Structure of superheavy elements reexamined.

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1. Motivation and introduction
2. Reexamining shell structure in covariant density functional theory
3. Confronting experimental data
4. Conclusions

In collaboration with S. Abgemava (MSU), P. Ring (TU Munich), T. Nakatsukasa (Tsukuba U), H. Abusara (MSU) and E. Litvinova (West Michigan U)
Density functional theories give the largest variations in the predictions of magic gaps at $Z=120$, 126 and 172, 184.
Covariant density functional theory (CDFT)

The nucleons interact via the exchange of effective mesons \( \rightarrow \) effective Lagrangian

\[
E_{\text{RMF}}[\hat{\rho}, \phi_m] = \text{Tr}[(\mathbf{a}\mathbf{p} + \mathbf{b}\mathbf{m})\hat{\rho}] \pm \int \left[ \frac{1}{2}(\nabla \phi_m)^2 + U(\phi_m) \right] \, d^3r + \text{Tr}[\{\Gamma_m \phi_m\} \hat{\rho}]
\]

density matrix \( \hat{\rho} \)

\[
\phi_m \equiv \{\sigma, \omega^{\mu}, \vec{\rho}^{\mu}, A^{\mu}\} - \text{meson fields}
\]

Mean field

\[
\hat{h} = \frac{\delta E}{\delta \hat{\rho}}
\]

Eigenfunctions

\[
\hat{h}\Phi_i = \varepsilon_i \Phi_i
\]
Two major differences between the state-of-the-art classes of covariant energy density functionals:

1. Range of interaction (finite => mesons are included) (zero => no meson, point-coupling models)

2. Effective density dependence
   - non-linear (through the power of sigma-meson)
   - explicit

Fitting protocol - another source of theoretical uncertainties in the definition of the functionals

All deformed calculations presented here were obtained in axial Relativistic Hartree-Bogoliubov (RHB) framework with separable pairing (see S. Agbemava et al, PRC 92, 054310 (2015)).
The basic idea comes from *ab initio* calculations. Density dependent coupling constants include Brueckner correlations and three-body forces.

Effectual interactions with medium-dependent couplings:

\[ g_\sigma(\rho), \quad g_\omega(\rho), \quad g_\rho(\rho) \]

Remove mesons $\rightarrow$ point coupling models with derivative terms.
Meson-exchange models

\[
\mathcal{L} = \bar{\psi} \left[ \gamma (i \partial - g_\omega \omega - g_\rho \bar{\rho} \bar{\tau} - eA) - m - g_\sigma \sigma \right] \psi \\
+ \frac{1}{2} (\partial \sigma)^2 - \frac{1}{2} m_\sigma^2 \sigma^2 - \frac{1}{4} \Omega_{\mu\nu} \Omega^{\mu\nu} + \frac{1}{2} m_\omega^2 \omega^2 \\
- \frac{1}{4} \bar{R}_{\mu\nu} R^{\mu\nu} + \frac{1}{2} m_\rho \bar{\rho}^2 - \frac{1}{4} F_{\mu\nu} F^{\mu\nu},
\]

Non-linear models

\[
U(\sigma) = \frac{1}{2} m_\sigma^2 \sigma^2 + \frac{1}{3} g_2 \sigma^3 + \frac{1}{4} g_3 \sigma^4
\]

Models with explicit density dependence

no nonlinear terms in the \( \sigma \) meson

\[
g_i(\rho) = g_i(\rho_{\text{sat}}) f_i(x) \quad \text{for} \quad i = \sigma, \omega, \rho
\]

\[
f_i(x) = a_i \frac{1 + b_i (x + d_i)^2}{1 + c_i (x + d_i)^2}
\]

\[
f_\rho(x) = \exp[-a_\rho (x - 1)]
\]

\[
x = \rho / \rho_{\text{sat}}
\]

