HOBET: The SM as an Effective Theory and its Direct Matching to LQCD
Nuclear Structure Calculations

- Configuration interaction calculations use an explicitly anti-symmetric 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 its 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 $H_{\text{eff}}$ can be reorganized, isolating $T$ …
The Bloch-Horowitz Equation

\[ P \text{ is projection operator to subspace to work in,} \quad Q = 1 - P \]

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

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

\[ \quad \hat{O}^\text{eff}_{ji} = \frac{E_j}{E_j - HQ} \hat{O} \frac{E_i}{E_i - QH} \]

- Eigenstates of \( H_{\text{eff}}(E) \) 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:
The Effective Theory Expansion

The Haxton-Luu form of the Bloch-Horowitz Equation

\[ H_{\text{eff}}(E) = P \frac{E}{E - TQ} \left[ T + T \frac{Q}{E} T + V + V \frac{1}{E - QH} QV \right] \frac{E}{E - QT} P \]
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\[ V_{IR} + V_\delta \quad ET \text{ Substitution} \]
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Far INFRA-RED

Regulated, NEAR IR

UV

\[ + \frac{\hbar \omega}{E} \quad + \quad \frac{V_{IR}^{\pi}}{} \quad + \quad a_{LO} + \left[ \frac{r_{SR}}{b} \right] a_{NLO} + \ldots \]
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.

\[
\left< j \left| \frac{E}{E - TQ} \left[ T + T \frac{QT}{E} \right] \frac{E}{E - QT} \right| i \right> = E \left( \delta_{ji} - b_{ji} \right)
\]

- A surprisingly simple result.

- A non-perturbative sum of kinetic energy scattering is key to a convergent ET expansion of the remaining parts.
The $V_\delta$ Expansion

- $V_\delta$ is described in terms of HO lowering operators.
  
  $\hat{c}$ lowers $L$, $\hat{a}$ lowers nodal $n$, $[\hat{c}, \hat{a}] = 0$

  $V^S_\delta = a^S_{LO} \delta(r) + a^S_{NLO} (\hat{a}^\dagger \delta(r) + \delta(r) \hat{a}) + ...$

  $V^{SD}_\delta = a^{SD}_{NLO} (\hat{c}^{\dagger 2} \delta(r) + \delta(r) \hat{c}^2) + a^{22,SD}_{NNLO} (\hat{c}^{\dagger 2} \delta(r) a + \hat{a}^\dagger \delta(r) \hat{c}^2)$

  $+ a^{40,SD}_{NNLO} (\hat{c}^{\dagger 2} \hat{a}^\dagger \delta(r) + \delta(r) \hat{a} \hat{c}^2) + ...$

- This is slightly simplified by absorbing a constant related to coupling spins to angular momentum into the LECs.
Matrix Structure: $^1S_0$, $\Lambda=8$

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

- 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 $(E_i, \text{Bdy}_i)$. 
Fitting LECs

- Principle: The BH equation is energy self consistent

\[ H_{\text{eff}}^{\text{full}} P |\psi_i\rangle = E_i P |\psi_i\rangle \]

- At fixed order we have a nearby eigenstate.

\[ H_{\text{eff}} (\text{LECs}) P |\psi'_i\rangle = \varepsilon_i P |\psi'_i\rangle \]

- The mismatch must be due to LEC values.

- Repair by minimizing \( \sum_{i \in \text{samples}} W(i) \frac{(\varepsilon_i - E_i)^2}{\sigma_i^2} \)

- 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.

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

- Operators can also be matched to an expansion.

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

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

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

- \( O_\delta \) 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.
A-Body ET Calculations

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

- Expanding and organizing yields

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

- \( H_{a}^{\text{eff}} \) 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 $\sin$ basis functions

- The kinetic energy operator is a bit complicated by the varying side lengths:

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

  with $\alpha_{i,m} = 2\pi |m_i| / L_i$

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

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

  $$
  = \lambda_{\bar{m}} \phi_{\bar{m}} (x,y,z)
  $$
Green’s Function for $E/(E-QT)$

- As before: $|i\rangle = \frac{E}{E-QT}|i\rangle = b_{ij} \frac{E}{E-T}|j\rangle$, $b_{ij} = \left\{ P \frac{E}{E-T} P \right\}_{ij}^{-1}$, $i,j \in P$

- $E/(E-T)$ is expressed as a bilinear eigenfunction expansion over the periodic basis functions.

$$G_T(E; r,r') = \sum_{\tilde{m}} \frac{E}{E - \lambda_{\tilde{m}} + i\epsilon} \phi_{\tilde{m}}(r)\phi_{\tilde{m}}(r')$$

$$b_{\tilde{n}\tilde{n}} = \langle \tilde{n}' | G_T | \tilde{n}\rangle = \sum_{\tilde{m}} \frac{E}{E - \lambda_{\tilde{m}}} \langle \tilde{n}' | \phi_{\tilde{m}}(r')\phi_{\tilde{m}}(r) | \tilde{n}\rangle = \sum_{\tilde{m}} \frac{E}{E - \lambda_{\tilde{m}}} \chi_{\tilde{n}'\tilde{m}}\chi_{\tilde{n}\tilde{m}}$$

where $\chi_{\tilde{n}\tilde{m}} = \chi_{n_x,m_x} \chi_{n_y,m_y} \chi_{n_z,m_z}$, $\chi_{n,m} = \int_{-\infty}^{\infty} dx \ H_n(x) \phi_m(x)$
Green’s Function for E/(E-QT)

