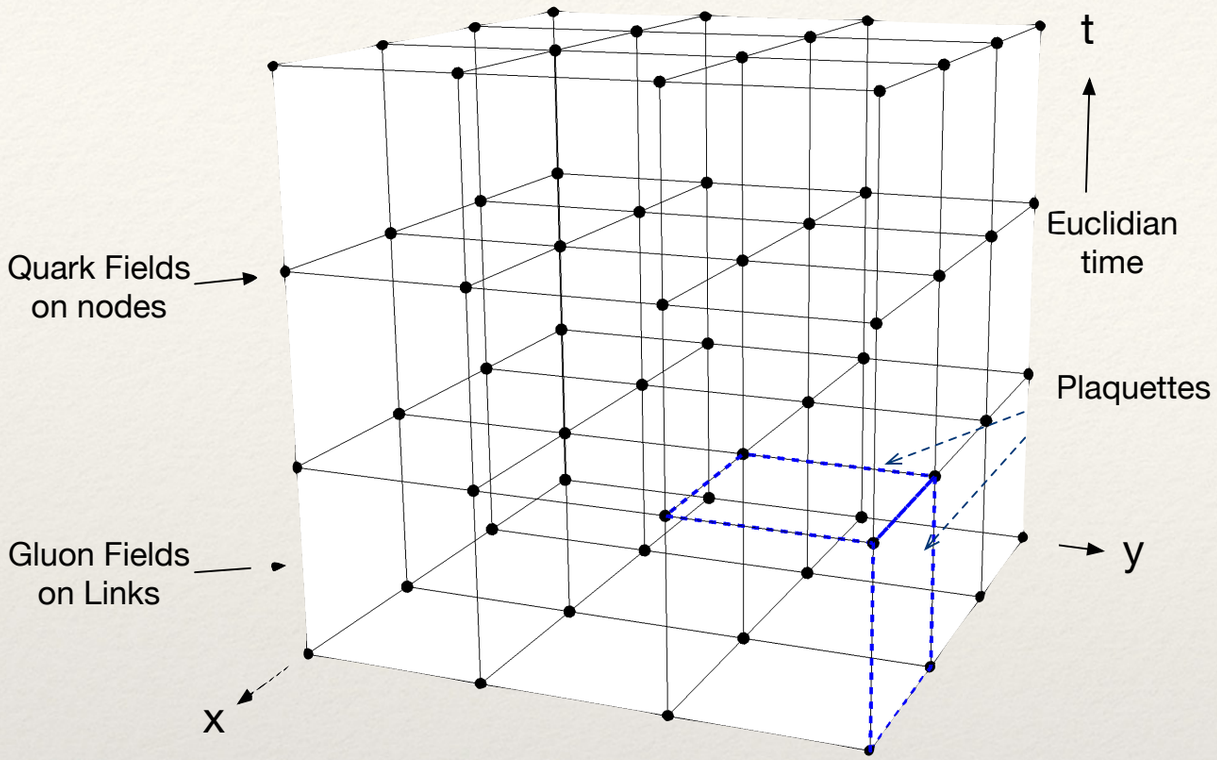

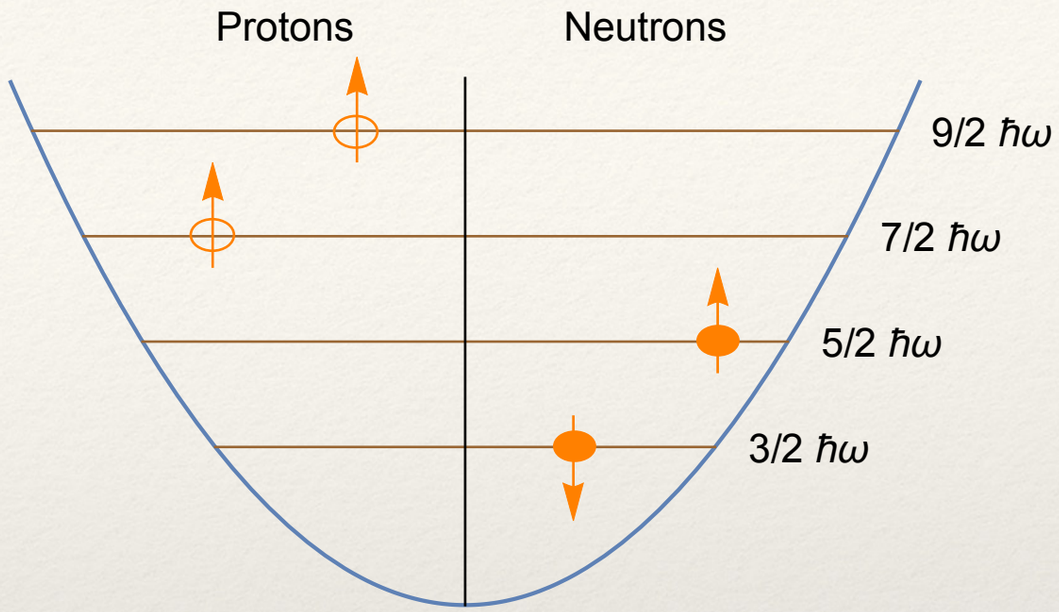

In collaboration with Wick Haxton

Connecting LQCD to Nuclear Structure via Harmonic-Oscillator-Based Effective Theory

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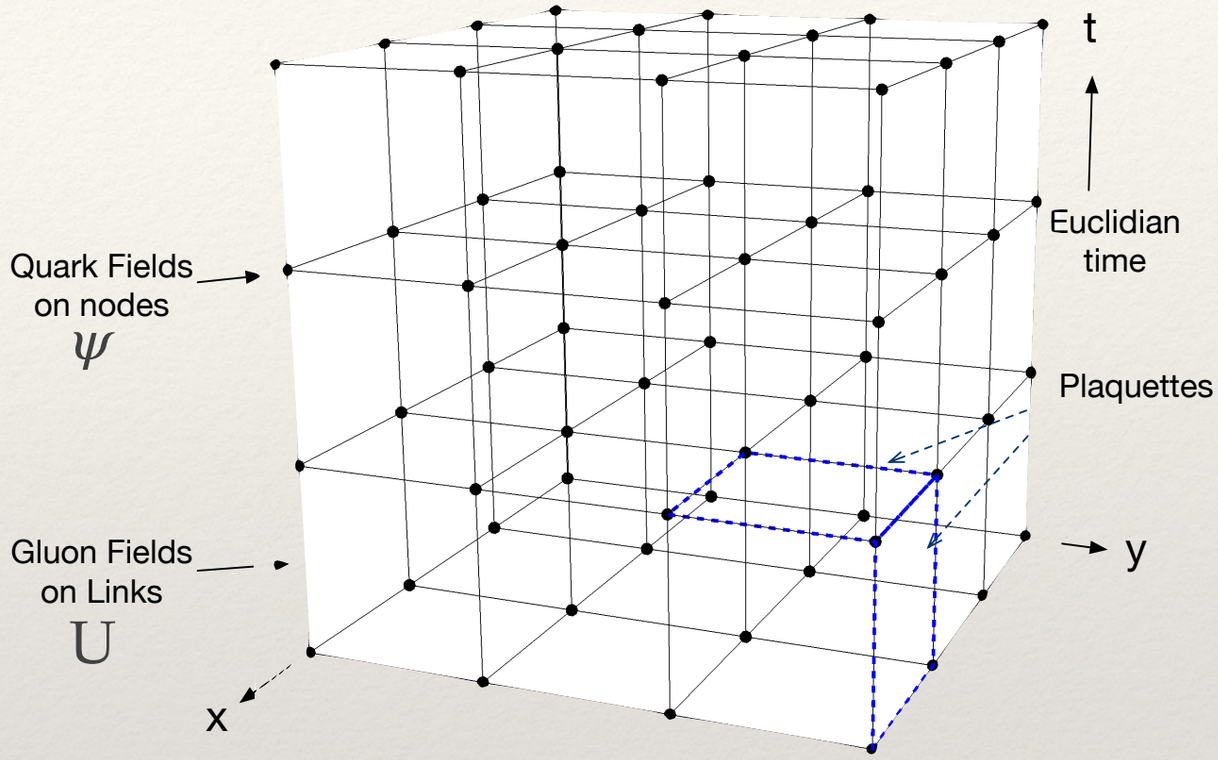
Timeline

