

Relativistic Models for Nuclear Structure Calculations: Comparative Study of Mean-Field and Hartree-Fock Approximation for Superheavy Nuclei

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The relevance of exchange effects for the stability of superheavy nuclei is examined within a linear QHD-II model by comparing Hartree-Fock with mean-field results. To allow a scan of the complete superheavy regime the recently developed local density approximation (LDA) for the exchange potential is employed for the Hartree-Fock level calculations. It turns out that, while many nuclear properties obtained with the LDA approach differ significantly from the corresponding mean-field results, the predictions of the two methods for shell closures are very similar. Furthermore, a comparison with a nonlinear variant of QHD-II shows that many nuclear properties obtained with the LDA in the framework of linear QHD-II are somewhere in-between the corresponding linear and nonlinear mean-field results. This indicates that the LDA exchange partially includes nonlinear contributions, which supports the interpretation of the meson self-coupling as a parametrization of many-body effects.

1. INTRODUCTION

Since the prediction of a doubly magic nucleus $^{298}_{184}114$,^(1, 2) the search for shell-stabilized superheavy nuclei has been an important topic of heavy-ion physics (see, e.g., Ref. 3). The recent experimental discovery of $^{270}_{162}\text{Hs}_{108}$ at GSI^(4, 5) and Dubna⁽⁶⁾ has fostered the hope that the existence of a doubly magic nucleus can be verified in the near future. The experimental progress has also stimulated renewed theoretical efforts,⁽⁷⁻⁹⁾ their main objective being a microscopic and self-consistent confirmation of the earlier shell model results (compare also Refs. 10, 11). Both relativistic mean-field (MF)

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models and the nonrelativistic Skyrme–Hartree–Fock (SHF) approach have been utilized in this context. While these models provide a realistic description of all known nuclei from ^{16}O on using only a modest number of parameters (see, e.g., Ref. 12), predictions for the regime of superheavy nuclei are a challenging task also on this more microscopic basis. In fact, the various self-consistent models do not give a unique answer for the shell closures of interest,⁽⁸⁾ both $Z = 120$, $N = 172$, and $Z = 126$, $N = 184$ being suggested in addition to the original nucleus $Z = 114$, $N = 184$.

At present, the precise microscopic origin of these contradicting results is not yet clear. The underlying models not only differ in their representation of the effective nucleon–nucleon interaction and their treatment of relativity, but also with respect to their many-body character. In particular, all systematic surveys of the superheavy regime with relativistic models, i.e., some variants of quantum hydrodynamics (QHD),^(13, 14) rely on the MF approximation^(8, 9) (a comparison of MF and density-dependent Dirac–Brueckner results for $^{298}_{184}114$ is given in Ref. 15). On the other hand, there is some evidence⁽¹⁶⁾ that at least for QHD models without nonlinear self-interaction terms the inclusion of exchange effects leads to a more consistent description of nuclear properties. As a consequence one would expect HF-based models also to be more reliable beyond the regime of those nuclei used to fix the models’ parameters. In view of these facts it seems worthwhile to extend the recent QHD-based studies of the superheavy regime^(8, 9) to the HF level.

In this contribution we thus present HF level results for superheavy nuclei obtained with the local density approximation (LDA) for the exchange potential^(17, 18) in the framework of QHD-II⁽¹⁴⁾ (while the LDA concept can also be applied to correlation contributions, we will use the abbreviation LDA for the exchange-only version in the following). The LDA, based on the density functional concept,⁽¹⁹⁾ provides an accurate local approximation to the nonlocal HF exchange potential: Both global nuclear properties like binding energies as well as more microscopic quantities like charge densities from LDA calculations^(17, 18) are very close to the corresponding full HF results,^(20, 21) so that LDA calculations can replace the full HF procedure without any relevant loss of information. On the other hand, due to its local exchange potential, the LDA approach is as efficient as MF models, in contrast to the computationally demanding full HF scheme.⁽²¹⁾ The LDA thus represents an ideal tool for systematic studies over a wide range of nuclei, like the present investigation of the stability of superheavy nuclei.

The paper is organized as follows: In Sec. 2 the density functional approach to QHD-II is briefly outlined, emphasizing the Kohn–Sham (KS) single-particle equations and the decomposition of the LDA exchange with

respect to the various mesonic degrees of freedom. Our LDA results for superheavy nuclei are presented in Sec. 3. Lacking any published HF parameter set for QHD-II including meson self-coupling, the LDA calculations are restricted to linear QHD-II, for which the parametrization ZJO⁽¹⁶⁾ seems most suitable for our purpose. By a comparison with MF results for linear QHD-II (using the parametrization LZ,⁽²²⁾ the role of exchange effects for the properties of individual nuclei as well as their relative stability is studied. In addition, a comparison with MF results for a nonlinear variant of QHD-II (NLZ⁽²²⁾) allows us to examine the relation between exchange and nonlinear contributions. Finally, a brief summary is given in Sec. 4.

2. THEORY

The meson exchange model on which the discussion will be based is characterized by the Lagrangian

