

#### HOBET: The SM as an Effective Theory and its Direct Matching to LQCD



#### Jun 1, 2018 CIPANP

#### Nuclear Structure Calculations

- Configuration interaction calculations use an explicitly antisymmetric basis of Slater determinants over a single particle basis.
- \* While the basis size grows very fast with the size of the single particle basis and A, the number of particles, fantastically efficient matrix techniques can be used to find the low lying spectrum.
- \* The required calculation cutoff on the basis ignores scattering through excluded states. This requires an *effective* interaction constructed in the HO basis that takes such scattering into account.

#### ET and The Harmonic Oscillator Basis

- \* We define a projection operator P for the states we will use in calculations and it's complement Q=1-P for the rest.
- \* An effective theory relies on a separation of scales or a weak coupling between P and Q.
- \* In a typical EFT using a momentum basis the kinetic energy T is diagonal and does not couple P & Q.
- \* In contrast, in the HO basis T is a hopping operator, strongly connecting the highest state in P to the lowest Q state.
  - \* Bad news for an ET expansion.
  - \* Maybe H<sub>eff</sub> can be reorganized, isolating T ...

#### The Bloch-Horowitz Equation

*P* is projection operator to subspace to work in, Q = 1 - P

$$H_{eff}(E_i)|\psi_i\rangle = P\left(H + H\frac{1}{E_i - QH}QH\right)P|\psi_i\rangle = E_iP|\psi_i\rangle$$

- \* Eigenstates of  $H_{eff}(E)$  are projections with the same eigenvalues.
  - \* All eigenstates that overlap P are included!
- \* It is continuous in energy, including across E=0. An effective theory based on the BH equation can be fit in the continuum and used to find bound states.
- \* Eigenstates are not orthogonal.
- \* Explicitly energy dependent: Must solve self consistently.
- \* Operators are formally renormalized as:

$$\hat{O}_{ji}^{eff} = \frac{E_j}{E_j - HQ} \hat{O} \frac{E_i}{E_i - QH}$$

#### The Effective Theory Expansion

The Haxton-Luu form of the Bloch-Horowitz Equation  $H_{eff}(E) = P \frac{E}{E - TQ} \left[ T + T \frac{Q}{E} T + V + V \frac{1}{E - QH} QV \right] \frac{E}{E - QT} P$ 

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$$V_{IR} + V_{\delta} ET Substitution$$

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$$V_{IR} + V_{\delta} ET Substitution$$

Far INFRA-RED

Regulated, NEAR IR Far INFRA-RED UV  $+ \frac{\hbar\omega/E}{V^{IR}} + \frac{1}{V^{IR}} +$ 



Far INFRA-RED

## E/(E-QT) Transform of Edge States



\* Acting on edge state with  $E/\hbar\omega = 1/2$ .

Recovers scattering wave function with phase shift.



\* Acting on edge state with  $E/\hbar\omega=-1/2$ .

Recovers bound state exponential decay from gaussian falloff of HO state.

\* E/(E-QT) with boundary condition recovers IR behavior.

### Sum T to All Orders

\* T contributions can be summed to all orders.

$$\left\langle j \left| \frac{E}{E - TQ} \left[ T + T \frac{Q}{E} T \right] \frac{E}{E - QT} \right| i \right\rangle = E\left(\delta_{ji} - b_{ji}\right)$$
  
$$b_{ij} = \left\{ P \frac{E}{E - T} P \right\}_{ij}^{-1}$$

\* A surprisingly simple result.

\* A non-perturbative sum of kinetic energy scattering is key to a convergent ET expansion of the remaining parts.

## The V<sub>s</sub> Expansion

\*  $V_{\delta}$  is described in terms of HO lowering operators.

 $\hat{c}$  lowers L,  $\hat{a}$  lowers nodal n,  $\left[\hat{c},\hat{a}\right] = 0$ 

$$V_{\delta}^{S} = a_{LO}^{S} \delta(r) + a_{NLO}^{S} \left( \hat{a}^{\dagger} \delta(r) + \delta(r) \hat{a} \right) + \dots$$

$$V_{\delta}^{SD} = a_{NLO}^{SD} \left( \hat{c}^{\dagger 2} \delta(r) + \delta(r) \hat{c}^{2} \right) + a_{NNLO}^{22,SD} \left( \hat{c}^{\dagger 2} \delta(r) a + \hat{a}^{\dagger} \delta(r) \hat{c}^{2} \right) + a_{NNLO}^{40,SD} \left( \hat{c}^{\dagger 2} \hat{a}^{\dagger} \delta(r) + \delta(r) \hat{a} \hat{c}^{2} \right) + \dots$$

 This is slightly simplified by absorbing a constant related to coupling spins to angular momentum into the LECs.

