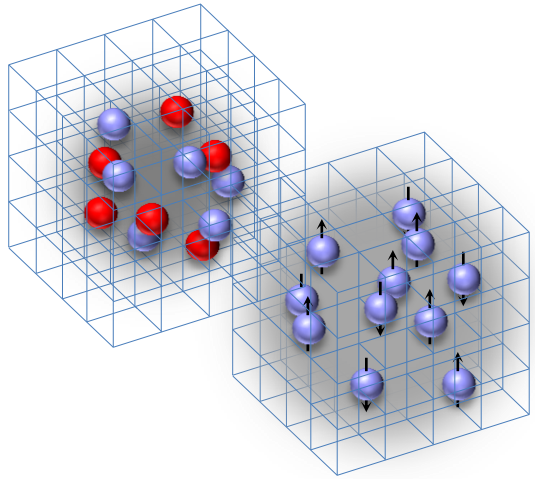
Adiabatic projection method for lattice scattering and reactions



Nuclear Lattice EFT Collaboration

Dean Lee (North Carolina State University)

Universality in Few Body Systems: Theoretical Challenges and New Directions

Institute for Nuclear Theory
University of Washington
May 16, 2014

Outline

Introduction to lattice effective field theory

Clusters in nuclei and universality

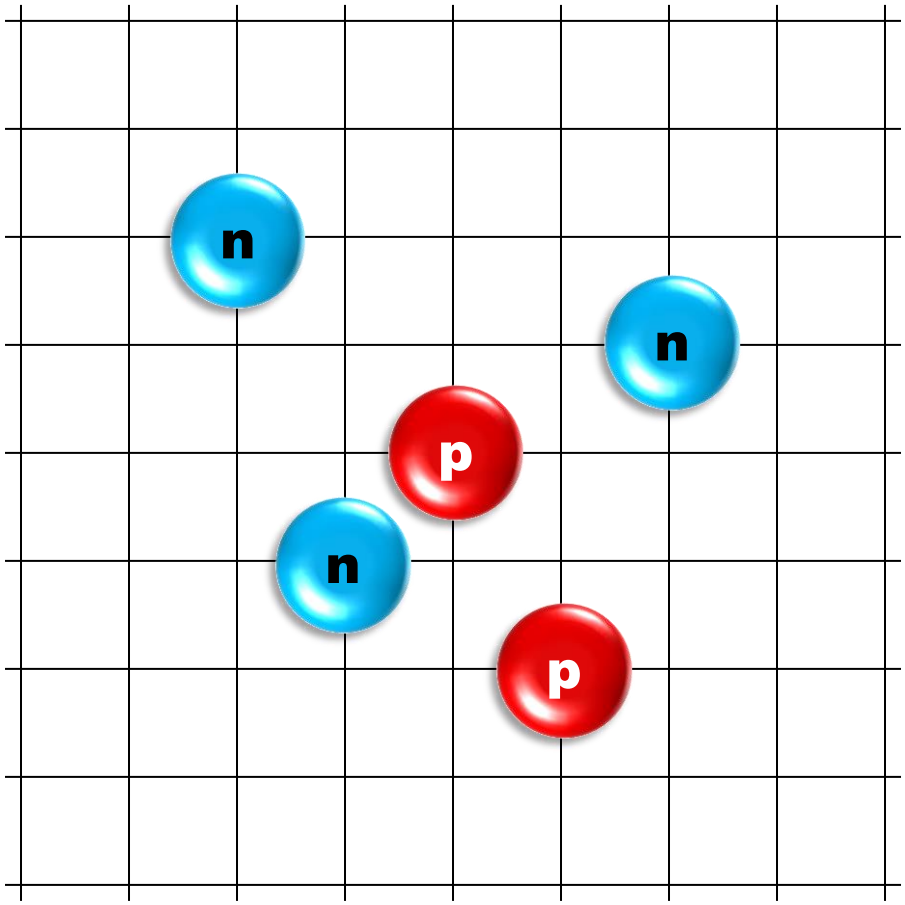
Adiabatic projection method

Elastic scattering on the lattice

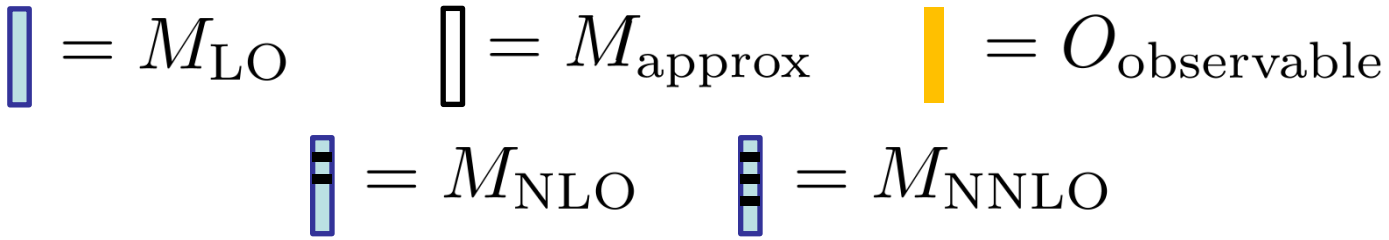
Reactions on the lattice

Summary and future direction

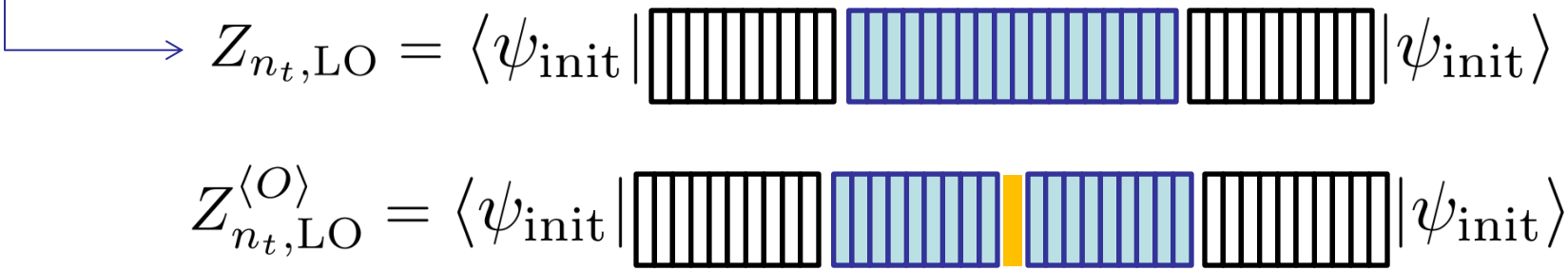
Lattice effective field theory



Schematic of lattice Monte Carlo calculation



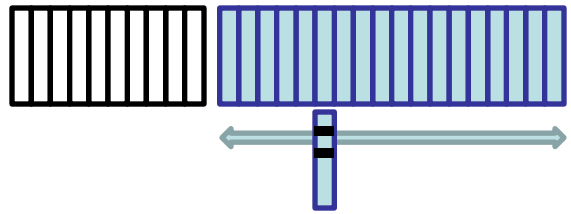
Hybrid Monte Carlo sampling



$$e^{-E_{0,\mathrm{LO}} a_t} = \lim_{n_t \to \infty} Z_{n_t+1,\mathrm{LO}} / Z_{n_t,\mathrm{LO}}$$

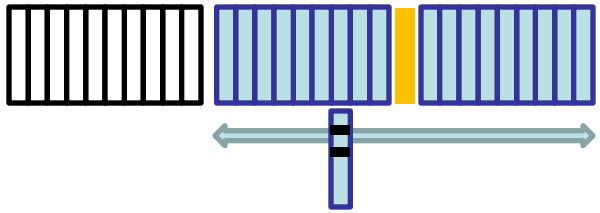
$$\langle O \rangle_{0,\mathrm{LO}} = \lim_{n_t \to \infty} Z^{\langle O \rangle}_{n_t,\mathrm{LO}} / Z_{n_t,\mathrm{LO}}$$

