Nuclear structure in the Quark-Meson Coupling (QMC) model

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Motivation
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Finite Nuclei in the Quark-Meson Coupling Model

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We report the first use of the effective quark-meson coupling (QMC) energy density functional (EDF),
derived from a quark model of hadron structure, to study a broad range of ground state properties of even-
even nuclei across the periodic table in the nonrelativistic Hartree-Fock + BCS framework. The novelty of
the QMC model is that the nuclear medium effects are treated through modification of the internal structure
of the nucleon. The density dependence is microscopically derived and the spin-orbit term arises naturally.
The QMC EDF depends on a single set of four adjustable parameters having a clear physics basis. When
applied to diverse ground state data the QMC EDF already produces, in its present simple form, overall
agreement with experiment of a quality comparable to a representative Skyrme EDF. There exist, however,
multiple Skyrme parameter sets, frequently tailored to describe selected nuclear phenomena. The QMC
EDF set of fewer parameters, derived in this work, is not open to such variation, chosen set being applied,
without adjustment, to both the properties of finite nuclei and nuclear matter.

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- The QMC model energy density functional (EDF) was successfully employed to investigate several ground state properties of even-even finite nuclei across the nuclear chart
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- A derivative-free optimization procedure (POUNDerS) is available to use to optimize nuclear EDFs.
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- A derivative-free optimization procedure (POUNDerS) is available to use to optimize nuclear EDFs.
- Several nuclear observables are left to be studied using the QMC model and further development in the model is sought for better predictions of such observables.
Motivation


The QMC Model
The QMC Model employs relativistic mean-field theory.
The QMC Model

- employs relativistic mean-field theory
- utilises the MIT bag model of a nucleon; assumes that nucleon bags do not overlap
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- interactions are described through the scalar $\sigma$ meson for the intermediate range attraction, vector meson $\omega$ for the short range repulsion, and vector-isovector $\rho$ for isospin dependence
The QMC Model

Nucleon effective mass:

\[ M_B^* = M_B - g_\sigma \sigma + \frac{d}{2}(g_\sigma \sigma)^2 \]
The QMC Model

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\[ M_B^* = M_B - g_\sigma \sigma + \frac{d}{2} (g_\sigma \sigma)^2 \]

The classical total energy

\[ E_{QMC} = \sum_{i=1,\ldots} \sqrt{P_i^2 + M_i^2(\sigma(\vec{R}_i))} + g_\omega^i \omega(\vec{R}_i) + g_\rho \vec{l}_i \cdot \vec{B}(\vec{R}_i) + E_\sigma + E_{\omega,\rho} \]
The QMC Model

To get the Hamiltonian, $H_{QMC}$, we eliminate the meson fields by solving the equations of motion:

$$\frac{\delta H_{QMC}}{\delta \sigma(\vec{r})} = \frac{\delta H_{QMC}}{\delta \omega(\vec{r})} = \frac{\delta H_{QMC}}{\delta B(\vec{r})} = 0$$
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HF calculation

$$\mathcal{E}_{QMC} = \langle \Phi | H_{QMC} | \Phi \rangle$$
The QMC Model

Method

Results

Conclusion

QMC model for finite nuclei

Densities

\[ \rho_m(\vec{r}) = \sum_{i \in F_m} \sum_{\sigma} \left| \phi^i(\vec{r}, \sigma, m) \right|^2, \quad \rho = \rho_p + \rho_n, \]

\[ \tau_m(\vec{r}) = \sum_{i \in F_m} \sum_{\sigma} \left| \nabla \phi^i(\vec{r}, \sigma, m) \right|^2, \quad \tau = \tau_p + \tau_n, \]

\[ \vec{J}_m = i \sum_{i \in F_m} \sum_{\sigma \sigma'} \vec{\sigma}_{\sigma' \sigma} \times \left[ \nabla \phi^i(\vec{r}, \sigma, m) \right] \phi^{i*}(\vec{r}, \sigma', m), \]

\[ \vec{J} = \vec{J}_p + \vec{J}_n \]
QMC model for finite nuclei

The contributions to the QMC Hamiltonian can be written as

\[ H_{QMC} = H_0 + H_3 + H_{\text{eff}} + H_{\text{fin}} + H_{\text{so}} + H_\pi \]

