\psi}} \frac{\partial_\mu}{2i} \Gamma_j \hat{\psi}, \quad \hat{C}_j = \partial_\mu \hat{\bar{\psi}} \Gamma_j \partial^\mu \hat{\psi},
$$

where $\partial_\mu = \overleftarrow{\partial}_\mu - \overrightarrow{\partial}_\mu$. These are the current operators from which actually only $\hat{J}_j$ is used at operator level. The associated currents are the expectation values

$$
J_j = \sum_\alpha \bar{\Psi}_\alpha \Gamma_j \Psi_\alpha, \quad A_{j\mu} = \partial_\mu J_j,
$$

$$
B_{j\mu} = \sum_\alpha \bar{\Psi}_\alpha \frac{\partial_\mu}{2i} \Gamma_j \Psi_\alpha, \quad C_j = \sum_\alpha \partial_\mu \bar{\Psi}_\alpha \Gamma_j \partial^\mu \Psi_\alpha,
$$

(1)

where the sum is running over occupied particle states only (anti-particles are neglected = no-sea approximation).

2.2 The Lagrangian

Starting point is the Lagrangian

$$
\hat{\mathcal{L}} = \hat{\mathcal{L}}_{\text{free}} + \hat{\mathcal{L}}_{\text{PC}} + \hat{\mathcal{L}}_{\text{NL}} + \hat{\mathcal{L}}_{\text{coul}}; \quad \hat{\mathcal{L}}_{\text{PC}} = \frac{1}{2} \sum_{j \in H} \left[ \alpha_j \hat{J}_j^2 + \delta_j \hat{A}_j^2 \right]; \quad \hat{\mathcal{L}}_{\text{NL}} = \frac{1}{3} \beta_3 \hat{\mathcal{J}}_3 \hat{\mathcal{J}}_3 + \frac{1}{4} \gamma_5 \hat{\mathcal{J}}_5^4.
$$

(2a)

(2b)

(2c)

At this point, replacing the current operators by their expectation values leads to a strict Hartree theory, as is mostly applied to nuclear structure problems.
But we are going here for a Hartree-Fock treatment. To this end we chose a Slater determinant $|0\rangle$ as the ground state with $A$ occupied single-nucleon levels (in the positive energy sector). It is defined by

$$b_i^\dagger |0\rangle = 0 \quad \forall \quad i \leq F,$$

($F$ indicates the fermi surface). We compute the expectation value of the Lagrangian (2) in standard manner and employ Fierz transformations to express exchange terms through simple currents. This yields

$$\langle 0 | \mathcal{L}^{PC}_L \mathcal{L}^{PC}_L | 0 \rangle = \mathcal{L}^{PC}_L - \mathcal{L}^{PC}_{Lx},$$

$$\mathcal{L}^{PC}_L = \sum_{i \in H} \left[ \frac{1}{2} \alpha_i J_i^2 + \frac{1}{2} \delta_i A_i^2 \right],$$

$$\mathcal{L}^{PC}_{Lx} = \sum_{i \in H} \sum_{j \in HF} \left[ C_{ji} \left( \frac{1}{2} \alpha_i J_j^2 + \delta_i \left( \frac{1}{4} A_j^2 - B_j^2 + J_j C_j \right) \right) \right].$$

The constants $C_{ji}$ stem from the Fierz transformation, their explicit form can be found in table 1.

Thus we have performed - by virtue of the Fierz transformation - a mapping from a Hartree Fock model to an effective Hartree model for all linear terms. The expectation value of non-linear term $\mathcal{L}_{NL}^{PC}$ has been calculated in Refs. [27,15]. The results are quite lengthy, therefore it is not useful to consider them explicitly here. The exchange terms emerging from the nonlinear part of the Lagrangian form a large variety of density-mixing terms, involving also products of isoscalar and isovector densities. This leads to modifications in both the isoscalar and the isovector channel of the effective interaction without introducing new parameters. Another feature of this result is that the contributions from the nonlinear exchange terms cannot be absorbed fully by a redefinition of the coupling constants into terms of $\mathcal{L}_{NL}^{PC}$ and they also cannot be considered as small corrections.

### 2.3 The Hartree-Fock equations

Variation of the effective Lagrangian density (4) with respect to the single-nucleon wavefunctions yields the effective mean-field equations
\[
C_{ji} \quad \Gamma_i=1 \quad \Gamma_i=\gamma_\mu \quad \Gamma_i=\gamma_\mu \tilde{\gamma}
\]

<table>
<thead>
<tr>
<th>(C_{ji})</th>
<th>(\Gamma_i=1)</th>
<th>(\Gamma_i=\gamma_\mu)</th>
<th>(\Gamma_i=\gamma_\mu \tilde{\gamma})</th>
</tr>
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<tr>
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<td>(\Gamma_j=\gamma_\mu \tilde{\gamma})</td>
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<tr>
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<tr>
<td>(\Gamma_j=\sigma_{\mu\nu} \tilde{\gamma})</td>
<td>(\frac{1}{16})</td>
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<tr>
<td>(\Gamma_j=\gamma_5)</td>
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<td>(-\frac{4}{8})</td>
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<td>(\Gamma_j=\gamma_5 \gamma_\mu \tilde{\gamma})</td>
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Table 1
The \(C_{ji}\) constants of equation (4).

\[
0 = \left[ -i \gamma_\mu \partial^\mu + m_B + V^j \Gamma_j + U^{j\mu} \Gamma_j \partial_\mu + W^j \Gamma_j \partial^\mu \partial_\mu \right] \Psi_\alpha \tag{5a}
\]

\[
V^j \Gamma_j = \tilde{S} + \gamma_\alpha \tilde{V}^\alpha \tag{5b}
\]

\[
U^{j\mu} \Gamma_j = U_\mu + \gamma_\alpha U_\alpha_\mu \tag{5c}
\]

\[
W^j \Gamma_j = W^1 + \gamma_\alpha W^{2\alpha} \tag{5d}
\]

\[
\tilde{S} = \alpha_a J_a - (\delta_a + \tilde{\delta}_a) \partial_\mu A_\mu a + \frac{2}{3} \tilde{\delta}_a (i \partial^\mu B_{\mu a} + C_a) \tag{5e}
\]

\[
\tilde{V}^\alpha = \alpha_b J_b^\alpha - (\delta_b + \tilde{\delta}_b) \partial_\mu A_\mu b + \frac{2}{3} \tilde{\delta}_b (i \partial^\mu B_{\mu b} + C_b^\alpha), \tag{5f}
\]

\[
U_\mu = \frac{4}{3} i \tilde{\delta}_a B_{\mu a}, \quad U_{\mu \alpha} = \frac{4}{3} i \tilde{\delta}_b B_{\mu b}, \tag{5g}
\]

\[
W_1 = -\frac{2}{3} \tilde{\delta}_a J_a, \quad W_{1\alpha} = -\frac{2}{3} \tilde{\delta}_b J_{ba}. \tag{5h}
\]

A double index \(a/b\) implies summations over S,D/V,R. The constants in front of the densities in Eq. (5h) \((\alpha_a/b, \delta_a/b, \tilde{\delta}_a/b)\) are functions of the meson coupling constants and masses. The \(\delta_a/b, \tilde{\delta}_a/b\) constants reflect the combinations of Fierz constants \(C_{ij}\), the meson coupling constants and masses of the mesons from the derivative exchange terms of Eq. (4) in the equation of motion. Because the formulas for the constants are lengthy and do not give particular insight, we do not show them. \(\tilde{S}, \tilde{V}^\alpha, W^1, W^{2\alpha}\) are of order \(< 1\) and \(U_\mu, U_{\alpha \mu}\) are of order \(v\). We can see here that the \(C_i\) densities give rise to the term with prefactor \(W^j\) and the \(B_{ij}\) term with prefactor \(U^{j\mu}\) in the equation of motion.

