Properties of infrared extrapolations in a harmonic oscillator basis

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PHYSICAL REVIEW C 86, 054002 (2012)

Convergence properties of *ab initio* calculations of light nuclei in a harmonic oscillator basis

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E.D. Jurgenson, P. Maris, R.J. Furnstahl, P. Navratil, W.E. Ormand, J.P. Vary, submitted to PRC; arXiv: 1302:5473

Outline

- History: HO shell model can provide a linear trial function for a variational calculation of few-body systems (energies, etc.)
- Review: How to extrapolate to infinite number of terms, based on functional analysis theorems
- Effective Field Theory concepts applied to a discrete basis suggest an alternative extrapolation approach respecting ultraviolet (UV) and infrared (IR) running of the results as the basis is extended.
- Examples: Two alternate proposals for IR running, two soft NN potentials (Idaho N3LO and JISP16), light nuclei A=2-6
- Conclusion: Extrapolation method is successful for energies and lo range operators such as radius and total dipole moment.

The No-Core Shell Model (NCSM)

Starting Hamiltonian is translationally invariant.

$$
H_A = \frac{1}{A} \sum_{i < j}^{A} \frac{(\vec{p_i} - \vec{p_j})^2}{2m} + \sum_{i < j}^{A} V_{\text{NN},ij}.
$$

Provided interaction is "soft" we don't need to do any renormalization of interaction,

It's that "simple".

NCSM has two parameters: Nmax and Ω

If we now use a single-particle basis, we have to remove the spurious CM states. Translational invariance is automatic if HO basis depends on Jacobi coordinates.

Advantage in m-scheme: Antisymmetry is easy to implement. Disadvantage in m-scheme: Number of basis states is much larger than JT basis

M-scheme basis dimensions

- But why stick with the HO basis? calculations all the time.
- Only basis where center of mass and intrinsic states can be completely decoupled.
- Size of the m-scheme basis grows rapidly with increasing Nmax.
- Switch to HO JT coupled basis? Possibly, but painful.
- Difficulties with such an approach, e.g. Jacobi coordinates or rewrite codes.
- Even if techniques like SRG potentials are used, you still can't perform converged

Slide from Michael Kruse

The Variational Approach

- One can view a shell model calculation as a variational calculation, and is thus expanding the configuration space merely serves to improve the trial wavefunction.
- The traditional shell-model calculation involves trial wavefunctions which are linear combinations of Slater determinants. Irvine, J. M. et al. "Nuclear Shell-Model Calculations and Strong Two-Body Correlations"

2.1.2. Linear Trial Functions
We next consider a trial function in the form of a linear expansion:

$$
\psi_T = \sum_{i=1}^{N} a_i \varphi_i
$$
(2.10)

Delves, L. M. Advances in Nuclear Physics Vol 5 1972 ($N \rightarrow N$ max)

The traditional shell-model calculation involves trial variational wave functions which are linear combinations of Slater determinants. Expanding the configuration space merely serves to improve the trial wave function. • J. M. Irvine, et al "Nuclear shell-model calculations and strong two-body correlations", Ann. Phys. 102, 129 (1976).
early appearance of the term "no-core shell model" (NCSM)

Use the HO eigenfunctions as a basis of a finite linear expansion to make a straightforward variational calculation of the properties of light nuclei.
M. Moshinsky, "The Harmonic Oscillator in Modern Physics: from Atoms to Quarks" (Gordon and Breach, New York, 1969).

$$
\Psi_T = \sum_{\nu} a_{\nu}^{(\mathcal{N})} h_{\nu}
$$

where $a_{\nu}^{(N)}$ are the parameters to be varied and h_{ν} are many-body states based on a summation over products of HO functions.

Theorems based upon functional analysis established the asymptotic convergence rate of these calculations as a function of the counting number N which characterizes the size of the expansion basis (or model space)

• inverse power laws in N for ``non smooth" potentials with strong short range correlations

• exponential in N for ``smooth" potentials such as gaussians

HO basis: I. M. Delves, "Variational Techniques in the Nuclear Three-body Problem" in Advances in Nuclear Physics, Volume 5, ed. M. Baranger and E. Vogt (Plenum Press, New York, 1972) p.1-224, Simen Kvaal, "Harmonic oscillator eigenfunction expansions, quantum dots, and effective interactions", Phys. Rev. B 80, 045321 (2009).

Hyperspherical Harmonics basis: T. R. Schneider, "Convergence of generalized spherical harmonic expansions in the three nucleon bound state", Phys. Lett. 40B, 439 (1972).