$$Z_{n_t,\mathrm{NLO}} = \langle \psi_{\mathrm{init}} |$$



$$| \psi_{\mathrm{init}} \rangle$$

$$Z^{\langle O \rangle}_{n_t,\mathrm{NLO}} = \langle \psi_{\mathrm{init}} |$$



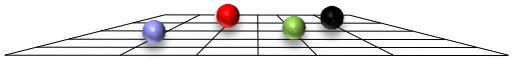
$$| \psi_{\mathrm{init}} \rangle$$

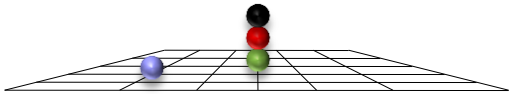
$$\langle O \rangle_{0,\mathrm{NLO}} = \lim_{n_t \to \infty} Z^{\langle O \rangle}_{n_t,\mathrm{NLO}} / Z_{n_t,\mathrm{NLO}}$$

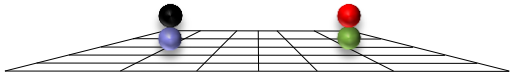
Low-energy 0^+ states for $N = Z$ = even

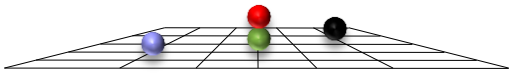
nuclear state	n	E_{4n}	$E_{4n} - nE_4$
$^4\mathrm{He}(0_1^+)$	1	-28.296 MeV	0
$^8\mathrm{Be}(0_1^+)$	2	-56.499 MeV	$+0.092$ MeV
$^{12}\mathrm{C}(0_1^+)$	3	-92.162 MeV	-7.275 MeV
$^{12}\mathrm{C}(0_2^+)$	3	-84.508 MeV	$+0.379$ MeV
$^{16}\mathrm{O}(0_1^+)$	4	-127.619 MeV	-14.437 MeV
$^{16}\mathrm{O}(0_2^+)$	4	-121.570 MeV	-8.387 MeV

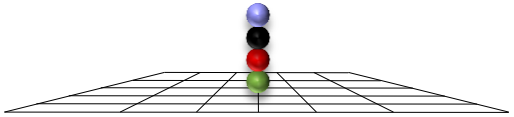
Particle clustering included automatically





