Hyperspherical Harmonics for Weakly Bound Systems

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 $8 \ {\rm March} \ 2010$

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Outline

1 Nuclear force models

- **2** Hyperspherical Harmonics
 - Short History
 - Construction
 - Summary

3 Symmetrization

4 Convergence

- Strategies
- The EIHH method

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Examples

5 Reactions

6 Conclusions

Background

• The underling theory for nuclear physics is QCD.



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- At low energy QCD is non-perturbative \longrightarrow lattice.
- Currently no reliable NN interactions can be derived from lattice calculations (this might change in the near future).
- Nuclear interaction is based on phenomenology.
- Effective Field Theory provides a consistent way to derive the nuclear interaction.



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 Long range - One Pion Exchange, Yukawa potential.



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1999 np database

Bin (MeV)	# of data	$N^{3}LO$	NNLO	NLO	AV18
0–100	1058	1.06	1.71	5.20	0.95
100 - 190	501	1.08	12.9	49.3	1.10
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- EFT potentials are naturally formulated in momentum space.





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The EFT expansion





The V8 potential

$$V_{NN}(r_{ij}) = \sum_{p} V_p(r_{ij}) \hat{O}_p(ij)$$

Central terms $p = 1, \ldots, 4$

$$1, (\sigma_i \cdot \sigma_j), (\tau_i \cdot \tau_j), (\sigma_i \cdot \sigma_j)(\tau_i \cdot \tau_j)$$

LS coupling p = 5, 6

$$LS, LS(\tau_i \cdot \tau_j)$$

Tensor force p = 7, 8

$$S_{ij}, S_{ij}(\tau_i \cdot \tau_j)$$

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	-Short	History	7

The HH were introduced in 1935 by Zernike and Brinkman.

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The "Tree" diagram



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- 5 All the rest of us ...

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Hyperspherical coordinates $x_1, x_2, x_3, \dots x_D \longrightarrow \rho = \sqrt{\sum x_i^2}, \Omega$

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$$\Delta = \frac{\partial^2}{\partial \rho^2} + \frac{D-1}{\rho} \frac{\partial}{\partial \rho} - \frac{\hat{K}^2}{\rho^2}$$

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 $\mathbf{B} \ \rho^K \mathcal{Y}_{[K]}(\Omega)$ is a Harmonic polynomial.

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Using the tree structure one can easily construct HH starting from the leafs and uniting branches.

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- **6** Each junction is associated with a quantum number.
- $\begin{array}{c} \hline \mathbf{Z} \quad \text{Each junction adds a factor} \\ N\cos^{K_R}(\theta)\sin^{K_L}(\theta)P^{(\alpha_R,\alpha_L)}_{(K-K_R-K_L)/2}(\cos(2\theta)) \\ \hline \end{array}$

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Removing the center of mass - The Jacobi coordinates

The normalized equal mass Jacobi coordinates

$$\begin{split} \eta_1 &= \sqrt{\frac{1}{2}} \Big(r_2 - r_1 \Big) \\ \eta_2 &= \sqrt{\frac{2}{3}} \Big(r_3 - \frac{1}{2} (r_2 + r_3) \Big) \\ & \cdots \\ \eta_{N-2} &= \sqrt{\frac{N-2}{N-1}} \Big(r_{N-2} - \frac{1}{N-2} (r_1 + r_2 + \cdots + r_{N-3}) \Big) \\ \eta_{N-1} &= \sqrt{\frac{N-1}{N}} \Big(r_{N-1} - \frac{1}{N-1} (r_1 + r_2 + \cdots + r_{N-1}) \Big) \end{split}$$



HH Weakly Bound L_{Hyperspherical} Harmonics

The common "Tree"



$$\begin{aligned} \mathcal{Y}_{[K]} &= \left[\prod_{j=1}^{N} Y_{\ell_j, m_j}(\hat{\eta}_j)\right] \\ &\times \left[\prod_{j=2}^{N} \mathcal{N}_{j, K_j}^{\ell_j, K_{j-1}}(\sin \alpha_j)^{\ell_j} (\cos \alpha_j)^{K_{j-1}} P_{\mu_j}^{(\ell_j + \frac{1}{2}, K_{j-1} + \frac{3j-5}{2})}(\cos(2\alpha_j))\right] \end{aligned}$$

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The Merits of the HH expansion

• A complete set of basis functions.