- 1973 - QCD introduced
  - Early successes in high energy scattering.
  - Nuclear physics in principle is also a consequence…
- 2012 - LQCD calculation of 2 nucleon states with non-physical heavy pions to reduce noise. - NPLQCD Beane et al., Phys. Rev. D85 (2012)
  - Early trial run.
- 2018 - “A per-cent-level determination of the nucleon axial coupling from quantum chromodynamics.” , Chang et al., Nature 558, 91-94 (2018)
  - Single nucleon calculation using a massive supercomputer!
- 202? - LQCD calculation of the spectrum of two nucleons at the physical point in a finite volume.
- LQCD computation are really hard!!

Lattice Quantum Chromo Dynamics (LQCD)

- A lattice calculation is non-perturbative, but …
- The no free lunch rule creates new problems.
  - Finite volume effects.
  - Discretization errors.
- Observables are evaluated by expensive Monte-Carlo integration over field configurations.
- Statistical uncertainty is $\propto N_{sample}^{-1/2}$



The z direction has been suppressed.
Space and time are periodic.

$$Lattice\ Size = L^3 \times T \times L_5 \times N_c \times N_s$$

$$\approx 3.5B \text{ lattice points}$$

$$L = 64, T = 96, L_5 = 12, N_c = 3, N_s = 4$$

Wick's Vision

Nonrelativistic Nuclear Structure
(model dependent)

Cold Lattice QCD (exact, but with a sign problem growing with A)

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δ^{LQCD}

A Controlled Nonrelativistic ET Applicable to Nuclei

Cold Lattice QCD focused on NN scattering observables

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Experimental Observables

Connect to Fundamental Theory

CalLat

Lattice QCD is Really Hard

- What is the minimum we can get away with computing?
  - NN Scattering states in a finite volume.
- Constructing a high momentum potential from this scattering data still takes way too much data.
- Answer: **Directly** fit a suitable low momentum effective theory (ET) to LQCD scattering data.

Effective Theory

- Ground Rules of Effective Theory
  - Formulated in a relevant subspace P (with complementary subspace Q) of the full Hilbert space. In the HO basis we use a quanta cutoff Λ for P.
  - Respects the symmetries of the underlying full theory.
  - Contains a systematic parameterized expansion such that controlled approximations to the full P+Q theory are calculable in P. Approximations are organized by order (power counting).
  - The parameters of the expansion, known as Low Energy Constants (LECs), are in principle determinable (in practice usually too hard) from the full theory, but importantly may also be fit to observables.
  - In the HO basis P is a function P(b,Λ) of the HO length scale and Λ
    - Results do not depend on b and Λ, but the order may have to be increased.

HOBET
Harmonic-Oscillator-Based Effect Theory

$$H^{eff} = PH\boxed{\frac{1}{E-QH}}QHP = P\frac{E}{E-TQ}\left[T - T\frac{Q}{E}T + V + V\frac{1}{E-QH}QV\right]\frac{E}{E-QT}P$$

- Tom Luu explained the the Bloch-Horowitz equation yesterday.
- The perturbative expansion of the boxed propagator has bad convergence, caused by the kinetic energy, T, which is a hopping operator in the HO basis. (Haxton, Song, Luu)
- The form on the right isolates this bad behavior so that kinetic energy scattering can be analytically computed.

HOBET
Harmonic-Oscillator-Based Effect Theory

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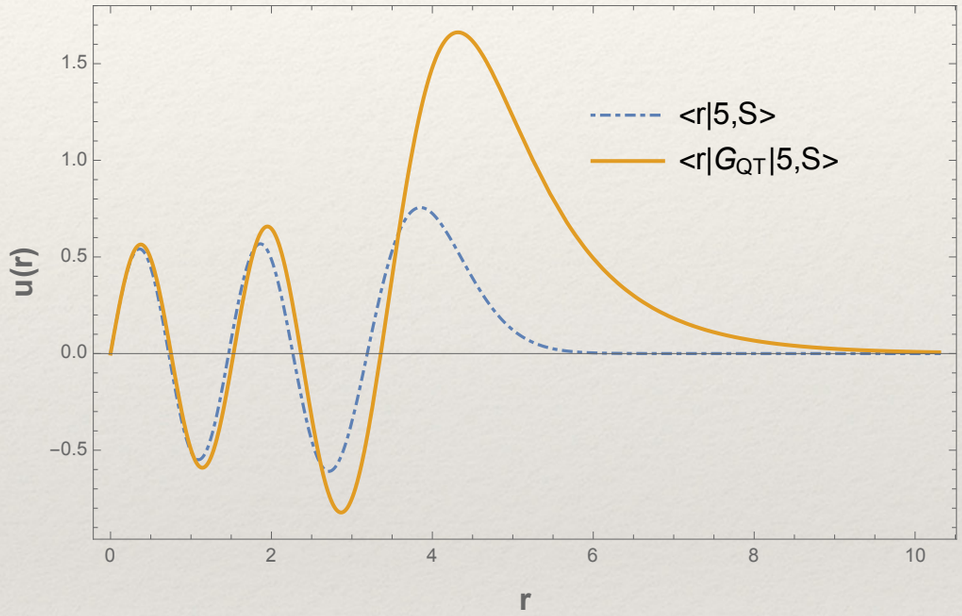
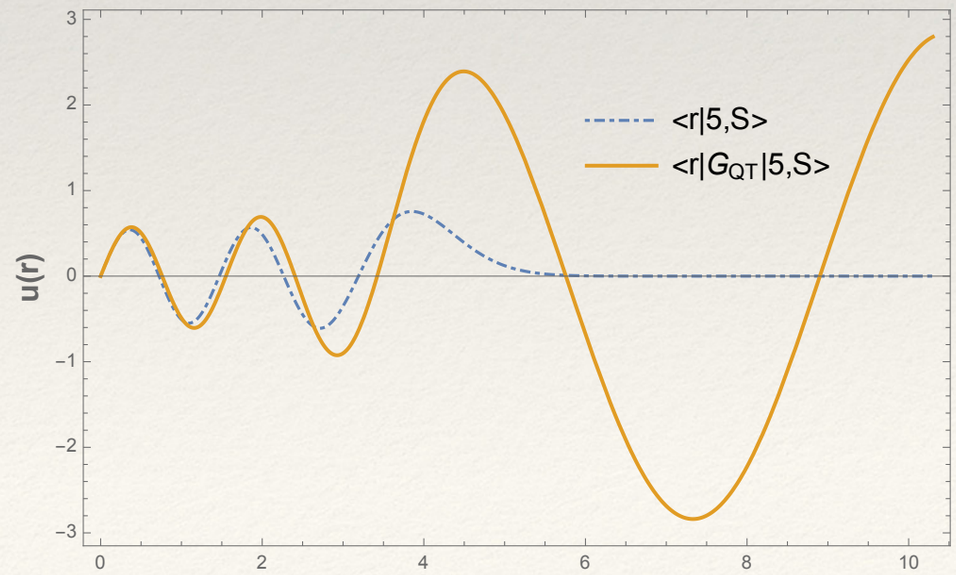
- Green's function acts only on edge states, producing a superposition of edge and higher quanta states.
- The Green's function boundary condition is the phase shift.



