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How should one formulate, extract and interpret 'non-observables' for nuclei?

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Abstract

Nuclear observables such as binding energies and cross sections can be directly measured. Other physically useful quantities, such as spectroscopic factors, are related to measured quantities by a convolution whose decomposition is not unique. Can a framework for these nuclear structure 'non-observables' be formulated systematically so that they can be extracted from experiment with known uncertainties and calculated with consistent theory? Parton distribution functions in hadrons serve as an illustrative example of how this can be done. A systematic framework is also needed to address questions of interpretation, such as whether short-range correlations are important for nuclear structure.

1. Nuclear observables and non-observables

In quantum mechanics, an observable is typically defined as a physical property that can be measured. The usual examples include energy, momentum and angular momentum. But what about familiar nuclear quantities such as momentum distributions and spectroscopic factors? Although one often says that momentum distributions are 'measured', in fact they must be extracted from data. The general structure is that a measured quantity such as a cross section is decomposed as a convolution of subsidiary pieces, usually based on a factorization principle. This decomposition is not unique, and so we refer here to the extracted quantities as 'non-observables'. The quotes are intended to soften the implication that it is improper to talk about them; nevertheless, unless the conventions (e.g. scale and scheme dependence) are controlled and specified, there will be ambiguities that will be entangled with the structure and reaction approximations. The challenge is to formulate and carry out experimental extractions and theoretical calculations of non-observables systematically and consistently.

The theoretical ambiguities for non-observables that take the form of a matrix element of an operator O (e.g. the momentum distribution $O(k) = a_k^\dagger a_k$) are manifested by considering

unitary transformations. We are free to apply a (short-range) unitary transformation U to O and to states $|\Psi_n\rangle$ with the result that matrix elements are invariant:

$$O_{mn} \equiv \langle \Psi_m | O | \Psi_n \rangle = (\langle \Psi_m | U^\dagger \rangle U\,O\,U^\dagger (U | \Psi_n \rangle)) = \langle \widetilde{\Psi}_m | \widetilde{O} | \widetilde{\Psi}_n \rangle. \qquad (1)$$

But the matrix elements of O itself between the transformed states are in general modified (unless O is a conserved charge):

$$\widetilde{O}_{mn} \equiv \langle \widetilde{\Psi}_m | O | \widetilde{\Psi}_n \rangle \neq O_{mn}. \qquad (2)$$

In a low-energy effective theory, there is no preferred set of states (equivalently, there is no preferred Hamiltonian) so transformations that modify short-range unresolved physics generate equally acceptable states. This is, for example, discussed in the context of nuclear forces in [1]. Thus to the extent that differences between O_{mn} and $\widetilde{O}_{mn}$ are important (which will depend on the process and kinematics), one cannot unambiguously refer to one as a measured quantity without specifying the basis states used and the corresponding Hamiltonian (including regularization and renormalization scheme)[5]. The same considerations apply to any sort of wavefunction overlap. A framework to specify the relevant conventions and relate different choices is well developed for parton distribution functions, but its counterparts do not yet exist for nuclear non-observables. The challenge is to formulate such frameworks.

These considerations are critically important for non-observables such as nuclear spectroscopic factors, which are extracted from experimental measurements and used to compare data to data and data to theory. In particular cases the extracted values may vary from essentially convention independence to highly scheme dependent; precision analysis of nuclear data requires a rigorous framework to assess these uncertainties and allow robust comparisons. Interpreting the physics implications of non-observables also requires knowing how they evolve with transformations of nuclear Hamiltonians that change the resolution.

2. Nuclear and other examples

In nuclear physics, there is a wealth of physics involved in analyzing spectroscopic factors. Examples include comparing the ratio of measured to calculated knock-out cross sections as a function of isospin; focusing on long-range characterizations of states, such as the Hoyle state as a triple-alpha cluster state (in a different basis this state may look very complicated); or using spectroscopic factors as a concept to gain understanding of the nature of single-particle dominated versus more complex states in nuclei. For a proper comparison and rigorous interpretation of spectroscopic factors it is important to have control over their extraction and calculation.

We can gain insight into the issues with spectroscopic factors by considering the simplest nucleus, the deuteron. The D-state probability of the deuteron is a non-observable; it depends on the short-range tensor strength that changes under unitary transformations of nuclear forces and the associated transformations of basis states. The D-state probability is a spectroscopic factor for the D-state part of the wavefunction, so this is an example of a general model dependence of spectroscopic factors. The deuteron example, with the resolution dependence of the S- and D-state probabilities (shown, e.g. in figure 57 of [1]), demonstrates that there may be a large theoretical uncertainty (roughly a factor of two for the D-state deuteron probability) associated with spectroscopic factors that are sensitive to short-range parts, and a significant theoretical uncertainty (of order 10% for the S-state deuteron probability) for spectroscopic factors that probe mainly the long-range parts of nuclear forces.