#### Matrix Structure: ${}^{1}S_{0}$ , $\Lambda = 8$

$$\left\langle \tilde{j} \middle| V_{\delta,a_{L0}} \middle| \tilde{i} \right\rangle^{S} = a_{L0}^{S} \pi^{-3/2} \begin{bmatrix} 1 & \sqrt{3/2} & \sqrt{15/8} & \sqrt{35/16} & 0.947 \\ \sqrt{3/2} & 3/2 & \sqrt{45/16} & \sqrt{105/64} & 1.160 \\ \sqrt{15/8} & \sqrt{45/16} & 15/8 & \sqrt{105/128} & 1.297 \\ \sqrt{35/16} & \sqrt{105/64} & \sqrt{105/128} & 35/16 & 1.401 \\ 0.947 & 1.160 & 1.297 & 1.401 & 0.898 \end{bmatrix}$$

- Edge state matrix elements in red vary with E due to Green's function action on edge states.
- \* Each such matrix corresponds to a pair (E<sub>i</sub>, Bdy<sub>i</sub>).

# Fitting LECs

- \* Principle: The BH equation is energy self consistent  $H_{eff}^{full} P | \psi_i \rangle = E_i P | \psi_i \rangle$
- \* At fixed order we have a nearby eigenstate.  $H_{eff}(LECs) P |\psi'_i\rangle = \varepsilon_i P |\psi'_i\rangle$
- \* The mismatch must be due to LEC values.
- Repair by minimizing

$$\sum_{i \in samples} W(i) (\varepsilon_i - E_i)^2 / \sigma_i^2$$

 The variance can be replaced by a full covariance matrix.

## S-Channel Eigenvalue Convergence



Test potential : hard core + well

#### P Channel Wave Function

ET Wave
 functions should
 match projections
 of numerical
 solutions.

1

2

3

r (fm)

 Colored lines are the projections of numerical solutions. Black dashed lines are the effective theory solutions at the same energies.

0

**Projection E=5MeV** 

5

4

#### **Operator Renormalization**

Operators can also be matched to an expansion.

$$\hat{O}_{ji}^{eff} = P \frac{E_j}{E_j - HQ} \hat{O} \frac{E_i}{E_i - QH} P$$

$$= P \frac{E_j}{E_j - TQ} \left[ \hat{O} + VQ \frac{E_j}{E_j - HQ} \hat{O} + \hat{O} \frac{E_i}{E_i - QH} QV + VQ \frac{E_j}{E_j - HQ} \hat{O} \frac{E_i}{E_i - QH} QV \right] \frac{E_i}{E_i - QT} P$$

$$\rightarrow P \frac{E_j}{E_j - TQ} \left[ \hat{O} + \hat{O}_{\delta} \right] \frac{E_i}{E_i - QT} P$$

\*  $O_{\delta}$  will have an expansion much like  $V_{\delta}$  with an expansion in harmonic oscillator quanta.

- \* Renormalizing the operator  $\hat{1}$  enables recovery of the projected state normalization!
  - \* An effective Hamiltonian in a P space may reproduce the spectrum, but if you don't know how much of the wave function is represented in P, operator evaluation is suspect.

$$H^{eff} = P \left[ H \frac{E}{E - QH} \right] P = P \left[ \left( \sum_{a \in pairs} H_a \right) \frac{E}{E - QH} \right] P$$

Expanding and organizing yields

$$H^{eff} = P \left[ \sum_{a} H_{a}^{eff} + \frac{1}{E} \sum_{a \neq b} H_{a}^{eff} Q H_{b}^{eff} + \frac{1}{E^{2}} \sum_{a \neq b, b \neq c} H_{a}^{eff} Q H_{b}^{eff} Q H_{c}^{eff} + \cdots \right] P$$

- \*  $H_a^{eff}$  is a spectator quanta dependent form of the effective interaction constructed previously.
- This expansion generalizes the effective interaction into an A-body effective Hamiltonian.

## Interactions from LQCD

- \* Lüscher's method can be used to map the spectrum of two nucleons to phase shifts.
  - \* Use traditional path: collect enough phase shift data in multiple channels and use to fit an effective theory or a model like a realistic potential.
- \* HAL QCD potential method, Doi et al. arXiv:1702.01600
  - \* Construct Nambu-Bethe-Salpeter wave function and infer non-local potential.
- \* Sources of error
  - \* Both: Tail of interaction exceeding L/2.
  - \* Lüscher's method: Divergences of zeta function in higher order terms.
  - \* HAL QCD potential: non-elastic excited state contamination.