$$E = +\hbar\omega/2$$



$$E = -\hbar\omega/2$$

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Harmonic-Oscillator-Based Effect Theory

$$H^{eff} = PH\boxed{\frac{1}{E-QH}}QHP = P\frac{E}{E-TQ}\left[T - T\frac{Q}{E}T + \underbrace{V + V\frac{1}{E-QH}QV}\right]\frac{E}{E-QT}P$$

- The fourth term is capped on both ends by the short range operator V and is therefore short range.

- We make The ET Substitution: $V + V\frac{1}{E-QH}QV \to V_\pi^{IR} + V_\delta$
- V_π^{IR} is the long range part of V not correctable by V_δ.
- V_δ is the systematic expansion.

$$V_\delta^S = a_{LO}^S\delta(r) + a_{NLO}^S\left(\hat{A}^\dagger\delta(r) + \delta(r)\hat{A}\right) + a_{NLO}^{S,02}\left(\hat{A}^{\dagger 2}\delta(r) + \delta(r)\hat{A}^2\right) + \cdots$$

$$V_\delta^{SD} = \left[a_{NLO}^{SD}\left[\left(a^\dagger \otimes a^\dagger\right)\delta(r) + \delta(r)\left(\tilde{a}\otimes\tilde{a}\right)\right]^{(2)} + \ldots\right]\odot\left[\sigma_1\otimes\sigma_2\right]^{(2)}$$

$$\bullet\ \bullet\ \bullet$$

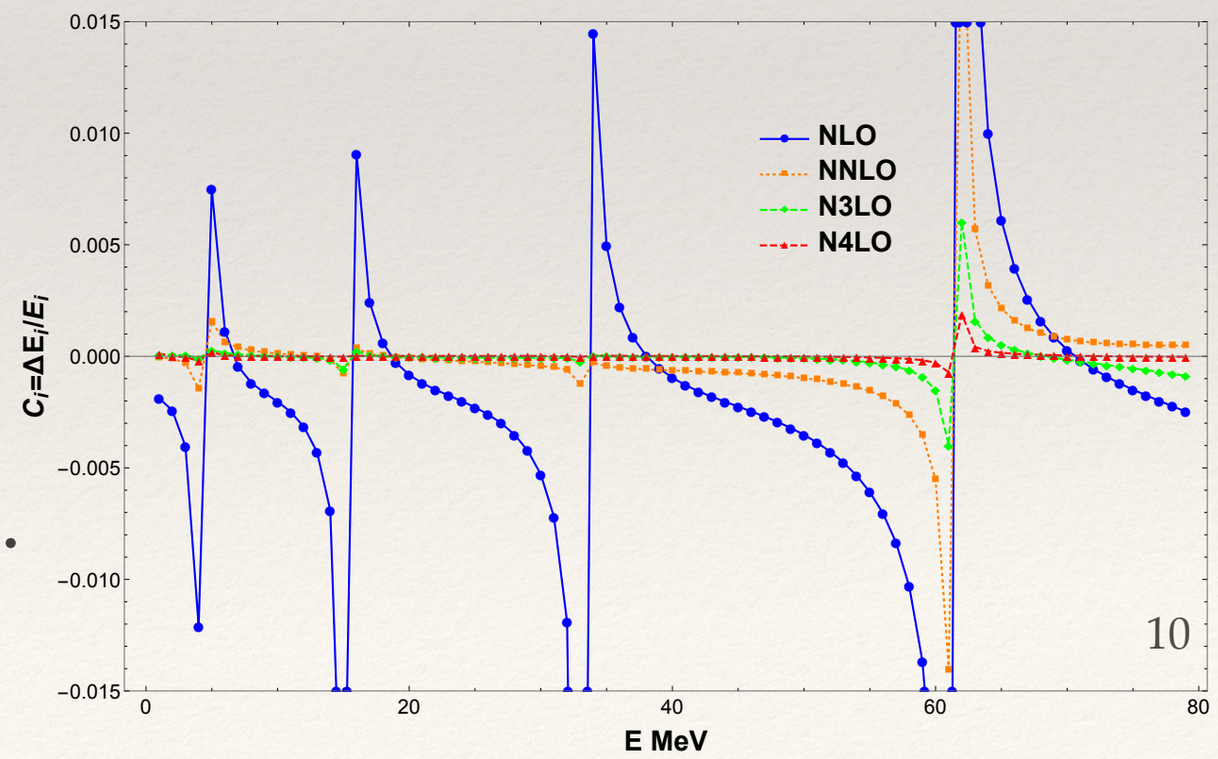
$\hat{A} = (\tilde{a}\odot\tilde{a})$ *lowers nodal n,* $a = (a_x, a_y, a_z)$ *is a vector lowering operator.*

Fitting LECs

- 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.