$$\begin{aligned}
 \mathcal{L} = & \bar{\Psi} [i\gamma^\mu \partial_\mu - M] \Psi + \frac{1}{2} [\partial_\mu \sigma \partial^\mu \sigma - m_\sigma^2 \sigma^2] \\
 & - \frac{1}{4} (\partial_\mu \omega_\nu - \partial_\nu \omega_\mu) (\partial^\mu \omega^\nu - \partial^\nu \omega^\mu) + \frac{1}{2} m_\omega^2 \omega_\mu \omega^\mu \\
 & + \frac{1}{2} [\partial_\mu \pi \cdot \partial^\mu \pi - m_\pi^2 \pi^2] \\
 & - \frac{1}{4} (\partial_\mu \rho_\nu - \partial_\nu \rho_\mu) \cdot (\partial^\mu \rho^\nu - \partial^\nu \rho^\mu) + \frac{1}{2} m_\rho^2 \rho_\mu \cdot \rho^\mu \\
 & - \frac{1}{4} (\partial_\mu A_\nu - \partial_\nu A_\mu) (\partial^\mu A^\nu - \partial^\nu A^\mu) - \frac{\lambda}{2} (\partial_\mu A^\mu)^2 \\
 & + g_\sigma \bar{\Psi} \sigma \Psi - g_\omega \bar{\Psi} \omega^\mu \gamma_\mu \Psi - \frac{f_\pi}{m_\pi} (\bar{\Psi} \gamma^5 \gamma^\mu \tau \Psi) \cdot \partial_\mu \pi \\
 & - g_\rho \bar{\Psi} \rho_\mu \cdot \tau \gamma^\mu \Psi - e \bar{\Psi} \gamma_\mu \frac{1}{2} (1 + \tau_3) A^\mu \Psi
 \end{aligned}$$

which represents the standard QHD-II model,^(13, 14) employing a pseudo-vector coupling for the pions. In MF calculations the Lagrangian is often extended by nonlinear meson self-interaction terms for the σ meson. Although it is possible to deal with these nonlinear contributions in the KS method,

we have not included them here, as no corresponding HF parametrization adjusted to nuclear ground state properties is available.

In Refs. 19, 17 it has been shown that any QHD-I ground state $|\Phi_0\rangle$ is uniquely determined by the proton and neutron ground state four-currents j_p^μ and j_n^μ and the ground state scalar density ρ_s , allowing one to interpret $|\Phi_0\rangle$ as a functional of these quantities. The extension of this basic DFT statement to QHD-II, requiring a reexamination of the basic variables of the DFT-scheme, has been discussed in Ref. 18. As far as the ρ mesons are concerned, no new density variable need to be introduced as long as only systems with a specified number of protons and neutrons are considered, to which we restrict ourselves here. The situation is more involved for the π mesons, for which

$$\Delta(\mathbf{x}) \equiv \nabla \cdot [\mathbf{j}_p^5(\mathbf{x}) - \mathbf{j}_n^5(\mathbf{x})] \quad (1)$$

has to be added to the set of basic variables known from QHD-I. As a consequence the total ground state energy E_0 can be written as a functional of j_p^μ , j_n^μ , ρ_s and Δ ,

$$E_0[j_p^\mu, j_n^\mu, \rho_s, \Delta] = \langle \Phi_0[j_p^\mu, j_n^\mu, \rho_s, \Delta] | \hat{H} | \Phi_0[j_p^\mu, j_n^\mu, \rho_s, \Delta] \rangle$$

Representing j_q^μ (where q characterizes either protons, $q=p$, or neutrons, $q=n$), ρ_s , and \mathbf{j}_q^5 in terms of auxiliary single-particle four-spinors $\varphi_{i,q}$,

$$\rho_s(\mathbf{x}) = \sum_{q=p,n} \left[\sum_{-M < \varepsilon_{i,q} \leq \varepsilon_{F,q}} \bar{\varphi}_{i,q}(\mathbf{x}) \varphi_{i,q}(\mathbf{x}) \right] \quad (2)$$

$$j_q^\mu(\mathbf{x}) = \sum_{-M < \varepsilon_{i,q} \leq \varepsilon_{F,q}} \bar{\varphi}_{i,q}(\mathbf{x}) \gamma^\mu \varphi_{i,q}(\mathbf{x}) \quad (3)$$

$$\mathbf{j}_q^5(\mathbf{x}) = \sum_{-M < \varepsilon_{i,q} \leq \varepsilon_{F,q}} \bar{\varphi}_{i,q}(\mathbf{x}) \gamma^5 \boldsymbol{\gamma} \varphi_{i,q}(\mathbf{x}) \quad (4)$$

(all vacuum corrections are neglected), one can decompose E_0 as

$$E_0 = T_S + E_H + E_{xc} \quad (5)$$

where T_S is the kinetic energy of the "KS quasi-nucleons,"

$$T_S = \sum_{q=p,n} \int d^3x \sum_{\varepsilon_{i,q} \leq \varepsilon_{F,q}} \varphi_{i,q}^\dagger (-i\boldsymbol{\alpha} \cdot \nabla + \beta M) \varphi_{i,q} \quad (6)$$

E_H is the mean-field (Hartree) energy,

$$\begin{aligned}
 E_H = & -\frac{g_\sigma^2}{2} \int d^3x d^3y \frac{e^{-m_\sigma |\mathbf{x}-\mathbf{y}|}}{4\pi |\mathbf{x}-\mathbf{y}|} \rho_s(\mathbf{x}) \rho_s(\mathbf{y}) \\
 & + \frac{g_\omega^2}{2} \sum_{q=p,n} \int d^3x d^3y \frac{e^{-m_\omega |\mathbf{x}-\mathbf{y}|}}{4\pi |\mathbf{x}-\mathbf{y}|} j_q^\mu(\mathbf{x}) j_{\mu,q}(\mathbf{y}) \\
 & + \frac{1}{2} \left(\frac{f_\pi}{m_\pi} \right)^2 \int d^3x d^3y \frac{e^{-m_\pi |\mathbf{x}-\mathbf{y}|}}{4\pi |\mathbf{x}-\mathbf{y}|} \Delta(\mathbf{x}) \Delta(\mathbf{y}) \\
 & + \frac{g_\rho^2}{2} \int d^3x d^3y \frac{e^{-m_\rho |\mathbf{x}-\mathbf{y}|}}{4\pi |\mathbf{x}-\mathbf{y}|} [j_n^\mu(\mathbf{x}) - j_p^\mu(\mathbf{x})][j_{\mu,n}(\mathbf{y}) - j_{\mu,p}(\mathbf{y})] \\
 & + \frac{e^2}{2} \int d^3x d^3y \frac{1}{4\pi |\mathbf{x}-\mathbf{y}|} j_p^\mu(\mathbf{x}) j_{\mu,p}(\mathbf{y})
 \end{aligned} \tag{7}$$

