Infrared and Ultraviolet Cutoffs: Convergence Strategies for Harmonic Oscillator Basis Expansion Methods

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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)

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

The traditional shell-model calculation involves trial variational wave functions which are linear combinations of Slater determinants. Expanding the conf guration 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 $a_{\nu}^{(\mathcal{N})}$ 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 \mathcal{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



2

0.5

0.2

0.1

2

E - E

MeV



0

50

8

20



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



"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'."

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Variational energy as a function of oscillator energy $\hbar\omega$ 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 $E_{\rho}(\varepsilon)$, 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 $\hbar \omega = (me^4/2\hbar^2)\varepsilon^2$.

2009 deuteron up to 20 quanta



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

The No-Core Shell Model (NCSM)

Starting Hamiltonian is translationally invariant.

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

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

Slide from Michael Kruse



Extrapolating with N_{Max}

Challenge: achieve numerical convergence for no-core Full Configuation calculations using finite model space calculations

- Perform a series of calculations with increasing N_{max} truncation (while keeping everything else fixed)
- **Solution** Extrapolate to infinite model space \longrightarrow exact results
 - binding energy: exponential in N_{max}

$$E_{\text{binding}}^N = E_{\text{binding}}^\infty + a_1 \exp(-a_2 N_{\text{max}})$$

- use 3 or 4 consecutive N_{max} values to determine $E_{binding}^{\infty}$
- use $\hbar\omega$ and N_{max} dependence to estimate numerical error bars

Maris, Shirokov, Vary, Phys. Rev. C79, 014308 (2009)

Slide by Pieter Maris



This truncation/extrapolation scheme is essentially that of the earlier few-body variational studies Assumes that the boundary of finite subspace is defined only by N_{max} implication: ħω is an inessential complication

Not the case! The use of HO single particle orbitals means that the system is limited to a region in coordinate space whose size is governed by the parameter of the HO basis: $\hbar\omega$

The finite model space is characterized by two parameters: $N_{_{max}}$ and $~\hbar\omega$

Troubles with N_{max} extrapolation



Chiral NN interaction, $\lambda = 2.5$ fm-1 Extrapolation A'



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

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. To limit the number of one-particle states introduce 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(λ) 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 or NCFC which utilize "realistic" nuclear interactions fit to data, not in a clearly defined model space, but in free space?



Popular examples







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 $\hbar\omega$ >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 .

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

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

Another discretization scheme: QCD on a 4-dimensional lattice

Continuum QCD simulated on a lattice has a model space with two cutoffs UV cutoff $\Lambda \sim 1/a$ where a is lattice spacing IR cutoff $\lambda \sim 1/L$ where L is the size of the lattice a must be small enough to simulate the continuum L must be large enough to contain the system

Suggests another possible IR cutoff for a HO basis

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

This IR cutoff is the inverse of the rms radius of the highest single particle state in the basis, i.e. the maximal radial extent needed to encompass the system



Test model space cutoffs with deuteron calculation done with defined N_{max} and $\hbar\omega$ convergence is clear as N_{max} goes to 238



$\lambda_{IR} \equiv \lambda$ acts as an IR cutoff should!



As the ultraviolet cutoff increases, the fractional difference between calculated $E(\Lambda, \lambda)$ and an accepted-as-converged E, decreases.

Alternatively, the plot can be read the other way, where if we fix the UV Λ , the results improve as we lower the IR cutoff λ .

 Λ acts as an UV cutoff should!



small λ

large λ



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

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

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.

$$rac{E(\lambda)-E(\lambda=0)}{E(\lambda=0)} \equiv rac{\Delta E}{E} = A \exp(-B/\lambda)$$

- B is a function of the UV cutoff Λ
- The IR cutoff *cannot* be aware of the UV cutoff.
- Remove dependence upon Λ

$$\begin{array}{l} \lambda = \sqrt{\Lambda \lambda_{sc}} \Longrightarrow \\ \bullet \\ \bullet \\ \bullet \end{array} \exp(-B/\lambda) = \exp(-B/\sqrt{\Lambda \lambda_{sc}}) = \exp\left(-\frac{B/\sqrt{\Lambda}}{\sqrt{\lambda_{sc}}}\right) \end{array}$$

 $B/\sqrt{\Lambda}$ (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).

Success! UV and IR cutoffs identified as $N_{max} \rightarrow 238$

Are cutoffs of any use for approachable N_{max} ?

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



Note: This is not the usual extrapolation in N_{max} (with some prescription for $\hbar\omega$) because

$$egin{aligned} 1/\lambda_{sc} &= \Lambda/\lambda^2 \ &= \sqrt{(N_{max}+3/2)/(m_N\hbar\omega)} \ &\propto \sqrt{N_{max}/(m_N\hbar\omega)} \end{aligned}$$

 N_{max} and $\hbar\omega$ on an equal footing



 $\Lambda > 700 \text{ MeV/c}$

 Λ < 700 MeV/c

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 λ_{sc} , which are defined only to leading order in λ_{sc}/Λ .



