Ab Initio Nuclear Structure Theory

James P. Vary Iowa State University

National Nuclear Physics Summer School **SUNY Stony Brook** July#2013

2. IR/UV Regulators and Renormalization Methods

- IR and UV properties of the Harmonic Oscillator (HO)
- IR and UV properties of NN interactions
- Okubo-Lee-Suzuki (OLS) renormalization scheme in the HO basis
- Similarity Renormalization Group (SRG) approach

Motivation: The 3D Harmonic Oscillator (HO) is both a pedagogical tool and the practical basis-of-choice in a variety of many-body theories

Notation for a single-particle system:

 $|\alpha\rangle \equiv 3D$ Harmonic Oscillator (HO) basis state

 α represents complete set of quantum numbers

$$
\alpha = \{n_{\alpha}, l_{\alpha}, j_{\alpha}, m_{j_{\alpha}}, \tau_{z_{\alpha}}\}
$$

Identity operator:

$$
I \equiv \sum_{\alpha} |\alpha\rangle\langle\alpha| \equiv \sum_{\alpha} |\alpha\rangle_{\omega}{}_{\omega}\langle\alpha|
$$

where ω represents the HO energy $\hbar \omega$ when used as a label

Identity operator in momentum representation:

$$
\langle \vec{k} | I | \vec{k} \rangle = \delta^3 (\vec{k} - \vec{k}')
$$

$$
\langle \vec{r} | \vec{k} \rangle = (2\pi)^{-3/2} e^{i\vec{k} \cdot \vec{r}}
$$

Recall some basic definitions for the HO

$$
H_{HO} = \frac{\hbar^2 k^2}{2m} + \frac{1}{2} m \omega^2 r^2
$$

\n
$$
H_{HO}|\alpha\rangle = E_{\alpha}|\alpha\rangle \qquad \alpha = \{n_{\alpha}, l_{\alpha}, m_{l_{\alpha}}\}
$$

\n
$$
E_{\alpha} = (2n_{\alpha} + l_{\alpha} + 3/2)\hbar\omega
$$

\n
$$
\langle \vec{r} | \alpha \rangle = \varphi_{\alpha}(\vec{r})
$$

With the normalized HO wavefunction in coordinate space defined In terms of the generalized Laguerre polynomials as

$$
\varphi_{\alpha}(\vec{r}) = N_{nl} \frac{R_{nl}(r)}{r} Y_{lm}(\Omega_r)
$$

\n
$$
R_{nl}(r) = \left(\frac{r}{b}\right)^{l+1} \exp\left(-\frac{r^2}{2b^2}\right) L_n^{l+\frac{1}{2}} \left(\frac{r^2}{b^2}\right)
$$

\n
$$
N_{nl} = \sqrt{\frac{2n!}{b\Gamma\left(n+l+\frac{3}{2}\right)}}, \qquad b = \sqrt{\frac{\hbar}{m\omega}}
$$

"Walkthrough" of HO wavefunctions nlm = 221 & superposition: 111+331

Challenge: Can you predict the locations of the zeroes (red)?

The normalized HO wavefunction in momentum space defined as

$$
\tilde{\varphi}_{\alpha}(\vec{k}) = N_{nl} \frac{\tilde{R}_{nl}(k)}{k} Y_{lm}(\Omega_k)
$$

$$
\tilde{R}_{nl}(k) = (kb)^{l+1} \exp\left(-\frac{k^2b^2}{2}\right) L_n^{l+\frac{1}{2}} \left(k^2b^2\right)
$$

$$
N_{nl} = (-1)^n \sqrt{\frac{2n!b}{\Gamma\left(n+l+\frac{3}{2}\right)}}
$$

Simple example of IR and UV regulators

=> What are the IR and UV regulators of an HO basis?