$$\sum_{[K]} \mathcal{Y}_{[K]}^*(\Omega') \mathcal{Y}_{[K]}(\Omega) \frac{\delta(\rho - \rho')}{\rho^{D-1}} = \prod_{i=1}^N \delta(\boldsymbol{\eta}_i - \boldsymbol{\eta}'_i)$$

Easy transformation between configuration and momentum space

$$e^{i\sum \eta_j q_j} = \frac{(2\pi)^{D/2}}{(Q\rho)^{D/2-1}} \sum_{[K]} i^K \mathcal{Y}^*_{[K]}(\Omega_q) \mathcal{Y}_{[K]}(\Omega) J_{K+D/2-1}(Q\rho)$$

- Good asymptotics.
- With appropriate choice of Jacobi coordinates and states clusterization can be "easily" treated.

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The HH expansion in 4 steps

1. Remove the center of mass

$$\vec{r}_1, \vec{r}_2, \dots \vec{r}_A \longrightarrow \vec{R}_{c.m.}, \vec{\eta}_1 \vec{\eta}_2 \dots \vec{\eta}_{A-1}$$

2. Introduce hyperspherical coordinates

$$\vec{\eta}_1\vec{\eta}_2\ldots\vec{\eta}_{A-1}\longrightarrow \rho=\sqrt{\eta_1^2+\eta_2^2+\ldots+\eta_{A-1}^2},\Omega$$

3. Expand the wave function using hyperspherical harmonics

$$\Psi(\rho, \Omega) = \sum_{K \le K_m ax} R_{[K]}(\rho) \mathcal{Y}_{[K]}(\Omega)$$

4. Solve the Schrödinger equation

$$H = -\frac{1}{2} \left(\frac{\partial^2}{\partial \rho^2} + \frac{3A - 4}{\rho} \frac{\partial}{\partial \rho} - \frac{\hat{K}^2}{\rho^2} \right) + \sum_{i < j} V_{ij} + \sum_{i < j < k} V_{ijk}$$

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Not so fast !!!



There are two Major obstacles

- The HH basis has no good permutational symmetry. (Anti)Symmetrization must be enforced.
- 2 For some nuclear forces the convergence of the HH expansion is notoriously slow and must be accelerated.

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Strategies

Apply the anti-symmetrization to the HH basis

$$\hat{A} = \sum_{g \in S_A} sign(g) \hat{g}$$

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At a cost of A! operations.

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Apply the anti-symmetrization to the HH basis

$$\hat{A} = \sum_{g \in S_A} sign(g)\hat{g}$$

At a cost of A! operations.

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2 Do it recursively in steps

$$\hat{A} = \begin{pmatrix} 1 - (1, A) - (2, A) - \dots (A - 1, A) \end{pmatrix}$$

$$\times \begin{pmatrix} 1 - (1, 3) - (2, 3) \end{pmatrix} \times \begin{pmatrix} 1 - (1, 2) \end{pmatrix}$$

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3 Generate HH states from HO Slater determinant.

$$det(HO) = e^{-\frac{1}{2}\rho^2} \rho^K \hat{A} \Big(\mathcal{Y}(\Omega) \mathcal{X}(s_i, t_i) \Big)$$

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4 Use the group of kinematic rotations $η_i → η'_i = \hat{g}η_i$

At a cost of A! operations.

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(Anti) Symmetrization via Kinematic rotations

Using the group of kinematic rotations $\eta'_i = \hat{g}\eta_i$, the HH symmetrization can be carried out in two steps

$$HH \longrightarrow O_{(A-1)}$$

and

$$O_{(A-1)} \longrightarrow S_A$$

In short we use the following group-subgroup chain

$$O_{3(A-1)} \subset O_3 \otimes O_{(A-1)} \subset O_3 \otimes S_A$$
$$K \qquad LM \quad \Lambda_{A-1} \qquad LM \quad Y_A$$

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6-body system: A comparison between direct symmetrization and symmetrization through the kinematical group O(A-1)

$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	Κ	$\mathrm{HH} \to S_A$	$\mathrm{HH} \to O_{(A-1)}$	$O_{(A-1)} \to S_A$	Ratio
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	2	198	56	108	1.21
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	4	11308	728	1528	5.01
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	6	516647	8771	16511	20.44
	8	10^{7}	84700	127544	47.12

HH Weakly Bound └─_{Convergence}

Convergence - Statement of the problem



- For potentials with Coulomb type singularities the HH expansion of Ψ converge as K_{max}^{-2}
- For Gaussian potentials Ψ converge as $e^{-cK_{max}}$.
- Actually. The **problem** is not the slow convergence rate but rather the fast growth in the number of HH states.