NL3*

DD-ME2, DD-ME\( \delta \)
Theoretical errors in the description of masses

<table>
<thead>
<tr>
<th>EDF</th>
<th>measured</th>
<th>measured + estimated</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$\Delta E_{\text{rms}}$</td>
<td>$\Delta E_{\text{rms}}$</td>
</tr>
<tr>
<td>NL3*</td>
<td>2.96</td>
<td>3.00</td>
</tr>
<tr>
<td>DD-ME2</td>
<td>2.39</td>
<td>2.45</td>
</tr>
<tr>
<td>DD-ME$\delta$</td>
<td>2.29</td>
<td>2.40</td>
</tr>
<tr>
<td>DD-PC1</td>
<td>2.01</td>
<td>2.15</td>
</tr>
</tbody>
</table>

Uncertainties in radii

<table>
<thead>
<tr>
<th>CEDF</th>
<th>$\Delta r_{ch}^{\text{rms}}$ [fm]</th>
</tr>
</thead>
<tbody>
<tr>
<td>NL3*</td>
<td>0.0283</td>
</tr>
<tr>
<td>DD-ME2</td>
<td>0.0230</td>
</tr>
<tr>
<td>DD-ME$\delta$</td>
<td>0.0329</td>
</tr>
<tr>
<td>DD-PC1</td>
<td>0.0253</td>
</tr>
</tbody>
</table>

S. Agbemava, AA, D, Ray, P. Ring, PRC 89, 054320 (2014) includes complete DD-PC1 mass table as supplement
Reexamining the structure of superheavy nuclei in CDFT

Detailed results in S. Agbemava et al, PRC 92, 054310 (2015)

**Covariant density functional theory: Reexamining the structure of superheavy nuclei**
Deformation effects on shell structure

→ Very important – deformed results differ substantially from spherical ones

Unusual feature: oblate shapes above the spherical shell closures

Results for PC-PK1 are very similar to the ones with NL3*
Open circles – experimentally observed nuclei

**DD-PC1:** Experimental $Z=116, 118$ nuclei are oblate

**PC-PK1:** Experimental $Z=118$ nucleus is spherical

Other experimental SHE are prolate
Potential energy surfaces in axially symmetric RHB calculations with separable pairing
The source of oblate shapes – the low density of s-p states
Confronting experimental data
**Table I:** Average deviations per state $\Delta \epsilon$ between calculated and experimental energies of the single-particle states for a proton (neutron) subsystem of a given nucleus. The results are shown for different nuclei and combinations of subshells:

<table>
<thead>
<tr>
<th>Nucleus/subsystem</th>
<th>$\Delta \epsilon_{def+TO}$ [MeV]</th>
<th>$\Delta \epsilon_{def+TO+PVC}$ [MeV]</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{56}$Ni/proton</td>
<td>0.76</td>
<td>0.77</td>
</tr>
<tr>
<td>$^{56}$Ni/neutron</td>
<td>0.89</td>
<td>0.71</td>
</tr>
<tr>
<td>$^{132}$Sn/proton</td>
<td>1.02</td>
<td>0.68</td>
</tr>
<tr>
<td>$^{132}$Sn/neutron</td>
<td>0.89</td>
<td>0.39</td>
</tr>
<tr>
<td>$^{208}$Pb/proton</td>
<td>1.53</td>
<td>0.84</td>
</tr>
<tr>
<td>$^{208}$Pb/neutron</td>
<td>1.00</td>
<td>0.47</td>
</tr>
</tbody>
</table>

**Key:**
- **Particle-vibration coupling** + TO, TE polarization effects
- **NL3* functional**
The description of deformed states at DFT level is better than spherical ones by a factor 2-3 (and by a factor ~1 (neutron) and ~2 (proton) as compared with spherical PVC calculations).