and the exchange-correlation energy E_{xc} is defined via Eq. (5). Minimization of E_0 with respect to the $\phi_{i,q}$'s leads to the single-particle equations (KS equations),

$$\begin{aligned}
 \{ & -i\boldsymbol{\alpha} \cdot \nabla + \beta[M - \phi_H - \phi_{xc} + \gamma_\mu(V_{q,H}^\mu + V_{q,xc}^\mu) \\
 & + \gamma^5 \boldsymbol{\gamma} \cdot (\mathbf{V}_{q,H}^5 + \mathbf{V}_{q,xc}^5)] \} \phi_{i,q} = \varepsilon_{i,q} \phi_{i,q}
 \end{aligned} \tag{8}$$

where ϕ_H , $V_{q,H}^\mu$ and $V_{q,H}^{5,i}$ are the Hartree potentials, and the local exchange-correlation potentials ϕ_{xc} , $V_{q,xc}^\mu$, and $V_{q,xc}^{5,i}$ are given by

$$V_{q,xc}^{\hat{\mu}}(\mathbf{x}) = \frac{\delta}{\delta j_q^\mu(\mathbf{x})} E_{xc}[j_p^\mu, j_n^\mu, \rho_s, \Delta] \tag{9}$$

$$\phi_{xc}(\mathbf{x}) = -\frac{\delta}{\delta \rho_s(\mathbf{x})} E_{xc}[j_p^\mu, j_n^\mu, \rho_s, \Delta] \tag{10}$$

$$V_{q,xc}^{5,i}(\mathbf{x}) = \partial^i \frac{\delta}{\delta [\nabla \cdot \mathbf{j}_q^5(\mathbf{x})]} E_{xc}[j_p^\mu, j_n^\mu, \rho_s, \Delta] \tag{11}$$

Equations (2-4) and (8-11) have to be solved self-consistently. Neglecting the xc-potentials ϕ_{xc} , $V_{q,xc}^\mu$, and $V_{q,xc}^{5,i}$ yields the MF equations. The Pauli correlation of the nucleons is included via the exchange contribution E_x to E_{xc} , so that the x-only limit of the KS scheme represents the DF equivalent of the HF approximation. Aiming at a comparison of mean-field and HF level results, we restrict ourselves to this x-only limit.

In order to obtain E_x as an explicit density functional the standard approximation applied in the case of electronic systems is the LDA (see, e.g., Ref. 23). In the present context the LDA amounts to utilizing the density-dependence of the exchange energy density of infinite nuclear matter (INM), e_x^{INM} , for the inhomogeneous systems of interest, i.e., nuclei, by locally replacing the nuclear matter densities by the actual densities $\rho_q(\mathbf{x}) = j_q^0(\mathbf{x})$ and $\rho_s(\mathbf{x})$,

$$E_x^{LDA}[\rho_p, \rho_n, \rho_s] = \int d^3x e_x^{INM}(\rho_p(\mathbf{x}), \rho_n(\mathbf{x}), \rho_s(\mathbf{x})) \quad (12)$$

The basic variable introduced by the π mesons does not show up in the LDA as for nuclear matter $\Delta = 0$ (the same holds for the spatial components of the nucleon currents). The x -only energy of nuclear matter can be decomposed with respect to the individual mesons,

$$e_x^{INM} = \sum_{q=p,n} [e_{x,\sigma}^{INM}(\rho_q, \rho_s) + e_{x,\omega}^{INM}(\rho_q, \rho_s)] + e_{x,\pi}^{INM}(\rho_p, \rho_n, \rho_s) + e_{x,\rho}^{INM}(\rho_p, \rho_n, \rho_s) \quad (13)$$

Note that the pions contribute to the exchange energy and potential, although Δ is not present in the LDA.

The exchange energy of nuclear matter can be evaluated analytically^(24, 17) as a function $\tilde{e}_x^{INM}(\rho_p, \rho_n, M^*)$ of the effective mass

$$M^* = M - \phi_H - \phi_x \quad (14)$$

rather than as a function of ρ_s . The connection between M^* and ρ_s is established by the standard mean-field relation

$$\rho_s = \frac{(M^*)^3}{2\pi^2} \sum_{q=p,n} [\beta_q \eta_q - \ln(\beta_q + \eta_q)] \quad (15)$$

where

$$\beta_q = (3\pi^2 \rho_q)^{1/3} / M^*; \quad \eta_q = [1 + \beta_q^2]^{1/2} \quad (16)$$

For nuclear matter the variables M^* and ρ_s are completely equivalent as the uniqueness of (15) allows the elimination of M^* from $\tilde{e}_x^{INM}(\rho_p, \rho_n, M^*)$ in favor of ρ_s . For inhomogeneous systems, however, the actual KS scalar density (2), to be used in (12), is not identical with the $\tilde{\rho}_s(\mathbf{x})$ obtained from the local $M^*(\mathbf{x})$ via (14, 15), so that an inversion of (15), using (2) as input, is required for the LDA.⁽²⁵⁾

For completeness the explicit expressions for the exchange energy functional in the LDA are summarized in the following. For σ and ω exchange one obtains

$$\tilde{e}_{x,\sigma}^{INM}(\rho_q, M^*) = \frac{g_\sigma^2 (M^*)^4}{(2\pi)^4} \left\{ \frac{1}{4} (\beta\eta - \ln \xi)^2 + \left(1 - \frac{w_\sigma}{4}\right) I(w_\sigma, \xi, \xi) \right\} \quad (17)$$

$$\tilde{e}_{x,\omega}^{INM}(\rho_q, M^*) = \frac{g_\omega^2 (M^*)^4}{(2\pi)^4} \left\{ \frac{1}{2} (\beta\eta - \ln \xi)^2 - \left(1 + \frac{w_\omega}{2}\right) I(w_\omega, \xi, \xi) \right\} \quad (18)$$

where $\xi = \beta + \eta$ (the index q is suppressed for brevity), $w_{\sigma,\omega} = (m_{\sigma,\omega}/M^*)^2$, and

$$I(w, \xi_1, \xi_2) = \int_1^{\xi_1} du \int_1^{\xi_2} dv \left(1 - \frac{1}{u^2}\right) \left(1 - \frac{1}{v^2}\right) \ln \frac{(uv-1)^2 + uvw}{(u-v)^2 + uvw} \quad (19)$$

