Shortcuts to nuclear structure: lessons in Hartree-Fock, RPA, and the no-core shell model

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While the no-core shell model is a state-of-the-art microscopic approach to low-energy nuclear structure, its intense computational requirements lead us to consider time-honored approximations such as the Hartree-Fock (HF) approximation and the random phase approximation (RPA). We review RPA and point out some common misunderstandings, then apply HF+RPA to the no-core shell model. Here the main issue is appropriate treatment of contamination by spurious center-of-mass motion.

1. Introduction

Don’t believe everything you read. Even recently written textbooks on introductory nuclear physics can leave the reader with the impression that our understanding of low-energy nuclear structure is ill-defined. A typical example is found in Dunlap,1 who opens with the time-independent Schrödinger equation, then states that for atomic and solid physics “the difficulty...lies, not in our lack of understanding of the fundamental properties of the electromagnetic interaction, but in the complexity of the mathematics... However, in nuclear physics the [potential] has not been uniquely determined and a phenomenological approach is usually adopted.” This statement is not really wrong, but it is not really correct either.

While it is fair to say that the nucleon-nucleon (NN) potential has not been uniquely determined, one can and should make a more careful statement: high-precision data does uniquely determine the on-shell behavior of the the NN inter-

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1First of all, because of the ”complexity of the mathematics” one almost always makes significant approximations in atomic, molecular, and solid state calculations. This footnote is too small to debate the justifications for those approximations.
action. As discussed during this symposium, it is the off-shell behavior, which is inextricably tied up with three-body on-shell interactions, that is not determined. This important distinction is often overlooked.

With the on-shell behavior of NN interactions firmly in hand, the last 10+ years have seen a variety of rigorous approaches to microscopic, ab initio calculations of the structure of light nuclei. One of these is based on the well-known interacting shell model, the “no-core shell model” of Bruce Barrett and collaborators. It is an irony of history that thirty years ago Barrett and Kirson’s work \(^3\) (on nonconvergence of particle-hole corrections to effective interactions was one of several bolides\(^4,5\), that caused a “mass extinction” of rigorous nuclear structure studies, by showing serious flaws in the then-current methodology. Twenty years later, the no-core shell model was proposed\(^6\) precisely to avoid those flaws.

We will not go deeply into the details\(^7\) of no-core calculations, but simply point out they are heavily computational, requiring bases with dimensions of millions, tens of millions, even hundreds of millions. For reductionist, ab initio calculations this is the right thing to do. On the other hand, it is useful to seek out approximations that, first, allow one to get preliminary results quickly and efficiently, and, second, illuminate the more detailed, precise results. Toward this end we turn to the Hartree-Fock approximation, extended by the random-phase approximation.

In the next section we review some common understandings about RPA, while in Section 3 we look at some common misunderstandings about RPA. While some material is a recitation of previous work, we present a new, nontrivial calculation illustrating the “collapse” of RPA, demonstrating the topic is more subtle than generally appreciated. Finally, in Section 4 we present and discuss preliminary results of applying deformed HF+RPA to the no-core shell model.

2. The Hartree-Fock and random phase approximations

The Hartree-Fock approximation is based on the variational principle; the trial wavefunction is a Slater determinant, an antisymmeterized product of single-particle wavefunctions. (For a good introduction we recommend the monograph of Ring and Schuck.\(^8\)) The advantage of Hartree-Fock is that one can interpret the many-body wavefunction in terms of single-particle degrees of freedom. The disadvantage is that one loses correlations.