Let us suppress the role of spin and isospin for the present so that

$$
\alpha\ =\ \left\{n_\alpha, l_\alpha, m_{l_\alpha}\right\}
$$

Define the projected identity operator (the completeness relation limited to a finite basis space (model space)) at a chosen omega. We further take the basis to consist of all states in all HO shells up to a cutoff N.

$$
I_{N,\omega} \equiv \sum_{\alpha}^{N} |\alpha\rangle_{\omega,\omega} \langle \alpha| \quad \text{where } N \equiv \max(2n+l)
$$

Now examine the momentum space matrix elements *k*

$$
\langle \overline{k}\Big| I_{N,\omega}\Big|\overline{k}^{\, \prime}\Big\rangle
$$

which satisfy

$$
\lim_{N \to \infty} \langle \vec{k} | I_{N,\omega} | \vec{k} \rangle = \delta^3(\vec{k} - \vec{k}) = \frac{\delta(k - k')}{k^2} \delta^2(\Omega_k - \Omega_{k'})
$$

Let us split up our truncated identity operator into contributions from each orbital angular momentum:

$$
{I}_{N, \omega} = \sum_{l_{\alpha}} \Biggl[\sum_{n_{\alpha} m_{\alpha}}^{N} \bigl| \alpha \bigr\rangle_{\omega-\omega} \bigl\langle \alpha \bigr| \Biggr] \! \equiv \sum_{l_{\alpha}} \! \bigl[I_{N, \omega, l_{\alpha}} \bigr]
$$

Then, let us select a single orbital angular momentum's contribution to the truncated completeness relation, put this into a momentum space representation, integrate over the angles and introduce the HO energy for a convenient scale factor. The resulting quantity is then defined as:

$$
\langle k|\overline{I}_{N,\omega,l}|k'\rangle \equiv \frac{\hbar\omega}{4\pi} \int d\Omega_k \, d\Omega_{k'} \langle \vec{k}|I_{N,\omega,l}|\vec{k}\rangle
$$

$$
= \hbar\omega(2l+1) \sum_{n}^{N=2n+l} \tilde{R}_{nl}(k)\tilde{R}_{nl}(k')
$$

Now observe the progression toward the delta function (times energy) in k as N increases towards the "infinite basis limit" in the next slide.

For simplicity, we examine the local limit in momentum space, perform an angle average, multiply by an integration measure $k²$ and define the resulting quantity as:

$$
I_{N,\omega}(k) \equiv k^2 \int d\Omega_k \langle \vec{k} | I_{N,\omega} | \vec{k} \rangle \equiv I_{\lambda\Lambda}(k) \qquad N \equiv \max(2n+l)
$$

which has a normalization = the number of single-particle states included in N+1 HO shells. Now, we evaluate that normalization:

$$
\int_{0}^{\infty} dk I_{N,\omega}(k) = \frac{1}{6}(N+1)(N+2)(N+3) \equiv \mathbb{N} = \text{number of sp states}
$$

For example, there is $\mathbb{N}=1$ state when N=0, $\mathbb{N}=4$ when N=1, $\mathbb{N}=10$ when N=2, $N=20$ when N = 3, $N=35$ when N = 4, etc.,

The quantity $I_{\lambda\Lambda}(k)$ defined above is labeled with alternative parameters representing the basis space parameters (N, ω) and will be examined below in more detail.

Recall the quantity defined above:

$$
I_{N,\omega}(k) \equiv k^2 \int d\Omega_k \langle \vec{k} | I_{N,\omega} | \vec{k} \rangle \equiv I_{\lambda\Lambda}(k)
$$

The indicated labels signify infrared (IR) and ultraviolet (UV) parameters of the 3D HO and are defined as follows:

$$
\lambda \equiv \sqrt{\frac{m\omega}{\left(N + \frac{3}{2}\right)\hbar}}
$$

$$
\Lambda \equiv \sqrt{\left(N + \frac{3}{2}\right)m\omega_{\hbar}}
$$

 $=$ inverse rms radius of state in N+1 HO shell, the adopted IR regulator implicit in the basis

= rms momentum of state in N+1 HO shell, a typical UV regulator implicit in the basis

Below, we will examine how well these IR and UV parameters track the momentum space region for the basis defined by (N, ω)

This UV regulator is defined as the momentum arising from an application of the virial theorem to any state in the N+1 HO shell:

$$
\left\langle \frac{\hbar^2 \Lambda^2}{2m} \right\rangle_N = \left(N + \frac{3}{2}\right) \frac{\hbar \omega}{2}
$$