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# Change: Boundary Conditions

- Phase shifts as boundary conditions are replaced by periodic boundary conditions.
- Small volumes limit the number of states in energy range of interest.
- ET construction should support
  - \* Multiple volumes to access more states.
  - Boosting

#### Periodic Momentum Basis

- Even and odd basis functions
- *m* ranges from -N/2 to
   N/2 with *m*<0 indicating</li>
   *sin* basis functions
- The kinetic energy operator is a bit complicated by the varying side lengths:

 $\phi_{i,s,m}(x) = \sqrt{2} / L_i \sin(\alpha_{i,m} x), \quad m = 1,...,N/2$   $\phi_{i,c,0}(x) = \sqrt{2} / L_i (1/\sqrt{2}), \quad m = 0$   $\phi_{i,c,m}(x) = \sqrt{2} / L_i \cos(\alpha_{i,m} x), \quad m = 1,...,N/2$ with  $\alpha_{i,m_i} = 2\pi |m_i| / L_i$ 

$$\phi_{\vec{m}}(x,y,z) = \phi_{m_x}(x) \phi_{m_y}(y) \phi_{m_z}(z)$$

$$\hat{T}\phi_{\vec{m}}(x,y,z) = 2\pi^2 \left(\sum_i \frac{m_i^2}{L_i^2}\right)\phi_{\vec{m}}$$
$$= \lambda_{\vec{m}}\phi_{\vec{m}}(x,y,z)$$

### Green's Function for E/(E-QT)

- \* As before:  $\left|\tilde{i}\right\rangle = \frac{E}{E QT} \left|i\right\rangle = b_{ij} \frac{E}{E T} \left|j\right\rangle, \quad b_{ij} = \left\{P \frac{E}{E T}P\right\}_{ij}, \quad i, j \in P$
- E/(E-T) is expressed as a bilinear eigenfunction expansion over the periodic basis functions.

$$G_{T}(E;\mathbf{r},\mathbf{r}') = \sum_{\vec{m}} \frac{E}{E - \lambda_{\vec{m}} + i\varepsilon} \phi_{\vec{m}}(\mathbf{r}) \phi_{\vec{m}}(\mathbf{r}')$$
  

$$b_{\vec{n}'\vec{n}} = \left\langle \vec{n}' \middle| G_{T} \middle| \vec{n} \right\rangle = \sum_{\vec{m}} \frac{E}{E - \lambda_{\vec{m}}} \left\langle \vec{n}' \middle| \phi_{\vec{m}}(\vec{r}') \phi_{\vec{m}}(\vec{r}) \middle| \vec{n} \right\rangle = \sum_{\vec{m}} \frac{E}{E - \lambda_{\vec{m}}} \chi_{\vec{n}'\vec{m}} \chi_{\vec{n}\vec{m}}$$
  
where  $\chi_{\vec{n},\vec{m}} = \chi_{n_{x},m_{x}} \chi_{n_{y},m_{y}} \chi_{n_{z},m_{z}}, \qquad \chi_{n,m} = \int_{-\infty}^{\infty} dx \ H_{n}(x) \phi_{m}(x)$ 

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3D basis overlap Calculated on the fly 1D basis overlap Stored

 $-\infty$ 

#### **Evaluate by Inserting Periodic Basis**

Sum T to all orders:

$$\left\langle \vec{n}' \left| \frac{E}{E - TQ} \left[ T + T \frac{Q}{E} T \right] \frac{E}{E - QT} P \left| \vec{n} \right\rangle = E \left( \delta_{\vec{n}'\vec{n}} - b_{\vec{n}'\vec{n}} \right)$$

\* V<sub>IR</sub> matrix elements are the most expensive part of H<sub>eff</sub>  $\left\langle \vec{n}' \middle| G_{TQ} V_{IR} G_{QT} \middle| \vec{n} \right\rangle = \sum_{\vec{m}', \vec{m}, \vec{s}, \vec{t}} b_{\vec{n}', \vec{s}} \frac{E}{E - \lambda_{\vec{m}'}} \left\langle \vec{s} \middle| \vec{m}' \right\rangle \left\langle \vec{m}' \middle| V_{IR} \middle| \vec{m} \right\rangle \left\langle \vec{m} \middle| \vec{t} \right\rangle \frac{E}{E - \lambda_{\vec{m}}} b_{\vec{t}, \vec{n}}$ 

All pieces are precomputed, but sum is still very large.
For *n*',*n* ∈ *P*<sup>-</sup> *G*<sub>QT</sub>=1, which can be used to check results.