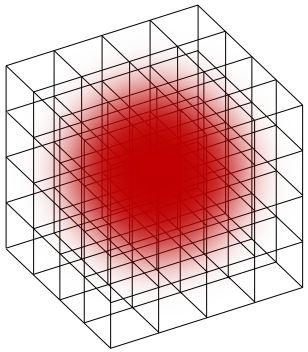






Projection Monte Carlo with initial/final state wavefunctions

$$\langle \psi_{\rm init} |$$  $$| \psi_{\rm init} \rangle$$



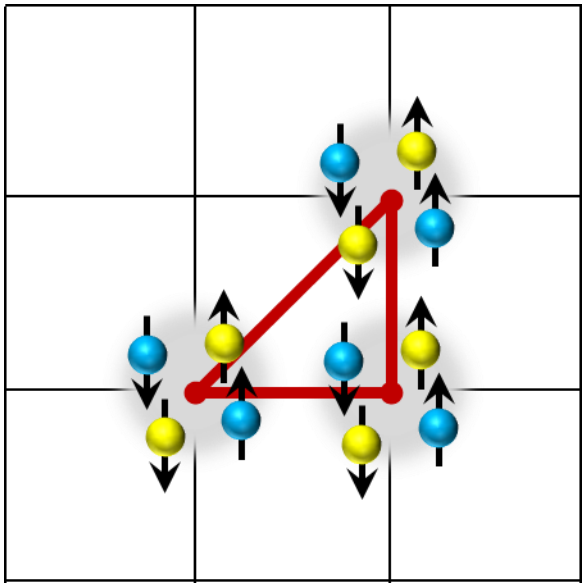
$$f_j(\vec{n}) \quad j = 1, \cdots A$$

Construct initial/final states as a Slater determinant

$$\psi_{\rm init}(\vec{n}_1, \cdots \vec{n}_A) \propto \sum_{\vec{m}} e^{i\vec{P}\cdot\vec{m}} \det_{i,j} f_i(\vec{n}_j - \vec{m})$$

Carbon-12 ground state and first 2^+

Strong overlap with compact triangle configuration



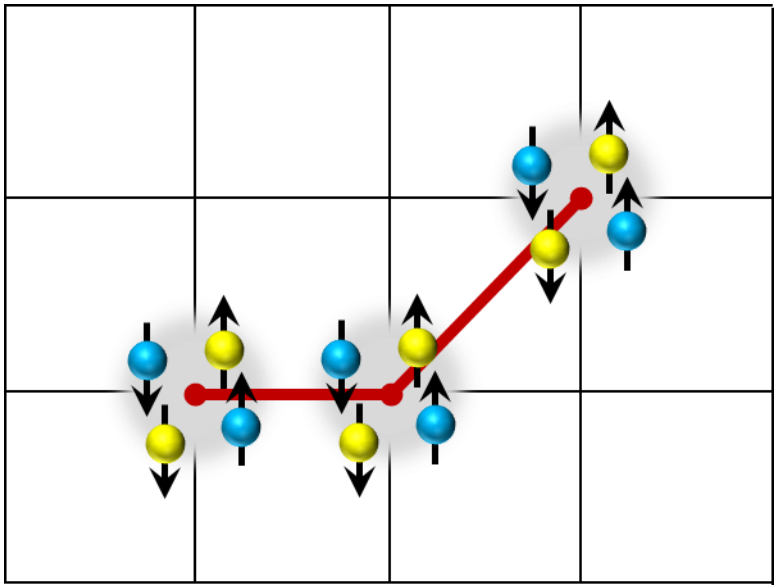
12 rotational orientations

$$b = 1.97 \text{ fm}$$

Epelbaum, Krebs, D.L, Meißner, PRL 106 192501 (2011),
Epelbaum, Krebs, Lähde, D.L, Meißner, PRL 109 252501 (2012)

Second 0^+ (Hoyle state) and second 2^+

Strong overlap with bent arm configuration



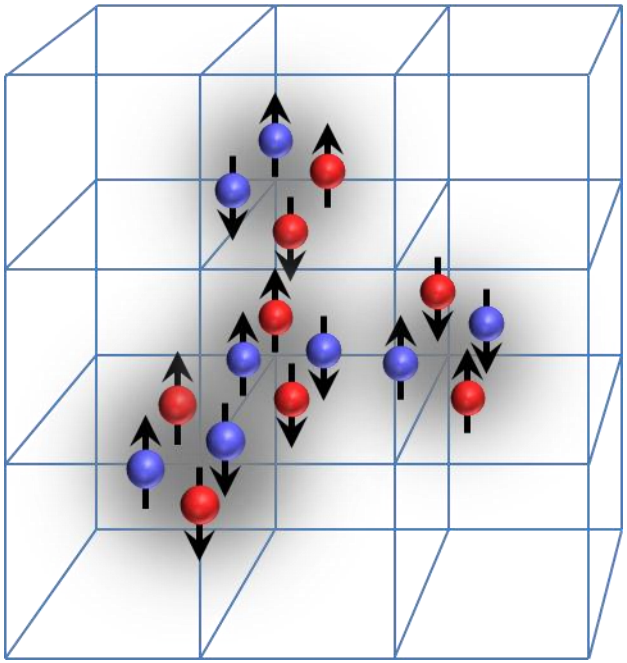
24 rotational orientations

$b = 1.97$ fm

Epelbaum, Krebs, D.L, Meißner, PRL 106 192501 (2011),
Epelbaum, Krebs, Lähde, D.L, Meißner, PRL 109 252501 (2012)