The random phase approximation is a generalization of Hartree-Fock that includes small amplitude correlations.\(^8,9,10\) It can be derived by different approaches: time-dependent Hartree-Fock, equations-of-motion, and the quasi-boson harmonic approximation, which we favor. There are two equivalent formulation of RPA: Green’s function and matrix. For the latter one solves

\[
\begin{pmatrix}
A & B \\
-B^* & -A^*
\end{pmatrix}
\begin{pmatrix}
\vec{X}_\lambda \\
\vec{Y}_\lambda
\end{pmatrix} = \hbar \Omega_{\lambda}
\begin{pmatrix}
\vec{X}_\lambda \\
\vec{Y}_\lambda
\end{pmatrix} \tag{1}
\]

In simple terms, \(A\) is the sub-matrix of the Hamiltonian \(\hat{H}\) taken between one-
particle, one-hole states, while $B$ is constructed from the matrix elements of $\hat{H}$ between the HF state and two-particle, two-hole states. If one ignores $B$, then one is simply diagonalizing $\hat{H}$ in a truncated basis; this is the Tamm-Dancoff approximation (TDA). TDA calculates only excited states; RPA implicitly calculates corrections to the ground state, but is not variational.

Hartree-Fock (HF) and the random-phase approximation (RPA) are old topics in nuclear structure, and there is much lore about HF and RPA in textbooks and monographs. You might think there is nothing new to be learned, at least not about the standard formulations. Nonetheless, it is important to pay attention to several technical issues if one wishes to apply HF+RPA to the no-core shell model:

(1) **Broken symmetries and their restoration.** Mean-field calculations can break exact symmetries such as translational and rotational invariance. By breaking an exact symmetry one often gets a surprising improvement: for example, deformed solutions can be lower in energy than spherical (rotationally invariant) solutions.

RPA and broken symmetries have a contentious relationship. It is often stated that RPA “restores” broken symmetries. More careful and accurate statements can be found in the literature: RPA “treats the inherent symmetries of the problem consistently.” What does this mean? Eq. (1) can be derived by a quadratic expansion of the energy about HF state. The vectors $\vec{X}_\lambda$ and $\vec{Y}_\lambda$ represent particle-hole and hole-particle perturbations, respectively, on the HF state; so for any perturbation corresponding to a generator of an exact symmetry, for example a rotation, the energy ought to be unchanged. In RPA the generators of broken symmetries are solutions of Eq. (1) with $\Omega_\lambda = 0$. By way of contrast, TDA does not correctly identify broken symmetries as zero-frequency modes. It is critical to note that the zero-frequency mode can only appear if the model space allows for exact restoration of symmetries, a fact that will return to haunt us.

(2) **“Collapse” of RPA.** A salient issue is the so-called “collapse” of RPA. RPA assumes small correlations, but in some calculations the RPA corrections are unphysically large. This can be seen when the HF state is near a transition from a symmetry-conserving state to a symmetry-breaking state, for example, from a spherical to a deformed state. The transition can be driven by changing a parameter, e.g. single-particle splitting. The classic illustration of collapse of RPA is the Lipkin-Meshkov-Glick model. Whenever one has symmetry breaking one worries about unphysically large RPA corrections.

(3) **Multi-shell calculations.** In a large, multi-shell model space, another symmetry that can be broken in HF is parity (i.e., by mixing, for example, $s_{1/2}$ and $p_{1/2}$ single-particle states). While most HF calculations enforce parity conservation, some recent papers report HF with parity mixing. Because of the possibility of “collapse” of RPA, however, it must be approached with concern. A specific question is: which is more vulnerable to collapse, deformation or parity mixing?
2.1. Implementation of RPA in the interacting shell model: SHERPA

We recently developed a code, SHERPA\(^{16}\) (SHell-model RPA), which implements Hartree-Fock and RPA in occupation space, solving the RPA matrix equations, Eq. (1). The only restriction is the Hartree-Fock wavefunction must be real; otherwise we allow for arbitrary deformation and mixing as allowed by the model space.

Using the code SHERPA and comparing with exact results from the Glasgow\(^{17}\) and REDSTICK\(^{18}\) shell model codes, we have written a series of papers carefully testing RPA in nontrivial shell-model systems.\(^{19,20,21,22}\) The shell-model interactions used had dozens of independent parameters, far more complicated than most previous tests (the Lipkin model has only two independent parameters).

3. Lessons from RPA

In the course of applying SHERPA to the shell model, we found that many of the common beliefs about RPA were not strictly true. Some we discovered through our calculations, others through a careful reading of the original literature.