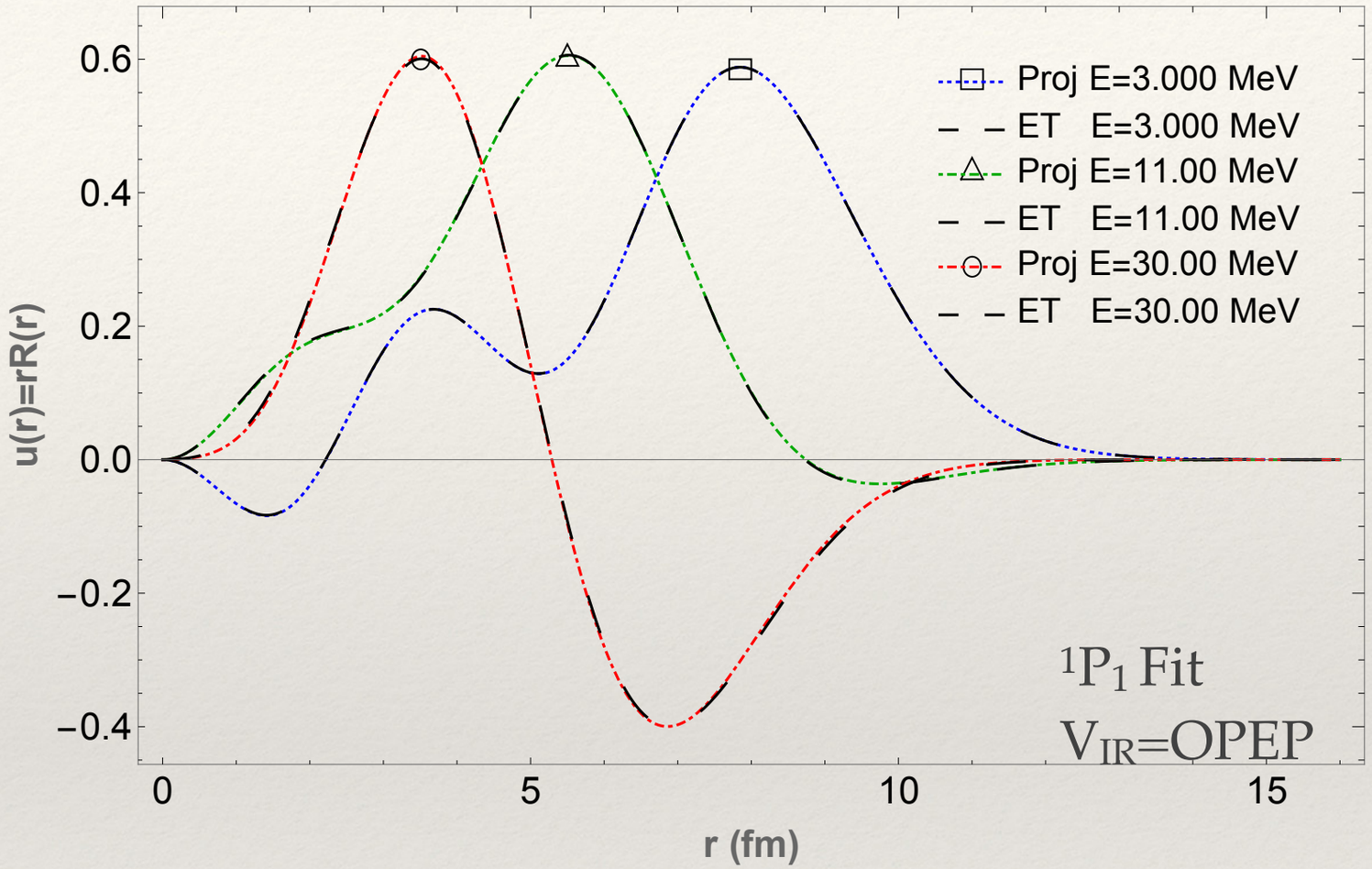
$$H_{eff}(LECs)\, P|\psi'_i\rangle = \varepsilon_i P|\psi'_i\rangle$$

- The mismatch must be due to LEC values.
- Repair by minimizing $\sum_{i \in samples} W(i)\left(\varepsilon_i - E_i\right)^2 / \sigma_i^2$
- This is a typical convergence plot showing the order by order improvement in the eigenvalue match.
- H_{eff} is continuous across E=0. continuum -> bound states



Continuum Wave Functions

- ET Wave functions (long black dashes) should match projections of numerical solutions with Av_{18} (dotted colored lines)

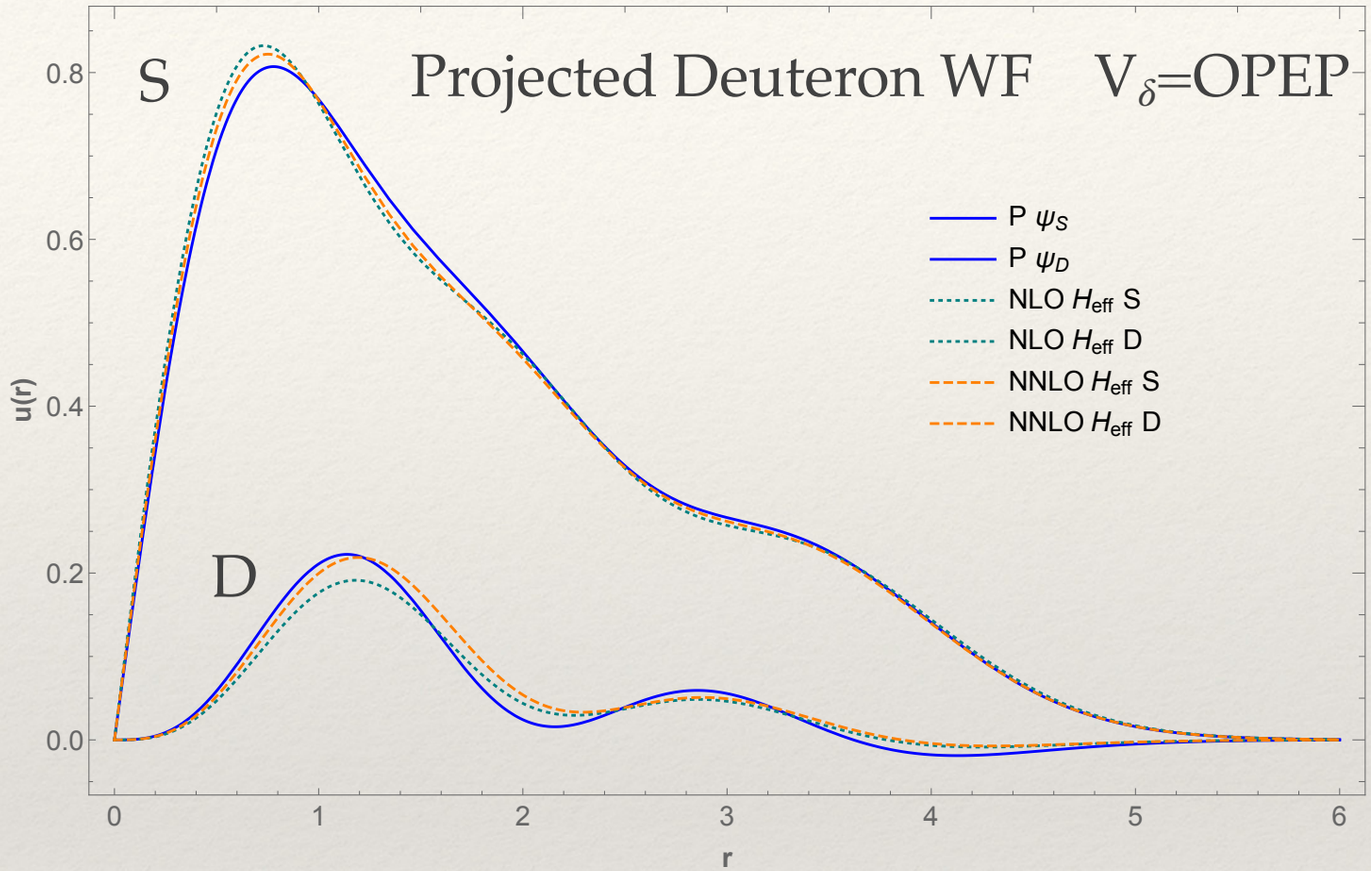


- The energies chosen in the plot are deliberately chosen to be distinct from the (E_i,δ_i) used in fitting the LECs.
- Phase shifts are recovered by solving for δ in