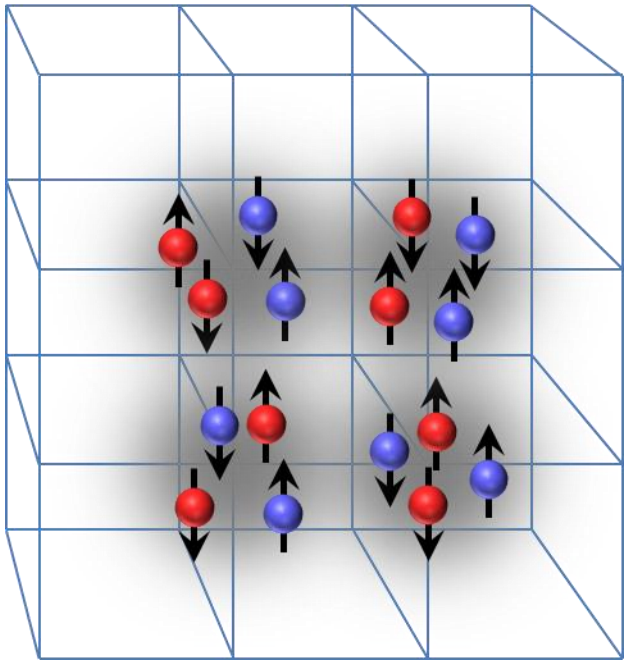
Oxygen-16

0_1^+



A - Tetrahedral structure

0_2^+



B,C - Square-like structure

Epelbaum, Krebs, Lähde, D.L, Meißner, Rupak, PRL112, 102501 (2014)

Scattering and reactions on the lattice

$$1 + 2 \to 1 + 2$$

$$1 + 2 \to 3 + \gamma$$

$$1 + 2 \to 3 + 4$$

$$1 + 2 \to 3 + 4 + 5$$

Hard problem: How to reconcile Euclidean-time evolution and finite volume needed for lattice simulations with infinite-volume real-time analytic structures connected with scattering and reactions

Big reward: Lattice Monte Carlo simulations have excellent scaling with particle number. A good lattice algorithm for point particle reactions can be scaled up to do calculations of large clusters.

Adiabatic projection method

Strategy: Divide the calculation into two parts

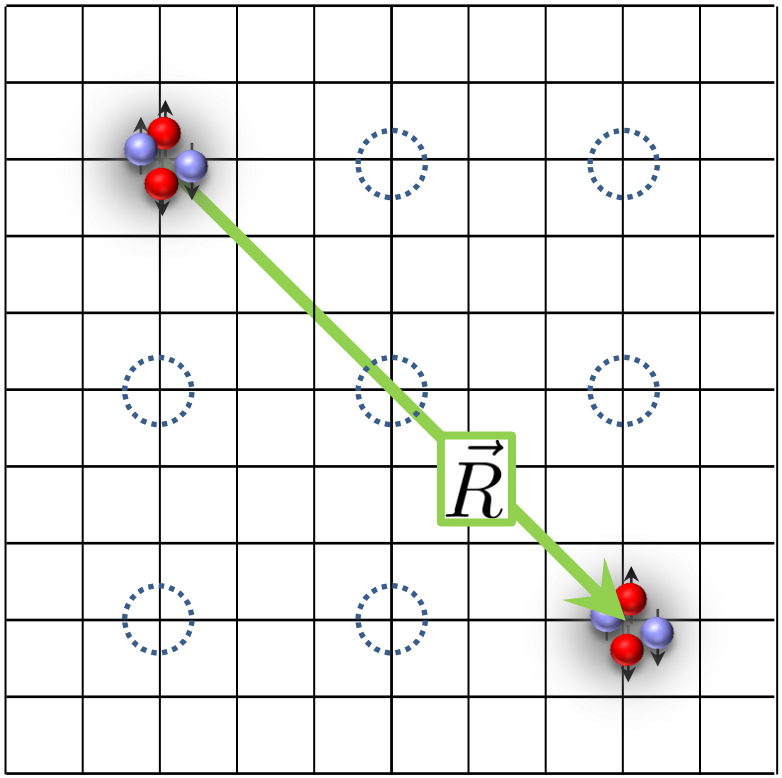
First - use lattice Monte Carlo simulations to get a good description of the low-energy states in a finite volume up to some desired energy scale.

Second - extract scattering matrix elements from this low-energy data. For elastic scattering, one can use Lüscher's method and needs only accurate determinations of the finite-volume energy levels. For inelastic reactions, one generally needs a matrix representation of the low-energy system in a basis of asymptotic in and out states.

See also recent work of Briceno and Davoudi [PRD (2013) 87, 094507; PRD (2014) 89, 074507] as well as Rusetsky, et al., [PLB (2009) 681, 439; EPJA (2012) 48, 67] for coupled channels and three-body systems via Lüscher's method.

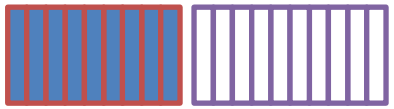
Adiabatic projection method

Use cluster wavefunctions for initial/final scattering states and then project in Euclidean time



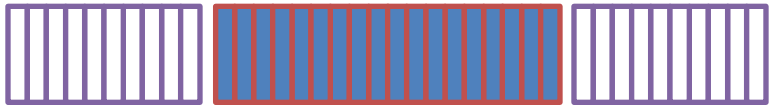
Use projection Monte Carlo to propagate cluster wavefunctions in Euclidean time

$$|\vec{R}\rangle_t = e^{-Ht}|\vec{R}\rangle$$

$|\vec{R}\rangle_t =$  $|\vec{R}\rangle$

Construct a norm matrix and matrix of expectation values

$$\langle N\rangle_t = {}_t\langle\vec{R}'|\vec{R}\rangle_t =$$

$\langle\vec{R}'|$  $|\vec{R}\rangle$

$$\langle O\rangle_t = {}_t\langle\vec{R}'|O|\vec{R}\rangle_t =$$

$\langle\vec{R}'|$  $|\vec{R}\rangle$

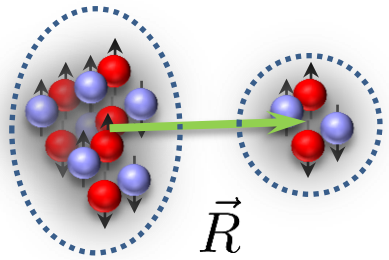
Compute the projected adiabatic matrix elements

$$\langle O \rangle_{\rm adiab} = \langle N \rangle_t^{-1/2} \langle O \rangle_t \langle N \rangle_t^{-1/2}$$

$$\langle H \rangle_{\rm adiab} = \langle N \rangle_t^{-1/2} \langle H \rangle_t \langle N \rangle_t^{-1/2}$$

Projected adiabatic Hamiltonian is now an effective two-body Hamiltonian. Similar in spirit to no-core shell model with resonating group method pioneered by Navratil and Quaglioni.