- As before: \[ |\tilde{i}\rangle = \frac{E}{E-QT} |i\rangle = b_{ij} \frac{E}{E-T} |j\rangle, \quad b_{ij} = \left\{ P \frac{E}{E-T} P \right\}_{ij}^{-1}, \quad i, j \in P \]
- \( E/(E-T) \) is expressed as a bilinear eigenfunction expansion over the periodic basis functions.

\[
G_T(E; r, r') = \sum_{\tilde{m}} \frac{E}{E - \lambda_{\tilde{m}} + i\epsilon} \phi_{\tilde{m}}(r) \phi_{\tilde{m}}(r')
\]

\[
b_{\tilde{n}\tilde{n}} = \langle \tilde{n}' | G_T | \tilde{n} \rangle = \sum_{\tilde{m}} \frac{E}{E - \lambda_{\tilde{m}}} \langle \tilde{n}' | \phi_{\tilde{m}}(\tilde{r}') \phi_{\tilde{m}}(\tilde{r}) | \tilde{n} \rangle = \sum_{\tilde{m}} \frac{E}{E - \lambda_{\tilde{m}}} \chi_{\tilde{n}\tilde{m}} \chi_{\tilde{n}\tilde{m}}
\]

where \( \chi_{\tilde{n}\tilde{m}} = \chi_{n_x,m_x} \chi_{n_y,m_y} \chi_{n_z,m_z} \), \( \chi_{n,m} = \int_{-\infty}^{\infty} dx \ H_n(x) \phi_m(x) \)

3D basis overlap
Calculated on the fly

1D basis overlap
Stored
Evaluate by Inserting Periodic Basis

Sum $T$ to all orders:

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

- $V_{IR}$ matrix elements are the most expensive part of $H_{\text{eff}}$

$$\langle \tilde{n}' | G_{TQ} V_{IR} G_{QT} | \tilde{n} \rangle = \sum_{\tilde{m}', \tilde{m}, \tilde{s}, \tilde{t}} b_{\tilde{n}' \tilde{s}} \frac{E}{E - \lambda_{\tilde{m}'}} \langle \tilde{s} | \tilde{m}' \rangle \langle \tilde{m}' | V_{IR} | \tilde{m} \rangle \langle \tilde{m} | \tilde{t} \rangle \frac{E}{E - \lambda_{\tilde{m}}} b_{\tilde{t} \tilde{n}}$$

- All pieces are precomputed, but sum is still very large.

- For $\tilde{n}', \tilde{n} \in P^-$ $G_{QT} = 1$, 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.

<table>
<thead>
<tr>
<th>LEC</th>
<th>operators</th>
</tr>
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<tbody>
<tr>
<td>$c000d000$</td>
<td>$\delta(r)$</td>
</tr>
<tr>
<td>$c100d100$</td>
<td>$(a_x^\dagger \delta(r)a_x + a_y^\dagger \delta(r)a_y + a_z^\dagger \delta(r)a_z)$</td>
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<tr>
<td>$c100d010$</td>
<td>$(a_x^\dagger \delta(r)a_y + a_x^\dagger \delta(r)a_z + a_y^\dagger \delta(r)a_z) + \text{h.c.}$</td>
</tr>
<tr>
<td>$c200d000$</td>
<td>$(a_x^\dagger + a_y^\dagger + a_z^\dagger) \delta(r) + \text{h.c.}$</td>
</tr>
<tr>
<td>$c110d000$</td>
<td>$(a_x^\dagger a_y^\dagger + a_x^\dagger a_z^\dagger + a_y^\dagger a_z^\dagger) \delta(r) + \text{h.c.}$</td>
</tr>
</tbody>
</table>
Testing Plan

1. Choose $V$
2. Solve $H\Psi = E\Psi$ in Box
3. Insert LECs in infinite volume $H_{\text{eff}}$
4. Filter to $A_1$ spectrum
5. Self consistency determines phase shifts
6. Fit LECs to reproduce spectrum
7. Traditional generation of phase shifts

$= ?$
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.

$L = 14.3 \text{ fm}$

$m_\pi L = 10$

<table>
<thead>
<tr>
<th>Rep</th>
<th>MeV</th>
<th>L=0</th>
<th>L=2</th>
<th>L=4</th>
<th>L=6</th>
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<td>$A_1^+$</td>
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</table>
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

\[
k \cot \delta_0 = \frac{2}{\sqrt{\pi} L} Z_{0,0}(1; \tilde{k}^2) + \frac{12288 \pi^7}{7 L^{10}} \frac{Z_{4,0}(1; \tilde{k}^2)^2}{k^9 \cot \delta_4} + O(\tan^2 \delta_4)
\]

Luu, Savage, arXiv:1101.3347

- An effective range expansion up to \(k^6\) is used to interpolate.

- For simplicity the second term is evaluated using the L=4 phase shift directly determined from V.
Phase Shift Results

The V column should be considered the reference.

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.

\[ L = 14.3 \text{ fm} \]
\[ m_\pi L = 10 \]

<table>
<thead>
<tr>
<th>E (MeV)</th>
<th>V</th>
<th>HOBET</th>
<th>Leading Lüscher</th>
<th>Next Order Lüscher</th>
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<td>74.691</td>
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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 \( \Lambda \) 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
End