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Reactions of exotic nuclei with the quark-meson coupling model

E. McRae[1,⋆], *C.* Simenel[1], *E. C.* Simpson[1], and *A. W.* Thomas[2]

[1]*Department of Nuclear Physics, Research School of Physics and Engineering, The Australian National University, Canberra, ACT 2601, Australia*
[2]*ARC Centre of Excellence for Particle Physics at the Terascale and CSSM, Department of Physics, The University of Adelaide, SA 5005, Australia*

Abstract. The nucleon-nucleon interaction is an important requirement for investigations of nuclear structure and reactions, as well as for astrophysical models such as r-process nucleosynthesis and neutron stars. The traditional approach to low-energy nuclear physics is to treat nucleons as immutable objects interacting via phenomenological forces. The use of phenomenological interactions, rather than one derived from a microscopic theory, raises questions as to the reliability of predictions for exotic regions of the nuclear chart. The quark-meson coupling (QMC) model uses a relativistic mean-field approach to provide a microscopically derived nucleon-nucleon interaction, which takes into account the quark structure of the nucleon.
The Skyrme energy density functional is a popular phenomenological tool in studies of nuclear structure and reactions. In this work, the QMC density functional was used to produce a set of Skyrme parameterisations, in the hopes that they will give more reliable predictions for exotic nuclei. In conjunction with Hartree-Fock-Bogoliubov (HFB) calculations, the Skyrme-QMC (SQMC) parameterisations have been used to model the ground-state properties of individual nuclei and nucleus-nucleus potentials for Ca + Sn reactions. The SQMC parameterisation performs with an accuracy comparable to modern phenomenological functionals. From this, one can investigate the importance of the isovector terms of the nucleon-nucleon interaction, which are particularly significant for exotic, neutron-rich regions of the nuclear chart.
One of the notable successes of the QMC model is its derivation of nuclear spin-orbit coupling. The isovector dependence of the spin-orbit equation of state is remarkably similar to that of the modern UNEDF1 phenomenological density functional. HFB calculations along the Sn isotopic chain reveal that the isovector properties of the spin-orbit term impact binding energies to a level that will be significant for astrophysical r-process modelling.

1 Introduction

The behaviour of exotic nuclear systems is an important question for nuclear, particle and astrophysics. While new experimental facilities and techniques are constantly expanding the limits of known nuclei, many regions remain largely out of reach, including the astrophysical r-process path, superheavy elements, and the neutron dripline.

Theoretically, one is faced with the quantum many-body problem posed by a system of strongly interacting nucleons. One of the most successful tools currently used is the Skyrme energy density functional. It gives the energy density at each point in the nuclear system, as a function of the local nucleon densities. The functional can be derived from the Skyrme interaction [1], which is the most general two-body, zero-range nucleon-nucleon interaction up to second-order in derivatives. The downside of the Skyrme density functional is that it is phenomenological. Its set of 10–17 parameters are typically determined by a fit to experimental masses and radii of nuclides near stability, calling into question the predictions for very exotic systems. A possible solution to this is to obtain the interaction between nucleons from the more fundamental, high-energy degrees-of-freedom of the system.

The quark-meson coupling (QMC) model is a relativistic mean-field approach which self-consistently accounts for the in-medium modification of the quark structure of bound nucleons. Proposed by P. A. M. Guichon in Ref. [2], and since developed in Refs. [3–5], it confines three quarks to a nucleon bag and allows the quarks of different bags to interact by exchanging σ, ω and ρ mesons. This results in an energy density functional with only four free parameters (a coupling constant for each meson field and the mass of the σ meson). The reduced number of parameters should make the QMC model more predictive than standard phenomenological approaches.

Thanks to its inclusion of quark degrees-of-freedom, the QMC model offers a possible explanation to the famous "European Muon Collaboration" (EMC) effect [6–8] and also gives a remarkably successful description of hypernuclei [9, 10].

While the QMC model assumes that nucleons move slowly, the quarks are treated relativistically and the model

⋆e-mail: ellen.mcrae@anu.edu.au

naturally includes certain relativistic corrections. Most notably, the model derives nuclear spin-orbit coupling, a relativistic effect essential for shell structure of nuclei and dissipation in collisions.