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[5] The field-theoretic counterpart to this argument in terms of field redefinitions is presented in the context of momentum distributions and occupation numbers in [2, 3].

In addition, spectroscopic factors rely on a convention for the long-range parts in nuclear Hamiltonians, such as pion exchanges or a pionless theory. Both describe very low-energy scattering with similar accuracy, but the corresponding long-range parts of wavefunctions will differ. We stress the importance of separating mid-range physics from short-range contributions in the discussion of spectroscopic factors. For example, mid-range will receive contributions from one- and multi-pion physics in chiral effective field theory (EFT).

In systems with a large separation of scale, spectroscopic factors are effectively measurable (that is, there are only small systematic uncertainties) because the unitary transformations that change spectroscopic factors lead to shifts of order $(kR)^n$, with $kR \ll 1$ (where k is a typical momentum scale and R denotes the range of interactions). An excellent example is a precision measurement of the closed-channel fraction of cold atom pairs across a broad Feshbach resonance, obtained from radio-frequency spectroscopy where initial and final state interactions are negligible [4]. Similarly, the momentum distribution for strongly interacting cold atom gases near the unitarity limit follows a universal power law $1/k^4$ as $k \to \infty$ as long as $kR \ll 1$. As for cold atoms near unitarity, when there is a large separation between the energy scales of interactions and the excitation of the composite particles, the impulse approximation will be good and the separation of the momentum distribution from experimental data will also be clean. But this is not the case for nuclei, which therefore require greater care.

3. Parton distribution functions as a paradigm

We propose the framework of parton distribution functions (PDFs) as a paradigm for nuclear non-observables. The general scenario is that experimental cross sections are expressed as a well-defined convolution. The PDF analysis is based on the expectation that part of the convolution can be calculated reliably for given experimental conditions so that the remaining part can be extracted as a universal quantity, which can then be related to other processes and kinematic conditions. In the case of hard-scattering processes with a large momentum transfer scale Q, factorization allows a separation of the momentum and distance scales in the reaction. (In short, the time scale for binding interactions in the rest frame is time dilated in the center-of-mass frame, so the interaction of an electron with a hadron in deep-inelastic scattering is with single non-interacting partons.) The short-distance part can be calculated systematically in low-order perturbative QCD and the long-distance part identified as PDFs, which are basically momentum distributions for partons (i.e. quarks and gluons) in hadrons.

The PDFs are typically extracted from global fits to experimental data. Related quantities to PDFs are fragmentation functions, parton distribution amplitudes, generalized parton densities, which all summarize the universal non-perturbative parts of the physics. Since they are universal, the same PDFs appear in all reactions, so once determined they can relate processes such as the deep inelastic scattering of leptons, Drell–Yan, jet production, and more. Thus, one can measure them in a limited set of reactions and then perturbative calculations of hard scattering and PDF evolution enable first principles predictions of cross sections for other processes [5].

The rigorous framework developed for PDFs and related functions offers important lessons for analogous low-energy nuclear quantities. The momentum distribution for a given hadron is not unique: there is dependence on Q^2, which serves as the resolution scale and can be changed by renormalization group (RG) evolution, and the PDF analysis at next-to-leading order must be performed in a specific renormalization and factorization scheme (typical choices are MS

and DIS) [6]. To maintain consistency, any hard-scattering cross section calculations that are used for the input processes or that use the extracted PDFs have to be implemented with the *same* scheme. There is careful treatment of the uncertainties in the PDFs. It is *not* considered sufficient to just compare different extractions. Instead, the Lagrange Multiplier and Hessian techniques have been developed to estimate PDF uncertainties (see [6] for brief explanations and original references). Finally, in expressing a PDF in terms of a quark correlation function there are non-trivial details that must be done correctly; as emphasized by Collins [5], naive factorization is not adequate.

Each of these features has an analog in calculating spectroscopic factors and other nuclear non-observables. Can we formulate our theory to have the same control as with PDFs using factorization? An underlying question is whether the necessary ingredients (corresponding to asymptotic freedom, infra-red safety and factorization for PDFs, see [7]) are present. If not, there will be intrinsic limitations that have to be quantified. The seeds for such a framework have been under development for some years. These include EFT methods to consistently calculate structure and operators [8] and RG methods that can change the resolution [1]. Extending these methods to the problems discussed here is an important open task for nuclear theory.