$$H^{eff}\left(E_i, LECs, \delta\right)P|\psi\rangle = E_i P|\psi\rangle.$$

Predicting the Deuteron

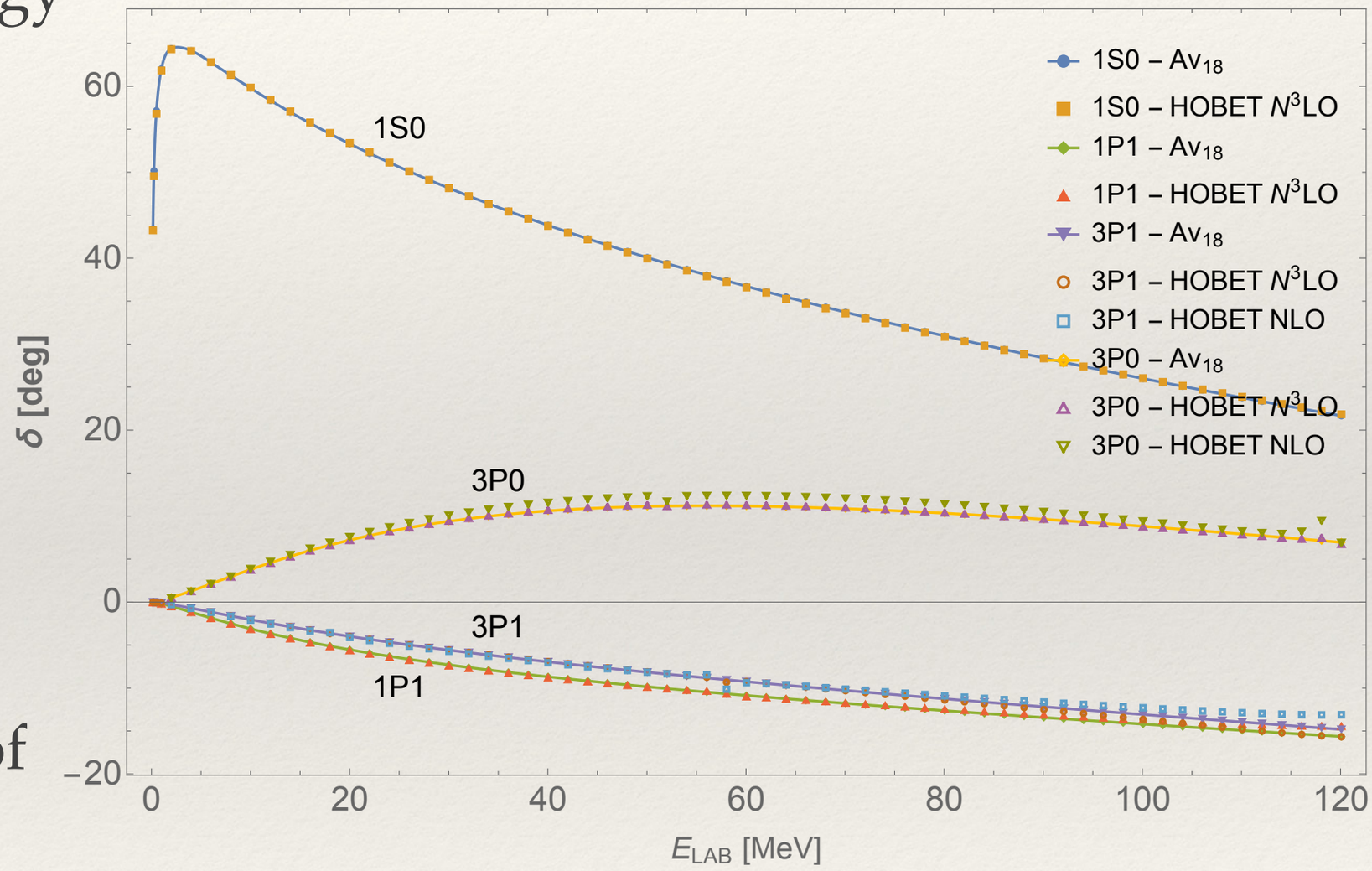
- Prediction of Deuteron WF from phase shift fit.
- ET Wave functions should match projections of numerical solutions with Av_{18} - solid blue lines



- The matrix elements are continuous in energy across E=0, one can fit V_δ in the continuum and determine bound states.
- Using the same phase shift data we get
  - With pionful V_{IR}=OPEP, at N3LO $E_{binding}$=-2.2278 MeV
  - With pionless V_{IR}=0, at N3LO $E_{binding}$=-2.0690 MeV

LECs →Phase Shifts

- Use fixed LECs at energy E, dial phase shift produce eigenvalue match to E.
- Even NLO 3P1 fit produces a good reproduction of phase shifts.
- A very small number of LECs reproduce phase shifts. P channel NLO has 1, other N3LO have 4.

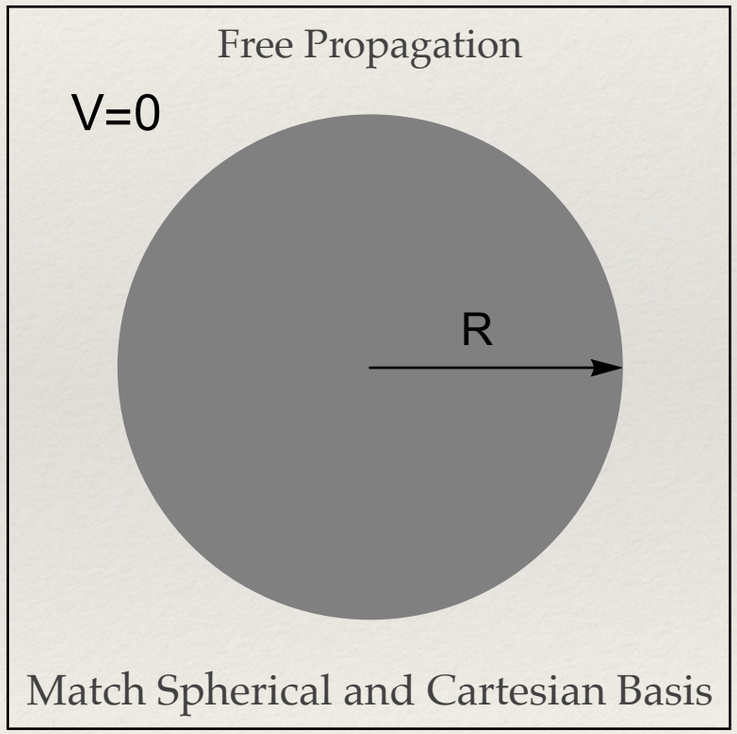


A lot of physics is in the Green's Functions

$$\frac{E}{E-QT} = EG_{QT}$$

Connecting to 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 it to fit the HOBET effective interaction.



- Sources of error
  - Tail of interaction exceeding L/2.
  - Divergences of the zeta function in higher order terms of Lüscher's formula.