The integral (19) can be calculated analytically; for the explicit expression we refer the reader to Ref. 17. $e_{x,\pi}^{INM}$ and $e_{x,\rho}^{INM}$ involve the isospin decomposition⁽²⁶⁾

$$e_{x,\pi,\rho}^{INM}(\rho_p, \rho_n, \rho_s) = \tilde{e}(\rho_p, \rho_p, M^*) + \tilde{e}(\rho_n, \rho_n, M^*) + 4\tilde{e}(\rho_n, \rho_p, M^*) \quad (20)$$

where for ρ exchange $\tilde{e}(\rho_1, \rho_2, M^*)$ is given by

$$\begin{aligned} \tilde{e}_\rho(\rho_1, \rho_2, M^*) = g_\rho^2 \frac{M^{*4}}{(2\pi)^4} & \left\{ (\beta_1 \eta_1 - \ln \xi_1)(\beta_2 \eta_2 - \ln \xi_2) \right. \\ & \left. + \left(1 - \frac{w_\rho}{4}\right) I(w_\rho, \xi_1, \xi_2) \right\} \end{aligned} \quad (21)$$

with $w_\rho = (m_\rho/M^*)^2$, while for π exchange one has

$$\begin{aligned} \tilde{e}_\pi(\rho_1, \rho_2, M^*) = \left(\frac{f_\pi}{m_\pi}\right)^2 \frac{M^{*6}}{(2\pi)^4} & \{ (\beta_1 \eta_1 - \ln \xi_1)(\beta_2 \eta_2 - \ln \xi_2) \\ & - w_\pi I(w_\pi, \xi_1, \xi_2) \} \end{aligned} \quad (22)$$

with $w_\pi = (m_\pi/M^*)^2$.

3. RESULTS

The KS equations (8) have been solved by a basis set expansion in terms of spherical harmonic oscillator functions. The same expansion

technique has been used for the meson field equations determining the Hartree potentials. Details of the numerical procedure can be found in Ref. 12. All results given in the following are based on an oscillator parameter of $\hbar\omega_0 = 41A^{-1/3}$ and 30 shells ($N_F = 30$). The numerical stability of our calculations has been verified by performing the convergence tests of Ref. 12.

Pairing correlations are treated in a constant-gap approximation using a schematic pairing in which the occupation numbers are calculated via

$$w_{i,q} = \frac{1}{2} \left(1 + \frac{\varepsilon_{F,q} - \varepsilon_{i,q}}{\sqrt{(\varepsilon_{F,q} - \varepsilon_{i,q})^2 + \Delta^2}} \right) \quad (23)$$

with

$$\Delta = 11.2 \text{ MeV}/\sqrt{A} \quad (24)$$

$\varepsilon_{F,q}$ is here determined by proton and neutron number conservation, thus extending the standard DFT formalism in analogy to the finite temperature case.

We start by comparing two linear models, i.e., the MF parametrization LZ⁽²²⁾ and the HF parametrization ZJO⁽¹⁶⁾ (listed in Table I). Both parameter sets were obtained by least-squares fits to nuclear ground state properties, the only conceptual difference being that the HF parametrization was optimized without pairing contributions. They thus can be viewed as being equivalent, allowing us to examine to what extent exchange contributions can be absorbed into MF potentials and energies by a

Table I. Linear Parameter Sets LZ and ZJO
Used for the MF and LDA Calculations

	MF (22)	LDA (16)
m_σ	551.31 MeV	525 MeV
g_σ^2	125.29	108.63
m_ω	780 MeV	760.69 MeV
g_ω^2	191.15	148.05
m_ρ	763 MeV	752.32 MeV
g_ρ^2	29.64	13.35
m_π		138.0 MeV
f_π^2		0.9771
M	938.9 MeV	938.9 MeV

