The microscopic modelling of odd-mass and odd-odd nuclei

Markus Kortelainen[*]
Department of Physics, University of Jyväskylä, 40014 Jyväskylä, Finland

Sophie Péru[†]
CEA,DAM,DIF, F-91297 Arpajon, France

Wouter Ryssens[‡]
Institut d'Astronomie et d'Astrophysique, Université Libre de Bruxelles, CP-226, 1050 Brussels, Belgium

Project of the *Espace de Structure et de réactions Nucléaires Théorique*
https://esnt.cea.fr

28/10/2024 - 31/10/2024

CEA Saclay, DPhN, Orme des Merisiers, b. 703, room 135, F-91191 Gif-sur-Yvette

I. MOTIVATIONS

The description of atomic nuclei in terms of its constituent neutrons and protons is demanding: the nuclear theorist faces both the residual nature of the strong force and the difficulty of the quantum many-body problem. Nuclei occupy a rather awkward spot in the many-body landscape: one one hand, their particle number is too small for a successful statistical description but the number of nucleons is for most of them too large for the systematic application of sophisticated many-body techniques that go beyond the mean-field approximation. One way this complexity manifests itself is in the competition between collective and single-particle excitations: both energy scales are generally comparable in most nuclei, which leads to a complicated competition between both types of excitations.

Luckily for theorists, the formation of pairs of nucleon is energetically favoured; this is why all known even-even nuclei have a $J^\pi = 0^+$ ground state. Nuclear pairing introduces a separation of scales for even-even nuclei: below the energy threshold of pair breaking - typically around 2 MeV - only collective excitations exist and the level density is low. As a result, the rather intuitive modelling of a nucleus in terms of collective excitations of a single intrinsic shape is quite successful for most even-even nuclei. Even when multiple shapes compete, this picture does not change although the calculations often become demanding.

The situation is rather different for nuclei that are *not* even-even: nuclei with an odd number of neutrons, protons or both have at least one unpaired nucleon. For simplicity, we will use the term "odd nuclei" in what follows to simultaneously refer to these three categories. Exciting an unpaired nucleon does not require breaking a pair; as a result single-particle and collective excitations strongly mix in odd nuclei. Consequently, the level density of an odd nucleus is typically more than an order of magnitude larger than that of its even-even neighbours at equal excitation energy. Reproducing such a tangled low-energy spectrum that consists of a large number of possible single-particle excitations mixed with (possibly multiple) collective excitations is an enormous challenge for the nuclear theorist; even ground state properties such as spins and magnetic moments cannot reliably be reproduced by any model that can be applied to more than a handful of nuclei [1]. This complexity also has practical consequences for several many-body techniques: the relevant equations typically allow for many solutions that barely differ in energy, rendering any automated attempt at solving them difficult [2]. Perhaps more problematic are conceptual issues with collective models: although they are widely used and often essential to access particular observables, such models have almost without exception been developed under assumptions that are only verified for even-even nuclei.

---

[*] Electronic address: `markus.kortelainen@jyu.fi`
[†] Electronic address: `sophie.peru-desenfants@cea.fr`
[‡] Electronic address: `wouter.ryssens@ulb.be`

The goal of this workshop is to start a discussion on all technical and conceptual problems - whether mentioned above or not - that affect the modelling of odd nuclei. Many, if not most, many-body approaches rely on the construction of reference mean-field many-body states at some point; we will thus naturally focus on how to best construct and interpret such states, but also discuss the ways they can best be used for post-processing via more elaborate many-body techniques or comparatively simple collective models to finally result in improved predictions for specific observables related to odd nuclei. We intend to gather the experts in this domain that have developed different mitigation strategies for these issues in the context of different many-body settings and targetting different observables; our goal is to gather this accumulated but - so far - dispersed expertise to empower future research.