Equation (5a) starts out like a Dirac equation and continues with very unconventional terms \(\propto \Gamma_j \partial_\mu\) and \(\propto \Gamma_j \partial^\mu \partial_\mu\). The latter are generated from the Fierz transformed exchange terms \(\propto B\) and \(C\) in Eq. (4). These terms are awkward
to handle. We would like to transform Eq. (5a) into a more standard form. This will be done in section 4 by means of a Gordon decomposition. Before that we first check the importance of the new terms. This will be done in the following section.

From the discussion above it is clear that, in contrast to the claim of Ref. [17], qualitatively, if a standard ansatz is used, a Lagrangian density $\mathcal{L}_{HF}$ can be determined in a relativistic Hartree-Fock sense that is not equivalent to that determined in a relativistic Hartree sense, $\mathcal{L}_H$. Of course, the Hartree or Hartree-Fock calculations belong to effective theories, where many details or ignored corrections can be hidden in the form of the effective interaction and in its fitted parameters. In this sense, the models can only be compared after refitting the parameters. Therefore, only quantitative calculations can actually distinguish the predictive capabilities of the models. Before embarking into the actual calculation, though, we present a rough approximation that gives physical insight into the exchange contributions.

3 Estimating the Densities $B_{j\mu}$ and $C_j$

For a first overview, we compare the order of magnitude of the energy density contributions of each term in Eq. (4) in the plane wave (nuclear matter) limit. The dominant contributions in the energy density come from the terms with $\Gamma_j = 1, \gamma_0$. The terms with $\Gamma_j = \gamma_0$ show a clear order counting and are easy to calculate. It is illustrative to examine their order of magnitude. They will be represented by:

$$
\epsilon_1 = -\frac{1}{2} \alpha_V J_V^2
$$
$$
\epsilon_2 = \frac{1}{2} \delta_V A_V^2
$$
$$
\epsilon_{ex1} = -\frac{c_v}{2} \alpha_V J_V^2
$$
$$
\epsilon_{ex2} = c_v \delta_V B_V^2
$$

$$
\approx -\frac{c_v}{4} \delta_V \sum_{\alpha\beta} [\bar{\Psi}_{\alpha} \gamma_0 (\vec{\nabla} \Psi_{\alpha}) - (\vec{\nabla} \bar{\Psi}_{\alpha}) \gamma_0 \Psi_{\alpha}] [\bar{\Psi}_{\beta} \gamma_0 (\vec{\nabla} \Psi_{\beta}) - (\vec{\nabla} \bar{\Psi}_{\beta}) \gamma_0 \Psi_{\beta}]
$$
$$
\epsilon_{ex2} = c_v \delta_V \mathcal{C}_V \approx c_v \delta_V \sum_{\alpha\beta} (\bar{\Psi}_{\alpha} \gamma_0 \Psi_{\alpha}) (\vec{\nabla} \bar{\Psi}_{\beta}) \gamma_0 (\vec{\nabla} \Psi_{\beta})
$$

$c_v$ is a constant due to the Fierz transformation. It is a function of the coupling constants and fulfills $c_v \leq 1$. Because the formula for $c_v$ is lengthy and does not give particular insight, we do not show it here. In the last two equations ($\epsilon_{ex2}$ and $\epsilon_{ex2}^2$), we neglect the energy dependent parts (retardation parts) by assuming that this contribution is small. Then in the plane-wave approximation
The order counting which is shown in Table 2 is obtained. We use

$$\bar{\rho}_0 \equiv \frac{(2S + 1)(2I + 1)}{(2\pi)^3} \int d^3k \bar{\Psi}_k \gamma_0 \Psi_k$$

where $S$ and $I$ denotes spin and isospin, respectively, and $p_F$ is the fermi momentum. If we define $p_F/m_v = v$, every exchange term in the derivative part gives a contribution of order $v^2$, where $v < 1$. Then in the nuclear matter limit, $\bar{\rho}_i \neq 0, \nabla \bar{\rho}_i = 0$, $|\vec{B}_i|/(m_B \bar{\rho}_i)$ is of order $v$ and $|\vec{C}_i|/(m_B^2 \bar{\rho}_i)$ is of order $v^2$, while in finite nuclei, we know that $\rho_i \neq 0$ and $\nabla \rho_i \neq 0$, where $|\vec{\nabla} \rho_i|/(m_i \rho_i)$ can be estimated to be of order $v$ or maybe even smaller [17] by comparing the direct and derivative terms in the Hartree level of the point-coupling model. Here the index $i$ denote V or S. If we consider the densities in finite nuclei as consisting of the nuclear matter value plus fluctuation corrections due to quantum effects, it seems reasonable to assume in finite nuclei that on the average $|\vec{B}_i|/(m_B \rho_i)$ is also of order $v$ and $|C_i|/(m_B^2 \rho_i)$ of order $v^2$.

In conclusion, it is reasonable to assume that the contribution from the derivative exchange terms could be similar or even a bit larger than the direct derivative terms, so that they cannot be neglected if the direct derivative terms, which are necessary for a reasonable description of the nuclear surface, are kept.

It should be noted that even the nonderivative exchange terms are larger than the derivative terms in order of magnitude, but their largest contributions (scalar-isoscalar, vector-isoscalar and vector-isovector) can be absorbed into the nonderivative terms through a redefinition of the coupling constants and refitting of the experimental data. The crucial difference between Hartree and Hartree-Fock calculations of the nonderivative terms is represented by the scalar-isovector term, which is usually omitted in most Hartree models. In the Hartree-Fock approach presented here, it emerges naturally without introducing an additional parameter.

As a further check of our procedure, we show a transformed form of the $B^\sigma$ terms through the Gordon decomposition [29] by using the exact equation
of motion in Eq. (5). Here we only calculate the scalar case; the vector case is similar but not as simple. In the limit of small \(v^2\) (for more details see Appendix (2)), we have

\[
B^\sigma \approx \sum_\alpha \left[ -\frac{1}{2} \partial_\mu (\bar{\Psi}_\alpha \sigma^{\mu \sigma} \Psi_\alpha) - \bar{m} \bar{\Psi}_\alpha \gamma^\sigma \Psi_\alpha - \bar{V}^\sigma \bar{\Psi}_\alpha \Psi_\alpha \right].
\]

(6)

The same result as above is obtained by using the equation of motion in the form of a Dirac equation with scalar potential \((\bar{m} - m)\) and vector potential \(\bar{V}^\sigma\). It means that in the limit of small \(v\) the \(B^\sigma\) can be determined from the Dirac equation (second-order differential equation).

A similar situation holds for all \(C_i\) and \(B_{i\mu}\), so that we can say that the transformed form of the exact \(C_i\) and \(B_{i\mu}\) consist of parts responsible for generating effects beyond the Dirac equation. The order of magnitude analysis above shows that these parts are small. Neglecting them everywhere (via projecting onto a Dirac-Hartree structure) will lead to the Dirac equation but neglecting these small parts means also neglecting the retardation and nonlocal effects. This is what we will do in the next section, where we map the exact Lagrangian including exchange onto a Dirac-Hartree structure.

4 The Approximate Lagrange Density

The aim of this chapter is to derive an effective Lagrangian which leads to a Dirac equation without extra derivative terms, i.e., we will formulate, by employing some approximations, a Dirac-Hartree model.