Next, we will consider an alternative to this UV regulator, which is a factor of Sqrt(2) larger and based on another property of any state in the N+1 HO shell. The alternative will be called Λ_a

The "Kallio momentum", k_N , defines the effective momentum for a spherical Bessel function that provides an accurate representation for a HO wavefunction near the origin in either momentum space (for a fixed radius) or coordinate space (for a fixed momentum. For example, as r -> 0 the HO potential energy vanishes so the Schroedinger solution locally resembles the free-particle equation. For the N+1 HO shell, the total energy is then the kinetic energy:

$$
\frac{\hbar^2 k_N^2}{2m} \equiv \left(N + \frac{3}{2}\right)\hbar\omega
$$

for which

$$
\frac{R_{nl}(r)}{r} = \sqrt{\frac{\Gamma(n+l+3/2)}{\pi n! l (N+3/2)}} 2^{l+2} j_l(k_N r)
$$

Ex: Verify this relation in relative coordinate space with $(n, l) = (3, 0)$ and hw = 40 MeV.

This leads to the definition of an alternative UV regulator

$$
\Lambda_a \equiv k_N = \sqrt{2\left(N + \frac{3}{2}\right) m\omega/\hbar} = \sqrt{2}\Lambda
$$

Let us investigate the connection between 3D HO wavefunctions and 3D plane waves in momentum space in more detail. We define

$$
b_N = b\sqrt{2(N+3/2)} = \sqrt{\frac{2(N+3/2)\hbar}{m\omega}}
$$

and we consider the specific case where

- m = reduced mass of 2 equal mass nucleons
- $k =$ relative momentum between the 2 nucleons

With these choices, we add a superscript "NN" to the regulators since NN interactions are defined in relative coordinates. In Fig. 1 below, we consider the specific case defined by:

$$
\lambda^{NN} = 0.225 \text{fm}^{-1}
$$

$$
\Lambda^{NN} = 2.141 \text{fm}^{-1}
$$

 $\Lambda_a^{NN} = 3.027$ fm⁻¹

Note that there is no need to discuss the CM motion of the two nucleons at the present time but we will return to this issue below when addressing 2-nucleon states

Figure 1a Comparison of 3D HO radial wavefunction with spherical Bessel function in momentum space. The related IR and UV regulators are listed.

Let us now consider a representative measure of how a truncated HO basis space spreads over a region of momentum space. We first take the specific case of $N = 8$ and examine how the IR and UV parameters indicate the spread of HO states in momentum space.

We then consider the spread in momentum space as a function of N at $\hbar \omega$ = 40 MeV.

Fig. 3 Integrands for projected identity operator ($N = 8$) vs relative momentum, normalized by the number of single-particle states (165). Rectangles represent the range from the IR to UV regulators.

Fig. 4 Integrands for projected identity operator vs k at three values of N, normalized by the number of single-particle states ($\mathbb N$). Vertical edges of rectangles represent IR & UV regulators as indicated.

Next, we consider the identity operator projected onto a finite space (N) in a particular orbital angular momentum channel so that

$$
I_{N,\omega}(k) \equiv \sum_{l} I_{N,\omega,l}(k)
$$

where

$$
I_{N,\omega,l}(k) = (2l+1) \sum_{n'}^{(N-l)/2} \left[\widetilde{R}_{n'l}(k) \right]^2
$$

In Figure 5 we present the particular L=0 case for N=8 and hw=40 MeV (normalized by the number of S-states in that HO basis = N/2 + 1) and compare with several additional quantities.

Fig. 5 Comparison of momentum-space integrands (see legend) as a function of relative momentum. Vertical lines represent regulators as labelled.