We believe that such a gathering is important and timely for several reasons; the first - and simplest - reason is that odd nuclei make up the majority of the nuclear chart. Models that only tackle even-even nuclei are not truly globally applicable; this deficiency becomes crippling if the motivation to provide input for astrophysical applications is taken seriously [3]. Secondly, many experimental techniques are indifferent to whether nuclei are even-even or not; and we feel that a significant body of existing experimental data is not utilised to its fullest potential. In particular, continued experimental progress in laser spectroscopy has challenged existing models with respect to magnetic moments [4], highlighted the physics content of the odd-even staggering of charge radii [5] and even promises access to hitherto unexplored observables [6]. Not only low-energy experiments challenge nuclear theory: relativistic collisions of odd-mass ^{197}Au have been shown to be sensitive to its deformation [7, 8], while the closely-lying excited states of heavy odd nuclei are crucial to different types of precision searches for beyond-standard-model physics [9], even if the systems are radioactive [10]. Finally, nuclear theory has progressed on this subject as well with important advances such as the large-scale application of beyond-mean-field techniques for systematic study of magnetic moments [11, 12], the first time-reversal breaking calculations covering the entire nuclear chart [13] and the prediction of product yields in the fission of odd-mass Uranium isotopes [14].

II. GOALS OF THE PROJECT

With this ESNT workshop, we aim to

1. gather experts in the field to discuss its current state and review recent progress,
2. discuss the conceptual issues inherent in modelling odd nuclei starting from mean-field reference states,
3. identify the technical limitations common to all approaches and discuss mitigation strategies.

III. SHORT-TERM VISITORS

We foresee no visitors beyond the duration of the program detailed below.

IV. LIST OF POTENTIAL SPEAKERS

For the two introductory lectures, we propose the following:

1. L. Robledo, Universidad Autonoma de Madrid (Spain)
   Modelling odd-mass and odd-odd nuclei.
2. T. Cocolios, KULeuven (Belgium)
   The experimental view on odd-mass and odd-odd nuclei.

The following list enumerates experts in the field (including lecturers and organisers) that have expressed a strong interest in participating in this workshop. Because of the meeting format we propose, we do not include a specific presentation topic for each person on this list.

1. A. Afanasjev, Mississippi State University (USA).
2. B. Bally, ESNT, IRFU, CEA, Université Paris-Saclay (France).
3. M. Bender, CNRS/IN2P3, IP2I Lyon (France).
4. T. Cocolios, KULeuven (Belgium).

5. J. Dobaczewski, University of York (UK).
6. M. Kortelainen, University of Jyväskylä (Finland).
7. K. Nomura, Hokkaido University (Japan).
8. S. Péru, CEA, DAM, DIF (France).
9. P.-G. Reinhard, Universität Erlangen-Nürnberg (Germany).
10. L. Robledo, Universidad Autonoma de Madrid (Spain).
11. W. Ryssens, Université Libre de Bruxelles (Belgium).
12. L. Bonneau, LP2I Bordeaux (France).
13. N. Pillet, CEA, DAM, DIF (France).
14. W. Younes, University of Berkeley (USA).

V. PRELIMINARY PROGRAM

We propose to forego a traditional schedule of talks and instead propose a schedule built around round table discussions with specific subjects. For each of these discussions, we will explicitly ask the subset of participants with relevant expertise to prepare material and indicate a chairman from among them. We hope to encourage all participants to interpret the subjects in the widest possible way and engage in free discussion, particularly since most subjects are naturally linked. We propose five discussion sessions; combined with two introductory lectures, these fill up four days of workshop as follows.

Monday 28 - 10	Tuesday 29 - 10	Wednesday 30 - 10	Thursday 31 - 10
	09h00 Round Table 1	09h00 Round Table 3	09h00 Round Table 4
	10h30 **Break**	10h30 **Break**	10h30 **Break**
12h Welcome	11h30 Round Table 1	11h30 Round Table 3	11h30 Round Table 4
12h30 **Lunch**	12h30 **Lunch**	12h30 **Lunch**	12h30 **Lunch**
13h30 Lecture 1: Prof. L. Robledo	13h30 Round Table **5**	13h30 Round Table **2**	13h30 End.
15h00 **Break**	15h30 **Break**	15h30 **Break**	
15h30 Lecture 2: Prof. T. Cocolios	16h00 Round table **5**	16h00 Round Table **2**	
17h00 **End**	17h00 **End**	17h00 **End**	

Round Table 1: Building mean-field reference states for odd nuclei.
Essentially all approaches require the construction of some reference many-body states, often taken as symmetry-broken Hartree-Fock-Bogoliubov states. One often needs large numbers of these: when exploring a collective subspace with either simple models or advanced beyond-mean-field calculations or even when describing many nuclei at the single-reference level. The automation of such calculations is commonplace today for even-even systems but essentially nonexistent for odd nuclei. Here, we will deal with the technical complexities of this initial modelling step for odd nuclei: among other things, the convergence of iterative procedures, the (in)stability of quasiparticle selection techniques and practical aspects of time-reversal symmetry breaking.

