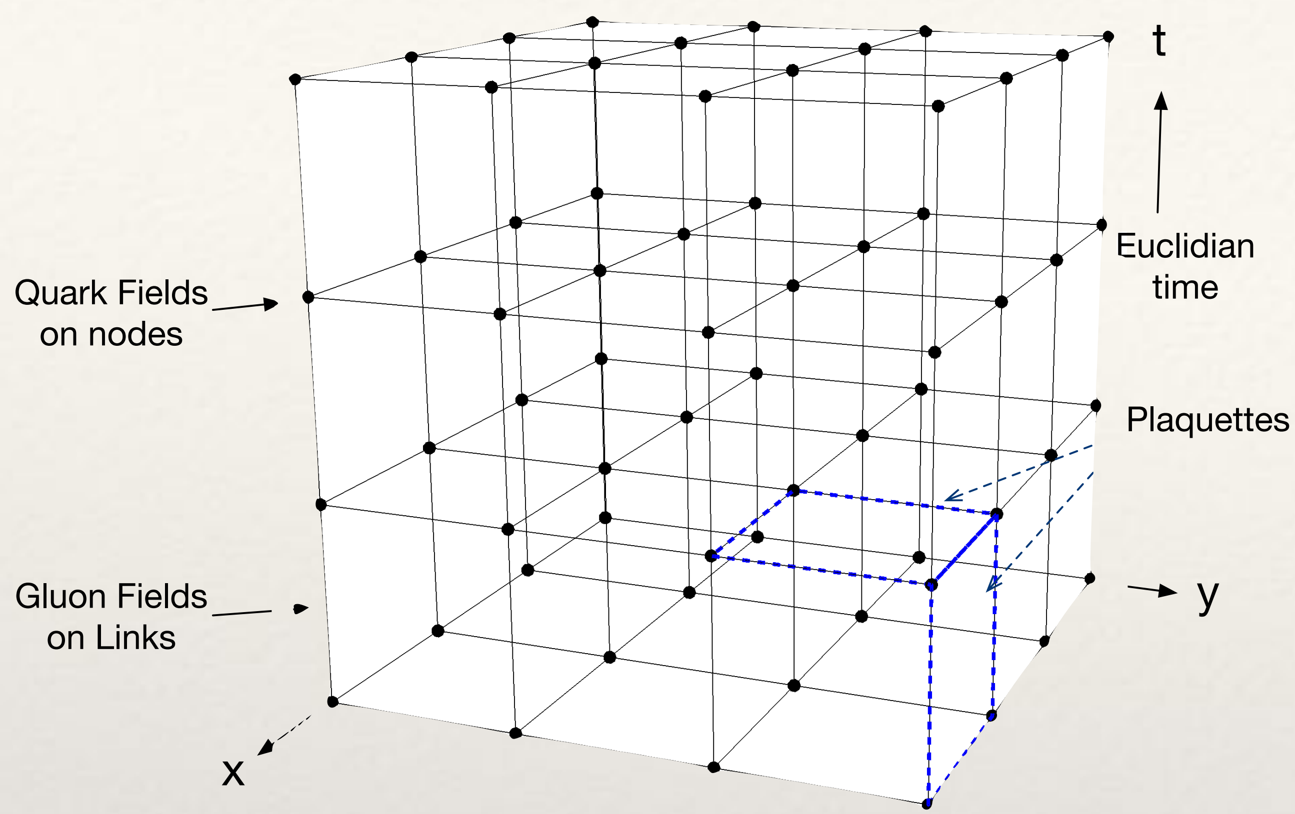

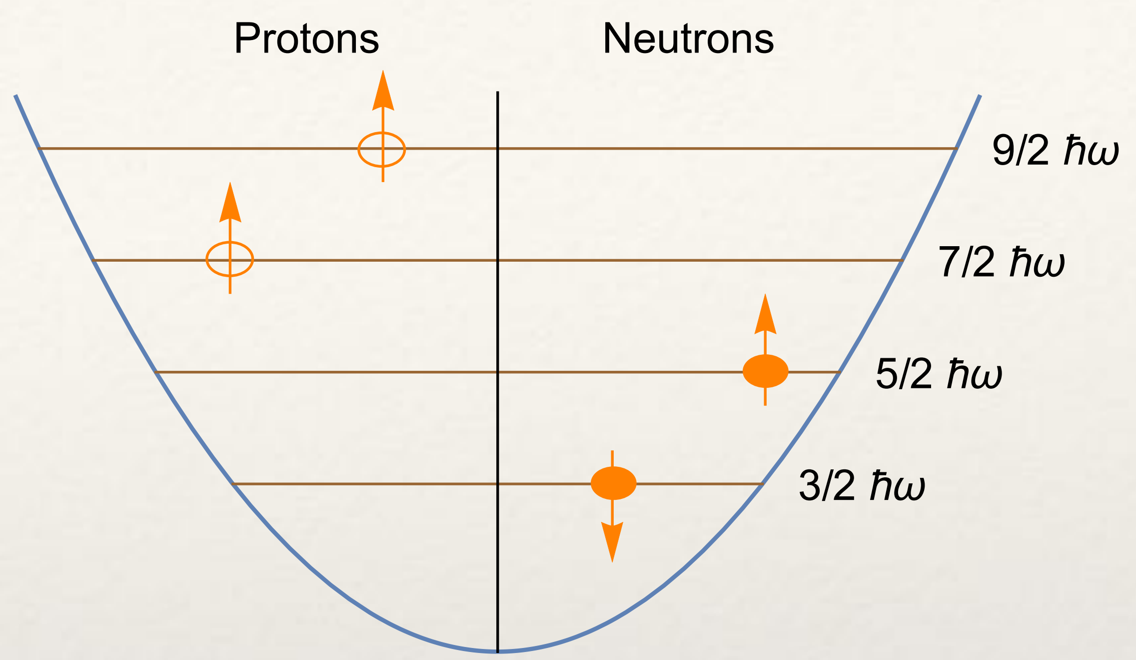

HOBET: Connecting LQCD to Nuclear Structure

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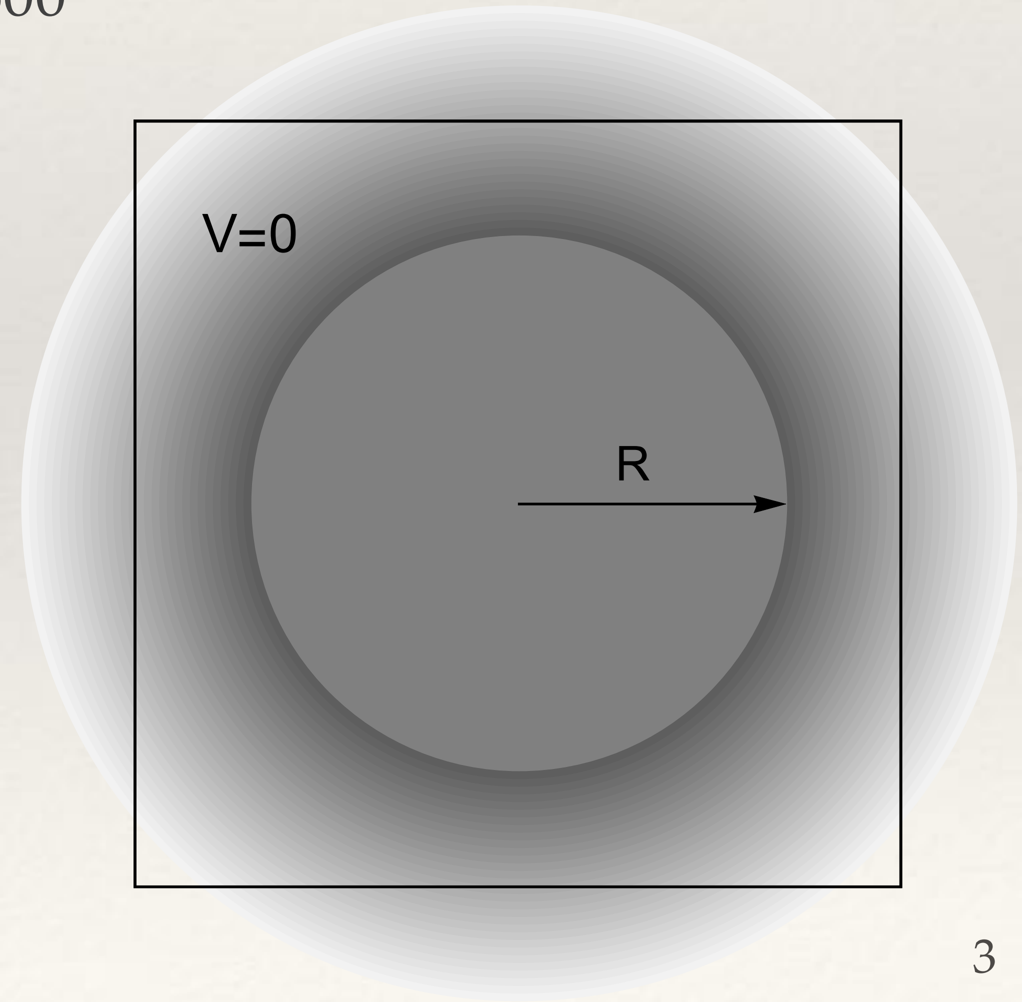
Outline

- Part 1: Construction of the HOBET (Harmonic Oscillator based Effective Theory) interaction from observables in spherical infinite volume form.
- Part 2: Construction of the HOBET interaction in Cartesian form from the spectrum in a periodic box.
    - The magic trick is that the LECs of the two forms can be related.

Interactions from LQCD

- Lüscher's method can be used to map the spectrum 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.



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.

The Bloch-Horowitz Equation

$$P \text{ is projection operator to space to work in}, \quad Q = 1 - P$$

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

- Eigenstates of $H_{eff}(E)$ are projections with the same eigenvalues.
  - All eigenstates that overlap P are included!
- Eigenstates are not orthogonal.
- Explicitly energy dependent: Must solve self consistently.
- Operators are formally renormalized as:

$$\hat{O}_{eff}(E) = \frac{E}{E - HQ}\hat{O}\frac{E}{E - QH}$$

ET and The HO Basis

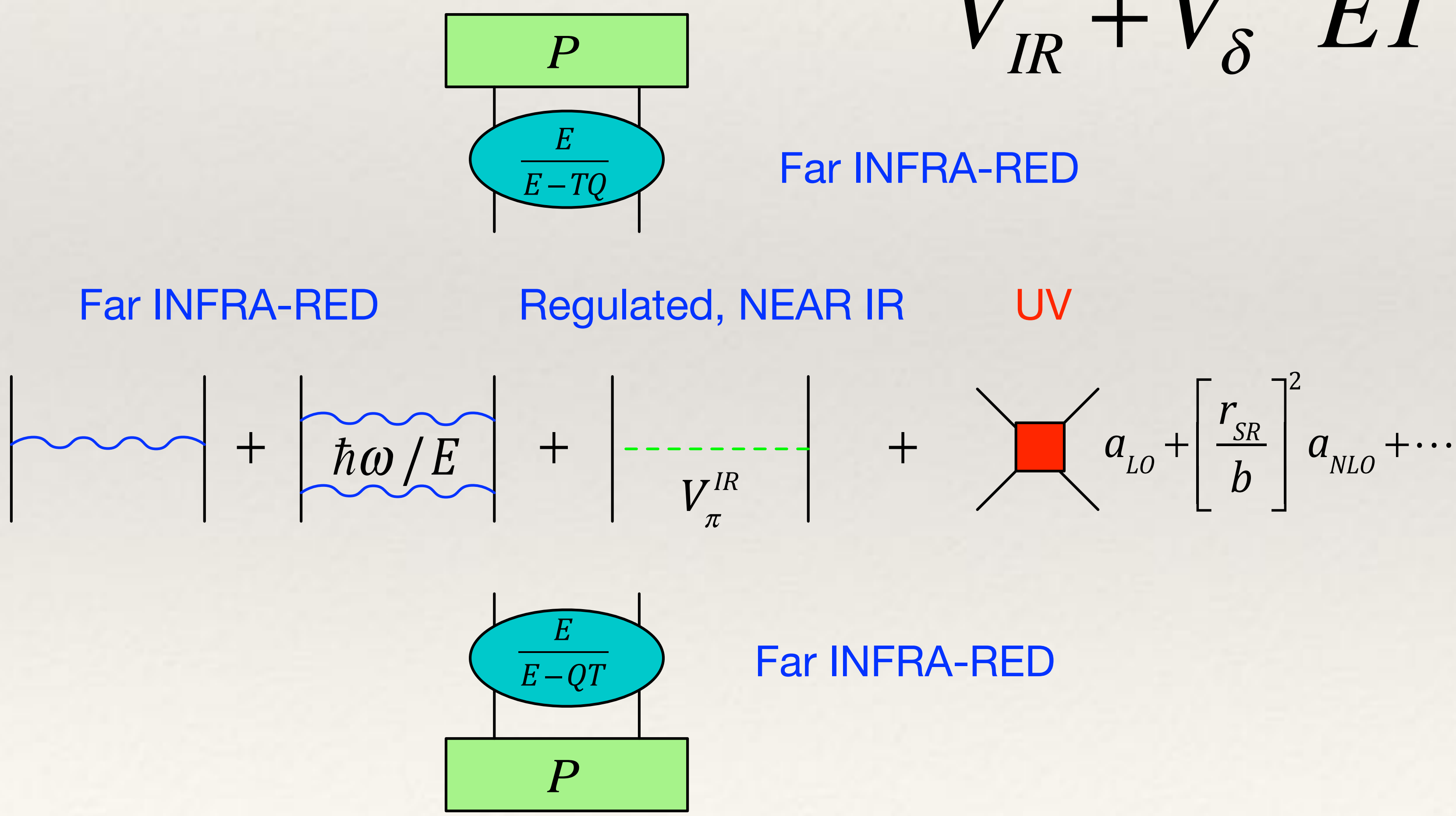
- In a typical EFT using a momentum basis T is diagonal and does not couple P & Q.
- In the HO basis T is a hopping operator, strongly connecting the last P state to the lowest Q state.
  - Bad news for an ET expansion.
  - Maybe H_{eff} can be reorganized, isolating T …

The Effective Theory Expansion

The Haxton-Luu form of the Bloch-Horowitz Equation

$$H_{eff}(E) = P\frac{E}{E-TQ}\left[T + T\frac{Q}{E}T + \underbrace{V + V\frac{1}{E-QH}QV}_{V_{IR}+V_{\delta}}\right]\frac{E}{E-QT}P$$

ET Substitution



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

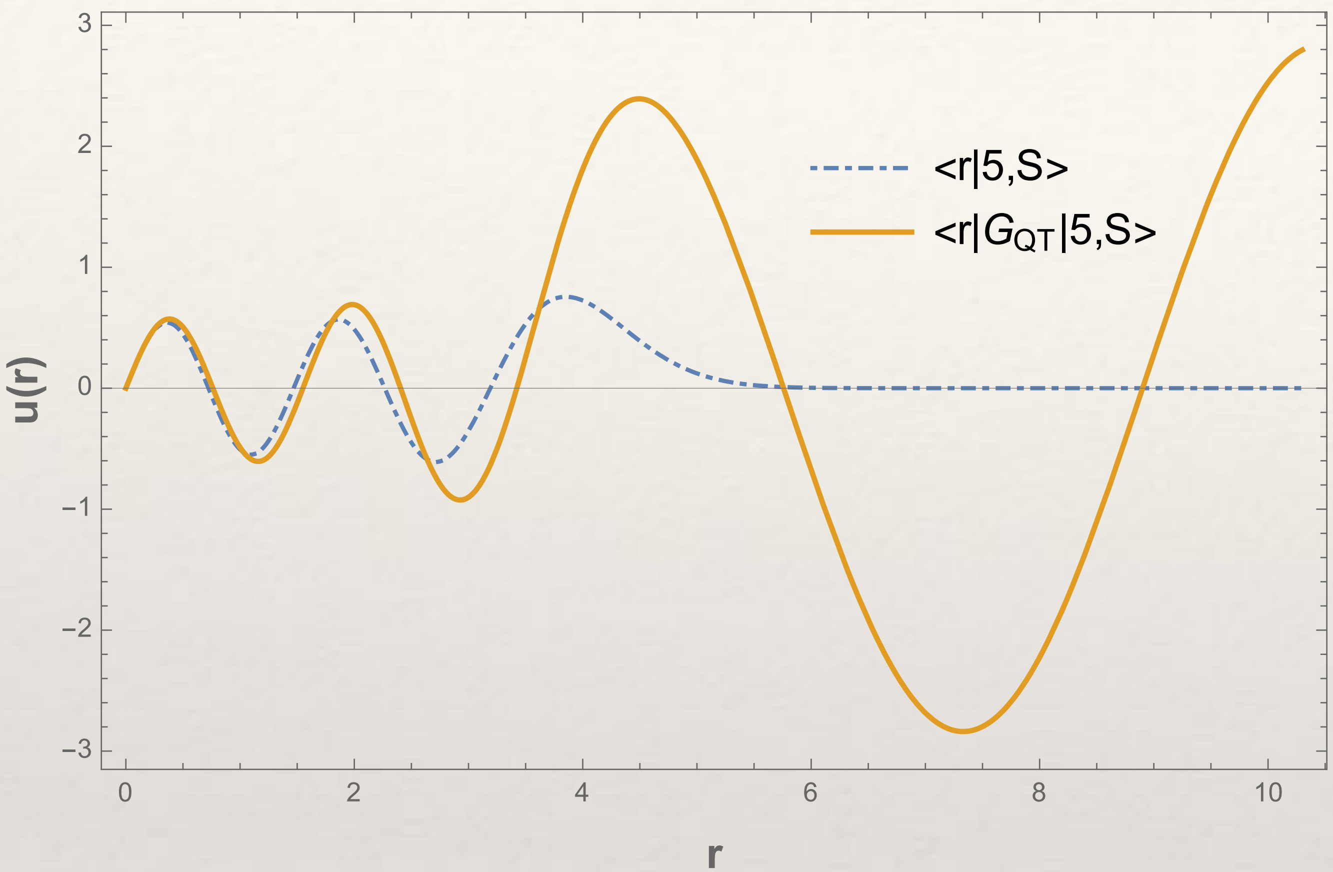
- Simplify: $\left|\tilde{i}\right\rangle = \frac{E}{E-QT}\left|i\right\rangle = b_{ij}\frac{E}{E-T}\left|j\right\rangle, \quad b_{ij} = \left\{P\frac{E}{E-T}P\right\}_{ij}^{-1}, \quad i,j \in P$
- GF for E/(E-T) is expressed in terms of solutions of (E-T)u=0