The approximate forms of the densities \(C_i\) and \(B_{i\mu}\) are not yet known. We expect to obtain from them an approximate Lagrangian density (with the approximate forms of the densities \(C_i\) and \(B_{i\mu}\)), which should lead to a Dirac equation of the form

\[
[\gamma_\mu \partial^\mu + i (m^* + \gamma_\alpha V^\alpha + \sigma_{\alpha \beta} T^{\alpha \beta})] \Psi_\alpha = 0,
\]

(7)

where \(m^*, V^\alpha\) and \(T^{\alpha \beta}\) are real functions. It implies a connection between the two types of functions: \(m^*, V^\alpha, T^{\alpha \beta}\) and \(J_i, A_{i\mu}, C_j, B_{j\mu}\). Therefore we will try to obtain the \(C^j\) and \(B_{j\mu}\) as functions of the \(m^*, V^\alpha, T^{\alpha \beta}\). This will be done in an iterative procedure starting from \(m^* - m, V, T = 0\) and generating successively terms with increasing orders. Finally, we use the approximate form of \(m^*, V^\alpha, T^{\alpha \beta}\) to calculate \(C^j\) and \(B_{j\mu}\) and from these approximate densities \(C^j\) and \(B_{j\mu}\) we obtain the approximate Lagrange density. These steps will now be done explicitly for the scalar case (\(\Gamma = 1\)).
Starting point is the Gordon decomposition [29] of Eq. (7) which leads to

\[ \Psi_\alpha [\gamma_\mu \not{\partial}^\mu - i (m^* + \gamma_\alpha V^\alpha + \sigma_{\alpha\beta} T^{\alpha\beta})] \Psi_\alpha \\
- \Psi_\alpha \mu [\gamma_\mu \not{\partial}^\mu + i (m^* + \gamma_\alpha V^\alpha + \sigma_{\alpha\beta} T^{\alpha\beta})] \Psi_\alpha = 0, \quad (8) \]

\[ \mu = a^\mu \gamma_\mu \text{ and } a^\mu \text{ is an arbitrary vector. Choosing } \mu = \gamma_\mu \text{ yields} \]

\[ B_S = \frac{-i}{2} \left( \not{\partial}_\mu \Psi_\alpha (\not{\partial}^\mu \Psi_\alpha) - (\not{\partial}^\mu \not{\partial}_\mu) \Psi_\alpha \right) \]

\[ = -i [\partial_\mu (\Psi_\alpha \sigma^{\mu\nu} \Psi_\alpha) + 2m^* \Psi_\alpha \gamma^\nu \Psi_\alpha + 2V^\nu \Psi_\alpha \Psi_\alpha + 2\epsilon^{\alpha\beta\mu\nu} T_{\alpha\beta} \Psi_\alpha \gamma^\mu \gamma^\nu \Psi_\alpha], \quad (10) \]

From Eq. (7) we deduce directly

\[ C_S = (\partial_\mu \Psi_\alpha) (\not{\partial}^\mu \Psi_\alpha) \]

\[ = [m^2 \Psi_\alpha \Psi_\alpha + 2m^* V^\mu \Psi_\alpha \gamma^\nu \Psi_\alpha + 1/2 \partial^\mu \partial_\mu (\Psi_\alpha \Psi_\alpha) \]

\[ + V^\nu V_\mu \Psi_\alpha \Psi_\alpha - \partial_\nu (V_\mu \Psi_\alpha \sigma^{\mu\nu} \Psi_\alpha) + \bar{\Psi}_\alpha f(T_{\alpha\beta}) \Psi_\alpha]. \quad (10) \]

Here \( f(T_{\alpha\beta}) \) denotes a complicated function of \( T_{\alpha\beta} \) which is zero for \( T_{\alpha\beta}=0 \) and the order of magnitude of this functions can be estimated as small therefore it is not necessary to show this function explicitly. These are the desired expressions for \( B_S \) and \( C_S \) in terms of \( m^* \), \( V \), and \( T \). We would like to express them in terms of standard currents. The construction for that proceeds as follows:

The iteration procedure leads to \( m^* = m_B + \tilde{\alpha}_S \rho_S(x) + \ldots, \)

\( V^\nu = \tilde{\alpha}_V J^\nu_V(x) \) + \ldots, and \( T^{\alpha\beta} = \ldots, \) where \( \tilde{\alpha}_S \) and \( \tilde{\alpha}_V \) are effective coupling constants. They are functions of \( \alpha_S, \alpha_V, \delta_S \) and \( \delta_V \), which come from the contribution of the direct and the exchange part in front of the nonderivative and the derivative of the scalar and vector densities, respectively. In the above equations, \( \ldots \) denotes contributions from the derivative, isovector, nonlinear and tensor correction parts. They will generate nonlinear terms in the Lagrangian density that consist of all possible combinations of the above mentioned densities and of all possible order. Now we obtain the approximate forms by neglecting \( \ldots \) (neglecting higher order terms) yielding

\[ B_S = -i [\partial_\mu (\bar{\Psi}_\alpha \sigma^{\mu\nu} \Psi_\alpha) + 2(m_B + \tilde{\alpha}_S \rho_S) \bar{\Psi}_\alpha \gamma^\nu \Psi_\alpha + 2\tilde{\alpha}_V J^\nu_V \bar{\Psi}_\alpha \Psi_\alpha], \quad (11a) \]

\[ C_S = [(m_B + \tilde{\alpha}_S \rho_S)^2 \bar{\Psi}_\alpha \Psi_\alpha + 2(m_B + \tilde{\alpha}_S \rho_S) \tilde{\alpha}_V J^\nu_V \bar{\Psi}_\alpha \gamma^\nu \Psi_\alpha + 1/2 \partial^\mu \partial_\mu (\bar{\Psi}_\alpha \Psi_\alpha) \]

\[ + (\tilde{\alpha}_V J^\nu_V)^2 \bar{\Psi}_\alpha \Psi_\alpha - \partial_\nu (\tilde{\alpha}_V J^\nu_V \bar{\Psi}_\alpha \sigma^{\mu\nu} \Psi_\alpha)]. \quad (11b) \]

Putting the pieces together yields
\[ \tilde{\mathcal{L}}_{S,Lx}^{PC(0)} = -\frac{1}{2} \partial_\mu \rho_S \partial^\mu \rho_S + 2m_B^2 \rho_S^2 - 2m_B^2 J_V^\mu J_V^\mu - 2m_B J_V^\mu \partial^\nu (J_{T \nu \mu}) - \frac{1}{2} \partial^\nu (J_{T \nu \mu}) \partial_\sigma (J_{T}^{\sigma \mu}), \]

\[ \tilde{\mathcal{L}}_{S,Lx}^{PC(1)} = 4m_B \tilde{\alpha}_S \rho_S^2 + 2\tilde{\alpha}_S^2 \rho_S^2 - 4m_B \tilde{\alpha}_S \rho_S J_V^2 + 2\tilde{\alpha}_V \rho_S J_{T \nu \mu} \partial^\nu (J_{T}^\mu) - 2\tilde{\alpha}_S \rho_S J_V^\mu \partial^\nu (J_{T \nu \mu}) - 2\tilde{\alpha}_S^2 \rho_S^2 J_V^2. \] (12)

The densities and currents appearing in these formulas are special cases of the displayed in Table 3. Inserting these results into Eq. (12) define the scalar case of the approximation for the derivative exchange yields:

\[ \rho_S(x) = \sum_\alpha \bar{\Psi}_\alpha \Psi_\alpha, \quad J_V^\mu(x) = \sum_\alpha \bar{\Psi}_\alpha \gamma^\mu \Psi_\alpha, \]

\[ \rho_tS(x) = \sum_\alpha \bar{\Psi}_\alpha \tau \Psi_\alpha, \quad \bar{J}_V^\mu(x) = \sum_\alpha \bar{\Psi}_\alpha \gamma^\mu \tau \Psi_\alpha, \]

\[ J_T^{\mu \nu}(x) = \sum_\alpha \bar{\Psi}_\alpha \sigma^{\nu \mu} \Psi_\alpha, \quad \bar{J}_{TT}^{\mu}(x) = \sum_\alpha \bar{\Psi}_\alpha \sigma^{\mu \nu} \tau \Psi_\alpha. \] (13)

We see that the approximate form of the interaction effects in \( \mathcal{C} \) and \( B_\mu \) corresponds to having all possible terms made up of products of different densities.