Round Table 2: The role of symmetries.
The spontaneous breaking of symmetries is a cornerstone of our understanding of atomic nuclei: each broken symmetry can be linked to a type of deformation, which in turn can explain specific aspects of nuclear phenomenology across the nuclear chart. In most approaches, the mean-field reference states do not respect at least one symmetry; while this technique is powerful, it also implies that quantum numbers cannot be assigned

and a connection to experiment is lost. The most advanced calculations today restore broken symmetries by constructing superpositions of several symmetry-broken states; the technology to perform such calculations for even-even nuclei is now somewhat established[1]. The same cannot be said for odd nuclei: beyond-mean-field calculations of any type for such nuclei are few and far between. Perhaps one reason is the role of time-reversal: odd nuclei do not exhibit this symmetry even in their ground states, which complicates again the description of these systems. In this round table we wish to discuss several questions related to all aspects of the spontaneous breaking and restoration of symmetries. Some examples: Which observables require the breaking of specific symmetries? Which ones require full-fledged symmetry restoration? What holds back symmetry-restoration techniques for odd nuclei as compared to even-even nuclei? How important is time-reversal symmetry breaking? How should one construct reference states to optimise the final superposition of them?

Round Table 3: Effective interactions and time-odd terms
It is today nigh-impossible to simulate nuclear structure starting from quarks, which is why all nuclear theorists employ effective interactions in one way or another. In this round table, we wish to explore how the description of odd nuclei is entangled with the construction of effective interactions: how do odd nuclei challenge existing interactions and how could we leverage an improved understanding of odd nuclei to build better interactions? Are aspects of our interactions sensitive to observables specific to odd nuclei? These questions are particularly relevant to approaches based on energy density functionals due to the breaking of time-reversal symmetry. First, it is now well known that many existing EDF parameterizations exhibit finite-size instabilities in such conditions [15]. Second, the absence of time-reversal implies that spin and current densities can take non-zero values and can contribute to the total energy of the nucleus; the resulting ‘time-odd’ terms are often omitted from the parameter adjustment protocol and are hence undetermined. What is the best way to determine these terms? How much do they affect predictions for different observables?

Round Table 4: Collective models for odd nuclei.
Collective models are widely used in nuclear structure but have almost without exception been derived only for even-even nuclei. In this round table, we mean to discuss the points where these models pose conceptual problems or fail to reach the desired accuracy when applied to odd nuclei. Arguably the most important questions concern the construction of collective spaces for odd nuclei: can one simply select a handful of multipole moments of the nuclear density as one does for even-even nuclei, despite the difficulties of quasiparticle blocking? If one does so, how seriously do (probably unavoidable) discontinuities affect the results? Can we cure such problems by breaking more symmetries and/or including hitherto unexplored collective degrees of freedom? If so, which ones? Furthermore, is this different for different types of collective motion? In the case of fission, for instance, we can ask whether the axial quantum number K should play a role in fission calculations of odd nuclei or should one allow for triaxial deformation as for even-even nuclei? Is it realistic to try and calculate a hindrance factor for odd nuclei? For models based on collective Hamiltonian of the Bohr type: how does one obtain the relevant inertial parameters, given that (i) essentially all formulas in the literature apply to even-even nuclei only and (ii) these parameters might depend on the blocked quasiparticle? Should we aim our sights lower and stick to models of the particle-core type?