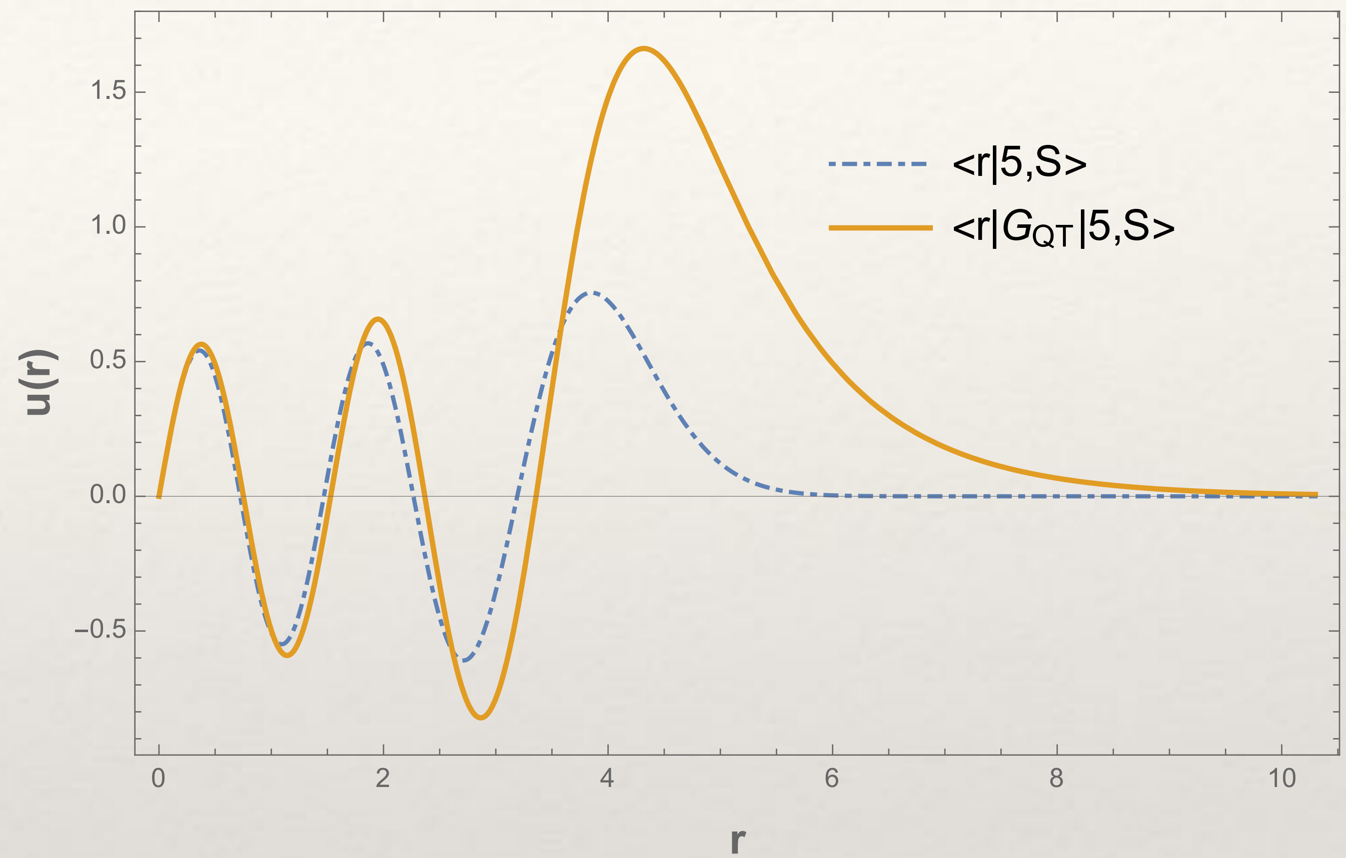
$$u_{in}(r) = kr\ j_\ell(kr),\ u_{out}(r) = kr\left(-\cot(\delta_\ell)\ j_\ell(kr) + \eta_\ell(kr)\right)$$

$$g(r,r') \propto \begin{cases} u_{in}(r)u_{out}(r') & r < r' \\ u_{out}(r)u_{in}(r') & r > r' \end{cases}$$

- For r > range(HO basis) the form of the transformed edge state is $u_{out}(r)$.
- The boundary condition at infinity is specified by δ_ℓ .

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 Operator Expansion

- Described in terms of HO lowering operators.

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

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

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

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

Matrix Structure: $^1S_0$, Λ=8

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

- 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, Bdy_i).