## Magic with $V_{\delta}$

- \* As long as  $V_{\delta}$  on *P* doesn't interact with the boundary it is the same object in both finite and infinite volume contexts.
- Spherical and Cartesian HO bases are simply representations related by brackets.

Cartesian ET
 expansion
 respecting parity
 invariance.

LEC	operators
c000d000	$\delta(r)$
c100d100	$\left(a_x^{\dagger}\delta(r)a_x + a_y^{\dagger}\delta(r)a_y + a_z^{\dagger}\delta(r)a_z\right)$
c100d010	$\left(a_x^{\dagger}\delta(r)a_y + a_x^{\dagger}\delta(r)a_z + a_y^{\dagger}\delta(r)a_z\right) + \text{h.c.}$
c200d000	$(a_x^{\dagger 2} + a_y^{\dagger 2} + a_z^{\dagger 2}) \delta(r) + \text{h.c.}$
c110d000	$(a_x^{\dagger}a_y^{\dagger} + a_x^{\dagger}a_z^{\dagger} + a_y^{\dagger}a_z^{\dagger})\delta(r) + \text{h.c.}$

Table 9.1: LECs and Cartesian operators

## Testing Plan



## Test Setup: Range(V)>L/2



- Periodic images of the potential make a contribution.
- Infinite volume bound state at -4.05 MeV.
- LECs are fit using states with
   L=0 overlap.

Rep	MeV	L=0	L=2	L=4	L=6
$A_1^+$	-4.4428	0.5	0	0.866	0
$A_1^+$	2.0314	0.155	0	0.988	0
$E^+$	7.5995	0	0.424	0.361	0.830
$E^+$	15.2980	0	0.474	0.393	0.788
$A_1^+$	21.6167	0.326	0	0.265	0.908
$E^+$	23.2423	0	0.468	0.597	0.651
$A_1^+$	29.4041	0.521	0	0.853	0.023
$E^+$	30.9457	0	0.567	0.428	0.704
$A_1^+$	35.2449	0.655	0	0.189	0.732
$E^+$	38.4043	0	0.882	0.176	0.437
$A_1^+$	45.1402	0.526	0	0.576	0.625

## Phase Shift Comparison Setup

- Reference phase shifts for L=0 and L=4 are directly calculated from V.
- HOBET S-channel phase shifts are computed from the N3LO LECs that reproduce the spectrum. The phase shift is found by dialing the phase shift to produce energy self consistency.
- \* Lüscher's method phase shifts come from the formula  $k \cot \delta_{0} = \frac{2}{\sqrt{\pi L}} \mathcal{Z}_{0,0}(1;\tilde{k}^{2}) + \frac{12288\pi^{7}}{7L^{10}} \frac{\mathcal{Z}_{4,0}(1;\tilde{k}^{2})^{2}}{k^{9}\cot \delta_{4}} + \mathcal{O}(\tan^{2}\delta_{4}) \qquad \begin{array}{c} \text{Luu, Savage,} \\ \text{arXiv:1101.3347} \end{array}$
- \* An effective range expansion up to k<sup>6</sup> is used to interpolate.
- \* For simplicity the second term is evaluated using the L=4 phase shift directly determined from V.

## Phase Shift Results

 $L = 14.3 \ fm$  $m_{\pi}L = 10$ 

				Leading	Next Order
	E MeV	V	HOBET	Lüscher	Lüscher
The V column	1	142.023	141.931	142.552	142.751
	2	128.972	128.860	129.571	129.823
should be	4	113.602	113.464	114.205	114.403
considered the	8	96.919	96.752	97.575	97.3135
constacted the	10	91.473	91.296	92.228	91.6403
reference.	15	81.672	81.480	82.852	81.3184
	20	74.876	74.691	76.667	74.0936

- \* A potential source of error for both HOBET and Lüscher 's method is the accuracy of the finite volume spectrum.
  - Solved three times with N=350,400,450 and made a continuum extrapolation. The 3 results showed a consistent and small evolution of the eigenvalues.

## Summary

- \* The HOBET interaction can be directly constructed from observables such as phase shifts in the continuum.
- \* Energy dependence is a virtue, enabling a complete sum of kinetic energy scattering, isolating short range physics for the ET expansion.
- \* The interaction can be used in an A-body context with the excitation of spectators determining *Λ* for the interaction.
- \* Operator renormalization is natural, including correct normalization of states one simply renormalizes the "1" operator.
- \* The same ET expansion is valid in a periodic volume, enabling matching to the LQCD spectrum with the same LEC values as in the infinite volume case!

Thanks to my collaborator on this project - Wick Haxton