- \( H_0 + H_3 \propto \rho^2 \): QMC density-dependent terms
- \( H_{\text{eff}} \propto \rho \tau \): effective mass term
- \( H_{\text{fin}} \propto \nabla^2 \rho \): finite size effect
- \( H_{\text{so}} \propto \nabla \cdot \vec{J} \): spin-orbit
- \( H_\pi \): single-pion exchange
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- \( H_{\pi} \) single-pion exchange

Model parameters: \( G_{\mu} = \frac{g_{\mu}}{m_{\mu}^2} \) (\( \mu = \sigma, \omega, \rho \)), \( m_\sigma \), and \( \lambda_3 \)
The pairing EDF

HF+BCS pairing

\[ \mathcal{E}_{\text{pair}, q} = \frac{1}{4} S_q(\vec{r}) \rho^2_q, \quad \chi_q(\vec{r}) = \sum_{\alpha \in q} u_\alpha v_\alpha |\phi_\alpha(\vec{r})|^2 \]

Pairing strength

\[ S_q(\vec{r}) = V_q \left[ 1 - \left( \frac{\rho(\vec{r})}{\rho_c} \right)^{\alpha} \right] \]

Volume pairing / Delta force (DF) pairing
Surface pairing / Density dependent delta interaction (DDDI)
The QMC Model

Method

Results

Conclusion

The QMC-derived pairing EDF

Pairing potential

\[ V(\vec{r} - \vec{r}') = - \left( \frac{G_\sigma}{1 + d' G_\sigma \rho(\vec{r})} - G_\omega - \frac{G_\rho}{4} \right) \delta(\vec{r} - \vec{r}') \]

\[ d' = d + \frac{1}{3} G_\sigma \lambda_3 \]
The QMC-derived pairing EDF

**Pairing potential**

\[
V(\vec{r} - \vec{r}') = - \left( \frac{G_\sigma}{1 + d' G_\sigma \rho(\vec{r})} - G_\omega - \frac{G_\rho}{4} \right) \delta(\vec{r} - \vec{r}')
\]

\[
d' = d + \frac{1}{3} G_\sigma \lambda_3
\]

**EDF parameters**

\[
V_q = G_\sigma - G_\omega - \frac{G_\rho}{4}, \quad \rho_c = \frac{V_q (1 + d' G_\sigma \rho)}{d' G_\sigma^2}, \quad \alpha = 1
\]
Coulomb and center-of-mass correction

\[ \mathcal{E}_{\text{Coulomb}} = e^2 \frac{1}{2} \int d^3r d^3r' \frac{\rho_p(\vec{r})\rho_p(\vec{r}')}{|\vec{r} - \vec{r}'|} - \frac{3}{4} e^2 \left( \frac{3}{\pi} \right)^{1/3} \int d^3r [\rho_p]^{4/3} \]

\[ \mathcal{E}_{\text{c.o.m.}} = -\langle \hat{P}_{\text{cm}}^2 \rangle / (2mA) \]
## QMC versions

<table>
<thead>
<tr>
<th>version</th>
<th>pion</th>
<th>$\tilde{m}_\sigma$</th>
<th>$\lambda_3$</th>
<th>full SO</th>
<th>$\tilde{J}$</th>
<th>pairing</th>
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<td>QMC-I$^{[1]}$</td>
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<td>✓</td>
<td></td>
<td></td>
<td></td>
<td>DF</td>
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<td>✓</td>
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<td></td>
<td>DF</td>
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<tr>
<td>QMC$\pi$-II$^{[8, 9]}$</td>
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<td>bare</td>
<td>✓</td>
<td>✓</td>
<td></td>
<td>DF</td>
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<tr>
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<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>DDDI (QMC)</td>
</tr>
</tbody>
</table>
Method
Parameter optimization