1) Broken symmetries and “restoration.” What the literature actually says is that RPA yields an “approximate restoration of the symmetry”\(^{8}\) (italics added); the restoration is not exact, because the RPA wave function is valid only in the vicinity of the HF state\(^{23}\). As a further investigation, we computed RPA corrections to \(J^2\) and other scalar operators.\(^{20}\) For a deformed, even-even nucleus, the HF value of \(J^2\) is nonzero. The RPA corrections typically bring this value closer to zero, but not exactly; and the RPA value of \(J^2\) for the ground state can even be negative. Such unphysical values arise because we have taken \(J^2\) only to RPA order, neglecting proper treatment of the Pauli principle, etc.

2) Phase transitions and “collapse” of RPA. Long ago, and mostly forgotten, Thouless already correctly pointed out two kinds of phase transitions.\(^{24}\) In first-order transition, one has coexisting solutions, each of which are locally stable HF, and there is no collapse of RPA. In a second-order transitions, there is no coexistence, and collapse can occur. Thouless also argues that a first-order transition will occur for even-parity modes, e.g., quadrupole deformation, while a second-order transition can occur for odd-parity modes.

We present two illustrations from the shell model. The first example, shown in the right side of Fig. 1, is in the \(1s_{1/2}-0d_{3/2}-0d_{5/2}\) or \(sd\) valence space with the Wildenthal interaction,\(^{25}\) examining the transition from deformed to spherical by lowering the \(d_{5/2}\) single-particle energy. We compute the RPA correlation energy\(^{19}\) and RPA corrections to scalar observables\(^{20}\). (RPA is usually an improvement over HF, but \(Q^2\) in the spherical regime of \(^{28}\)Si is an exception. For other scalars in \(^{28}\)Si RPA is an improvement for both spherical and deformed regimes\(^{20}\).) RPA does not collapse in this case: it is a second-order transition, because at the transition point both the spherical and deformed HF solutions are local minima and thus stable.

In the second example, entirely new, we work in the \(0p_{1/2}-0d_{5/2}\) space with
Fig. 1. First- and second-order phase transitions in RPA. Left side panels are $^{28}$Si in the $sd$-shell. As the $0d_{5/2}$ single-particle energy is lowered, the HF state transitions (first order) from deformed to spherical; there is no collapse in either $\langle Q^2 \rangle$ (a) or g.s. correlation energy (b). Right side panels are $^{16}$O in a $0p_{1/2}-0d_{5/2}$ space. As the $0p_{1/2}-0d_{5/2}$ splitting increases, the HF state transitions (second order) from mixed parity to pure parity. Both $\langle Q^2 \rangle$ (d) and g.s. correlation energy (d) show unphysical contribution from, or “collapse” of, RPA.

a combination of interactions. Here the transition is between HF states of good and mixed parity. (This turns out to be similar to the Lipkin model, where the so-called “deformed” state is in fact a state of mixed parity.) We show our results for $^{16}$O, but have similar results for a variety of nuclides both in the $0p_{1/2}-0d_{5/2}$ space and in a larger $0p_{1/2}-0p_{3/2}-1s_{1/2}-0d_{3/2}-0d_{5/2}$ space. The RPA corrections grow unphysically large, a classic but nontrivial illustration of “collapse.”

This demonstrates that, at least in an explicit $0\hbar\Omega$ space a quadrupole shape transition is first order. It seems plausible that Thouless' analysis will continue to hold in multi-shell spaces and that the threat to multi-shell HF+RPA calculations will likely come not from quadrupole deformations but from cross-shell, parity-mixing (although we have not yet found explicit examples in multi-$\hbar\Omega$ spaces).

4. HF+RPA calculations for the no-core shell model

We are not the first to apply HF to the no-core shell model. The pioneering calculations of Hasan, Vary, and Navrátíl (HVN) looked at $^4$He and $^{16}$O in spherical Hartree-Fock, with second-order corrections similar to RPA. They compared their mean-field calculations to large-basis interacting shell-model (SM) calculations in a multi-shell space: for $^4$He their full interacting shell-model calculations included up to $10\hbar\Omega$ excitations, while for $^{16}$O the full calculations included up to $6\hbar\Omega$ excita-
tions. Complete $N\hbar\Omega$ shell-model spaces, when used with translationally invariant interactions, allows one to exactly separate out spurious center-of-mass motion.