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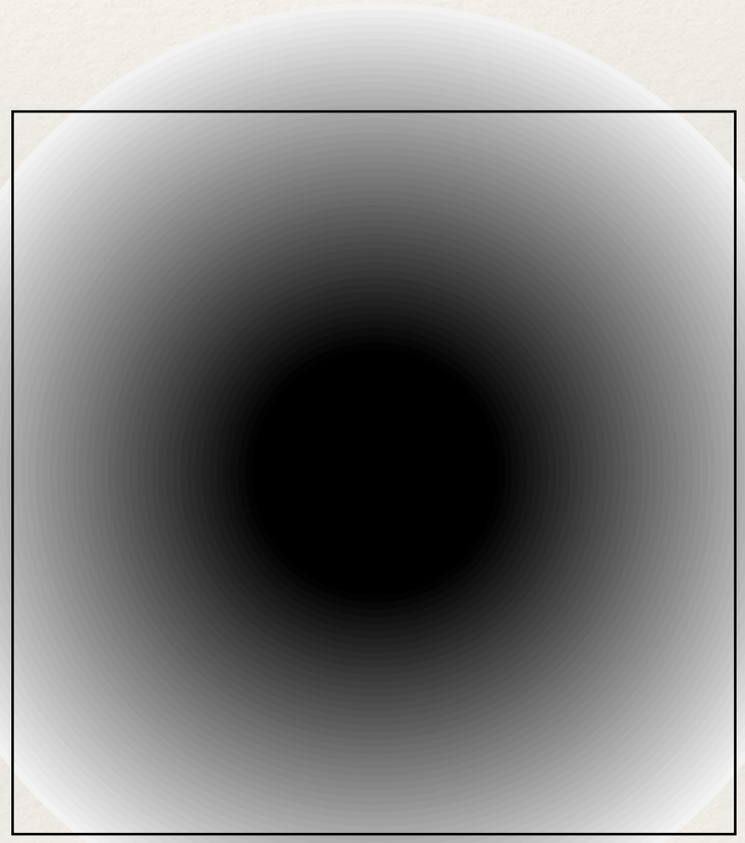

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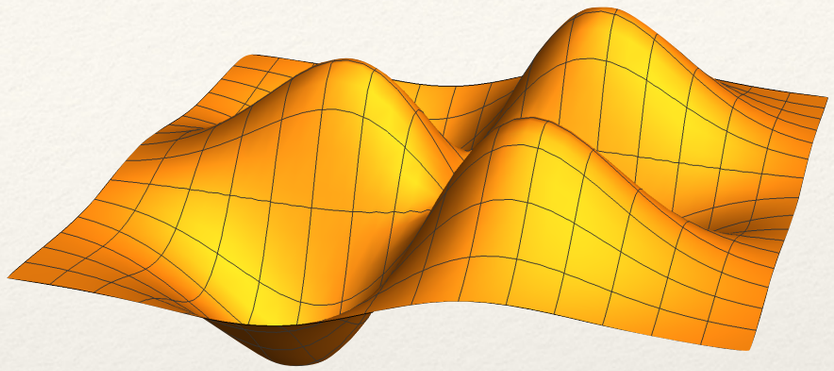
HOBET in Periodic Volumes

- Phase shifts as boundary conditions are replaced by periodic boundary conditions.
- Easier to construct in Cartesian HO basis.



Slice of 3D Cartesian State

- Key Observation: V_δ is short range and isolated from the boundary conditions by Green's functions. It is the same object in infinite volume, or periodic volumes.
  - We can use Cartesian-spherical brackets to relate V_δ in both domains. The Cartesian V_δ can be written in terms of the infinite volume spherical LECs!
- If V_{IR} is longer range than $L/2$, introduce images of V_{IR}.
  - This is a key advantage over Lüscher's method which requires a free propagation region outside the range of V, but inside the volume.

Evaluate by Inserting Periodic Basis

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

$$b_{ij} = \left\{ P\frac{E}{E-T}P \right\}^{-1}_{ij}$$

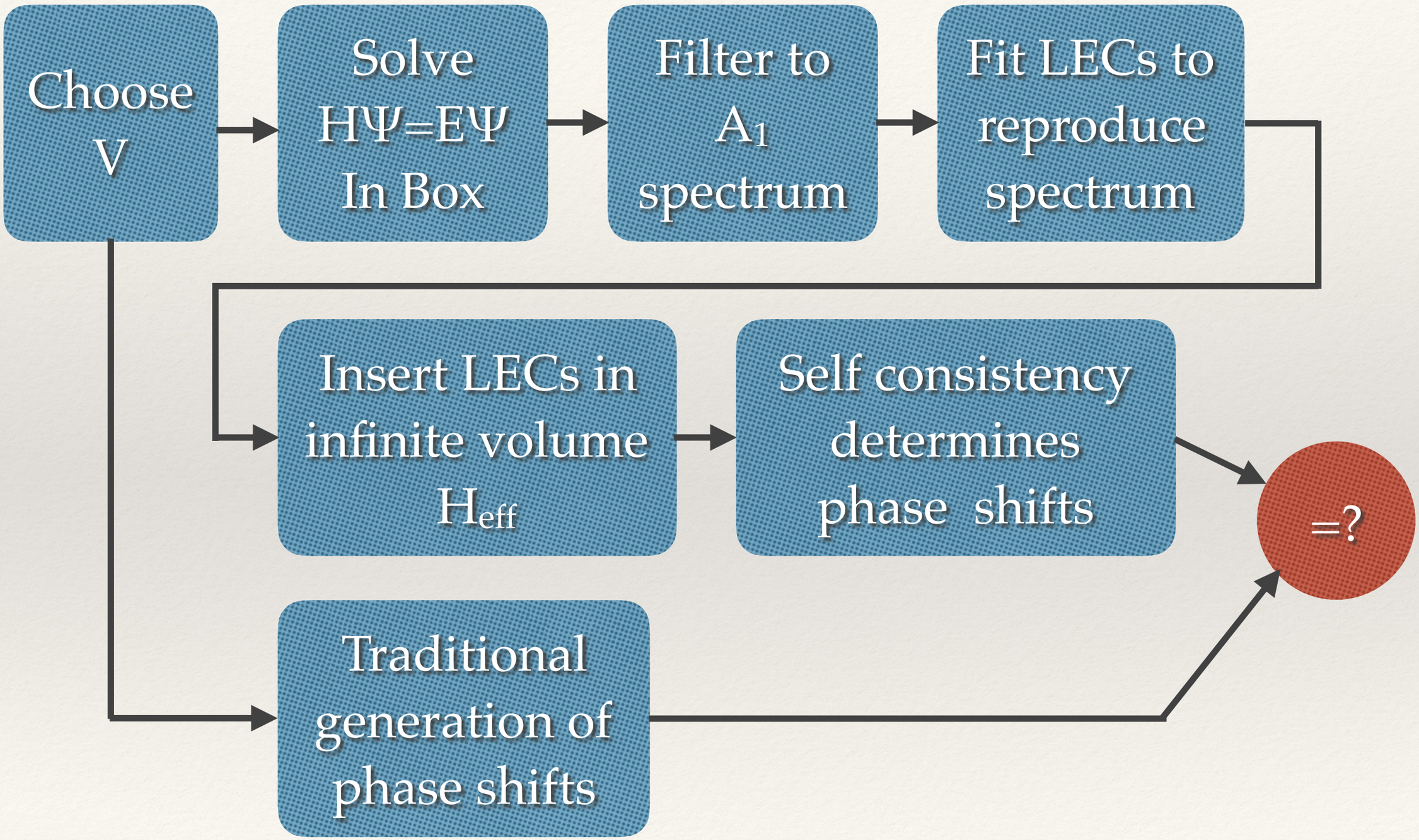
- V_{IR} matrix elements are the most expensive part of H_{eff}