2 Spin-orbit energy density functional

2.1 The QMC model

The spin-orbit energy density functional from the QMC model is given by [4]

$$\mathcal{H}_{\rm SO}^{\rm QMC} = \frac{-1}{4M_N^2}\Big[\left(G_\sigma + G_\omega\left(2\mu_s - 1\right)\right)\rho\nabla\cdot\boldsymbol{J} + \left(\frac{G_\sigma}{2} + \frac{G_\omega}{2}\left(2\mu_s - 1\right) + \frac{3G_\rho}{8}\left(2\mu_v - 1\right)\right) \times \sum_{q=n,p}\rho_q\nabla\cdot\boldsymbol{J}_q\Big], \quad (1)$$

where ρ_n (ρ_p) is the neutron (proton) particle density and ρ is the total particle density, $\rho = \rho_n + \rho_p$; similarly for the spin-orbit density, $\boldsymbol{J}$. The coefficients are formed from the meson coupling constants (G_σ, G_ω, G_ρ), the isoscalar and isovector nucleon magnetic moments (μ_s and μ_v, respectively), and the free nucleon mass (M_N). Though not strictly necessary, the ω and ρ meson fields can be identified with real particles and their experimental masses used. This leaves only four free parameters in the QMC model, G_σ, G_ω, G_ρ and the σ meson mass, all of which are fixed by the central terms of the functional. Unlike non-relativistic approaches such as Skyrme, the QMC spin-orbit functional has no extra spin-orbit parameters to adjust. The small number of free parameters in the QMC model is expected to make it more predictive than a standard Skyrme functional, particularly for the spin-orbit term.

2.2 Skyrme

The most general form of the Skyrme density functional [11],

$$\mathcal{H}_{\rm SO}^{\rm Skyrme} = -\frac{1}{2}\Big[W_0\rho\nabla\cdot\boldsymbol{J} + W_0'\sum_{q=n,p}\rho_q\nabla\cdot\boldsymbol{J}_q\Big], \quad (2)$$

takes the same form of the nucleon densities but now with free coefficients W_0 and W_0'. As the Skyrme interaction is non-relativistic, obeying Galilean rather than Lorentz invariance, the coefficients of the spin-orbit term are completely unknown and must be adjusted to experiment.

2.3 Isovector dependence

The isovector dependence of the spin-orbit functionals quantifies how they are affected by differences between proton and neutron densities, which become increasingly important for studying very neutron rich nuclei. It is controlled by the second term of equations 1 and 2, as the proton and neutron densities appear individually. Therefore, the ratio of the two coefficients can be used to compare the isovector properties of different approaches, as done in Table 1.

Table 1. Ratio of the spin-orbit coupling constants illustrating the isovector dependence of spin-orbit energy density functionals.

W_0'/W_0	Model
1	Standard Skyrme
1.86	Modern Skyrme: UNEDF1 [12]
1.78	QMC
0.1	Standard relativistic mean-field (RMF) [13]
0.2	QMC, Hartree terms only, Dirac μ

Table 2. Parameters of the spin-orbit functional.

Model	W_0 (MeV fm^5)	W_0' (MeV fm^5)
QMC	82.8602	147.4411
UNEDF1	76.736144	142.63304

Traditionally, Skyrme functionals only had one spin-orbit parameter, W_0. The modern Universal Nuclear Energy Density Functional (UNEDF1) [12] released this constraint, and from its state-of-the-art fitting procedure, had actually derived a much stronger isovector dependence. The QMC model, with its more fundamental, relativistic basis gives a very similar value.

On the other hand, a standard relativistic mean-field (RMF) model of inert nucleons, neglecting exchange (Fock) terms, gives a substantially weaker isovector dependence. By keeping only the direct (Hartree) terms of the QMC spin-orbit functional and setting the nucleon magnetic moments to their Dirac ($\mu_s = \mu_v = 1$) rather than experimental ($\mu_s = 0.88$, $\mu_v = 4.7$) values, one would obtain a similarly weak isovector dependence. This implies that the weak isovector dependence of RMF is primarily due to these two approximations, neglect of exchange terms and use of Dirac magnetic moments. These are approximations which are not required in the QMC model.

There is a remarkable similarity between the spin-orbit functionals of UNEDF1 and the QMC model (see Tab. 2). However, the significance of this fact is dependent upon whether the isovector dependence of the spin-orbit term alone has any impact on Hartree-Fock calculations of nuclei. The following section investigates the use of a Skyrme parameterisation from the QMC model and the importance of the isovector properties of the spin-orbit term.