Eq. (12) define the scalar case of the approximation for the derivative exchange terms in Eq. (4). The other cases can be derived similarly. The results are displayed in Table 3. Inserting these results into \( \mathcal{L}_{L \text{ eff}}^{PC} = \langle \phi_0 | : \tilde{\mathcal{L}}_{L}^{PC} : | \phi_0 \rangle \) yields:

\[ \mathcal{L}_{L \text{ eff}}^{PC} = \sum_{\alpha = A} \bar{\Psi}_\alpha (i \gamma_\mu \partial^\mu - m_B) \Psi_\alpha \]

\[ \frac{1}{2} \tilde{\alpha}_S \rho_S^2 - \frac{1}{2} \tilde{\alpha}_tS \rho_tS^2 - \frac{1}{2} \tilde{\alpha}_V J_V^2 - \frac{1}{2} \tilde{\alpha}_{tv} \bar{J}_{IV}^2 \]

\[ \frac{1}{2} \tilde{\alpha}_t \rho_tS \partial^\mu \rho_S \rho_tS - \frac{1}{2} \tilde{\alpha}_t \rho_tS \partial^\mu \rho_tS \rho_tS - \frac{1}{2} \tilde{\alpha}_v \partial_\mu J_V^\mu \partial^\nu J_{T \nu \mu} \]

\[ -\tilde{\alpha}_{tv} \partial_\nu \bar{J}_{IV}^\mu \partial^\nu \bar{J}_{IV}^\mu - \frac{1}{2} \tilde{\alpha}_{tT} \bar{J}_{IV}^\mu \partial^\nu (J_{T \nu \mu}) - \frac{1}{2} \tilde{\alpha}_{tT} \bar{J}_{IV}^\mu \partial^\nu (J_{T \nu \mu}) \]

\[ + \mathcal{L}_{Lx}^{PC(1)} + \mathcal{L}_{T \text{ corr}} + \mathcal{L}_A, \]

\[ \mathcal{L}_{Lx}^{PC(1)} = c_S \tilde{\mathcal{L}}_{S,Lx}^{PC(1)} + c_V \tilde{\mathcal{L}}_{V,Lx}^{PC(1)} + c_tS \tilde{\mathcal{L}}_{tS,Lx}^{PC(1)} + c_{tv} \tilde{\mathcal{L}}_{tV,Lx}^{PC(1)} \]

\[ \mathcal{L}_{T \text{ corr}} = \frac{1}{16} \tilde{\alpha}_S (\frac{1}{2} \partial_\mu (J_{T \alpha \beta}) \partial^\mu (J_{T \alpha \beta}) + \frac{1}{2} \partial_\mu (J_{T \alpha \beta}) \partial^\mu (J_{T \alpha \beta})) \]

\[ + \frac{1}{16} \tilde{\alpha}_S (J_{T \nu \mu} J_{T}^{\nu \mu} + J_{T \nu \mu} J_{T}^{\nu \mu}) \]

\[ + \frac{1}{2} \tilde{c}_S \partial^\nu (J_{T \nu \mu}) \partial_\sigma (J_{T}^{\nu \mu}) + c_tS \partial^\nu (J_{T \nu \mu}) \partial_\sigma (J_{T}^{\nu \mu}), \] (14)
The different terms (except the scalar term) of the approximate Lagrange density.

with primed coupling constants \( \tilde{\alpha}_i, \tilde{\delta}_i, \tilde{\theta}_i \). These are not new parameters but can be related uniquely by a linear transformation to the given original coupling parameters of the model

\[
(\tilde{\alpha}_S, \tilde{\alpha}_{tS}, \tilde{\alpha}_V, \tilde{\alpha}_{tV}, \tilde{\delta}_S, \tilde{\delta}_{tS}, \tilde{\delta}_V, \tilde{\delta}_{tV}, \tilde{\theta}_T, \tilde{\theta}_{tV}) \quad \Leftarrow \quad (\alpha_S, \alpha_V, \alpha_{tV}, \delta_S, \delta_V, \delta_{tV})
\]

The actual transformation is a bit lengthy. It is given explicitly in appendix A.3.

Finally, \( \mathcal{L}_A \) is an electromagnetic Lagrangian density with an exchange correction, it just remains to approximate the exchange part by the local density (Slater) approximation [30]. We have seen that in the Gordon decomposition representation, the dominant part of the \( \mathcal{B}_{j\mu} \) and \( \mathcal{C}_j \) densities can be replaced effectively by tensor terms and all possible mixings or combinations of nonlinear terms in all orders. It means that if we perform Hartree calculations by taking into account tensor terms and all possible mixings or combinations of nonlinear terms of all orders, the effect of the dominant part of \( \mathcal{B}_{j\mu} \) and \( \mathcal{C}_j \) is already represented effectively, but still a part which manifests itself as an effect beyond the Dirac equation and retardation effects are not yet represented. A strict Hartree theory including these additional effects can be constructed by starting off with the appropriate terms, but at the cost of introducing new parameters (the details about the mapping from Hartree-Fock to Hartree can

<table>
<thead>
<tr>
<th>Term</th>
<th>Expression</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \mathcal{L}_{V,Lx}^{PC(0)} )</td>
<td>(-\frac{1}{2}\partial_\mu J_\nu^V \partial^\mu J_{\nu V} + 2m_B^2 J_\nu^V J_{\nu V} )</td>
</tr>
<tr>
<td>( \mathcal{L}_{V,Lx}^{PC(1)} )</td>
<td>(-2\tilde{\alpha}<em>V^2 J</em>\nu^V + 4m_B \tilde{\alpha}<em>S \rho S J</em>\nu^2 + 2\tilde{\alpha}<em>S^2 \rho S^2 J</em>\nu^2 )</td>
</tr>
<tr>
<td>( \mathcal{L}_{T,Lx}^{PC(0)} )</td>
<td>(\frac{1}{2} \partial_\mu (J_{\alpha \beta}^\alpha \delta) \partial^\mu (J_{\alpha \beta}^\delta) )</td>
</tr>
<tr>
<td>( \mathcal{L}_{T,Lx}^{PC(1)} )</td>
<td>0</td>
</tr>
<tr>
<td>( \mathcal{L}_{tS,Lx}^{PC(0)} )</td>
<td>(-\frac{1}{2} \partial_\mu \tilde{\rho}_S \partial^\mu \tilde{\rho}_S + 2m_B^2 \tilde{\rho}<em>S^2 - 2m_B^2 j</em>{1V}^2 )</td>
</tr>
<tr>
<td>( \mathcal{L}_{tS,Lx}^{PC(1)} )</td>
<td>(-2m_B j_{1V}^2 \partial^\mu (\tilde{J}<em>{IT\nu \mu}) - \frac{1}{2} \partial^\mu (\tilde{J}</em>{IT\nu \mu}) \partial_{\sigma} (\tilde{J}_{IT\nu}^{\mu}) )</td>
</tr>
<tr>
<td>( \mathcal{L}_{tV,Lx}^{PC(0)} )</td>
<td>(-4\tilde{\alpha}<em>S m_B \rho S (\tilde{J}</em>{1V}^2 - \tilde{\rho}_S^2) - 2\tilde{\alpha}<em>S^2 \rho S^2 (\tilde{J}</em>{1V}^2 - \tilde{\rho}_S^2) )</td>
</tr>
<tr>
<td>( \mathcal{L}_{tV,Lx}^{PC(1)} )</td>
<td>(-2\tilde{\alpha}<em>S \partial</em>{\sigma} (\tilde{J}<em>{IT\sigma \mu}) \rho S \tilde{J}</em>{1V}^\mu + \tilde{\alpha}<em>V \tilde{\rho}<em>S \tilde{J}</em>{IT\sigma \mu} \partial</em>{\sigma} (\tilde{J}_{1V}^\mu) )</td>
</tr>
<tr>
<td>( \mathcal{L}_{tV,Lx}^{PC(0)} )</td>
<td>(-\frac{1}{2} \partial_\mu \tilde{J}<em>{1V}^\nu \partial^\mu \tilde{J}</em>{1V}^\nu + 2m_B^2 j_{1V}^2 )</td>
</tr>
<tr>
<td>( \mathcal{L}_{tV,Lx}^{PC(1)} )</td>
<td>(4\tilde{\alpha}<em>S m_B j</em>{1V}^2 \rho S + 2\tilde{\alpha}<em>S^2 \rho S^2 j</em>{1V}^2 )</td>
</tr>
<tr>
<td>( \mathcal{L}_{tT,Lx}^{PC(0)} )</td>
<td>(-2\tilde{\alpha}<em>V (\tilde{J}</em>{1V}^\nu J_{\nu V})^2 - 2\tilde{\alpha}<em>S \rho S \partial^\nu (\tilde{J}</em>{IT\nu \mu} \tilde{J}_{1V}^\mu) )</td>
</tr>
<tr>
<td>( \mathcal{L}_{tT,Lx}^{PC(1)} )</td>
<td>(\frac{1}{2} \partial_\mu (\tilde{J}<em>{1T}^\nu \partial^\nu (\tilde{J}</em>{1T}\alpha \beta)) )</td>
</tr>
<tr>
<td>( \mathcal{L}_{tT,Lx}^{PC(1)} )</td>
<td>0</td>
</tr>
</tbody>
</table>
be seen in Appendix (3)).