For reference – recall JISP16 S-wave Gaussian regulators $(N = 8, \hbar \omega = 40 \text{ MeV})$

$$
\lambda_{a}^{NN} = 0.225 \text{fm}^{-1} < m_{\pi} = 0.684 \text{fm}^{-1}
$$

$$
\Lambda_{a}^{NN} = 3.027 \text{fm}^{-1}
$$

Also recall the chiral N3LO exponential regulators

$$
\lambda_{a}^{NN} \sim m_{\pi} = 0.684 \,\text{fm}^{-1}
$$

$$
\Lambda_{a}^{NN} \sim 3.0 \,\text{fm}^{-1}
$$

Converting to Gaussian regulators (HO representation) as performed by the Trento group*

$$
\lambda^{NN} = 0.129 \text{fm}^{-1}
$$

$$
\Lambda_a^{NN} = 3.940 \text{fm}^{-1}
$$

*N. Barnea, W. Leidemann and G. Orlandini, Phys. Rev. C 81, 064001 (2010)

Combined IR and UV extrapolation: HO-basis regulator definitions

$$
E(\Lambda,\lambda) \thickapprox E_{\infty} + B_0 e^{-2\Lambda^2/B_1^2} + B_2 e^{-2k_{\infty}/\lambda}
$$

1S.A. Coon, M.I. Avetian, M.K.G. Kruse, U. van Kolck, P. Maris, and J.P. Vary, Phys. Rev. C 86, 054002 (2012); arXiv: 1205.3230 2R.J. Furnstahl, G. Hagen, T. Papenbrock, Phys. Rev. C 86 (2012) 031301 3E.D. Jurgenson, P. Maris, R.J. Furnstahl, P. Navratil, W.E. Ormand, J.P. Vary, Phys. Rev. C 87, 054312(2013); arXiv 1302.5473

 $E(\Lambda_{UV} L) \approx E_{\infty} + B_0 e^{-2\Lambda_U^2 V/B_1^2} + B_0 e^{-2k_{\infty}L}$

The above discussion has simplified the full 3D space to a 1D slice of that space. For a more complete discussion of the fully non-local 3D operators, see A. Negoita, PhD thesis, Iowa State University, 2010.

We will work in a HO basis to solve for the eigenstates of nuclear Hamiltonians using realistic NN + NNN interactions.

How do we obtain interactions with IR and UV regulators matched to our choice of basis space ("model space")?

In other words, how do we derive the effective interactions appropriate to the basis space in which we solve the problem?

No Core Shell Model

A large sparse matrix eigenvalue problem

$$
H = T_{rel} + V_{NN} + V_{3N} + \bullet \bullet \bullet
$$

\n
$$
H|\Psi_i\rangle = E_i|\Psi_i\rangle
$$

\n
$$
|\Psi_i\rangle = \sum_{n=0}^{\infty} A_n^i |\Phi_n\rangle
$$

\nDiagonalize $\{\langle \Phi_m | H | \Phi_n \rangle\}$

- Adopt realistic NN (and NNN) interaction(s) & renormalize as needed retain induced many-body interactions: Chiral EFT interactions and JISP16
- Adopt the 3-D Harmonic Oscillator (HO) for the single-nucleon basis states, α , β ,...
- Evaluate the nuclear Hamiltonian, H, in basis space of HO (Slater) determinants (manages the bookkeepping of anti-symmetrization)
- Diagonalize this sparse many-body H in its "m-scheme" basis where $[\alpha = (n,1,j,m,\tau)$]

$$
|\Phi_n\rangle = [a_\alpha^* \bullet \bullet a_\varsigma^+]_n |0\rangle
$$

$$
n = 1, 2, ..., 10^{10} \text{ or more!}
$$

• Evaluate observables and compare with experiment

Comments

- Straightforward but computationally demanding => new algorithms/computers
- Requires convergence assessments and extrapolation tools
- Achievable for nuclei up to A=20 (40) today with largest computers available

ab initio **NCSM Effective Hamiltonian for A-Particles Okubo-Lee-Suzuki Method plus Cluster Decomposition**

P. Navratil, J.P. Vary and B.R. Barrett, Phys. Rev. Lett. 84, 5728(2000); Phys. Rev. C62, 054311(2000) C. Viazminsky and J.P. Vary, J. Math. Phys. 42, 2055 (2001); S. Okubo, Progr. Theor. Phys. 12 (1954) 603; K. Suzuki and S.Y. Lee, Progr. Theor. Phys. 64, 2091(1980); K. Suzuki, *ibid***, 68, 246(1982);**