But some differences. Distortion of the nucleus wavefunctions is automatic due to projection in Euclidean time.



Rupak, D.L., PRL 111 (2013) 032502; Pine, D.L., Rupak, EPJA (2013) 49, 151

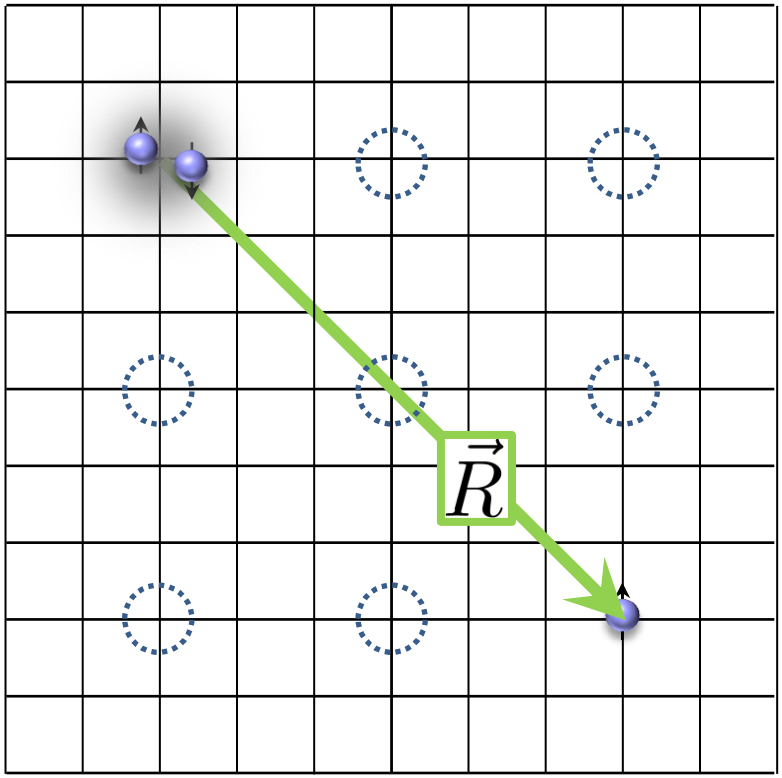
Example: Elastic fermion-dimer scattering

Two component fermions in 3D with attractive zero-range interactions

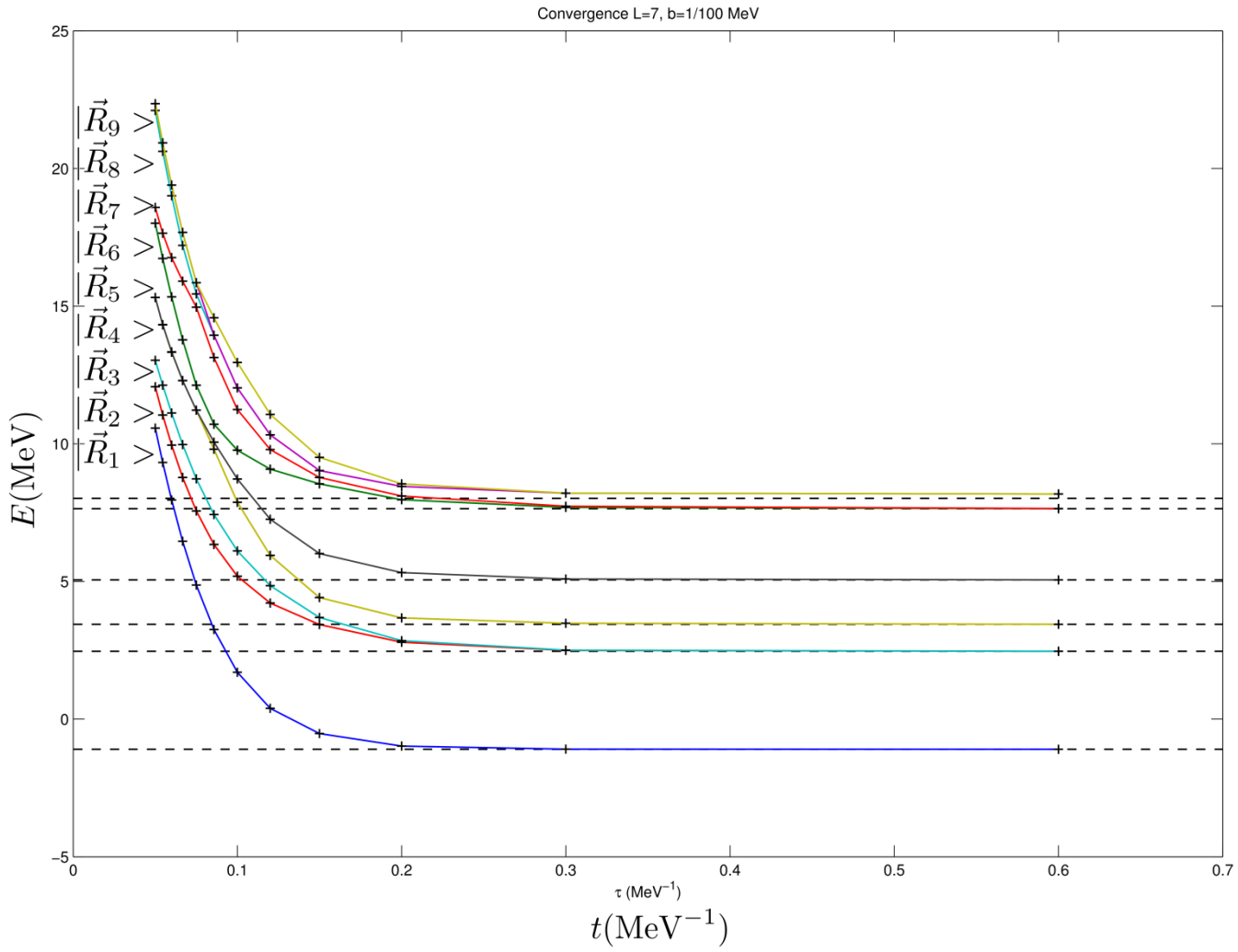
$$\mathcal{H}_{\rm int} = c\psi_1^\dagger \psi_1 \psi_2^\dagger \psi_2$$