Round Table 5: Observables and pseudo-observables.
Not all nuclear (pseudo-)observables are equally impacted by whether a nucleus is even-even or not; some - like ground state magnetic moments - are only relevant to odd nuclei, some - like absolute binding energies - can very roughly be interpolated from even-even neighbours and some - like nuclear level densities - can change dramatically by adding a single nucleon. In this session, we wish to discuss the (limited) performance of existing models for these quantities, investigating what factors hold them back and determining what degree of accuracy can reasonably be expected from future models. Another goal is identifying areas where theoretical work is missing: are there observables that have not so far not been tackled, either because the modeling is too difficult or the experimental data too recent [6]? Are there any areas where nuclear experimentalists or other communities are in urgent need of our support? If so, what theoretical developments are necessary? Have we exhausted all possibilities of the (comparatively plentiful) data on masses and charge radii or can we learn more from the odd-even staggering of both [5, 16, 17]? Finally, how can we best leverage the available experimental data to improve future models?

---

[1] "Somewhat established" here does not imply that symmetry-restoration techniques for even-even nuclei are widely practiced nor that they are completely free of issues.

[1] L. Bonneau, P. Quentin, and P. Möller, Phys. Rev. C **76**, 024320 (2007).

[2] N. Schunck, J. Dobaczewski, J. McDonnell, J. Moré, W. Nazarewicz, J. Sarich, and M. V. Stoitsov, Phys. Rev. C **81**, 024316 (2010).

[3] M. Arnould and S. Goriely, Progress in Particle and Nuclear Physics **112**, 103766 (2020), 2001.11228.

[4] A. R. Vernon, R. F. Garcia Ruiz, T. Miyagi, C. L. Binnersley, J. Billowes, M. L. Bissell, J. Bonnard, T. E. Cocolios, J. Dobaczewski, G. J. Farooq-Smith, et al., Nature **607**, 260 (2022).

[5] R. P. de Groote, J. Billowes, C. L. Binnersley, M. L. Bissell, T. E. Cocolios, T. Day Goodacre, G. J. Farooq-Smith, D. V. Fedorov, K. T. Flanagan, S. Franchoo, et al., Nat. Phys. **16**, 620 (2020).

[6] R. P. de Groote, J. Moreno, J. Dobaczewski, I. Moore, M. Reponen, B. K. Sahoo, and C. Yuan, Physics Letters B **827**, 136930 (2022), 2005.00414.

[7] STAR Collaboration, L. Adamczyk, J. Adkins, G. Agakishiev, M. Aggarwal, Z. Ahammed, I. Alekseev, J. Alford, A. Aparin, D. Arkhipkin, et al., Physical Review Letters **115**, 222301 (2015).

[8] B. Bally, G. Giacalone, and M. Bender, Eur. Phys. J. A **59**, 58 (2023).

[9] V. V. Flambaum, Physical Review C **99**, 035501 (2019).

[10] G. Arrowsmith-Kron, M. Athanasakis-Kaklamanakis, M. Au, J. Ballof, R. Berger, A. Borschevsky, A. A. Breier, F. Buchinger, D. Budker, L. Caldwell, et al., Rep. Prog. Phys. **87**, 084301 (2024).

[11] P. L. Sassarini, J. Dobaczewski, J. Bonnard, and R. F. G. Ruiz, J. Phys. G: Nuclear and Particle Physics **49**, 11LT01 (2022).

[12] J. Bonnard, J. Dobaczewski, G. Danneaux, and M. Kortelainen, Physics Letters B **843**, 138014 (2023).

[13] W. Ryssens, G. Scamps, S. Goriely, and M. Bender, Eur. Phys. J. A **58**, 246 (2022).

[14] N. Schunck, M. Verriere, G. Potel Aguilar, R. C. Malone, J. A. Silano, A. P. D. Ramirez, and A. P. Tonchev, Phys. Rev. C **107**, 044312 (2023).

[15] V. Hellemans, A. Pastore, T. Duguet, K. Bennaceur, D. Davesne, J. Meyer, M. Bender, and P.-H. Heenen, Phys. Rev. C **88**, 064323 (2013).

[16] W. Ryssens, G. Scamps, G. Grams, I. Kullmann, M. Bender, and S. Goriely (2022), arXiv:2211.03667.

[17] S. Geldhof, M. Kortelainen, O. Beliuskina, P. Campbell, L. Caceres, L. Cañete, B. Cheal, K. Chrysalidis, C. S. Devlin, R. P. de Groote, et al., Phys. Rev. Lett. **128**, 152501 (2022).