Fitting LECs

- Principle: The BH equation is energy self consistent

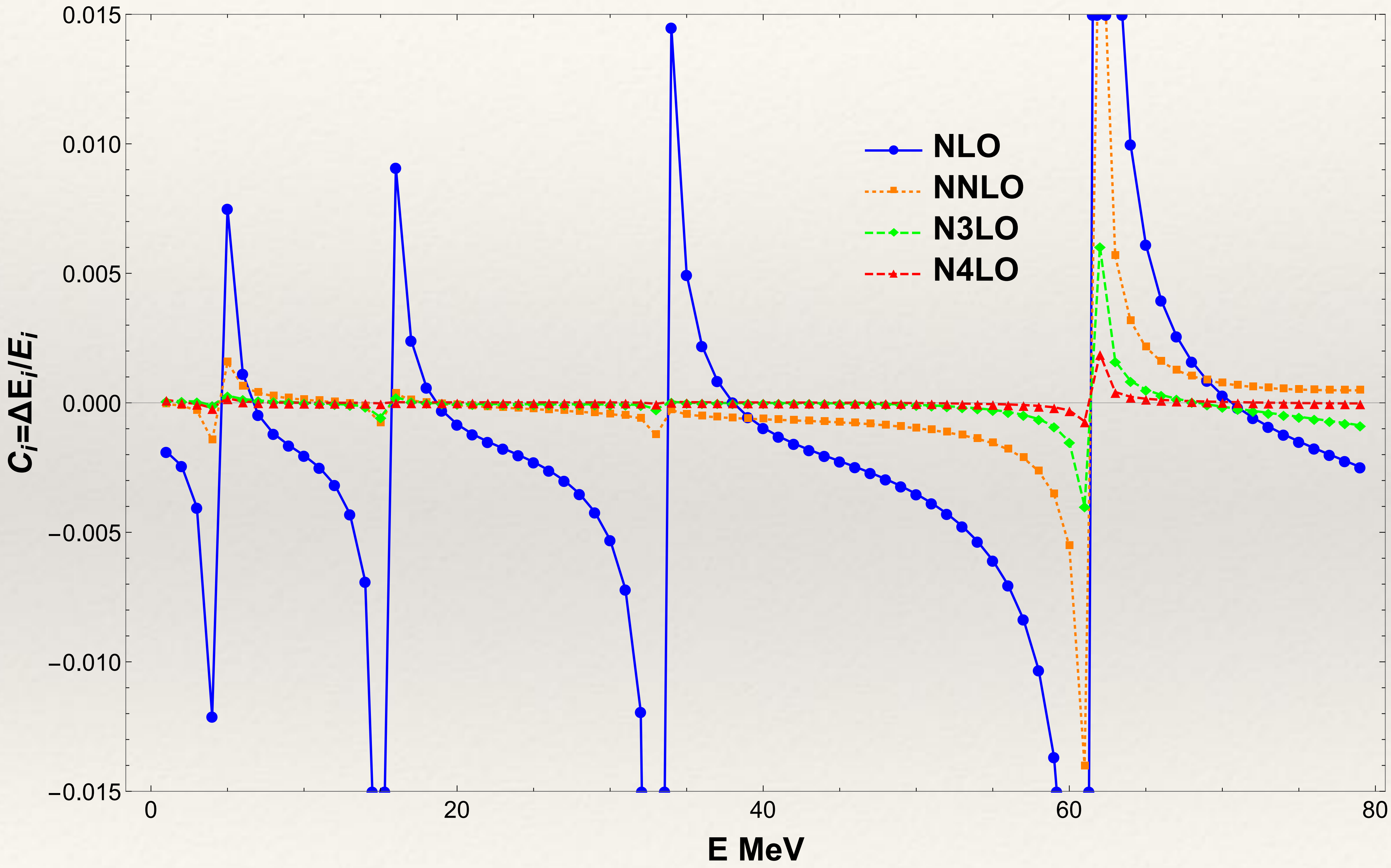
$$H_{eff}^{full}\, P\left|\psi_i\right\rangle = E_i P\left|\psi_i\right\rangle$$

- At fixed order we have a nearby eigenstate.

$$H_{eff}\left(LECs\right) P\left|\psi_i'\right\rangle = \varepsilon_i P\left|\psi_i'\right\rangle$$

- The mismatch must be due to LEC values.
- Repair by minimizing $\sum_{i\in samples} W(i)\left(\varepsilon_i - E_i\right)^2 / \sigma_i^2$
- The variance can be replaced by a full covariance matrix.