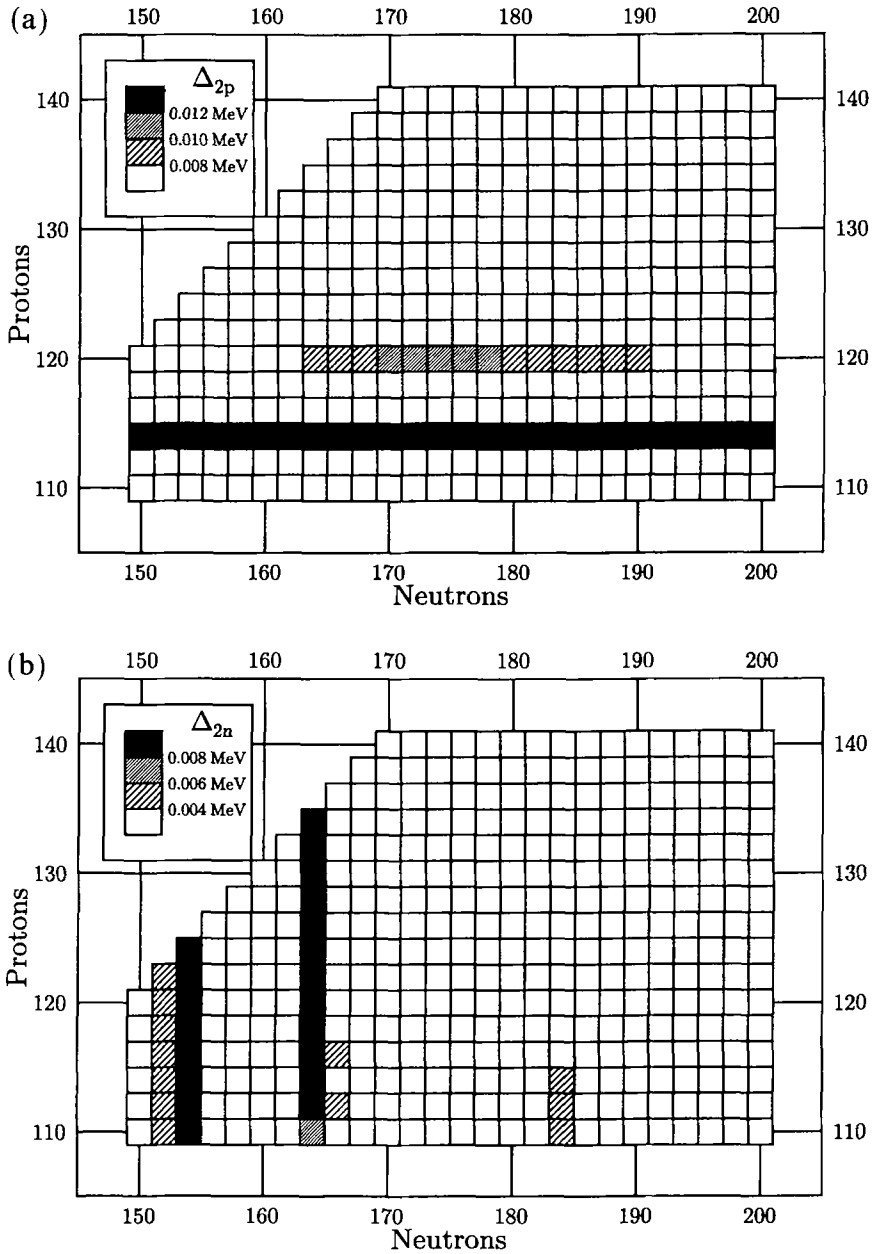


Fig. 1. Second derivatives of binding energy per nucleon with respect to proton and neutron numbers in the superheavy regime from LDA-ZJO calculations: (a) Δ_{2p} , Eq. (25), (b) Δ_{2n} , Eq. (26).

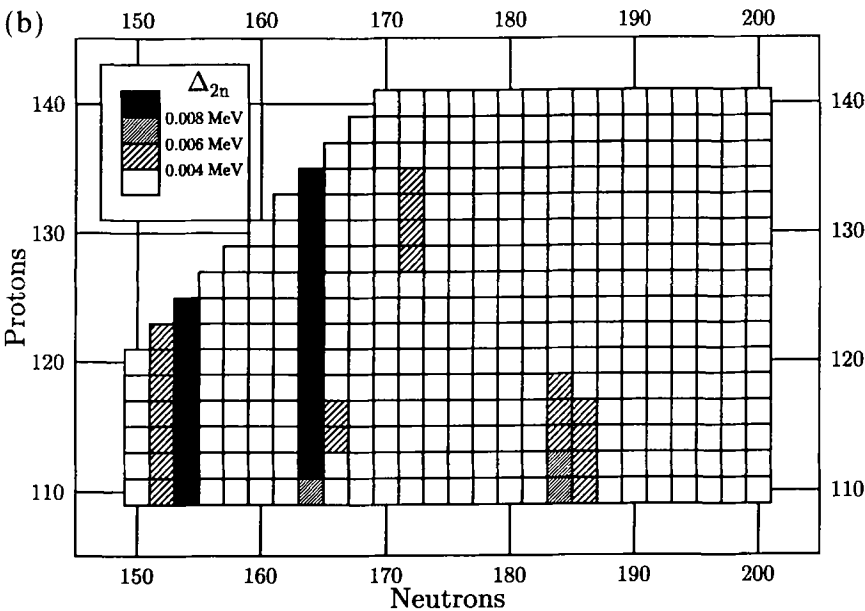
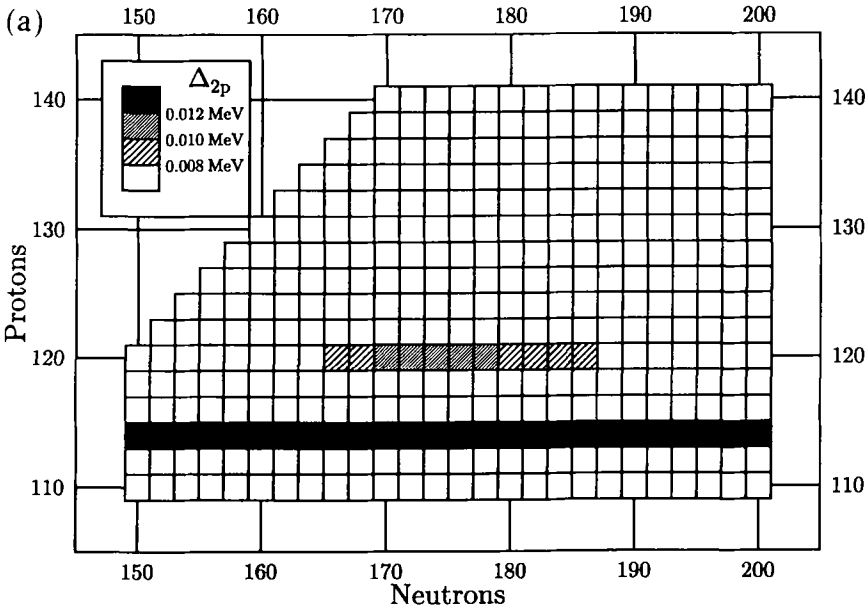


Fig. 2. Same as Fig. 1 for MF-LZ model.

reparametrization. For both models the ground states of all even–even nuclei with $110 \leq Z \leq 140$ and $Z + 40 \leq N \leq Z + 90$ have been calculated, restricting to spherical symmetry. While most of these nuclei are expected to be deformed (for the case of ${}^{264}_{156}\text{Hs}_{108}$ see Ref. 8), the neglect of deformation seems justified for our purpose of comparing the predictions of the two models for shell closures.