Figure 1: Doubly-magic and semi-magic nuclei included in the fit. The nuclear observables and number of data points per nucleus entering the fitting procedure are indicated.
POUNDerS algorithm

Objective function $F(\hat{x})$ for minimisation

$$F(\hat{x}) = \sum_{i}^{n} \sum_{j}^{o} \left( \frac{\bar{s}_{ij} - s_{ij}}{w_{j}} \right)^{2}$$

where

- $n$ total number of nuclei
- $o$ total number of observables
- $s_{ij}$ experimental values
- $\bar{s}_{ij}$ fitted values
- $w_{j}$ effective error

$w_{BE} = 1.0 \text{ MeV}$
$w_{R_{ch}} = 0.02 \text{ fm}$
$w_{\Delta_{p,n}} = 0.12 \text{ MeV}$
Results
QMC and pairing parameters

<table>
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<tr>
<th></th>
<th>QMC_(\pi)-III</th>
<th>QMC_(\pi)-II</th>
<th>QMC_(\pi)-I</th>
<th>QMC-I</th>
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<tr>
<td>(G_\sigma) [fm(^2)]</td>
<td>9.62</td>
<td>9.66</td>
<td>11.16</td>
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<td>(G_\omega) [fm(^2)]</td>
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<td>5.23</td>
<td>8.00</td>
<td>8.27</td>
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<tr>
<td>(G_\rho) [fm(^2)]</td>
<td>4.71</td>
<td>4.75</td>
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<td>7.68</td>
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<td>(M_\sigma) [MeV]</td>
<td>503</td>
<td>493</td>
<td>712</td>
<td>722</td>
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<td>(\lambda_3) [fm(^{-1})]</td>
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<td>0.05</td>
<td>-</td>
<td>-</td>
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<td>(V_p) [MeV]</td>
<td>-</td>
<td>258</td>
<td>302</td>
<td>284</td>
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<tr>
<td>(V_n) [MeV]</td>
<td>-</td>
<td>237</td>
<td>291</td>
<td>326</td>
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Correlation matrix

Figure 2: Correlation matrix for QMCπ-II and QMCπ-III
## QMC nuclear matter properties

<table>
<thead>
<tr>
<th>NMP</th>
<th>QMC(\pi\text{-III} )</th>
<th>QMC(\pi\text{-II} )</th>
<th>QMC(\pi\text{-I} )</th>
<th>QMC-I</th>
<th>SV-min</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\rho_0 \text{ (fm}^{-3})</td>
<td>0.15</td>
<td>0.15</td>
<td>0.15</td>
<td>0.16</td>
<td>0.16</td>
</tr>
<tr>
<td>(E_0 \text{ (MeV)})</td>
<td>-15.7</td>
<td>-15.7</td>
<td>-15.8</td>
<td>-15.9</td>
<td>-15.9</td>
</tr>
<tr>
<td>(a_0 \text{ (MeV)})</td>
<td>29</td>
<td>29</td>
<td>30</td>
<td>30</td>
<td>31</td>
</tr>
<tr>
<td>(L_0 \text{ (MeV)})</td>
<td>43</td>
<td>40</td>
<td>17</td>
<td>23</td>
<td>93</td>
</tr>
<tr>
<td>(K_0 \text{ (MeV)})</td>
<td>233</td>
<td>230</td>
<td>319</td>
<td>340</td>
<td>222</td>
</tr>
</tbody>
</table>
Even-even nuclei across the nuclear chart

Figure 3: QMCπ-III predictions for (a) BE residuals and (b) absolute BE % deviation for even-even nuclei with known masses. Magic numbers are specified with solid lines while symmetric nuclei, $Z = N$, are shown with dashed lines.
Even-even nuclei across the nuclear chart

Figure 4: QMC$\pi$-III predictions for (a) $R_{ch}$ residuals and (b) $R_{ch}$ % deviation for even-even nuclei with known radii. Magic numbers are specified with solid lines while symmetric nuclei, $Z = N$, are shown with dashed lines.
Even-even nuclei across the nuclear chart