One of the main issues of applying Hartree-Fock to the no-core shell model is the incongruency of model spaces. (If one works in a $0\hbar\Omega$ space there is no incongruency.) In the interacting shell model, one can limit the many-body basis to include all $N\hbar\Omega$ excitations. This is not possible for mean-field theory; instead one can only define the single-particle space. For example, $^{16}$O in a complete $4\hbar\Omega$ space includes, among others, 4p-4h excitations from the $0p$ shell into the $1s0d$ as well as 1p-1h excitations from the $0p$ up to $2p1f0h$. But if the single-particle space for the HF calculation includes the $2p1f0h$ shell, then the model implicitly includes not only $4\hbar\Omega$ excitations but also 6, 8, 10, ... $\hbar\Omega$ as well; but not all $10\hbar\Omega$ excitations, that is, the HF space is not a complete $N\hbar\Omega$ space.

This has three consequences. First, it makes comparison between the interacting shell model and HF (+RPA) calculations problematic. Second, there exist “out-of-space” two-body matrix elements that appear in the HF space that do not arise in the SM model space; what value should one assign them? Third, because the HF+RPA space is not a complete $N\hbar\Omega$ space, spurious center-of-mass motion cannot be separated out and will not appear as a zero-frequency mode in RPA.

HVN made several choices, all plausible but not inarguable. They made the HF single-particle space smaller in extent than that for the SM calculation (see their Figure 1). Because of this they had few “out-of-space” two-body matrix elements, and these were assigned, again plausibly but not inarguably, the relative kinetic energy. HVN obtained good values for the ground state energies, although with large second-order corrections.

Compared to HVN our calculations with SHERPA have both an advantage and a disadvantage. We allow for deformations (and odd numbers of nucleons, although we did not exploit that here), so we can in principle treat any light nucleus. This leads to a larger computational burden, however, so that in our initial results described here we could only tackle up to $2\hbar\Omega$ spaces.

We also made different choices for the HF+RPA space, taking the same single-particle span as for the SM calculation, and for the out-of-space two-body matrix elements: we set them $= 0$. We considered a number of 0s- and 0p-shell nuclei: $^4$He, $^8$Be, $^{10}$B, $^{12,14}$C, $^{14}$N, and $^{16}$O, all in a $2\hbar\Omega$ space, using an effective interaction derived from the bare Argonne $V8'$ interaction.29

We present our results in Fig. 2 for $^{12}$C; results for other nuclides were similar. The ordinate axis is the value of $\hbar\Omega$ for the harmonic oscillator basis, which sets the length scale (in no-core methodology one typically scans $\hbar\Omega$ for best convergence7). The shell-model (SM) calculations were performed in an exact $2\hbar\Omega$ space. It may seem surprising that even the HF values were lower than the exact SM values, but this can happen because the HF calculation can mix in spurious motion.

One signal of the mixing of higher-order excitations is that the HF and RPA states will have spurious center-of-mass contamination, signaled by $\langle H_{c.m.} \rangle > \frac{3}{2}\hbar\Omega$. Although we cannot exactly project out center-of-mass motion, we tried constrained
5. Conclusion and Summary

We have discussed the Hartree-Fock and random phase approximations, focusing on some hidden bits of lore regarding RPA, and applied HF+RPA to the ab initio no-core shell model. In particular we have presented two new results: (1) comparing, for the first time, in a non-trivial framework (the interacting shell model) both first- and second-order transitions, thus illuminating the so-called “collapse” of RPA; and (2) applying HF+RPA to the no-core shell model with arbitrary deformation and...
mixing of parity. The latter is not as successful as previous, spherical calculations, but the failure is likely due to inadequate treatment of center-of-mass and matrix elements in incongruency model spaces.

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