4. Interpreting non-observables for nuclei

A rigorous framework for extracting nuclear non-observables is needed to offer clear interpretations. A case in point are recent experiments that are interpreted as providing definitive evidence for the effects of short-range correlations in nuclei. This interpretation raises many questions, as these correlations are features of the nuclear wavefunction at short distances, which are particularly dependent on the choice of the Hamiltonian (e.g. the resolution). How is this physics reconciled with approaches using chiral EFT or low-momentum interactions, for which short-range correlations are greatly suppressed, or with 'mean-field' energy-density functionals? For low-momentum interactions, the unitary transformations leave observable cross sections unchanged by construction. Does one then simply have different interpretations at different resolutions (e.g. simple operator and complicated wavefunction versus complicated operator and simple wavefunction) or are there basic limitations to what can be concluded? Is the extraction from experiment better controlled at certain resolutions? Does factorization work better for a range of resolutions in nuclear Hamiltonians? The challenge is to develop a systematic framework that can be applied at different resolutions, to address these questions and enable the theoretical ambiguities involved in non-observables to be quantified.

While implications from high-momentum components in nuclear wavefunctions have been claimed for nuclear structure at both normal and higher densities (e.g. neutron stars), one should be cautious about attributing too much to resolution-dependent quantities. After all, with parton distributions one would not talk about the results at a particular Q^2 as being 'the' quark or gluon momentum distribution also for lower or higher Q^2. In addition, we note the importance of distinguishing short-range versus long-range (or mid-range) correlations. The issue is whether one understands the physics at the corresponding resolution scale, which makes it possible to attribute the result to the correct physics. This is relevant for recent experiments at Jefferson Lab that measure the differences in correlations between proton–proton and proton–neutron pairs by looking at the ratio of differential cross sections $d\sigma(e, e'pn)/d\sigma(e, e'pp)$, which shows a pronounced preference for *pn* pairs over *pp* pairs [9]. It is important to disentangle what is due to effects of long-range (low-momentum) pion-exchange tensor forces

as opposed to the high-momentum reaction physics or short-range effects usually associated with a strong short-range repulsion in nucleon-nucleon (NN) interactions.

It is sometimes said (e.g. see [10]) that short-range correlations are 'hidden' in the parameters of low-energy effective theories (e.g. an EFT). Presumably 'hidden' is in the sense of integrated out; that is, contributions from loop momenta are shifted into coupling constants as the resolution is decreased. When is it necessary (or at least desirable) to 'unhide' this physics when doing low-energy nuclear physics? In particular, is it relevant when calculating low-energy nuclear structure, such as binding energies and low-lying excitations? A systematic framework is needed to disentangle what is hidden but known from what is unconstrained short-distance physics.

In interpreting occupation numbers or momentum distributions extracted from experiment, a comparison is often made to independent-particle models, where occupation numbers are either zero or one. This in turn sometimes leads to criticism of mean-field energy-density functionals (EDF) because of the apparent contradiction of fractional occupation numbers extracted and those in the EDF being equal to zero or one (ignoring pairing here). However, the theoretical underpinning of EDF approaches is Kohn–Sham density functional theory (DFT), for which (without pairing) the occupation numbers *are* zero or one, regardless of the degree of correlation. At the same time, there are issues with using Kohn–Sham single-particle wavefunctions for non-Kohn–Sham observables (although calculations of single-particle levels in DFT have shown promise, even if not fully justified by the theory). How can we resolve these conflicting views? A key development would be a unified framework for DFT and experiments such as $(e, e'p)$. This would also help to distentangle the role of short-range versus long-range correlations in the theoretical calculation of occupation numbers. Recent results for the quenching of spectroscopic factors suggest that long-range correlations may be more dominant than previously realized [11]. Being able to make robust comparisons at different resolutions will be essential in addressing these issues.

A final example of a non-observable that requires careful treatment is the extraction of NN potentials from recent lattice QCD calculations. In this case it is computational rather than experimental data that is analyzed. We first note that the short-range NN interaction is a non-observable, which is immediately evident from the experience with unitary transformations [1]. In the case of the lattice calculations, a choice has to be made of quark fields that are to be used as interpolating operator for the nucleon (which is chosen to have a non-zero overlap with a nucleon state that will dominate at large Euclidean times). Different choices will lead to different potentials so one must be cautious in drawing conclusions. Nevertheless, this could be a powerful tool to gain physical insight, in particular given the many knobs to change QCD parameters on the lattice.

5. Final comments

The systematic formulation of 'non-observables' such as spectroscopic factors and related quantities is an important open problem for nuclear structure theorists. The analogy to parton distribution functions seems to us to be a promising avenue to pursue. However, the development and application of corresponding frameworks that can address questions such as the validity of factorization approximations with different Hamiltonian resolutions will require progress on other open questions of nuclear structure outlined in this volume. Finally, we note that resolution dependence for a given non-observable does not mean that a particular choice of conventions cannot be advantageous, just as in field theory contexts the choice of a particular gauge may be most illuminating or predictive. But having a rigorous framework will enable this choice to be made in a controlled way.

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