However, the HO expansion basis has an intrinsic scale parameter $\hbar\omega$ which does not naturally fit into an extrapolation scheme based upon N . Indeed the model spaces of these NCSM approaches are characterized by the ordered pair $(\mathcal{N}, \hbar\omega)$ where the basis truncation parameter $\mathcal N$ and the HO energy parameter $\hbar\omega$ are variational parameters. It is the purpose of this talk to summarize the properties of another ordered pair which more physically describes the nature of the model spaces and provides extrapolation tools which use $\mathcal N$ and $\hbar\omega$ on an equal footing

L.M Delves; in Advances In Nuclear Physics vol 5 1972

 $E_{N_{max}} = E + P(N_{max})^{-2}$ "nonsmooth potentials" like Yukawa

 N_{max}

"These results are independent of the dimensionality of the problem, that is, of the number of particles, provided that the appropriate N_{max} is used. ... The extrapolated results of these authors have been used for E. On the logarithmic scale used, these differences are predicted by our crude theory to lie on a straight line of slope 2 for the Reid potential; it is not clear to what extent we should expect the nonlocal [separable] Yamaguchi potential to be `smooth'."

Variational energy as a function of oscillator energy ħω for fixed number of quanta Number of quanta increases by two for each curve

FIG. 1. Energy of the ground state of the H atom as a function of the parameter ε for the variational analysis discussed in Section 3. This energy $E_p(\varepsilon)$, $p = 0, 1, 2, 3, 4, 5$ is associated with a trial wave function $\psi_p = \sum_{n=0}^{p} a_n^{(p)} |n00\rangle$, where $|n00\rangle$ is a harmonic-oscillator state
of frequency $\hbar \omega = (me^4/2\hbar^2)e^2$.

No-core full configuration method of Maris,Vary,Shirokov

The current method is to seek the minimum of E(Nmax, $\hbar \omega$).

Extrapolation A of Maris et al PRC 79, 014308 (2009)

Current Method is Unsatisfactory...

- ... from an effective field theory point of view.
- Results are oscillator frequency dependent.
- No clear control of ultra-violet or infra-red nuclear physics.
- The goal is to investigate an alternate way from a more formal view point.

UV & IR CUTOFFS INTRODUCED

Construction of an effective field theory within the No Core Shell Model

-> calculation at Leading order: two N-N contact interactions in the 3S_1 ¹S₀ channel and a threebody contact interaction in the 3nucleon $S_{1/2}$ channel

-> coupling constants fitted to the binding energy of the deuteron, triton and 4 He.

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Physics Letters B 653 (2007) 358-362

PHYSICS LETTERS B

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No-core shell model in an effective-field-theory framework

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Received 5 March 2007; received in revised form 8 July 2007; accepted 31 July 2007

Effective Field Theory (EFT)

In a field theory one *never* has access to the "full" Hilbert space. Experiments only probe a region of momenta. Nature is quantum mechanical. So to develop a theory for such a region we must pose a model space. For smallest errors the model space should be as big, if possible, as the region one is interested in.

The parameter of the projection operator P into the model space must have a dimension. Call the parameter Λ , the ultraviolet cutoff and take it to be a momentum.

Model space can be arbitrary but observables calculated within it cannot.

The Hamiltonian operator of the model space must depend on Λ in such a way that observables at momenta Q<<Λ are independent of how P is chosen, and in particular, independent of Λ.

Arizona program: formulate a nuclear EFT in an HO basis as an efficient way of reaching larger nuclei. The HO basis also introduces into the model space a parameter λ , an infrared cutoff in addition to Λ , so that observables at momenta Q>> λ are independent of λ . That is, the values of Λ and λ control the size of the model space and the projection operators P(Λ) and $P(\lambda)$ define the boundaries of the model space.

van Kolck, Barrett, Stetcu, Rotureau, Yang

My more modest goal: can EFT motivate and shape an extrapolation to the infinite basis limit for the HO basis calculations called NCSM which utilize "realistic" nuclear interactions fit to data, not in a clearly defined model space, but in free space?

Define a UV momentum cutoff Λ analogous to continuum Λ in which the particles are not confined:

$$
\Lambda=\sqrt{m_N(N_{Max}+3/2)\hbar\omega}
$$

A high momentum cutoff corresponding to the maximal non-infinite momentum in the bound system.

Interpret behavior of variational energy of system as more basis states are added as the running of an observable with the variation (increase) of the UV cutoff of model space

Confinement to a volume because ħω>0 means the energy levels are quantized. The associated momenta cannot take on continuous values so that the model space has an infrared (IR) momentum cutoff λ.

$$
\text{Define }\quad \ \lambda=\sqrt{(m_N\hbar\omega)}
$$

A low momentum cutoff corresponding to the minimal non-zero momentum in the bound system.