Equivalent to spin-quartet deuteron-neutron scattering in leading-order pionless effective field theory

We apply the adiabatic projection method to this system. We first start with a set of fermion-dimer cluster states with different separation vectors.



Next step is to project the initial cluster states in Euclidean time

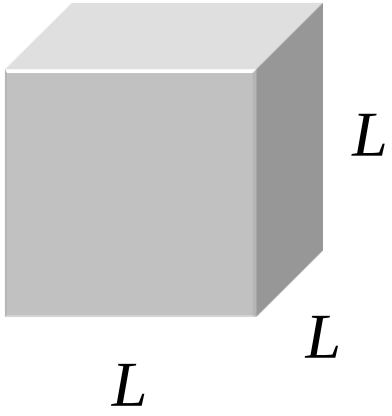


Pine, D.L., Rupak, EPJA (2013) 49, 151

Lüscher's finite-volume formula

Lüscher, Comm. Math. Phys. 105 (1986) 153; NPB 354 (1991) 531

Two-particle energy levels near threshold
in a periodic cube related to phase shifts



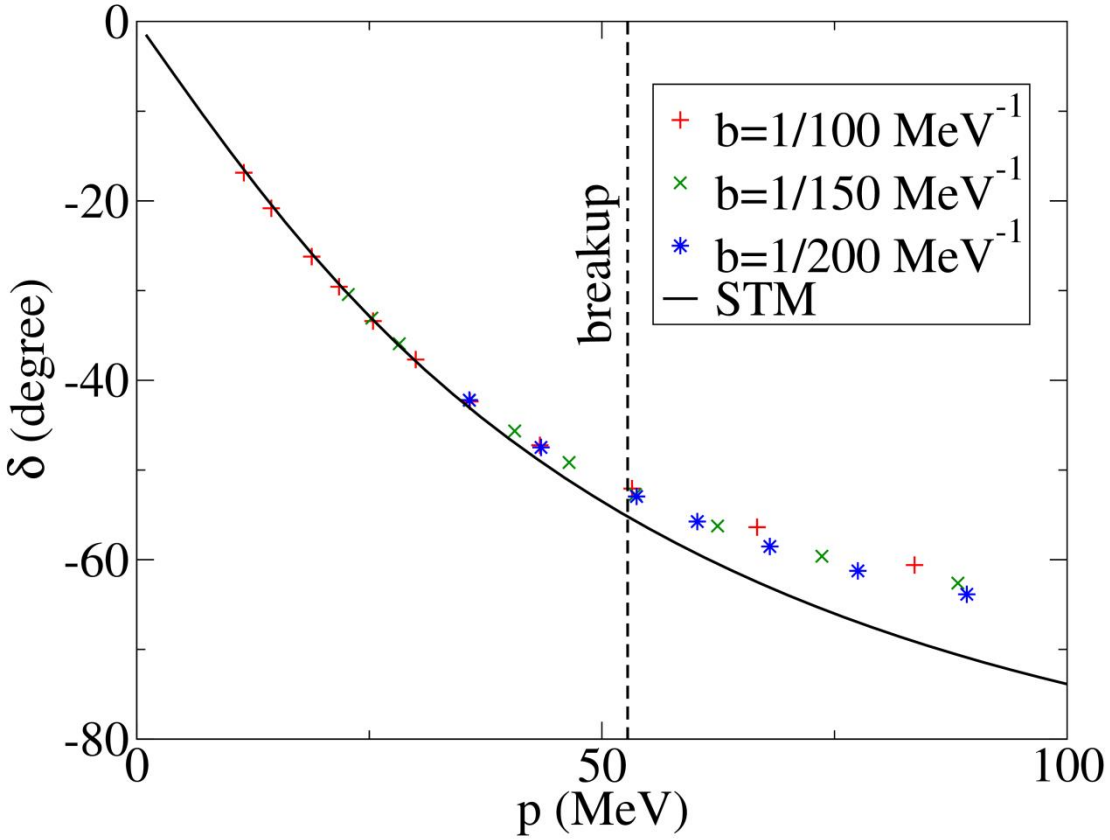
$$p \cot \delta_0(p) = \frac{1}{\pi L} S(\eta), \qquad \eta = \left(\frac{Lp}{2\pi}\right)^2$$

$$S(\eta) = \lim_{\Lambda \to \infty} \left[\sum_{\vec{n}} \frac{\theta(\Lambda^2 - \vec{n}^2)}{\vec{n}^2 - \eta} - 4\pi\Lambda \right]$$