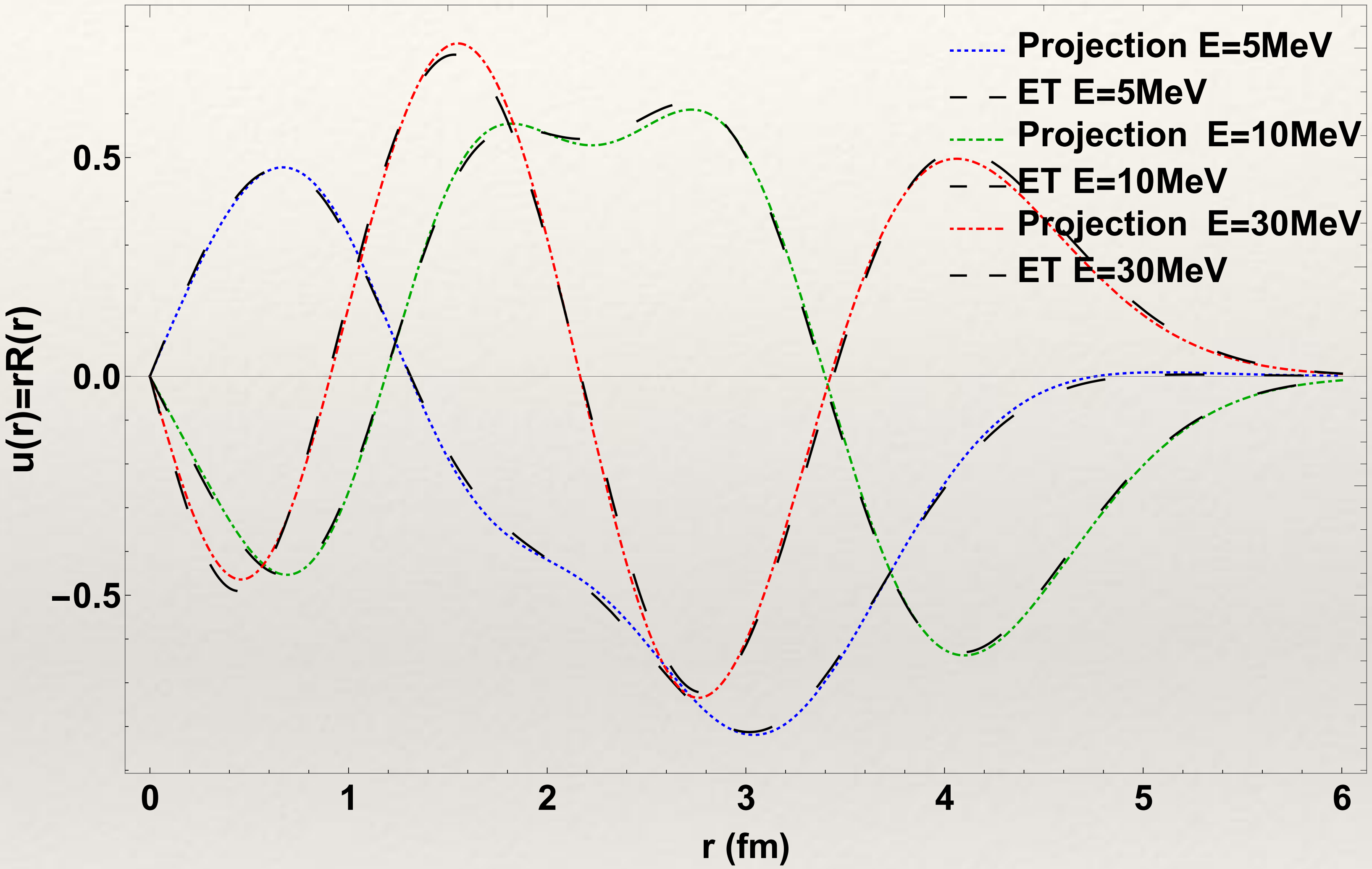
S-Channel Eigenvalue Convergence



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.

Part 1 Conclusions

- The HOBET interaction can be directly constructed from observables such as phase shifts in the continuum
- LQCD can produce nuclear phase shifts, subject to statistical errors and uncorrected finite volume effects.
- In combination, a nuclear effective interaction is produced that can be used in A-body calculations.

Outline

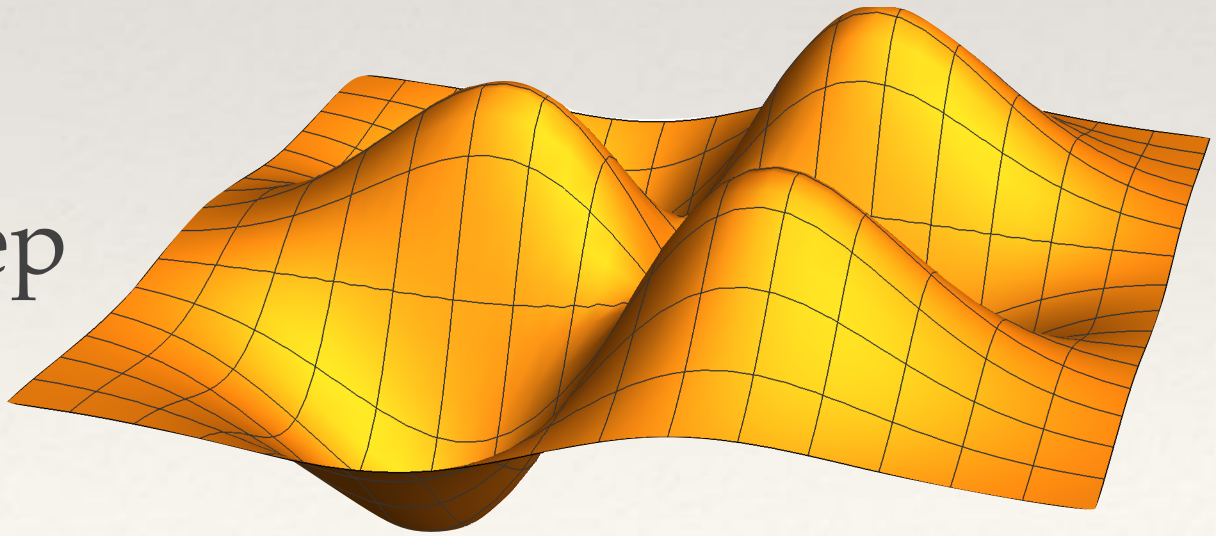
- Part 1: Construction of the HOBET (Harmonic Oscillator based Effective Theory) interaction from observables in spherical infinite volume form.
- Part 2: Construction of the HOBET interaction in Cartesian form from the spectrum in a periodic box.
  - The magic trick is that the LECs of the two forms can be related.

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

Cartesian Harmonic Oscillator

- 3D harmonic oscillator can be equivalently represented in spherical or Cartesian form.
  - Brackets $\langle n_x n_y n_z | n\ell m \rangle$ relate states in each energy level.
  - Quanta based cutoff is consistent - key
- The Cartesian form will be convenient for the periodic boundary conditions.
- Pick HO length scale to keep the basis away from edges in all volumes.



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:

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

$$\phi_{i,c,0}(x) = \sqrt{2/L_i}\,(1/\sqrt{2}), \quad m = 0$$

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

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

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

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

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

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

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

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

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

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

Evaluate by Inserting Periodic Basis

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

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

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

- All pieces are precomputed, but sum is still very large.
- For $\vec{n}',\vec{n} \in P^-$ $G_{QT}=1$, which can be used to check results.