The new terms that emerge in our investigation lead to modifications of a) the spin-orbit force due to tensor terms, b) the isovector channel due to products of isoscalar and isovector terms and the inclusion of isovector-scalar terms and c) the density dependence of the model. They in turn lead to a different density dependence of the effective mass. A similar change of the spin-orbit force and the effective mass might allow a larger effective mass closer to the values predicted by Skyrme forces. It is interesting to discover the effect of the modified density dependence in both the isoscalar and the isovector channel. All these contributions arise without introducing new parameters.

This unavoidably complicated mapping of the original exchange terms into a manageable Lagrangian in this rough approximation will now be applied to typical nuclear systems.

5 Finite Nuclei

Since the model discussed in this paper is meant to be applied to finite nuclei, observables connected with them should be considered when evaluating the consequences of our approximate treatment of exchange terms. We will take a look at a variety of different observables. The calculations are performed in spherical symmetry.

As a preliminary step, we will apply further approximations. Let us take the following Lagrange density:

\[ \mathcal{L}_{\text{NL eff}}^{\text{PC}} = \mathcal{L}_{\text{free}} + \tilde{\mathcal{L}}_{L}^{\text{PC}} + \mathcal{L}_{\text{Lx eff}}^{\text{PC}(0)} + \mathcal{L}_{\text{NL}}^{\text{PC}} + \mathcal{L}_{A} + \mathcal{L}_{Ax}, \]  

with

\[ \mathcal{L}_{\text{free}} = \sum_{\alpha = A} \bar{\Psi}_{\alpha} (i \gamma_{\mu} \partial^{\mu} - m_{B}) \Psi_{\alpha}, \]

\[ \tilde{\mathcal{L}}_{L}^{\text{PC}} = -\frac{1}{2} \tilde{\alpha}_{S} \rho_{S}^{2} - \frac{1}{2} \tilde{\alpha}_{V} J_{V}^{2} - \frac{1}{2} \tilde{\alpha}_{tV} \tilde{J}_{tV}^{2} - \frac{1}{2} \delta_{S} \partial_{\mu} \rho_{S} \partial^{\mu} \rho_{S} \]

\[ -\frac{1}{2} \delta_{V} \partial_{\mu} J_{V}^{\mu} J_{V}^{\nu} \partial^{\nu}, \]

\[ \mathcal{L}_{\text{Lx eff}}^{\text{PC}(0)} = -\frac{1}{2} \alpha_{tS} \rho_{tS}^{2} - \frac{1}{2} \delta_{S} \partial_{\mu} \rho_{tS} \partial^{\mu} \rho_{tS} - \frac{1}{2} \delta_{T} J_{T}^{\mu} \partial^{\mu} \rho_{T} \partial^{\nu} \tilde{J}_{tV}^{\nu} - \frac{1}{2} \delta_{tT} \tilde{J}_{tV}^{\mu} \partial^{\mu} \rho_{tT} \partial^{\nu} \tilde{J}_{tW}^{\nu}, \]

\[ \mathcal{L}_{A} = \frac{1}{2} \partial_{\mu} A^{\mu} \partial^{\nu} A_{\nu} + e \sum_{\alpha} \bar{\Psi}_{\alpha} \gamma^{\mu} A_{\mu} \frac{1}{2} (1 + \tau_{3}) \Psi_{\alpha}, \]

and

\[ \mathcal{L}_{\text{Ax}} = \frac{1}{2} \partial_{\mu} A^{\mu} \partial^{\nu} A_{\nu} + \sum_{\alpha} \bar{\Psi}_{\alpha} \gamma^{\mu} A_{\mu} \frac{1}{2} (1 + \tau_{3}) \Psi_{\alpha}, \]
\[ \mathcal{L}_{\text{NL}}^{PC} = -\frac{1}{3} \beta_S \rho_S^3 - \frac{1}{4} \gamma_S \rho_S^4. \]

Thus now \( \mathcal{L}_{Lx}^{PC(1)} \), \( \mathcal{L}_T^{corr} \), and \( \mathcal{L}_{NLx}^{PC} \) in Eq. (17) are neglected. \( \mathcal{L}_T^{corr} \) can be considered to give a small contribution, and it is assumed that parts of \( \mathcal{L}_{Lx}^{PC(1)} \) and \( \mathcal{L}_{NLx}^{PC} \) are already absorbed effectively in \( \mathcal{L}_{NL}^{PC} \), of course, this assumption is not really true in the strict sense. We will study the following Lagrange densities for which we will determine parameter sets as described in the next section:

(i) LH: Point-coupling model, no nonlinear terms, exchange omitted

\[ \mathcal{L}_{\text{LH}} = \mathcal{L}_{\text{free}} + \tilde{\mathcal{L}}_L^{PC} + \mathcal{L}_A. \]  

(18)

(ii) LHx : Point-coupling model, no nonlinear terms, approximate exchange included

\[ \mathcal{L}_{\text{LHx}} = \mathcal{L}_{\text{LH}} + \mathcal{L}_{Lx}^{PC(0)} + \mathcal{L}_{Ax}. \]  

(19)

(iii) NLH : Point-coupling model, nonlinear terms, exchange omitted

\[ \mathcal{L}_{\text{NLH}} = \mathcal{L}_{\text{LH}} + \mathcal{L}_{NL}^{PC}. \]  

(20)

(iv) NLHx : Point-coupling model, nonlinear terms, nonlinear exchange omitted but linear exchange terms included

\[ \mathcal{L}_{\text{NLHx}} = \mathcal{L}_{\text{LHx}} + \mathcal{L}_{NL}^{PC}. \]  

(21)

Comparing these four versions should shed light on both the role of nonlinear terms and of exchange for realistic applications.