Review: B.R. Barrett, P. Navratil and J.P. Vary, Prog. Part. Nucl. Phys. 69, 131 (2013)

Preserves the symmetries of the full Hamiltonian: Rotational, translational, parity, etc., invariance

$$
H_{A} = T_{rel} + V = \sum_{i < j}^{A} \left[\frac{(\vec{p}_i - \vec{p}_j)^2}{2mA} + V_{ij} \right] + V_{NNN}
$$

Select a finite oscillator basis space (P-space) and evaluate an - body cluster effective Hamiltonian: *a*

$$
H_{\text{eff}} = P\big[T_{\text{rel}} + V^a(N_{\text{max}}, \hbar\Omega)\big]P
$$

Guaranteed to provide <u>exact</u> answers as $a \rightarrow A$ or $a s P \rightarrow 1$.

Effective Hamiltonian in the NCSM Okubo-Lee-Suzuki renormalization scheme

$$
H: E_1, E_2, E_3, \dots E_{d_p}, \dots E_{\infty}
$$

\n
$$
H_{\text{eff}}: E_1, E_2, E_3, \dots E_{d_p}
$$

\n
$$
QX H X^{-1} P = 0
$$

\n
$$
H_{\text{eff}} = P X H X^{-1} P
$$

- *n*-body cluster approximation, 2≤*n*≤*A*
- $H^{(n)}_{\text{eff}}$ *n*-body operator
- Two ways of convergence:
	- $-$ For $P \rightarrow 1$ *H*⁽ⁿ⁾_{eff} \rightarrow *H*
	- *→* For *n* → *A* and fixed *P:* $H^{(n)}_{\text{eff}}$ → H_{eff}

Controlling the center-of-mass (cm) motion in order to preserve Galilean invariance

Add a Lagrange multiplier term acting on the cm alone so as not to interfere with the internal motion dynamics

$$
H_{eff}(N_{\text{max}}, \hbar\Omega) \equiv P[T_{rel} + V^a(N_{\text{max}}, \hbar\Omega)]P
$$

\n
$$
H = H_{eff}(N_{\text{max}}, \hbar\Omega) + \lambda H_{cm}
$$

\n
$$
H_{cm} = \frac{P^2}{2M_A} + \frac{1}{2}M_A\Omega^2 R^2
$$

\n
$$
\lambda \sim 10 \text{ suffices}
$$

Along with the N $_{\sf max}$ truncation in the HO basis, $\qquad \qquad \Big|\, \lambda \hbar \Omega\,$ the Lagrange multiplier term guarantees that all low-lying solutions have eigenfunctions that factorize into a 0s HO wavefunction for the cm times a translationaly invariant wavefunction.

Key equations to solve at the a-body cluster level

Solve a cluster eigenvalue problem in a very large but finite basis and retain all the symmetries of the bare Hamiltonian

$$
P_a = \sum_{P \in P} |\alpha_P \chi \alpha_P|
$$

$$
Q_a = \sum_{Q \in Q} |\alpha_Q \chi \alpha_Q|
$$

$$
P_a + Q_a \approx 1_a
$$

$$
H_a^{\Omega} |k\rangle = E_k |k\rangle
$$

\n
$$
\langle \alpha_{\Omega} | \omega | \alpha_{P} \rangle = \sum_{k \in K} \langle \alpha_{\Omega} | k \rangle \langle \hat{k} | \alpha_{P} \rangle
$$

\nwhere: $\langle \hat{k} | \alpha_{P} \rangle = Inverse \langle \langle k | \alpha_{P} \rangle \rangle$

 $\mathcal{H}^{(a)} = (P_a + \omega^T \omega)^{-1/2} (P_a + P_a \omega^T Q_a) H_a^{\Omega} (Q_a \omega P_a + P_a) (P_a + \omega^T \omega)^{-1/2}$