Root-mean-square residuals:

\[
\sqrt{\frac{1}{d} \sum_i^n \sum_j^o (\bar{s}_{ij} - s_{ij})^2}
\]

<table>
<thead>
<tr>
<th>Model</th>
<th>$BE$ (MeV)</th>
<th>$R_{ch}$ (fm)</th>
<th># of parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td>QMC$\pi$-III</td>
<td>1.59</td>
<td>0.024</td>
<td>5</td>
</tr>
<tr>
<td>QMC$\pi$-II</td>
<td>2.34</td>
<td>0.029</td>
<td>5+2</td>
</tr>
<tr>
<td>SV-min</td>
<td>3.64</td>
<td>0.024</td>
<td>11+3</td>
</tr>
<tr>
<td>UNEDF1</td>
<td>2.06</td>
<td>0.029</td>
<td>11+2</td>
</tr>
<tr>
<td>DD-ME$\delta$</td>
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<td>0.035</td>
<td>14+2</td>
</tr>
<tr>
<td>FRDM</td>
<td>0.89</td>
<td>-</td>
<td>17</td>
</tr>
</tbody>
</table>
Two-neutron separation energy

Figure 5: Two-neutron separation energies for calcium ($Z = 20$) and nickel ($Z = 28$) isotopes as a function of the neutron number.
Two-neutron shell gap

**Figure 6:** Two-neutron shell gaps for Ca, Ni, Sn, and Pb isotopes.
Driplines

Figure 7: Neutron driplines for Ca, Ni, Sn, and Pb isotopes predicted by QMCπ-III.
Figure 8: Charge density plots from various QMC versions compared to data from elastic scattering experiment.
Skin thickness

Figure 9: Skin thickness for nuclei included in the QMC fit as a function of the neutron excess.

Δ$r_{np}$ fit to expt. data
Antiprotonic x-ray expts.
Hadron scattering expts.
SVmin-HFBTHO
UNEDF1
DD-MEδ
QMCπ-II
QMCπ-III
Skin thickness and the slope of symmetry energy

Figure 10: Neutron skin thickness plotted against $L_0$ for isotopes $^{48}$Ca (red) and $^{208}$Pb (blue) from various nuclear models.
Nuclear deformations

Figure 11: QMCπ-III predictions for (a) quadrupole deformation parameter, $\beta_2$, and (b) corresponding residuals upon comparison with available data [11]. Magic numbers are specified with solid lines while symmetric nuclei, $Z = N$, are shown with dashed lines.
Binding energies of even-even superheavy elements (SHE)

Figure 12: SHE binding energy residuals for nuclei with $Z \geq 100$ plotted against mass number $A$. 
Subshell closures in the SHE region

Figure 13: Two-neutron separation energies plotted against neutron number. Results from QMCπ-III are shown as filled symbols and connected by lines while experimental data and errors are shown as empty symbols with vertical errorbars. Subshell closures at \( N = 152 \) and \( N = 162 \) are indicated with dashed lines. Inset shows the \( S_{2n} \) values plotted against \( N \) for SHE with \( Z \geq 112 \).
Nuclear deformations in the SHE region

Figure 14: Comparison of deformation parameter, $\beta_2$, values along the Fm, No, Rf, and Sg isotopic chains from several nuclear models. For QMC$\pi$-III, the first minima are shown as filled red symbols, while the other minima, which are very close to the first, are shown as empty red symbols and labelled ‘QMC$\pi$-III*’.
Conclusion
Summary and conclusions

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- QMC$\pi$-II and QMC$\pi$-III were optimised, parameter errors and correlations were presented and the final parameter set was used to calculate various nuclear observables
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- Ground state properties of even-even nuclei across the nuclear chart were computed and were shown to be comparable with those of other well known nuclear models
- Calculations were extended to other nuclear observables which had not been part of the fit
Thank you for your attention.
References I


References II