3 Skyrme-QMC parameterisation

There exist many codes based on Hartree-Fock approximations which can be used to compute properties of nuclear structure [14–16] and reactions [17–24]. The majority of them are based on Skyrme functionals. While the QMC functional has a similar form to the Skyrme functional, it is not identical.

We have constructed a Skyrme functional which is as close as possible to that of the QMC model, called Skyrme-QMC (SQMC) [25]. For the central part of the

functionals there is a difference in the density dependence and they are matched around the saturation point of nuclear matter. But for the spin-orbit term, SQMC and the QMC model are identical, making SQMC a convenient tool to test the isovector dependence of the original QMC functional.

A similar SQMC was obtained in Ref. [26], however with $W_0 = W_0'$. Here, our SQMC has $W_0'/W_0 = 1.78$ as in the original QMC model.

4 Hartree-Fock calculations

Hartree-Fock-Bogoliubov codes are well-suited to the study of exotic nuclear structure as the treatment of pairing remains robust for weakly bound nuclei. Also, long isotopic chains provide a large range of neutron excesses, useful for revealing trends in the isovector properties of the functionals. The axial Hartree-Fock-Bogoliubov code, HFBTHO [15], was used to calculate the ground-state binding energies of tin ($Z = 50$) nuclei.

Relative to experimental data [27], as seen in Figure 1, the SQMC functional performs at a level comparable to UNEDF1, especially away from stability. This is particularly remarkable when one recalls that the stable tin masses were included in the fit of UNEDF1, while no experimental masses were used to derive the SQMC functional.

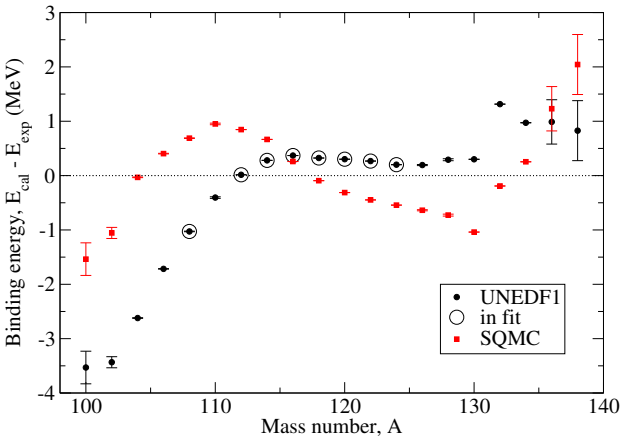

Figure 1. Difference between calculated and experimental binding energies for ^{A}Sn nuclei. The error bars are from the experimental data ($E_{\rm exp}$).

It is possible to extract the impact of only the isovector dependence of the spin-orbit term by comparing a SQMC parameterisation with the isovector dependence of the QMC model ($W_0'/W_0 = 1.78$), against a baseline which has only one spin-orbit parameter ($W_0 = W_0' = 104.3872$ MeV fm^5) but is otherwise identical. Calculations along the Sn isotopic chain out to the dripline, as shown in the upper panel of Figure 2, reveal that the isovector dependence of the spin-orbit term leads to a change of approximately 1 MeV in the region of the r-process ($^{134-152}$Sn). A change half this size is expected to have a significant impact on r-process abundances [28]. This illustrates that it is crucial to properly account for the isovector properties of the spin-orbit functional, as predicted by the QMC model for example.

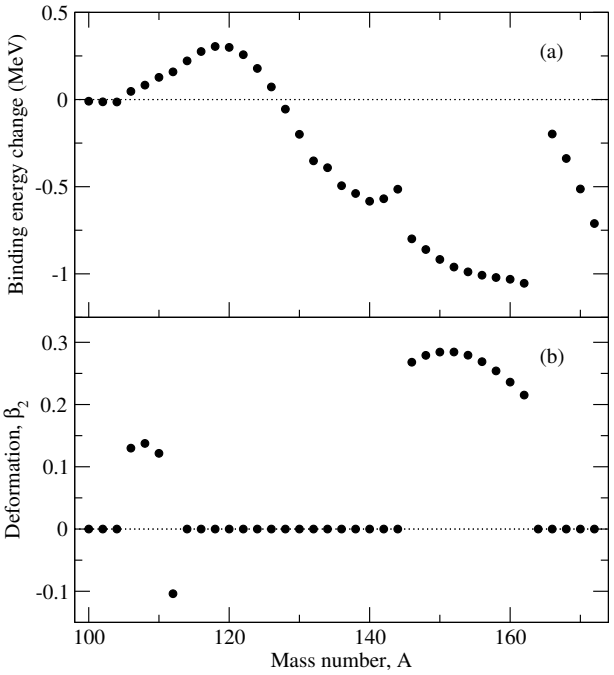

Figure 2. (a) Binding energy difference between SQMC with $W_0'/W_0 = 1.78$ and SQMC with $W_0'/W_0 = 1$, for ^{A}Sn nuclei. (b) Quadrupole deformation, β_2, predicted by the SQMC parameterisation.