Magic with V_δ

- As long as V_δ 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 9.1: LECs and Cartesian operators

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

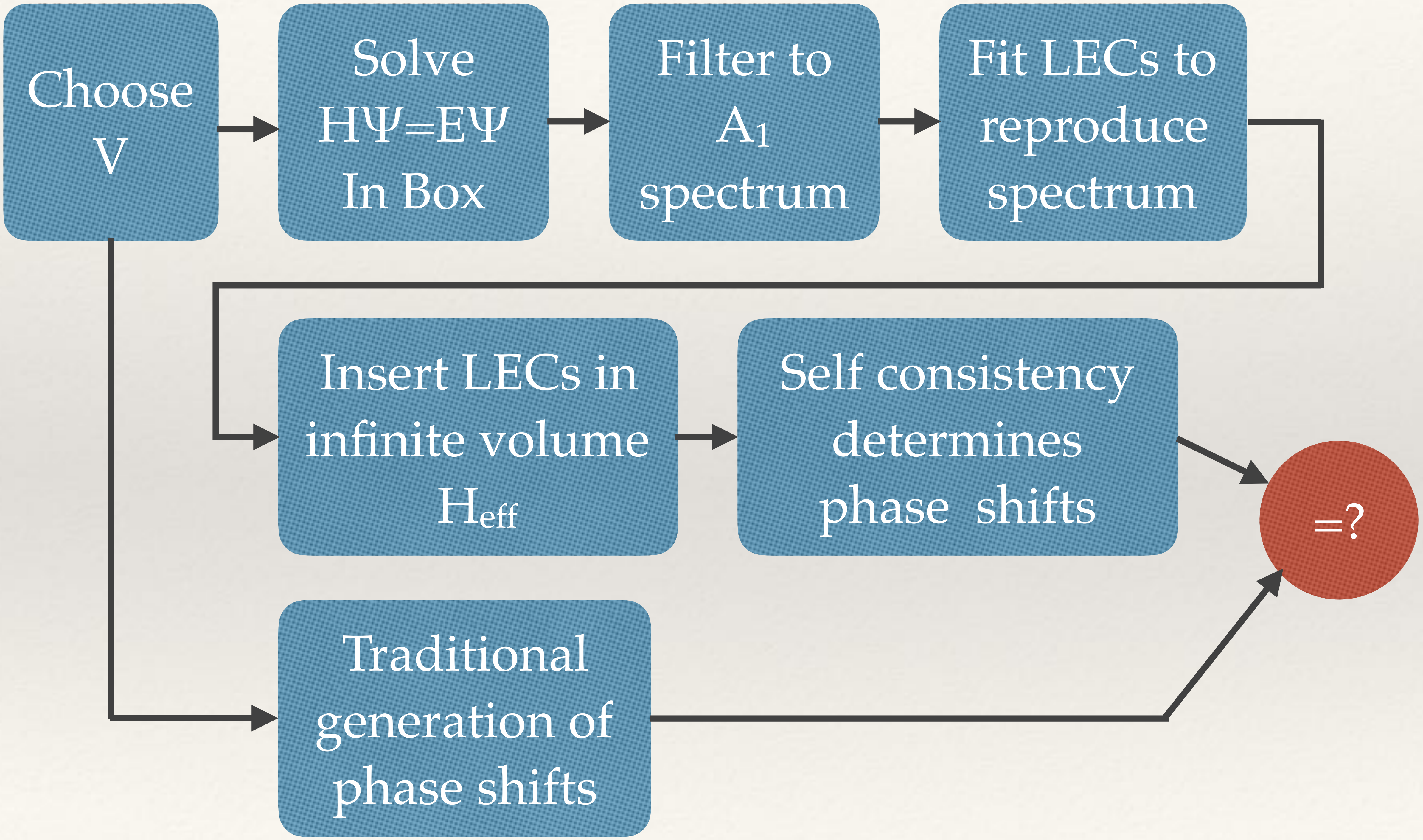
Relating Spherical to Cartesian V_δ

- Symmetries:
  - Cartesian construction: parity invariance.
  - Spherical construction: parity and rotational invariance.
- Setting $V_{\delta,cart}$=$V_{\delta,sph}$ on P^- imposes rotational invariance.
- Cartesian LECs are replaced by linear comb of spherical LECs, including in edge state matrix elements.

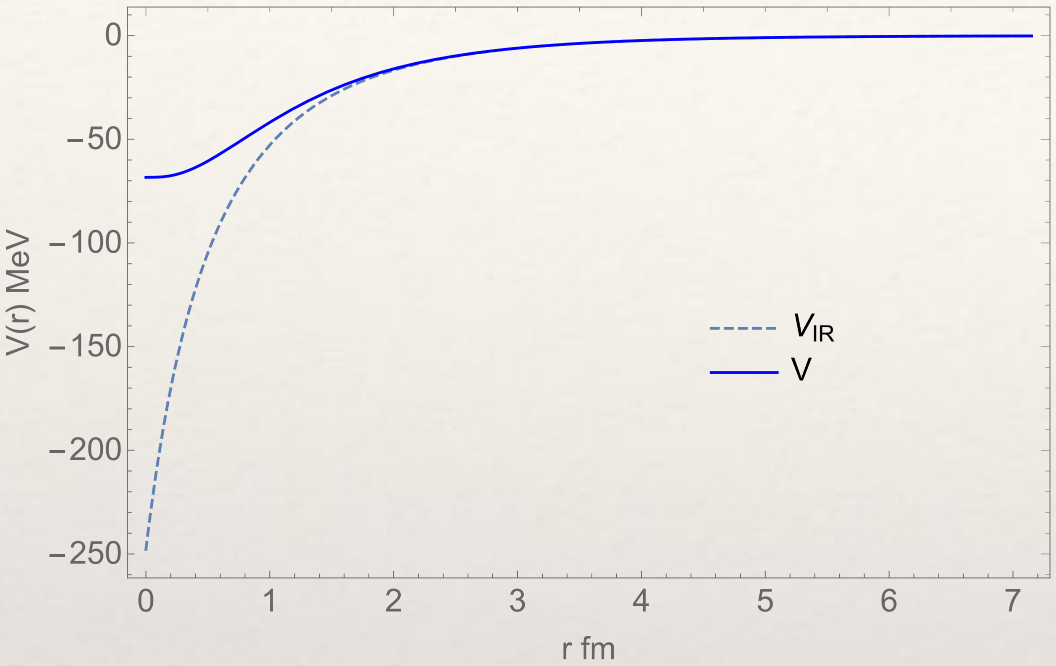
Example:

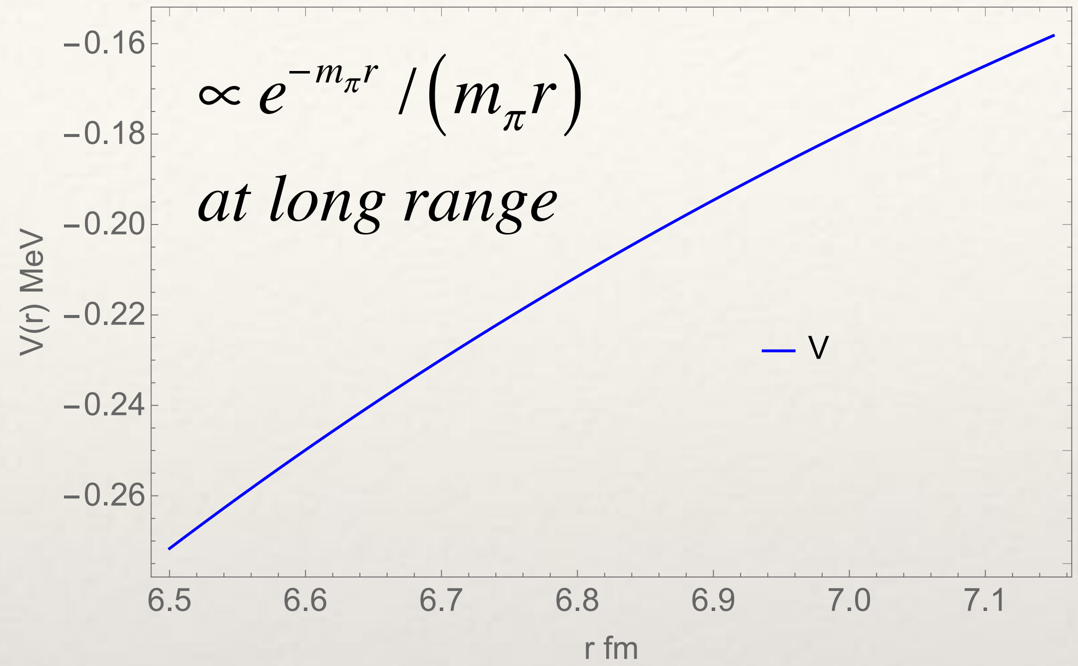
$$c200d200 = a^{1S0}_{NNLO22} + (2/3)a^{1D2}_{NNLO}$$
$$c200d020 = a^{1S0}_{NNLO22} - (1/3)a^{1D2}_{NNLO}$$

Testing Plan



Test Setup: Range(V)>L/2





$L = 14.3\ fm$

$m_\pi L = 10$

- 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 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

$$k\cot\delta_0 = \frac{2}{\sqrt{\pi}L}\mathcal{Z}_{0,0}\left(1;\tilde{k}^2\right) + \frac{12288\pi^7}{7L^{10}}\frac{\mathcal{Z}_{4,0}\left(1;\tilde{k}^2\right)^2}{k^9\cot\delta_4} + \mathcal{O}\left(\tan^2\delta_4\right)$$

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

$L = 14.3\ fm$

$m_\pi L = 10$

The V column should be considered the reference.

E MeV	V	HOBET	Leading Lüscher	Next Order Lüscher
1	142.023	141.931	142.552	142.751
2	128.972	128.860	129.571	129.823
4	113.602	113.464	114.205	114.403
8	96.919	96.752	97.575	97.3135
10	91.473	91.296	92.228	91.6403
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.

Observations on Errors

- Images double the potential contribution at the center of the faces.
- For HOBET the impact is suppressed by two powers of V in $V\left(1/\left(E-QH\right)\right)QV$.
- The second order correction for Lüscher's method is significant. In this trial parts of the spectrum fell near the divergences of $\mathcal{Z}_{4,0}$.

New Idea - Better Isolation

$$V = V_{UV} + V_{IR}$$ e.g. V_{UV} - unknown, V_{IR}=OPEP

$$V\frac{1}{E-QH}QV = \left(V_{UV}+V_{IR}\right)\frac{1}{E-QT-QV_{IR}-QV_{UV}}Q\left(V_{UV}+V_{IR}\right)$$

$$= V_{IR}\frac{1}{E-QT-QV_{IR}}QV_{IR} + V_{UV}[\dots] + [\dots]V_{UV}$$

- This motivates a new ET substitution.

$$V + V\frac{1}{E-QH}QV \rightarrow V_{IR} + V_{IR}\frac{1}{E-QH_{IR}}QV_{IR} + V_{\delta}$$

- V_{δ} becomes much shorter range, enabling the use of even smaller volumes.

Part 2: Conclusions

- The Cartesian finite volume HOBET interaction LECs are directly fit to the spectrum in a set of volumes.
- The same LECs are used in both infinite and finite volume forms.
- Finite volume effects are isolated from the ET expansion.
  - Issues common to other methods with the range of V are suppressed.
    - Allows smaller volumes for LQCD calculations.
- A direct test of both HOBET and Lüscher's method was made.
- Future: A 3-body interaction can be fit to a 3-body spectrum.

End