5.1 Determination of Parameters

We follow the \( \chi^2 \) fitting procedure of Refs. [3,2], choosing the same set of physical observables (binding energies, diffraction radii and surface thicknesses of \( ^{16}O, ^{40}Ca, ^{48}Ca, ^{58}Ni, ^{90}Zr, ^{116}Sn, ^{124}Sn, \) and \( ^{208}Pb \) ) and weights (0.2% relative error for the binding energies, 0.5% for the diffraction radii and 1.5% for the surface thicknesses) using the constant gap pairing correlation [3,2]. Our parameters are \( \delta_S, \delta_V, \alpha_{SV}, \delta_S, \delta_V \) and \( \delta_{TV} \) (six parameters) for LHx and LH and additionally \( \beta_S \) and \( \gamma_S \) for NLH and NLHx.
\[ \chi^2 \text{ results from the models defined by Eqs. (18-21). } E_B \text{ denotes the binding energies, } R_d \text{ the diffraction radii and } \sigma \text{ the surface thicknesses.} \]

<table>
<thead>
<tr>
<th>Model</th>
<th>( \chi^2_{E_B} )</th>
<th>( \chi^2_{R_d} )</th>
<th>( \chi^2_{\sigma} )</th>
<th>( \chi^2_{\text{Total}} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>LH</td>
<td>872.21</td>
<td>70.09</td>
<td>1250.96</td>
<td>2193.27</td>
</tr>
<tr>
<td>LHx</td>
<td>89.31</td>
<td>18.58</td>
<td>429.31</td>
<td>537.20</td>
</tr>
<tr>
<td>NLH</td>
<td>27.65</td>
<td>6.57</td>
<td>75.79</td>
<td>110.01</td>
</tr>
<tr>
<td>NLHx</td>
<td>21.93</td>
<td>6.91</td>
<td>59.51</td>
<td>88.35</td>
</tr>
</tbody>
</table>

Table 4

5.2 Results

Table 4 collects the \( \chi^2 \) results from the four model variations. Here LHx, LH, NLHx, NLH denote parameter sets from Eqs. (18-21). \( E_B, R_d \) and \( \sigma \) denote the binding energy, diffraction radius, and surface thickness.

To see the difference among the four parameter sets clearly in binding energies of finite nuclei, we use the error in the binding energies (\( \mathcal{E}_{E_B} \)) and the two-neutron (\( S_{2n} \)) and the two-proton (\( S_{2p} \)) separation energies from some isotopic and isotonic chains. The error in the binding energy is defined as

\[ \mathcal{E}_{E_B} = \frac{E_B^{\text{th}} - E_B^{\exp}}{E_B^{\exp}}, \]

while \( S_{2p} \) and the \( S_{2n} \) are defined as

\[ S_{2n} = E_B(N, Z) - E_B(N - 2, Z), \]
\[ S_{2p} = E_B(N, Z) - E_B(N, Z - 2) \]

respectively, with \( E_B(N,Z) \) being the calculated binding energy. Fig. 1 shows that in the isotope chains, LHx has better \( \mathcal{E}_{E_B} \) results than LH, but in the isotonic chains, LH performs better. Thus even though LHx has a better \( \chi^2_{E_B} \) than LH, it does not mean it must have better binding energy predictions for
all spherical nuclei. Although the $\chi^2_{EB}$ of NLH and NLHx are not drastically different from that of LHx, they yield much better predictions than LHx for these isotopic and isotonic trends. We see here that the role of nonlinear terms for an acceptable $E_{EB}$ prediction is more important than that of the tensor terms, which in this case partly represents the exchange effect of the linear point-coupling model. NLH has a quality in $E_{EB}$ as good as NLHx.

Fig. 2 shows that on the average, $S_{2n}$ and $S_{2p}$ from LHx are better than the ones from LH. Here we can see an important role of the nonlinear terms for the prediction of binding energies, because only NLH and NLHx can reproduce the $S_{2n}$ and $S_{2p}$ experimental data for almost all represented isotopes and isotones. The NLHx results are closer to the experimental data than NLH. The effect of the presence of tensor terms in the nonlinear model cannot be seen from $E_{EB}$, but $S_{2n}$ and $S_{2p}$ show better trends.
Fig. 2. Two-neutron separation energies ($S_{2n}$) for lead and tin isotopes (top) and two-proton separation energies ($S_{2p}$) for N=82 and N=126 isotope chains N=82 (bottom).

Errors in the diffraction radii ($E_{Rd}$) and the surface thicknesses ($E_{\sigma}$) are defined similarly as for the binding energies. The left picture of figure 3 shows that LH has an $E_{\sigma}$ of more than 20 %. Lhx has an $E_{\sigma}$ value in the range below 20 %. It is still a bad result compared to NLHx and NLH which have an $E_{\sigma}$ value below 10 %. Although the $\chi^2_{\sigma}$ of NLHx is considerably better than for NLH, they yield similar predictions for the surface thicknesses. This confirms the result of Ref. [19], namely that the relativistic linear Hartree-Fock calculation still cannot give acceptable surface thickness predictions. Here it is clearly shown that the exchange effect has an important role in the surface thickness prediction. This figure also shows that only models which include the nonlinearities can give acceptable predictions. The right picture of figure 3 shows that the $E_{Rd}$ results
of the parameter sets behave quite differently in each isotopic chain, but as the difference is not really significant, they may basically be considered to yield similar predictions in $E_{Rd}$.

The definition of the error in spin-orbit splitting is the same as in the previous cases. For the neutron case, all models give a bad prediction for $^{90}Zr(2p)$ and $^{48}Ca(1d)$. Only LH gives acceptable results in $^{208}Pb(3p)$, LHx and NLH in $^{16}O(1p)$ and $^{40}Ca(1d)$, and NLHx in $^{208}Pb(3p)$, $^{16}O(1p)$ and $^{40}Ca(1d)$. For protons, LH cannot give acceptable results. LHx and NLH have three acceptable results while NLHx has four, all parameter sets cannot reproduce the experimental result of $^{48}Ca(1d)$ for protons. LHx is intermediate in quality between LH, on the one hand, and NLH and NLHx on the other for the single-particle spectra. From these facts it is clear that the exchange effects from the linear terms are important for the shell structure though quantitatively still insufficient, while the nonlinearity in the relativistic mean-field model clearly appears necessary for shell structure predictions. For the case of $^{208}Pb$, LHx shows strong fluctuations in the surface part of the density and yields quite a large value of $\rho_P(r)$ in the center. This fact is probably due to the rough approximation used for the exchange of the derivative terms. We can see the role of the nonlinearity in NLHx which remedies the central density in comparison to LHx.

The above results can be understood from the nonrelativistic analysis [32] as follows: the nonlinear models (NLH, NLHx) exhibit better predictions for finite nuclei observables than the linear ones (LH, LHx) because they have an adequate density dependence in the central and spin-orbit potentials. LHx shows better predictions than LHx in shell structure related observables be-
cause LHx contains a density dependence in the spin-orbit potential. LHx has better predictions than LH in binding energy and surface thickness, but the result is still far from acceptable (in contrast to NLH, NLHx) because LHx gets the density dependence in the central potential not from the dominant part \( C_1 \) but from the minor part \( C_6 \).

In summary, it is found that the exchange effect in the linear Hartree-Fock point-coupling model cannot be absorbed effectively into the coupling constants of a Hartree calculation. In agreement with Refs. [19,20] where the linear Walecka model was used, a similar situation happens in the linear point-coupling model, namely that Hartree and Hartree-Fock calculations cannot give predictions which are close to experimental data. The nonlinear terms are needed to remedy this. Upon introducing the nonlinear terms, the exchange
effect from the linear terms does not drastically show up. Thus it seems that
the nonlinear terms are more important than the exchange effect from the lin-
ear terms. The validity of this presumption still needs to be checked, however,
by the exact calculation, namely taking into account the exchange of both the
linear and nonlinear terms exactly.

6 Conclusion

We have shown that formally, a Lagrangian density $\mathcal{L}^{HF}$ of the standard
ansatz can be determined in a relativistic point-coupling Hartree-Fock sense
that is not equivalent to that determined in a relativistic point-coupling strict
Hartree sense, $\mathcal{L}^{H}$ due to the exchange of the linear derivative terms and ex-
change of the nonlinear terms. The equivalency can be obtained if we use a
“complete” ansatz, but the cost we must pay is introducing more parameters.
The exchange of the linear derivative terms is created by the densities $C_i$ and
$B_{i\mu}$. By using the Gordon decomposition, we can separate these densities into
two parts. The role of the first part can be replaced effectively by tensor terms
and all possible nonlinear terms, while the second part is a genuine feature of
these densities. This second part is responsible for creating effects beyond the
Dirac equation, nonlocal and retardation effects. An order of magnitude anal-
ysis of the $C_i$ and $B_{i\mu}$ densities in the Gordon decomposition representation of
these densities shows that these parts are expected to be small, yet the actual
role of these parts in finite nuclei observables is still interesting to investigate.
Also, as discussed before, taking into account the nonlinear exchange terms
might alter the picture significantly.