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Convergence

1 Correlations: CHH, PHH, CFHHM ...

$$\Psi(\rho, \Omega) = F(r_{ij}) \sum_{K \le K_m ax} R_{[K]}(\rho) \mathcal{Y}_{[K]}(\Omega)$$

Basis Reduction: The potential basis (Fabre de-la Ripple), The Pisa Group, Efros.For a Bose-system this expansion may take the following form

$$\Psi(\rho, \Omega) = \sum_{ij} \sum_{[K]} R^{(2)}_{[K]}(\rho) \mathcal{Y}_{[K]}(\Omega_{ij}) + \sum_{ij,kl} \sum_{[K]} R^{(2,2)}_{[K]}(\rho) \mathcal{Y}_{[K]}(\Omega_{ij,kl}) + \dots$$

B Effective interaction for the HH expansion. Replace the bare potential by an effective one:

$$V^{(2)} \longrightarrow V^{(2)}_{eff}$$
$$V^{(3)} \longrightarrow V^{(3)}_{eff}$$

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The Effective Interaction Hyperspherical Harmonics (EIHH)

The $V_{eff}^{(2)}$ is derived from a "2-body" Hamiltonian

$$H_2(\rho) = \frac{1}{2m} \frac{\hat{K}^2}{\rho^2} + V(\vec{r} = \sqrt{2}\rho \sin \alpha_N \cdot \hat{\eta}_N) ,$$

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The effective Hamiltonian is constructed through the Lee-Suzuki similarity transformation

$$H_{2\,eff}(\rho) = U^{\dagger}(\rho)H_2(\rho)U(\rho) \quad ; \quad U = \frac{1+\omega}{\sqrt{P(1+\omega^{\dagger}\omega)P}}$$

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The operator $\omega = Q\omega P$ is given by

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Finally the effective interaction is given by

$$V_{2\;eff}(\rho) = H_{2\;eff}(\rho) - \frac{1}{2m}\frac{\hat{K}^2}{\rho^2}$$

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4-body ground-state - Bare vs Effective



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HH Weakly Bound

4-body ground-state

Convergence of the **EIHH** method for ⁴He binding energy E_b [MeV] and root mean square matter radius $\langle r^2 \rangle^{\frac{1}{2}}$ [fm] with AV18 and AV18+UIX potentials.

	AV18		AV18+UIX	
K_{max}	$E_b \qquad \langle r^2 \rangle^{\frac{1}{2}}$		E_b	$\langle r^2 \rangle^{\frac{1}{2}}$
6	25.312	1.506	26.23	1.456
8	25.000	1.509	27.63	1.428
10	24.443	1.520	27.861	1.428
12	24.492	1.518	28.261	1.427
14	24.350	1.518	28.324	1.428
16	24.315	1.518	28.397	1.430
18	24.273	1.518	28.396	1.431
20	24.268	1.518	28.418	1.432

HH Weakly Bound

4-body ground-state

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18	24.273	1.518	28.396	1.431
20	24.268	1.518	28.418	1.432
FY [Nogga]	24.25		28.50	
FY [Lazauskas]	24.22	1.516		
HH [Viviani]	24.21	1.512	28.46	1.428
GFMC [Wiringa]			28.34	1.44

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BENCHMARK for ⁴He ground state with AV8' potential

H. Kamada et al., PRC 64 044001 (2001)

Method	$\langle T \rangle$	$\langle V \rangle$	E_b	$\sqrt{\langle r^2 \rangle}$
FY	102.39(5)	-128.33(10)	-25.94(5)	1.485(3)
CRCGV	102.25	-128.13	-25.90	1.482
SVM	102.35	-128.27	-25.92	1.486
HH	102.44	-128.34	-25.90(1)	1.483
GFMC	102.3(1.0)	-128.25(1.0)	-25.93(2)	1.490(5)
NCSM	103.35	-129.45	-25.80(20)	1.485
EIHH	100.8(9)	-126.7(9)	-25.944(10)	1.486