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

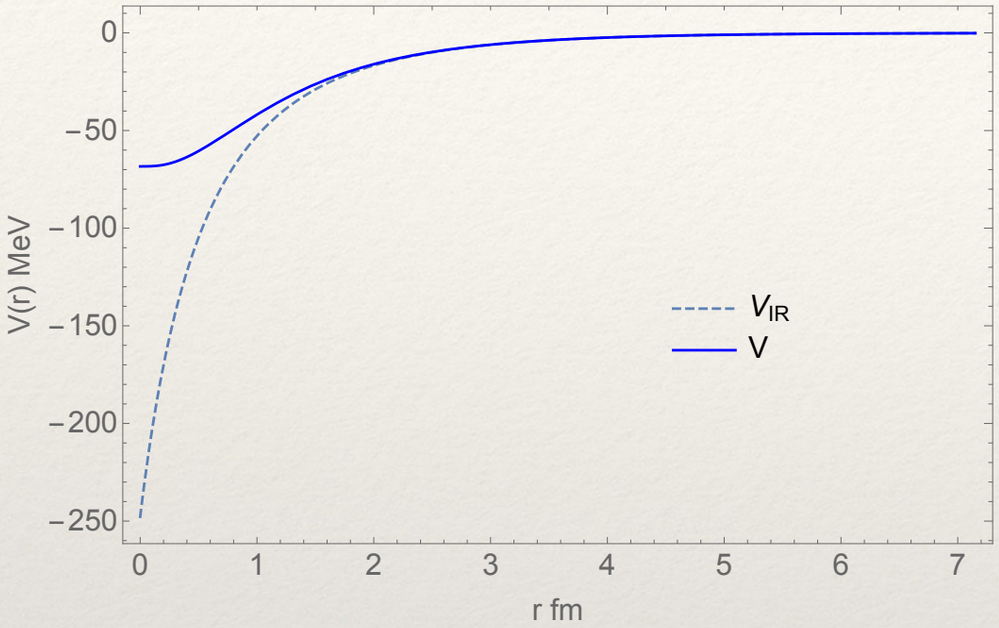
$\vec{m},\vec{m}'$ are discrete momentum states; s,t are HO states

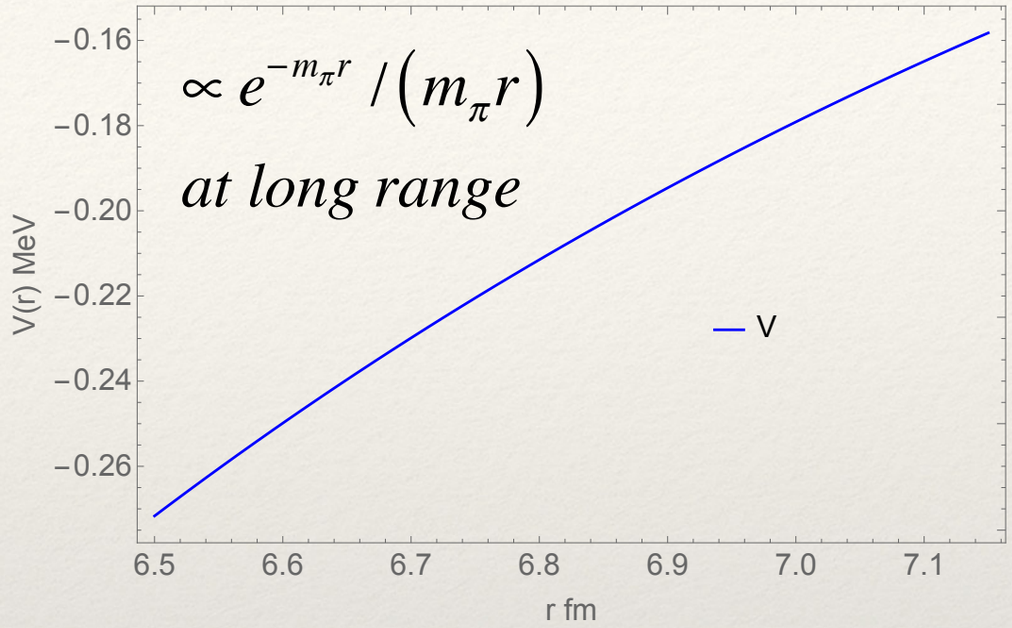
- All pieces are precomputed, but sum is still very large.
- For $\vec{n}',\vec{n} \in P^-$ $G_{QT}=1$, which can be used to check results.

Testing Plan



Test Setup: Range(V)>L/2





$L = 14.3\ fm$

$m_\pi L = 10$

- Periodic images of the potential make a contribution.
- Continuum extrapolation done on N^3 lattice with N={350,400,450}.
- Infinite volume bound state at -4.052 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

$$\det\left[\begin{pmatrix} \cot\delta_0 & 0 \\ 0 & \cot\delta_4 \end{pmatrix}\begin{pmatrix} \overline{F}_{0;0}^{(FV,A_1^+)} & \overline{F}_{0;4}^{(FV,A_1^+)} \\ \overline{F}_{4;0}^{(FV,A_1^+)} & \overline{F}_{4;4}^{(FV,A_1^+)} \end{pmatrix}\right] = 0$$

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_{test} column should be considered the reference.

E [MeV]	From V_{test}	From HOBET	Leading Lüscher	Next Order Lüscher
1	142.023	141.931	142.498	142.269
2	128.972	128.860	129.515	129.166
4	113.602	113.464	114.159	113.552
8	96.919	96.752	97.552	96.330
10	91.473	91.296	92.212	90.651
15	81.672	81.480	82.849	80.398
20	74.876	74.691	76.670	73.303

- ET bound state found at -4.066 MeV v.s. -4.052 MeV (directly from V).
- HOBET errors are from FV solution + Momentum basis cutoff.
- Lüscher errors are from Range(V) > L/2 and magnification of errors by Zeta function poles.

A-Body Effective Hamiltonian

- We want the same thing at the A-body level as at the 2-body level

$$H_A^{\text{eff}} P_A \left|\Psi_i\right\rangle = E_i P_A \left|\Psi_i\right\rangle \qquad P_A(\Lambda) - \text{total quanta cutoff}$$

- The effective potential has the same form as in the two body case

$$V_A^{\text{eff}} = P_A^{\Lambda_{\text{SM}}} EG_{TQ_A^{\Lambda_{\text{SM}}}} \left[V_A + V_A \frac{1}{E - Q_A^{\Lambda_{\text{SM}}} H_A} Q_A^{\Lambda_{\text{SM}}} V_A \right] EG_{Q_A^{\Lambda_{\text{SM}}} T} P_A^{\Lambda_{\text{SM}}}$$

- Now pick out the contribution purely of particles 1 and 2. (sum over pairs later)

$$V_{A,12}^{\text{eff}} = P_A^{\Lambda_{\text{SM}}} EG_{T_{12}Q_A^{\Lambda_{\text{SM}}}} \left[V_{12} + V_{12} \frac{1}{E - Q_A^{\Lambda_{\text{SM}}} H_{12}} Q_A^{\Lambda_{\text{SM}}} V_{12} \right] EG_{Q_A^{\Lambda_{\text{SM}}} T_{12}} P_A^{\Lambda_{\text{SM}}}$$

- The projection operators have a decomposition. With χ fixed, Q_A and P_A Become statements about the {1,2} pair.