Our study, by using rough approximations in the Lagrangian densities, has
shown gradual improvements in prediction for the finite nuclei. These results
and the possibility that the effect of the exchange of the nonlinear terms
and some neglected effects in the approximate forms of the densities $C_i$ and
$B_{i\mu}$, which could reveal more improvements or even give a different picture
in finite nuclei, support the importance of exact Hartree-Fock point-coupling
calculations.

Another interesting feature of such Hartree-Fock point-coupling calculations is
the possibility to take into account terms which cannot appear in the Hartree
calculation, for example the pionic degrees of freedom will contribute via the
exchange terms.

A reexamination of the ansatz is needed to improve the effectivity of the model
and a careful optimization procedure will be mandatory for fitting the model,
both need elaborate and extensive work. For these reasons, we postpone the
study of the complete quantitative Hartree-Fock model to future work.
A Appendix

A.1 From the Walecka to the Point-Coupling Model

The advantages and disadvantages of both models in the context of the Hartree-Fock calculation are discussed. A Lagrangian density operator for the Walecka (W) model is chosen as in [21]:

\[ \mathcal{L}^W = \mathcal{L}^W_L + \mathcal{L}^W_{NL} \]  

(A.1)

with

\[ \mathcal{L}^W_L = \bar{\Psi}(i\gamma_\mu \partial^\mu - m_B)\Psi \]

\[ \quad + \sum_{i=S,V,R,A...} s_i \left[ \frac{1}{2}(\partial_\nu \hat{\phi}_i^{\mu}\partial^\nu \hat{\phi}_i^{\mu} - m_i^2 \hat{\phi}_i^{\mu}\hat{\phi}_i^{\mu}) - g_i \bar{\Psi}\Gamma_i^{\mu}\hat{\phi}_i^{\mu}\Psi \right], \]  

(A.2)

and

\[ \mathcal{L}^W_{NL} = -\frac{1}{3}b_2\hat{\phi}^3 - \frac{1}{4}b_3\hat{\phi}^4. \]  

(A.3)

where the meson contents can be seen in table A.1.

<table>
<thead>
<tr>
<th>Meson</th>
<th>( \hat{\phi}_{i\mu} ) (Field)</th>
<th>( g_i ) (Coupling Const)</th>
<th>( m_i ) (Mass)</th>
<th>( \Gamma_i^{\mu} ) (Coupling terms)</th>
<th>si</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \sigma )</td>
<td>( \hat{\phi}(x) )</td>
<td>( g_S )</td>
<td>( m_S )</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>( \omega )</td>
<td>( \hat{V}_\mu(x) )</td>
<td>( g_V )</td>
<td>( m_V )</td>
<td>( \gamma_\mu )</td>
<td>-1</td>
</tr>
<tr>
<td>( \rho )</td>
<td>( \hat{R}_\mu(x) )</td>
<td>( g_R )</td>
<td>( m_R )</td>
<td>( \gamma_\mu\tilde{\tau} )</td>
<td>-1</td>
</tr>
<tr>
<td>photon</td>
<td>( \hat{A}_\mu(x) )</td>
<td>( e )</td>
<td>0</td>
<td>( \frac{1}{2}\gamma_\mu(1 + \tau_3) )</td>
<td>-1</td>
</tr>
</tbody>
</table>

Table A.1
The meson contents of equation (A.2).

For the \( \hat{\phi}_{i\mu} \), the fields used are \( \hat{\phi}(x) \), \( \hat{V}_\mu(x) \), \( \hat{R}_\mu(x) \) and \( \hat{A}_\mu(x) \), denoting a scalar-isoscalar, a vector-isoscalar, a vector-isovector and the electromagnetic field operators, respectively. \( g_i \) and \( m_i \) are the coupling constants and masses of each field operator \( \hat{\phi}_{i\mu} \). We find that a difficulty appears to determine the scalar field operator due to the nonlinearities making it different from a simple Yukawa form. Some approximations have been done to overcome this problem [22–24] but as far as we know there is not yet an exact Hartree-Fock calculation including mesonic nonlinear terms. Replacing
we can avoid the above problem and the standard definition for the linear field operators can be used as \[21\]

\[
\hat{\phi}_{i\mu}(x) = \hat{\phi}_{i\mu}^0(x) + g_i \int d^4y D(x - y, m_i) \hat{\Psi}_{i\mu} \hat{\Gamma}_i \hat{\Psi},
\]

\[
\hat{\phi}_{j\mu}^0(x) = \sum_{\alpha} (f_{\alpha j\mu}(x) \hat{a}_{\alpha j} + f_{\alpha j\mu}^\dagger(x) \hat{a}_{\alpha j}^\dagger),
\]

\[
\hat{\Psi}(x) = \sum_{\alpha} (\Psi_{\alpha}(x) \hat{b}_{\alpha} + \tilde{\Psi}_{\alpha}(x) \hat{d}_{\alpha}^\dagger),
\] (A.4)

where \(\Psi_{\alpha}(x), \tilde{\Psi}_{\alpha}\) and \(f_{\alpha i\mu}\) denote a nucleon, an antinucleon, and a meson wavefunction with \(\alpha\) enumerating the states. The operators \(\hat{a}_{\alpha j}, \hat{b}_{\alpha}\) and \(\hat{d}_{\alpha}\) annihilate a free meson, a nucleon and an antinucleon with a momentum \(k_{\alpha}\), with the conjugate operators the corresponding creation operators. \(D(x,y)\) is the meson propagator which is defined as a solution of

\[
(\partial_\mu \partial^\mu + m_i^2)D(x - y, m_i) = \delta^4(x - y).
\] (A.5)

The necessity to introduce an extra density dependence in Dirac-Brueckner-Hartree-Fock calculations that allows a simultaneous fit of the NN phase shift and the nuclear matter equilibrium point \[25,26\] provides a physical motivation for this replacement.

Further on, we can study the connection between the Walecka and point-coupling models by replacing the meson propagators with their low-order expansion plus additional parameters \(k_i\) as

\[
-\int \frac{d^4p}{(2\pi)^4} \frac{e^{-ip(x-y)}}{p^2 - m_i^2 + i\epsilon} \rightarrow \frac{1}{m_i^2} \delta^4(x - y) - \frac{k_i}{m_i^2} \partial_\mu \partial^\mu \delta^4(x - y),
\] (A.6)

to arrive at the Lagrangian density operator of the point-coupling (RMF-PC) \[17\] model in section 1.