Definition of Momentum Cutoffs

Ultraviolet momentum cutoff

 $\Lambda = \sqrt{m_N(N+3/2)}\hbar\omega$ Stetcu et al. PLB **653** (2007) "Kallio momentum" $\Lambda_a = \sqrt{2}\Lambda$ JPVary lectures (2012) Furnstahl et al. PRC **86** (2012)

Infrared momentum cutoff defined by discrete energy levels of the HO

 $\lambda = \sqrt{(m_N \hbar \omega)}$

Stetcu et al. PLB **653** (2007)

Alternate infrared cutoff defined by maximal radial extent of highest sp state

of model space
 $\lambda_{SC} = \sqrt{(m_N \hbar \Omega)/(N + 3/2)}$ $\lambda_{SC} = \lambda^2/\Lambda$

Jurgenson et al. PRC (2011)

Alternate $\lambda_{_{\rm sc}}$ in Furnstahl et al. PRC **86** (2012), More et al. PRC **87** (2013), Furnstahl et al. ArXiv:1312.6876

Strategy: minimize $E(\Lambda,\lambda)$ or $E(\Lambda,\lambda_{\text{sc}})$

Works only if the answer improves as we lower the infrared cutoff at a fixed ultraviolet cutoff

Or if answer improves as we raise UV cutoff at a fixed ir cutoff

Remove IR effects by decreasing value of IR momentum cutoff in the function chosen as an extrapolator whilst keeping the UV cutoff undisturbed.

Extrapolator is clearly the exponential function.

$$
\bullet \quad \tfrac{E(\lambda)-E(\lambda=0)}{E(\lambda=0)} \equiv \tfrac{\Delta E}{E} = A \, \exp(-B/\lambda)
$$

- B is a function of the UV cutoff
- The IR cutof*f annothe* aware of the UV cutoff.
- Remove dependence upon

•
$$
\lambda = \sqrt{\Lambda \lambda_{sc}} \Longrightarrow
$$

\n
$$
\exp(-B/\lambda) = \exp(-B/\sqrt{\Lambda \lambda_{sc}}) = \exp\left(-\frac{B/\sqrt{\Lambda}}{\sqrt{\lambda_{sc}}}\right)
$$

 $B/\sqrt{\Lambda}$ (i.e., multiplier of $1/\sqrt{\lambda_{sc}}$) is constant to within 5 %.

The momentum cutoff λ will remove IR effects. Indeed, any momentum cutoff $\lambda_{sc} \leq \lambda_{IR} \leq \Lambda$ will remove IR effects, but the IR regulator which is independent of the UV cutott is some function of λ_{sc} . It is λ_{sc} which causes the IR effects and one does not need to decrease a IR cutoff below that of λ_{sc} to remove IR effects (i.e. extrapolate to zero).

Result scales with $1/\lambda_{sc} = \Lambda/\lambda^2$ almost a universal behavior

1/ $\lambda_{\rm sc}$ has units of a length. 1/ $\lambda_{\rm SC}$ is the maximal radial extent needed to encompass the system. One could call this radius ``L" if one wanted a different name for $1/\lambda_{\text{sc}}$.

 Λ > 700 MeV Λ < 700 MeV

Running of $|\Delta E/E|$ with IR cutoff suggests an intrinsic UV scale of the NN interaction

 $|\Delta E/E|$ does not go to zero unless $\Lambda > \Lambda^{NN}$ where Λ^{NN} is some uv regulator scale of the NN interaction For $\Lambda < \Lambda^{NN}$ there are missing contributions of size $\|\Lambda - \Lambda^{NN}\|/\Lambda^{NN}$ so "plateaus" appear as ir cutoff approaches 0. Rise of plateaus suggests corrections are needed to Λ and $\lambda_{_{\rm sc}}$, which are defined only to leading order $\,$ in $\lambda_{_{\rm sc}}\!/\Lambda.$

Intrinsic UV scale depends on the NN interaction

Running of $|\Delta E/E|$ with UV cutoff suggests an intrinsic IR scale of the NN interaction

Plateau's ascribed to another "missing contributions" argument.

 $|\Delta E/E|$ does not go to zero unless where λ_{ac}^{NN} is some ir regulator scale of the NN interaction. Value of λ_{sc}^{NN} is consistent with lowest energy configuration described by NN interaction;

e.g. deuteron binding momentum $Q = 45$ MeV/c, or average of inverse scattering lengths \approx 16 MeV/c

How do intrinsic regulator scales control needed values of N and hbar-omega for a converged result?

Conclusion: One must extrapolate for all but the lightest nuclei

Single curve for $\lambda_{sc} \leq \lambda_{sc}^{NN}$ and $\Lambda \leq \Lambda^{NN}$

167

40

Momentum of nucleus Q to demonstrate universal (i.e., independent of particle number) nature of the Gaussian fits to low values of UV cutoff Λ

Extrapolated energies do NOT agree with independent calculations but are *lower*: 2 keV for deuteron, 300 keV (or 4%) for triton and 620 keV (or 2.4%) for alpha

UV extrapolations with $\Lambda < \Lambda^{NN}$

1) Extrapolation agrees with independent calculations only for SRG transformed potential.