Figures 1 and 2 show the resulting second derivatives of the binding energy per particle with respect to proton and neutron numbers,

$$\Delta_{2,p} = \frac{E_0(Z+2, N)}{Z+2+N} - 2 \frac{E_0(Z, N)}{Z+N} + \frac{E_0(Z-2, N)}{Z-2+N} \quad (25)$$

$$\Delta_{2,n} = \frac{E_0(Z, N+2)}{Z+N+2} - 2 \frac{E_0(Z, N)}{Z+N} + \frac{E_0(Z, N-2)}{Z+N-2} \quad (26)$$

which we use as a measure for shell closures. Compared with the two nucleon gaps like $E_0(Z+2, N) - 2E_0(Z, N) + E_0(Z-2, N)$ considered in Ref. 8, Δ_2 has the advantage that it is only weakly dependent on the size of the nuclei (Δ_2 is also often applied to identify shell closures in the context of atomic clusters—see, e.g., Ref. 27). The similarity of the LDA and the MF results is remarkable. In particular, both models suggest $Z=114$, $N=164$ to be the “magic” nucleus, and indicate a much less prominent double shell closure for $Z=114$, $N=184$.

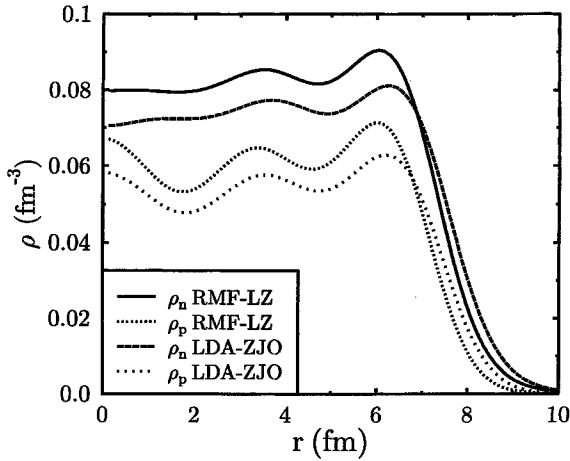


Fig. 3. Proton (ρ_p) and neutron (ρ_n) densities for ${}^{278}_{164}114$ obtained from LDA-ZJO and MF-LZ calculations.

This similarity is somewhat surprising as the corresponding ground state and single-particle energies as well as density profiles show notable differences. As an example the proton and neutron densities of the “magic” nucleus $^{278}_{164}114$ are plotted in Fig. 3. Both the densities inside the nucleus and the surface thicknesses differ substantially. Differences of similar size are found for the single-particle energies. In Fig. 4 the proton and neutron spectra obtained for $^{278}_{164}114$ are given. It is obvious that when going from a MF to a LDA description the spectra are compressed and the protons are destabilized relative to the neutrons. The ordering of the levels and the relative size of the level spacings, however, remain essentially unchanged, thus offering an explanation for the insensitivity of shell closures to exchange effects.

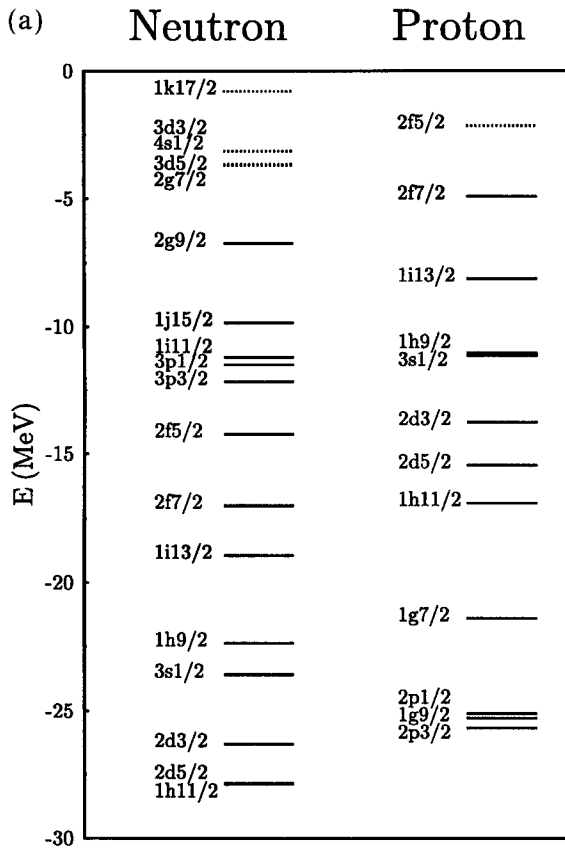


Fig. 4. Single-particle spectrum of $^{278}_{164}114$: (a) LDA-ZJO calculation, (b) MF-LZ calculation.

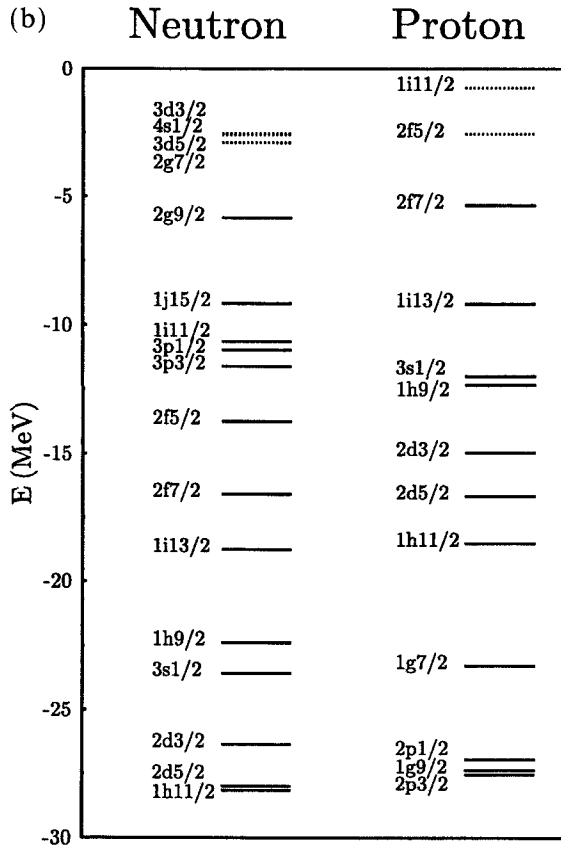


Fig. 4. (Continued)