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 L_2 doesn't remove plateaus either

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 $\lambda_{sc} \leq \lambda_{sc}^{NN}$ where λ_{sc}^{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 16 MeV/c



Are deduced values of intrinsic Λ and λ_{sc} consistent with expectations?

S wave parts of JISP16 potential f t to data in a HO space of N=8 and $\hbar\omega$ = 40 MeV. JISP16 regulator scales of $\lambda_{sc}^{NN} \sim 63 \text{ MeV/c}$ and $\Lambda^{NN} \sim 600 \text{ MeV/c}$. In practice, UV region seems already captured at $\Lambda > 500-550 \text{ MeV/c}$.

Idaho N³LO potential f t to data in momentum space. Gaussian regulator function with cutoff parameter of 500 MeV/c

How to compare apples and oranges?

Represent this potential in a HO basis. Barnea et al PRC 81, 064001 (2010) Nir Barnea, private communication

Idaho N³LO regulator scales of $\lambda_{sc}^{NN} \sim 21\text{-}42 \text{ MeV/c}$ $\Lambda^{NN} \sim 900\text{-}1100 \text{ MeV/c}.$

In practice, UV region seems already captured at Λ > 800 MeV.





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

$\Lambda/\lambda_{sc}~=~N+3/2$				
$(\Lambda\lambda_{sc})/m_N~=~\hbar\omega$				
,				
L	$\Lambda \ge \Lambda^{NN} = 800$)		
$\lambda_{sc}pprox 10$	$\lambda_{sc}pprox 20$	$\lambda_{sc}pprox 40$		
$N \ge 80$	$N \ge 40$	$N \ge 20$		
$\hbar\omega \succeq 8$	$\hbar\omega \succeq 16$	$\hbar\omega \succeq 32$		
1	$\Lambda \ge \Lambda^{NN} = 500$)		
$\lambda_{sc}pprox 10$	$\lambda_{sc}pprox 20$	$\lambda_{sc}pprox 40$		
$N \ge 50$	$N \ge 25$	$N \ge 12$		
$\hbar\omega \succeq 5$	$\hbar\omega \succeq 10$	$\hbar\omega \succeq 20$		

Conclusion: One must extrapolate for all but the lightest nuclei

For fixed λ_{sc} result does NOT improve with increasing Λ , if $\Lambda \ge \Lambda^{NN} \sim 800$ MeV/c !



Result independent of nucleus

Universal curve at $\Lambda \leq \Lambda^{\text{NN}}$ for low $\lambda_{_{\text{sc}}}$



Scale each model space cutoff by binding momentum of nucleus Q to demonstrate universal (i.e., independent of particle number) nature of the Gaussian f ts 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 λ_{sc} is neither reliable nor robust.

IR extrapolations with

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}



IR extrapolations with λ



We fit the ground state energy with three adjustable parameters using the relation $E_{gs}(\hbar\omega) = a \exp(-b/\hbar\omega) + E_{gs}(\hbar\omega = 0)$ 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.

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	$\Lambda = 700 \text{ MeV/c}$	E(0) = -7.798 MeV
	Λ =800 eV/c	E(0) = -7.844 MeV
	Λ =900 MeV/c	E(0) = -7.844 MeV
•	$\Lambda = 1000 \text{ MeV/c}$	E(0) = -7.843 MV
	$\Lambda = 1100 \text{ MeV/c}$	E(0) = -7.841 MeV
٠	$\Lambda = 1200 \text{MeV/c}$	E(0) = -7.847 MeV
	NCSM (Navratil)	E= -7.85(1) MeV
	Faddeev (Machl	eidt) E= -7.85 MeV
	HH (Pisa)	E= -7.854 MeV

IR extrapolations with

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,ħ ω) onto (Λ , λ_{sc}) holding N fixed



Accepted extrapolation is -28.68(22) MeV

Of the 6 extrapolations only the three with $N \ge 13$ 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.

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 ($\hbar\omega$).

Effective Field Theory concepts applied to a discrete basis suggest an alternative extrapolation approach based upon (Λ, λ_{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 λ_{sc}/Λ) corrections to these lowest order λ_{IR} and Λ_{UV}

Happy Birthday, James



Extra slides

One can use this universal scaling behavior to make an extrapolation which is independent of particle number



Data points are fit to $y = A \exp(-B/\lambda_{sc})$



Figure 8: (Color online) Dependence of the ground-state energy of ³H upon $\hbar\omega = \lambda^2/m_N = \lambda_{sc}^2/[m_N(N+3/2)]$ for fixed $N = \Lambda^2/\lambda^2 - 3/2 = \Lambda/\lambda_{sc} - 3/2$. Curves are not fits but spline interpolations to guide the eye.