A.2 Gordon decomposition of the exact equation of motion

After a straightforward Dirac matrix algebra calculation we have from the Gordon decomposition of the exact equation of motion that \(A_1 + A_2 + A_3 = 0\), with
\[ A_1 = -\frac{1}{2i}[(\partial^\alpha \bar{\Psi}_\alpha) \Psi_\alpha - \bar{\Psi}_\alpha (\partial^\alpha \Psi_\alpha)] \]
\[ + \frac{1}{2} U_\mu [(\partial^\mu \bar{\Psi}_\alpha) \gamma^\sigma \Psi_\alpha - \bar{\Psi}_\alpha \gamma^\sigma (\partial^\mu \Psi_\alpha)] \]
\[ + \frac{1}{2} W_1 \partial_\mu [(\partial^\mu \bar{\Psi}_\alpha) \gamma^\sigma \Psi_\alpha - \bar{\Psi}_\alpha \gamma^\sigma (\partial^\mu \Psi_\alpha)] \]
\[ + \frac{1}{2} U_\sigma [\partial^\mu (\bar{\Psi}_\alpha) \Psi_\alpha] \]
\[ - \frac{1}{2} W_1 \partial_\mu [(\partial^\mu \bar{\Psi}_\alpha) \Psi_\alpha - \bar{\Psi}_\alpha (\partial^\mu \Psi_\alpha)], \quad (A.7) \]

\[ A_2 = \frac{1}{2} \partial_\mu (\bar{\Psi}_\alpha \sigma^{\mu \sigma} \Psi_\alpha) - \frac{1}{2} i U_\alpha \mu \partial^\mu (\bar{\Psi}_\alpha \sigma^{\alpha \sigma} \Psi_\alpha) \]
\[ - \frac{1}{2} i W_2 \partial_\mu (\bar{\Psi}_\alpha \sigma^{\mu \alpha} \Psi_\alpha), \quad (A.8) \]

\[ A_3 = \bar{m}^* \bar{\Psi}_\alpha \gamma^\sigma \Psi_\alpha + \bar{\Psi}_\alpha \gamma^\sigma \Psi_\alpha. \quad (A.9) \]

Let us define \( \bar{m}^* \equiv \bar{m}^* + \Delta m^* \) and \( \bar{V}_\alpha \equiv \bar{V}_\alpha + \Delta V_\alpha \), where \( \Delta m^* \) and \( \Delta V_\alpha \) are the parts of \( \bar{m}^* \) and \( \bar{V}_\alpha \) of order \( v^2 \). Note that up to this point the treatment of exchange is still exact. Now, if we apply the order-of-magnitude estimation of section 3 to study the magnitude in every term in \( A_1 \) through \( A_3 \) and assume that the terms of order \( \geq v^2 \) are small and can be neglected, it is obvious that only the first term in \( A_1 \) and \( A_2 \) will survive and the \( \Delta m^* \) and \( \Delta V_\alpha \) contributions vanish in \( A_3 \). Therefore in this limit we will obtain Eq. (6) of section (3).
A.3 The coupling constants of the approximate Lagrangian

\[ \tilde{\alpha}_S = \alpha_S - \left( \frac{1}{8} \alpha_S + \frac{4}{8} \alpha_V + \frac{12}{8} \alpha_{tV} \right) - 2m_B^2 \left( \frac{1}{8} \delta_S + \frac{4}{8} \delta_V + \frac{12}{8} \delta_{tV} \right), \quad (A.10a) \]

\[ \tilde{\alpha}_V = \alpha_V + \left( -\frac{1}{8} \alpha_S + \frac{2}{8} \alpha_V + \frac{6}{8} \alpha_{tV} \right) + 2m_B^2 \left( -\frac{1}{8} \delta_S + \frac{2}{8} \delta_V + \frac{6}{8} \delta_{tV} \right) 
+ 2m_B^2 \left( \frac{1}{8} \delta_S + \frac{4}{8} \delta_V + \frac{12}{8} \delta_{tV} \right), \quad (A.10b) \]

\[ \tilde{\alpha}_{tS} = \left( -\frac{1}{8} \alpha_S - \frac{4}{8} \alpha_V + \frac{4}{8} \alpha_{tV} \right) + 2m_B^2 \left( -\frac{1}{8} \delta_S - \frac{4}{8} \delta_V + \frac{4}{8} \delta_{tV} \right) \quad (A.10c) \]

\[ \tilde{\alpha}_{tV} = \alpha_{tV} + \left( -\frac{1}{8} \alpha_S + \frac{2}{8} \alpha_V - \frac{2}{8} \alpha_{tV} \right) + 2m_B^2 \left( -\frac{1}{8} \delta_S + \frac{2}{8} \delta_V - \frac{2}{8} \delta_{tV} \right) 
- 2m_B^2 \left( \frac{1}{8} \delta_S - \frac{4}{8} \delta_V + \frac{4}{8} \delta_{tV} \right), \quad (A.10d) \]

\[ \tilde{\delta}_S = \delta_S + \left( \frac{1}{16} \delta_S + \frac{4}{16} \delta_V + \frac{12}{16} \delta_{tV} \right) \quad (A.10e) \]

\[ \tilde{\delta}_V = \delta_V - \left( -\frac{1}{16} \delta_S + \frac{2}{16} \delta_V + \frac{12}{32} \delta_{tV} \right) \quad (A.10f) \]

\[ \tilde{\delta}_{tS} = \left( \frac{1}{16} \delta_S + \frac{4}{16} \delta_V - \frac{4}{16} \delta_{tV} \right) \quad (A.10g) \]

\[ \tilde{\delta}_{tV} = \delta_{tV} - \left( -\frac{1}{16} \delta_S + \frac{2}{16} \delta_V - \frac{4}{32} \delta_{tV} \right) \quad (A.10h) \]

\[ \tilde{\theta}_T = 4m_B \left( \frac{1}{16} \delta_S + \frac{4}{16} \delta_V + \frac{12}{16} \delta_{tV} \right) \quad (A.10i) \]

\[ \tilde{\theta}_{tT} = 4m_B \left( \frac{1}{16} \delta_S + \frac{4}{16} \delta_V - \frac{4}{16} \delta_{tV} \right) \quad (A.10j) \]

\[ c_S = \left( \frac{1}{16} \delta_S + \frac{4}{16} \delta_V + \frac{12}{16} \delta_{tV} \right), \quad (A.10k) \]

\[ c_V = \left( -\frac{1}{16} \delta_S + \frac{2}{16} \delta_V + \frac{12}{32} \delta_{tV} \right), \]

\[ c_{tS} = \left( -\frac{1}{16} \delta_S + \frac{4}{16} \delta_V - \frac{4}{16} \delta_{tV} \right), \]

\[ c_{tV} = \left( -\frac{1}{16} \delta_S - \frac{2}{16} \delta_V + \frac{4}{32} \delta_{tV} \right), \]

A.4 A complete mapping from Hartree-Fock to Hartree

It has been shown that the usual ansatz for the point-coupling RMF model, when considered within the Hartree-Fock approximation, leads to equations
that deviate from the structure of a Dirac-equation. The source for these differences are the exchange terms with derivatives, leading to densities that do not occur in the standard Dirac-Hartree model.

It should be mentioned, however, that the reason for these deviations is the form of the Lagrange density operator, with which we start off. We could as well choose a Lagrangian meant for a strict Hartree treatment, which would lead to the same structure as we obtained it in this investigation. A similar situation holds for the Skyrme-Hartree-Fock theory. The mapping can be achieved by adding terms that lead to the new densities in the Hartree-Fock case. The Lagrangian density would have to be complemented by the following terms:

$$\Delta \hat{L}_{\text{derivative}} = \sum_{j \in H} \left[ \frac{1}{2} \alpha_j \hat{A}_{j\mu} \hat{B}^{j\mu} + \frac{1}{2} \beta_j \hat{B}_{j\mu} \hat{B}^{j\mu} + \frac{1}{2} \theta_j \hat{J}_j \hat{C}^j \right], \quad (A.11)$$

here $\alpha_j$, $\beta_j$ and $\theta_j$ are free parameters. This would include, however, the introduction of additional parameters, whereas in the HF case, no new parameters arise. The ansatz complemented by Eq. (A.11) leads to the same type of equation in both the Hartree and the Hartree-Fock approximations.

Though the mapping of the Hartree-Fock (and the corresponding effective Hartree) theory to a related strict Hartree theory can be done in principle, it would be at the cost of introducing and motivating new terms and additional coupling constants. If we also consider higher order terms [27], a complete mapping to a Hartree theory would introduce many new parameters. Experience will tell which ansatz for the effective interaction will prove to be most adequate for a Hartree-Fock theory for finite nuclei.

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