The lower panel of Fig. 2 shows the deformation of the mean-field ground-states in the tin isotopes. We observe that the effect of the isovector contribution to the spin-orbit functional is clearly enhanced by the presence of prolate deformation in neutron-rich nuclei ($^{146-162}$Sn). A more detailed investigation of the interplay between deformation and the isovector contribution to the spin-orbit functional will be the focus of a future study.

5 Fusion

The SQMC parameterisation can also be used to investigate any effect the isovector dependence of the spin-orbit term has on nucleus-nucleus potentials and fusion cross-sections. Ref. [29] showed that isovector terms (central and spin-orbit) were significant for density-constrained time-dependent Hartree-Fock (DC-TDHF) calculations of the nucleus-nucleus potential of the ^{40}Ca + ^{132}Sn system. As a preliminary study, frozen Hartree-Fock (FHF) [30–33] was used with the SQMC parameterisation for the same system. FHF calculations provide the bare nucleus-nucleus potential from the Hartree-Fock ground-states, with no polarisation effects from dynamics.

Again we compare the two SQMC functionals with different spin-orbit isovector dependences ($W_0' = W_0 = 104.3872$ MeV fm^5 and $W_0'/W_0 = 1.78$), shown in Figure 3. While SQMC is in good agreement with the phenomenological UNEDF1 functional, the isovector dependence of the spin-orbit interaction has no impact on the

fusion barrier of ^{40}Ca + ^{132}Sn. Similar results were obtained for the ^{40}Ca + ^{100}Sn and ^{48}Ca + ^{100,132}Sn systems.

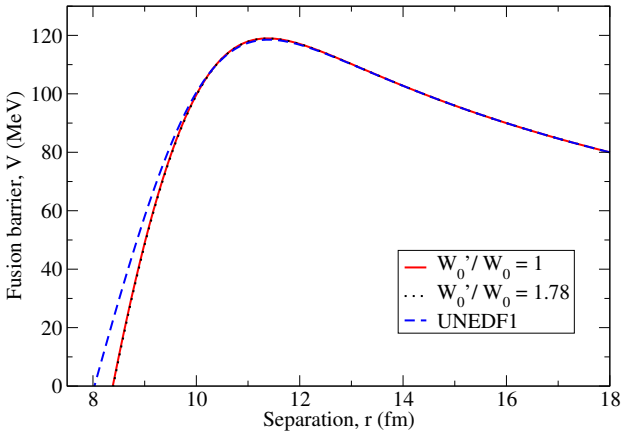

Figure 3. Nucleus-nucleus potential for ^{40}Ca + ^{132}Sn.

Future work will involve calculations using TDHF [34, 35] and the DC-TDHF technique [36], which self-consistently treats dynamical effects and nuclear structure, to investigate any potential impact of the isovector dependence of the spin-orbit term coupling to the dynamics or deformation of the system.

6 Conclusions

The isovector dependence of the spin-orbit term from the QMC model, with its high-energy degrees of freedom, is remarkably similar to that of UNEDF1. This is significant because, while no change to bare fusion potentials was observed, this dependence is an important factor that should be accounted for in r-process calculations [25].

A Skyrme functional from the QMC model can successfully reproduce ground-state binding energies. In the future, the SQMC functional will be used to study further exotic structure effects or, using a time-dependent Hartree-Fock code, dynamic processes including reactions with exotic nuclei, fusion barriers, transfer and fission.

It will also be possible to perform similar investigations using the original QMC functional, rather than the SQMC parameterisation, by modifying Skyrme-based Hartree-Fock codes to accept the more complicated density dependence of the central terms. Stone *et al.* [5] modified the static SKYAX code [37] in this way and used nuclear data to fix the few free parameters of the QMC model. A similar implementation in a time-dependent code will allow for a study of the giant monopole resonance [38, 39] to explore the effects of the unique density dependence of the QMC model.

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