In contrast, a MF calculation based on the nonlinear NLZ model⁽²²⁾ leads to a completely different picture, predicting $Z = 120$, $N = 172$ to be a double shell closure, as can be seen from Fig. 5. Our results for NLZ are in close agreement with the findings of Ref. 8 using the parametrization PL40. As all parametrizations considered here were obtained following the same principles, this demonstrates that exchange contributions, in spite of their nonlinear character, cannot serve as a substitute for the nonlinear meson self-interactions. This can be seen on a more microscopic level in Figs. 6 and 7 where the LZ, ZJO, NLZ and experimental charge densities of ^{48}Ca and ^{208}Pb are plotted. In particular, for ^{48}Ca the LDA-ZJO density differs substantially from both the experimental and the MF-NLZ result. Also, the LDA-ZJO binding energies are less accurate than the MF-NLZ values (see Table II).

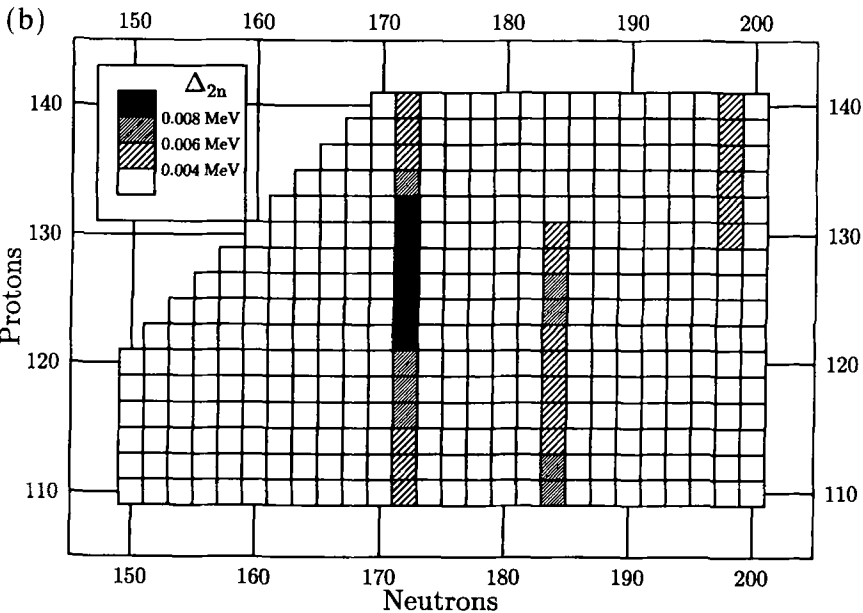
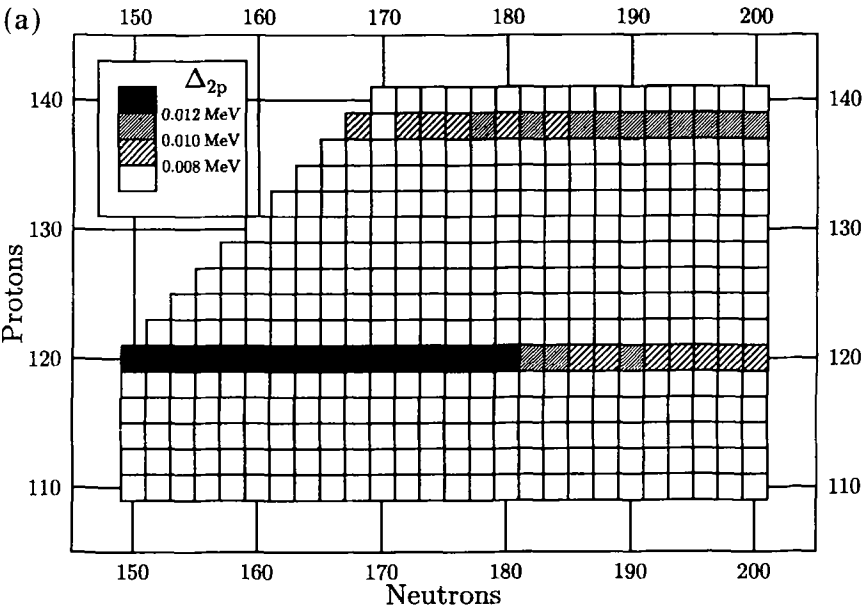


Fig. 5. Same as in Fig. 1 for MF-NLZ model.

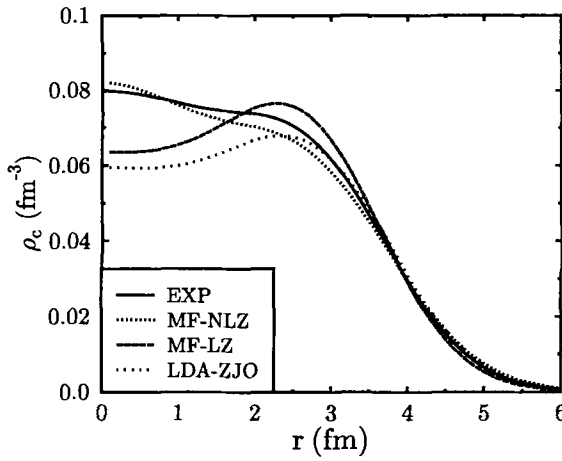


Fig. 6. Charge densities for ^{48}Ca obtained from LDA-ZJO, MF-LZ, and MF-NLZ calculations in comparison with experimental result.