2) Extrapolation with other values of fixed $\lambda_{_{\mathrm{sc}}}$ is neither reliable nor robust.

IR extrapolations with $λ$ sc

 $E(\lambda_{sc}) = A \exp(-B/\lambda_{sc}) + E(\lambda_{sc} = 0)$

If UV cutoff is large enough, all extrapolations agree with each other and with the accepted value of -7.85 MeV

IR extrapolations with λ sc

 $\Lambda > \Lambda^{NN}$ ~ 500 MeV/c for this SRG transformed interaction

IR extrapolations of energy, radius, and total dipole moment operator

Convergence of all three operators is the same with $\lambda_{\textrm{sc}}^{\textrm{}}$ extrapolation

Plot all results at $\hbar \omega$ = 22 and 28 MeV and Nmax up to 18

Data from M. D. Schuster, S. Quaglioni, C. W. Johnson and P. Navratil, ArXiv:1304:5491 "Ab Initio many-body calculation of the 4He photo-absorbtion cross section"

Universal property of IR extrapolation is nucleus dependent

Universal property of IR extrapolation is potential dependent

 $\Delta E = E(\lambda_{sc}) - E(\lambda_{sc} = 0) = a \exp(-b/\lambda_{sc})$

Single nucleon separation energies and slopes of $\Delta E/E$ vs $1/\lambda_{sc}$ plots

Alternate defs of $\lambda_{\textrm{sc}}$ in Furnstahl et al. PRC **86** (2012), More et al. PRC **87** (2013), Furnstahl et al. ArXiv:1312.6876 model the slope "b" in the table by the momentum which corresponds to the separation energy of a single nucleon from the nucleus.

E.D. Jurgenson, P. Maris, R.J. Furnstahl, P. Navratil, W.E. Ormand, J.P. Vary, submitted to PRC; arXiv: 1302:5473

Summary

HO shell model provides a linear trial function for a variational calculation of few-body systems.

Traditional extrapolation from finite model space $(N, \hbar\omega)$ is based upon extension of basis (N) "guided by" considerations of non-linear scale parameter (ħω).

Effective Field Theory concepts applied to a discrete basis suggest an alternative extrapolation approach based upon ($\Lambda,\!\lambda_{_{\mathrm{sc}}}\!$) which respects ultraviolet (UV) and infrared (IR) running of the results as the basis is extended.

Intrinsic UV and IR scales of the NN interaction are identified.

Extrapolation in UV with IR cutoff of model space below intrinsic IR scale is neither robust nor reliable.

Extrapolation in IR with UV cutoff of model space above intrinsic UV scale is quite successful.

Continuing need for higher order (in $\lambda_{\rm sc}/\Lambda$) corrections to these lowest order $\lambda_{\rm_{IR}}$ and $\Lambda_{\rm_{UV}}$

Extra Slides

IR extrapolations with λ

We fit the ground state energy with three adjustable parameters using the relation $E_{qs}(\hbar\omega)$ = $a \exp(-b/\hbar\omega) + E_{as}(\hbar\omega = 0)$ five times, once for each "fixed" value of Λ . It is readily seen that one can indeed make an ir extrapolation by sending $\hbar\omega \to 0$ with fixed Λ as first advocated in Ref. [35] and that the five ir extrapolations are consistent. The spread in the five extrapolated values is about 500 keV or about 2% about the mean of -28.78 MeV. The standard deviation is 200 keV.

> S. A. Coon, M. I. Avetian, M. K. G. Kruse, U. Van Kolck, P. Maris, J. P. Vary Archive:1205.3230, PRC 86, 054002 (2012)

IR extrapolations with λ_{α} **SC**

In conclusion, our extrapolations in the ir cutoff λ of $-28.78(50)$ MeV or the ir cutoff λ_{sc} of 28.68(22) MeV are consistent with each other and with the independent calculations.

Map (N,ħω) onto $(\Lambda,\lambda_{\rm sc})$ holding N fixed

Accepted extrapolation is -28.68(22) MeV

Of the 6 extrapolations only the three with N≥13 are consistent with this number.

But mean of these three large N extrapolations is -28.54 MeV with standard deviation of 0.11 MeV.

Naively concentrating on large N gives a worse extrapolation than using all points with $\Lambda > 500$ MeV/c.

Moral: results with low N can usefully stabilize and bound an extrapolation to the IR limit.

Figure 1: The plot shows the famous plateaus for $\Lambda = 650$ MeV/c. Note that there is no difference between using the original IR definition L_0 or the 'corrected' IR L .

Michael Kruse-private communication $\mathsf{L}\xspace_{_{2}}$ doesn't remove plateaus either