$\bar{P}_{12}^A(\chi)$ is 1 when $\dot{\Lambda}_2 + \ldots + \dot{\Lambda}_{A-1} = \chi$

$$P_A^{\Lambda_{\text{SM}}} = \sum_{\chi=0}^{\Lambda_{\text{SM}}} \bar{P}_{12}^A(\chi) P_{12}(\Lambda_{\text{SM}} - \chi)$$

$$V_{A,12}^{\text{eff}} = \sum_{\chi=0}^{\Lambda_{\text{SM}}} \bar{P}_{12}^A(\chi) P_{12}(\Lambda_{\text{SM}} - \chi) EG_{T_{12}Q_{12}(\Lambda_{\text{SM}}-\chi)} \left[V_{12} + V_{12} \frac{1}{E - Q_{12}(\Lambda_{\text{SM}} - \chi) H_{12}} Q_{12}(\Lambda_{\text{SM}} - \chi) V_{12} \right] EG_{Q_{12}(\Lambda_{\text{SM}}-\chi)T_{12}} P_{12}(\Lambda_{\text{SM}} - \chi)$$

- $\rightarrow \sum_{\chi=0}^{\Lambda_{\text{SM}}} \bar{P}_{12}^A(\chi) V_{12}^{\text{eff}}(\Lambda_{\text{SM}} - \chi)$ - Substituting the HOBET 2-body effective interaction

Conclusion

- Wick's vision of building a bridge between QCD and nuclear physics is nearing realization
  - Minimization of LQCD calculations to 2, and possibly 3 body finite volume scattering spectra

- Fit HOBET LECs in finite volumes to match spectra.
- The same LEC values configure the infinite volume spherical effective interaction.
- The shell model effective Hamiltonian can be constructed as a cluster expansion from the 2 and 3 body effective interactions.

Phys. Lett. B 987, McElvain, Haxton (2019)
arXiv:1910.07961, Drischler, Haxton, McElvain, Mereghetti, Nicholson, Vranas, Walker-Loud (2019)

Backup Slides

Higher Body Contributions

- How do we include the induced 3-body contributions?

$$V_A = \sum_{i<j<k} \frac{1}{A-2}\left(V_{ij} + V_{jk} + V_{ik}\right) + V_{ijk}$$

- The same steps work again, this time with spectators to the involved 3 particles.
- The sum of the resulting 3 body contributions will contain the 2-body contributions + induced 3-body + the effective interaction associated with V_{123}.
- Dropping already included 2-body pieces yields

$$V_{123}^{\text{eff}}(\Lambda) = P_{123}^{\Lambda} \frac{E}{E - T_{123} Q_{123}^{\Lambda}} \left[V_{123}^{IR} + V_{\delta 123} \right] \frac{E}{E - Q_{123}^{\Lambda} T_{123}} P_{123}^{\Lambda}$$

- The LECs of $V_{\delta 123}$ would be fit to 3-body observables not fully predicted by the 2-body part of the cluster expansion.
- The kinetic energy part should be calculated once at the highest cluster level.
  - For modest A the Green's functions can be evaluated via matrix inversion in **P**, for larger A there are Lanczos methods available.

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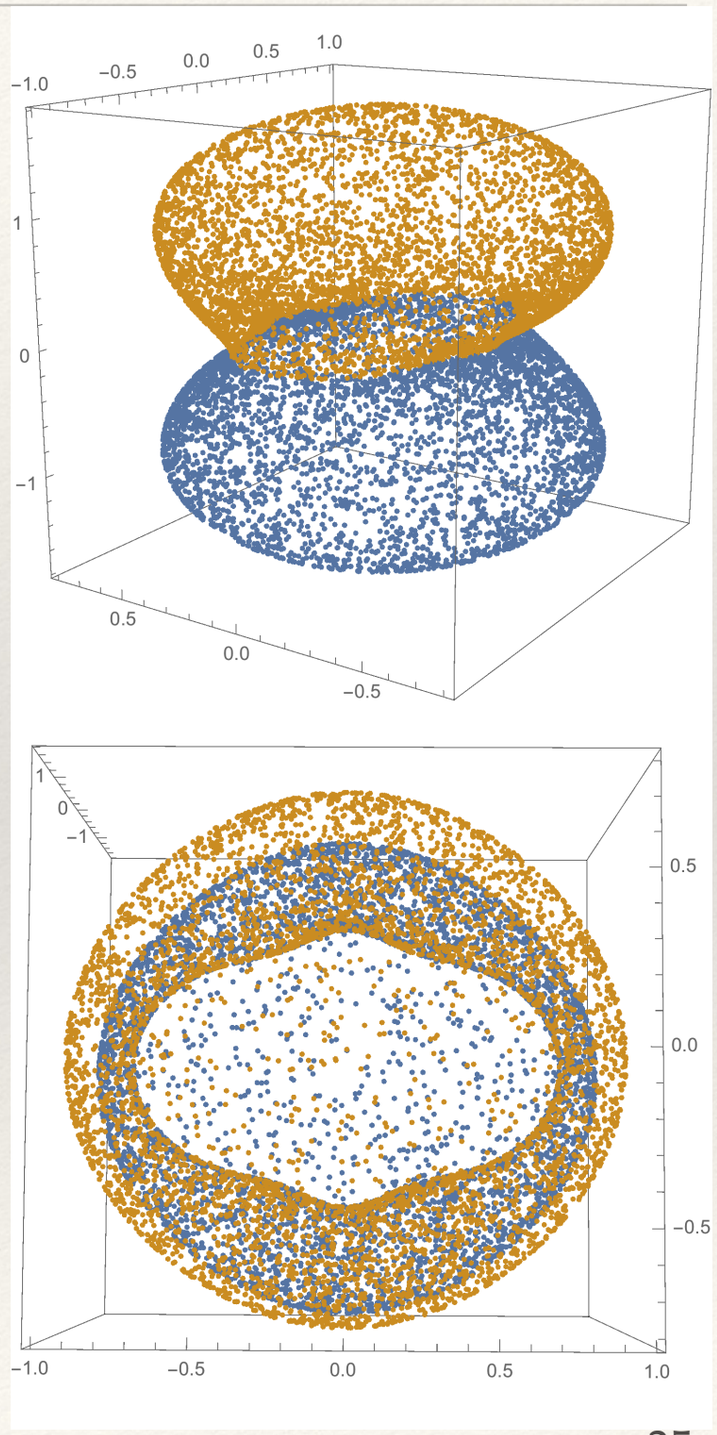
Induced Mixing

- Setup: spherical well potential in a periodic finite volume.
- The wave function is sampled on sphere outside potential and displayed as a radial displacement from a unit sphere.
- Higher order structure induced by periodic boundary conditions is obvious.
- All this mixing is isolated in E/(E-QT) Green's functions.



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Generating V^{eff} for Multiple Λ

- Suppose $\Lambda_{SM} = 6$, then we can fit the HOBET interaction in $\Lambda = 10$ and then use the BH equation to reduce to all needed spaces.

$$H^{eff}(\Lambda-\chi) = P(\Lambda-\chi) H_{\Lambda}^{eff} \frac{E}{E - Q(\Lambda-\chi) H_{\Lambda}^{eff}} P(\Lambda-\chi)$$

- It seems like there may be an advantage in fitting the ET expansion in a larger P that will be used …