However, this comparison also demonstrates that the LDA-ZJO results are more realistic than their MF-LZ counterparts, the LDA-ZJO density always being somewhat closer to the experimental result. This is corroborated by Table II, in which the charge radii and surface thicknesses obtained for a number of magic nuclei are compared with experimental

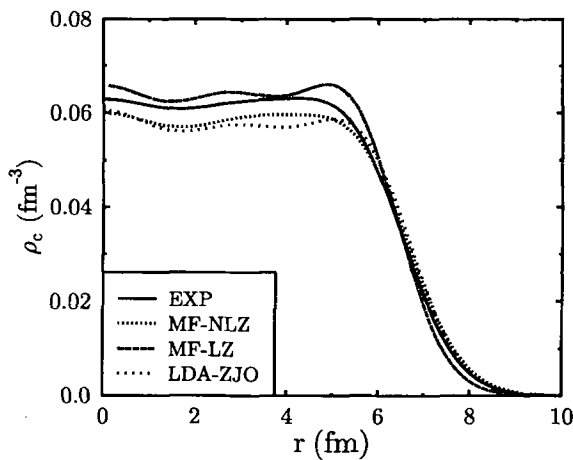


Fig. 7. Same as in Fig. 6 for ^{208}Pb .

Table II. Binding Energy per Nucleon (E/A), rms (r_p —Protons, r_n —Neutrons) and Charge (r_c) Radii as well as Surface Thickness (σ) Obtained from Linear MF-LZ and LDA-ZJO Models in Comparison with Results from Nonlinear MF-NLZ Parametrization and Experimental Data (Taken from Refs. 28, 22)

Nucleus	Method	E/A (MeV)	$r_n(fm)$	$r_p(fm)$	$r_c(fm)$	$\sigma(fm)$
^{48}Ca	MF-LZ	-8.62	3.83	3.34	3.43	0.762
	LDA-ZJO	-8.56	3.94	3.50	3.59	0.805
	MF-NLZ	-8.66	3.98	3.49	3.59	0.834
	exp	-8.67			3.45	0.868
^{90}Zr	MF-LZ	-8.84	4.28	4.11	4.19	0.679
	LDA-ZJO	-8.77	4.43	4.27	4.35	0.734
	MF-NLZ	-8.73	4.42	4.26	4.33	0.934
	exp	-8.71			4.26	0.949
^{116}Sn	MF-LZ	-8.60	4.67	4.43	4.50	0.691
	LDA-ZJO	-8.56	4.82	4.60	4.67	0.731
	MF-NLZ	-8.53	4.81	4.60	4.67	0.909
	exp	-8.52			4.63	0.925
^{124}Sn	MF-LZ	-8.46	4.83	4.48	4.55	0.688
	LDA-ZJO	-8.46	4.97	4.66	4.73	0.729
	MF-NLZ	-8.47	4.99	4.64	4.70	0.915
	exp	-8.47			4.68	0.891
^{208}Pb	MF-LZ	-7.82	5.72	5.33	5.39	0.764
	LDA-ZJO	-7.87	5.89	5.54	5.60	0.810
	MF-NLZ	-7.88	5.97	5.54	5.60	0.942
	exp	-7.88			5.50	0.885

data. For all nuclei considered the surface thicknesses (σ) found with the LDA-ZJO are somewhere in-between the MF-LZ and the MF-NLZ values, the latter being closest to the experimental σ 's. In addition, the LDA-ZJO proton and neutron rms radii are in very good agreement with the MF-NLZ values, in contrast to the MF-LZ radii (see Table II). Also, the proton shell closure at $Z = 120$, which dominates in the case of the MF-NLZ calculation, is more pronounced for the LDA-ZJO than for the MF-LZ model. So, while the inclusion of exchange does not allow one to drop the nonlinear self-interactions completely, there is a clear tendency to approach the NLZ model, indicating a partial incorporation of nonlinear contributions. Finally, it is obvious from Figs. 3, 4, 6, and 7 and Table II that on a local level exchange effects cannot be absorbed into mean-field models by a suitable choice of the parametrization.

4. CONCLUDING REMARKS

In summary, we have examined the relevance of exchange contributions for the description of superheavy nuclei within a linear QHD-II model. It turned out that their effect on shell closures is negligible. On the other hand, for the detailed properties of nuclei one observes significant differences between the MF-LZ and the LDA-ZJO model, the latter consistently improving over the former. Moreover, while the overall performance of the linear model including exchange cannot compete with that of the nonlinear MF approach, all individual nuclear properties develop into the direction of the nonlinear MF results when going from the linear MF to the linear LDA model. This partial representation of nonlinear contributions by the LDA exchange raises the question whether the meson self-coupling can be interpreted as a parametrized form of exchange-correlation effects on a microscopic level. It thus seems worthwhile to investigate whether the inclusion of many-body corrections beyond the HF level can bridge the presently remaining gap between linear LDA and nonlinear MF results.

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25. Unfortunately, this inversion leads to numerical difficulties in the asymptotic regime with its exponentially decaying densities. To deal with this problem one resorts to a perturbative evaluation of $e_x^{INM}(\rho_p, \rho_n, \rho_s)$, in which the difference between ρ_s and $\tilde{\rho}_s$ is taken into account to first order,

$$e_x^{INM}(\rho_s) \approx \tilde{e}_x^{INM}(M^*) + \frac{d\tilde{e}_x^{INM}}{dM^*}(M^*) \left(\frac{d\tilde{\rho}_s}{dM^*}(M^*) \right)^{-1} (\rho_s - \tilde{\rho}_s)$$

with $M^*(x)$ taken from (14) (for fixed ρ_p and ρ_n , which are here suppressed for brevity).

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