SRG Similarity Renormalization Group

F. Wegner Ann. Phys. (Leipzig) 3, 77 (1994)

SRG flow: series of unitary transformations

$$
H_s = U(s)HU^+(s) \equiv T_{rel} + V_s
$$

As evolves according to
$$
\frac{dH_s}{ds} = [\eta(s), H_s]
$$

with
$$
\eta(s) = \frac{dU(s)}{dV}(s) = -\eta^+(s)
$$

ds

Choice for η (s), specifies the transformation: $\eta(s) = [T_{rel}, H_s]$

The actual flow equation is:
$$
\frac{dH_s}{ds} = [[T_{rel}, H_s], H_s]
$$

More convenient flow parameter $\lambda = s^{-4}$ $-\frac{1}{4}$ $\lambda = s^{-4}$ which we use as the UV regulator **NOIC possible source of comasion nere as we generally use 2x as the line of the the UV regular but here, we defer to conventional practice** Note possible source of confusion here as we generally use $|\Lambda|$ as the for SRG of using λ . The final SRG potential is then:

$$
V_s = V_{s=0} + \int \frac{dV}{ds} ds
$$

Similarity Renormalization Group - NN interaction

- drives interaction towards band-diagonal structure
- SRG shifts strength between 2-body and many-body forces
- Initial chiral EFT Hamiltonian power-counting hierarchy A-body forces

$$
V_{NN} \gg V_{NNN} \gg V_{NNNN}
$$

key issue: preserve hierarchy of many-body forces

Changing the resolution: The (Similarity) Renormalization Group

• common choice for generator

relative kinetic energy operator $\; G_{\lambda} = T$:

SRG evolution slides from Kai Hebeler, ECT* workshop, June 2013

Changing the resolution: The (Similarity) Renormalization Group

Eventually, we reach a convenient softened interaction as shown below:

• common choice for generator

relative kinetic energy operator $\; G_{\lambda} = T$:

SRG evolution slides from Kai Hebeler, ECT* workshop, June 2013

Improve convergence rate by applying SRG to N3LO

(Bogner, Furnstahl, Maris, Perry, Schwenk, Vary, NPA801, 21 (2008), arXiv:0708.3754)

Effect of three-body forces

(Jurgenson, Navratil, Furnstahl, PRC83, 034301 (2011), arXiv:1011.4085)

- Induced 3NF significantly reduce dependence on SRG parameter
- N₂LO_{3NF}
	- binding energy in agreement with experiment
	- may need induced 4NF?
- See cited paper $A = 7 12$ results

An Important Message

Chiral EFT generates a sequence of terms for any observable starting from the standard model (SM). Take, for example, electroweak (EW) couplings to the Quarks in the SM. Chiral perturbation theory defines how pions and nucleons couple with these EW operators – that is, it provides consistent one-body, two-body, etc., current operators.

Note, that previous discussions of scheme dependence carry through to these operators as well.

If we go to lower scales with renormalization (e.g. OLS, SRG) we need to perform these transformations on the chiral EFT operators to maintain consistency in the evaluation of EW observables. This renormalization gives rise to additional "induced" currents.

A number of applications have appeared where chiral EFT is used to generate EW operators through some order (e.g. NLO) but very few have appeared that carry out the additional renormalizations when SRG or OLS renormalizations were used for the Hamiltonian $=$ lots of work lies ahead!

Coupling to External Probes in Chiral EFT

Nuclear Current Operators \Box

¹⁴C beta decay - detailed results and estimated corrections due to chiral 2-body currents

TABLE I. Decomposition of p-shell contributions to M_{GT} in the LS scheme for the beta decay of ¹⁴C without and with 3NF. The 3NF is included at two values of c_D where $c_D \approx -0.2$ is preferred by the ³H lifetime and $c_D \approx -2.0$ is preferred by the ¹⁴C lifetime. The calculations are performed in the $N_{\text{max}} = 8$ basis space with $\hbar\Omega = 14$ MeV.

Table I from: P. Maris, J.P. Vary, P. Navratil, W.E. Ormand, H. Nam and D.J. Dean. Phys. Rev. Lett. 106, 202502 (2011)

*J. Menéndez, D. Gazit and A. Schwenk, Phys. Rev. Lett. 107 (2011) 062501 (estimated using their effective density-dependent 1-body operator)

Questions?