There are analogous results for higher partial waves

See also talk by Amy Nicholson

Fermion-dimer scattering



Pine, D.L., Rupak, EPJA (2013) 49, 151

Fermion-dimer system using adiabatic projection calculated via Monte Carlo simulations

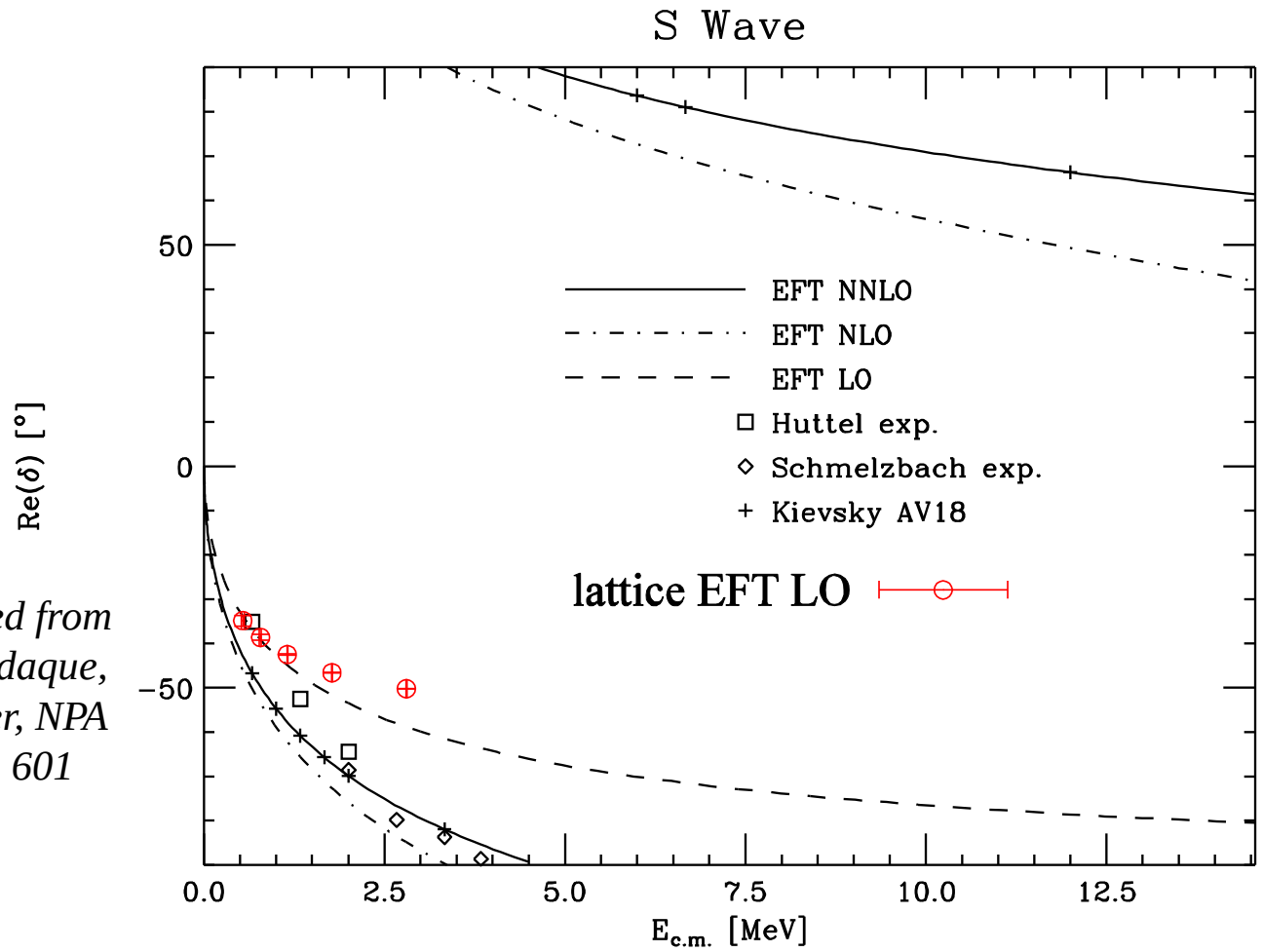


Figure adapted from Gabbiani, Bedaque, Griesshammer, NPA (2000) 675, 601

S. Elhatisari, D. L., in preparation

Fermion-dimer system using adiabatic projection calculated via Monte Carlo simulations