HH Weakly Bound	
Convergence	
Examples	

The effective 3-body force

Convergence of $^6\mathrm{Li}$ ground state with the AV8' NN potential

K_{max}	B.E $V^{(2)}eff$	B.E. $(K_Q^{(3)} = 16)$	B.E. $(K_Q^{(3)} = 20)$
2	39.80	38.83	
4	33.43	30.37	30.27
6	31.02	31.11	30.94
8	31.13	31.17	30.94
10	30.23	31.22	30.88

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10	30.23	31.22	30.88
NCSM [Navratil]	30.30		
GFMC [Pieper]	29.70(5)		

HH Weakly Bound

EIHH for Non-local interactions

Local potential: $V_{eff}^{(2)}(\rho)$ was derived using the fact that V is diagonal in configuration space.

Non-local potential: (or in general) we can construct EI from a "2-body" Hamiltonian of the form:

$$\langle n|H_2|n\rangle = \frac{1}{2m}\hat{K}^2\langle n|\frac{1}{\rho^2}|n\rangle + \langle n|V_{A,A-1}|n\rangle$$

In this case

$$\langle n|V_{eff}^{(2)}|n'\rangle = \delta_{n,n'} \langle n|H_{eff}^{(2)} - \frac{1}{2m} \frac{\hat{K}^2}{\rho^2}|n\rangle + (1 - \delta_{n,n'}) \langle n|V^{(2)}|n'\rangle$$



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The nuclear response function

$$R(\omega) = \int d\psi_f |\langle \psi_i \mid \hat{O} \mid \psi_f \rangle|^2 \delta(E_f - E_i - \omega)$$

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Transformed with Lorentzian kernel

$$L(\sigma) = \int d\omega \frac{R(\omega)}{(\omega - \sigma)^2 + \Gamma^2}$$

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The transform can be written as

$$L(\sigma) = \int d\psi_f \langle \psi_i \mid \hat{O} \mid \psi_f \rangle \frac{1}{E_f - E_i - \sigma - i\Gamma} \frac{1}{E_f - E_i - \sigma + i\Gamma} \langle \psi_f \mid \hat{O} \mid \psi_i \rangle$$

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 \mathbf{Or}

$$L(\sigma) = \int d\psi_f \langle \psi_i \mid \hat{O} \frac{1}{H - E_i - \sigma - i\Gamma} \mid \psi_f \rangle \langle \psi_f \mid \frac{1}{H - E_i - \sigma + i\Gamma} \hat{O} \mid \psi_i \rangle$$

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Using closure

$$L(\sigma) = \langle \psi_i \mid \hat{O} \frac{1}{H - E_i - \sigma - i\Gamma} \frac{1}{H - E_i - \sigma + i\Gamma} \hat{O} \mid \psi_i \rangle = \langle \tilde{\psi} \mid \tilde{\psi} \rangle$$

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$$(H - E_0 - \sigma + i\Gamma) \mid \tilde{\psi} \rangle = \hat{O} \mid \psi_0 \rangle.$$

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Few comments

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- I The LIT equation can be solved using bound state methods !!!

Using closure

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- **B** Since the source is localized $\tilde{\psi} \longrightarrow 0$ as $r \longrightarrow \infty$.
- I The LIT equation can be solved using bound state methods !!!
- **5** $R(\omega)$ is obtained trough inversion of the transform, $L(\sigma)$.

Using closure

$$L(\sigma) = \langle \psi_i \mid \hat{O} \frac{1}{H - E_i - \sigma - i\Gamma} \frac{1}{H - E_i - \sigma + i\Gamma} \hat{O} \mid \psi_i \rangle = \langle \tilde{\psi} \mid \tilde{\psi} \rangle$$

 $| \tilde{\psi} \rangle$ is the solution of the Schrödinger like equation

$$(H - E_0 - \sigma + i\Gamma) \mid \tilde{\psi} \rangle = \hat{O} \mid \psi_0 \rangle.$$

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V. Efros, W. Leidemann, and G. Orlandini, PLB 238,

130 (1994).

Photoabsorption of Nuclei

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Bacca, Marchisio, Barnea, Leidemann, Orlandini, PRL 89 (2002)



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Giant Dipole Mode



Soft Dipole Mode







HH Weakly Bound └─_{Reactions}

Six-body Photoabsorption - Comparison with experiment



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S. Bacca, N. Barnea, W. Leidemann, and G. Orlandini, PRC **69**, 057001 (2004)

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Thanks, and enjoy the workshop !!!

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