<table>
<thead>
<tr>
<th>Region</th>
<th>calculated states (#)</th>
<th>compared states (#)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Actinides (NL3*)</td>
<td>415</td>
<td>209</td>
</tr>
<tr>
<td>Actinides (NL1)</td>
<td>444</td>
<td>217</td>
</tr>
<tr>
<td>Rare-earth (NL1)</td>
<td>360</td>
<td>149</td>
</tr>
</tbody>
</table>

Triaxial CRHB; fully self-consistent blocking, time-odd mean fields included, NL3*, Gogny D1S pairing, AA and S.Shawaqfeh, PLB 706 (2011) 177

Two sources of deviations:
1. Low effective mass (stretching of the energy scale)
2. Wrong relative energies of the states

Similar problems in Skyrme and Gogny DFT
Accuracy of the description of experimental data in $Z>94$ nuclei

<table>
<thead>
<tr>
<th>CEDF</th>
<th>$\Delta E_{rms}$ [MeV]</th>
<th>$\Delta (S_{2n})_{rms}$ [MeV]</th>
<th>$\Delta (S_{2p})_{rms}$ [MeV]</th>
<th>$\Delta (Q_\alpha)_{rms}$ [MeV]</th>
</tr>
</thead>
<tbody>
<tr>
<td>NL3*</td>
<td>3.02/3.39</td>
<td>0.71/0.68</td>
<td>1.33/1.34</td>
<td>0.68/0.75</td>
</tr>
<tr>
<td>DD-ME2</td>
<td>1.39/1.40</td>
<td>0.45/0.54</td>
<td>0.85/0.90</td>
<td>0.51/0.65</td>
</tr>
<tr>
<td>DD-MEδ</td>
<td>2.52/2.45</td>
<td>0.60/0.51</td>
<td>0.45/0.48</td>
<td>0.39/0.51</td>
</tr>
<tr>
<td>DD-PC1</td>
<td>0.59/0.74</td>
<td>0.30/0.32</td>
<td>0.41/0.42</td>
<td>0.36/0.47</td>
</tr>
<tr>
<td>PC-PK1</td>
<td>2.82/2.63</td>
<td>0.25/0.23</td>
<td>0.36/0.33</td>
<td>0.32/0.38</td>
</tr>
</tbody>
</table>

With exception of the DD-MEδ, the deformed $N=162$ gap is well reproduced in all CEDF’s.
The $Q_\alpha$-values

(a) NL3*

(b) DD-ME2

(c) DD-MEδ

(d) DD-PC1
Fission barriers: theory versus experiment [state-of-the-art]

Mac+mic, LSD model

Mac+mic, FRDM model

Gogny DFT,


No fit of functionals (parameters) to fission barriers or fission isomers only in mac+mic (Kowal) and CDFT
A. Staszczak et al, PRC 87, 024320 (2013) – Skyrme SkM*
Inner fission barrier heights as obtained in axially symmetric RHB with separable pairing provides upper limit for inner barrier height.
Conclusions

1. The accuracy of the description and theoretical uncertainties have been quantified for
   - **deformations** [PRC 88, 014320 (2013) and PRC 92, 054310 (2015)]
   - masses, separation energies [PRC 89, 054320 (2014), 92, 054310 (2015)]
   - α-decays [PRC 92, 054310 (2015)]
   - fission barriers [PLB 689, 72 (2010), PRC 82, 044303 (2010), PRC 85, 024314 (2012), also in progress]
   - pairing [PRC 88, 014320 (2013) and PRC 89, 054320 (2014)] in actinides and superheavy nuclei.

2. Detailed analysis with deformation included does not confirm the importance of the N=172 spherical shell gap. On the contrary, a number of functionals show important role of the N=184 shell gap.

3. Some functionals do not predict spherical SHE around Z=120 and N=184 lines !!!
Conclusions

4. Available experimental data in actinides and SHE does not allow to give a clear preference to a specific functional predictions in the $Z \sim 120, N \sim 184$ region.

5. Be careful with the predictions based on $\delta_{2n}(Z,N)$ and $\delta_{2p}(Z,N)$ quantities obtained in spherical calculations !!!

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