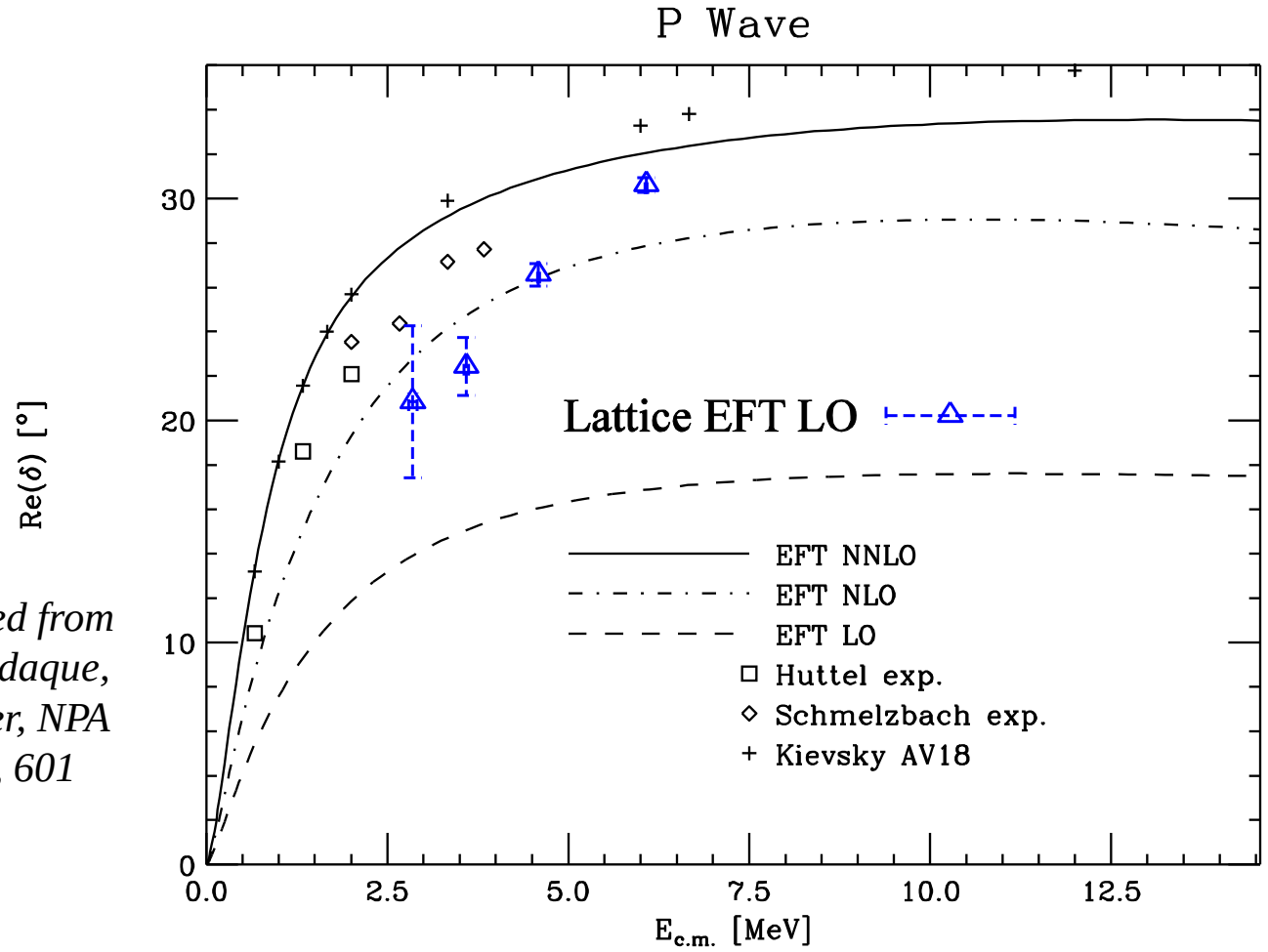
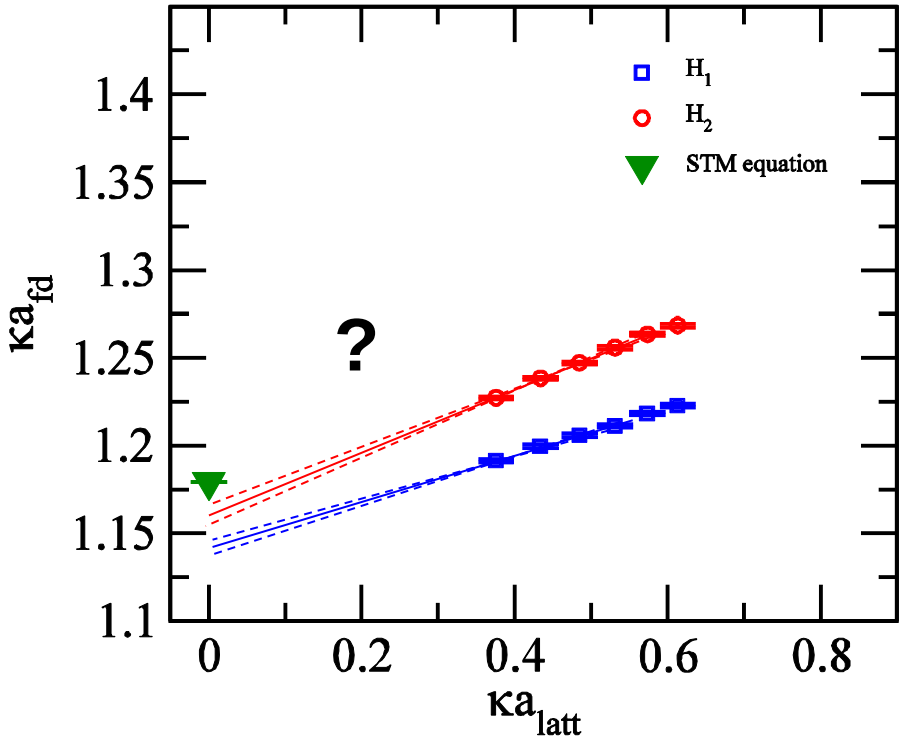


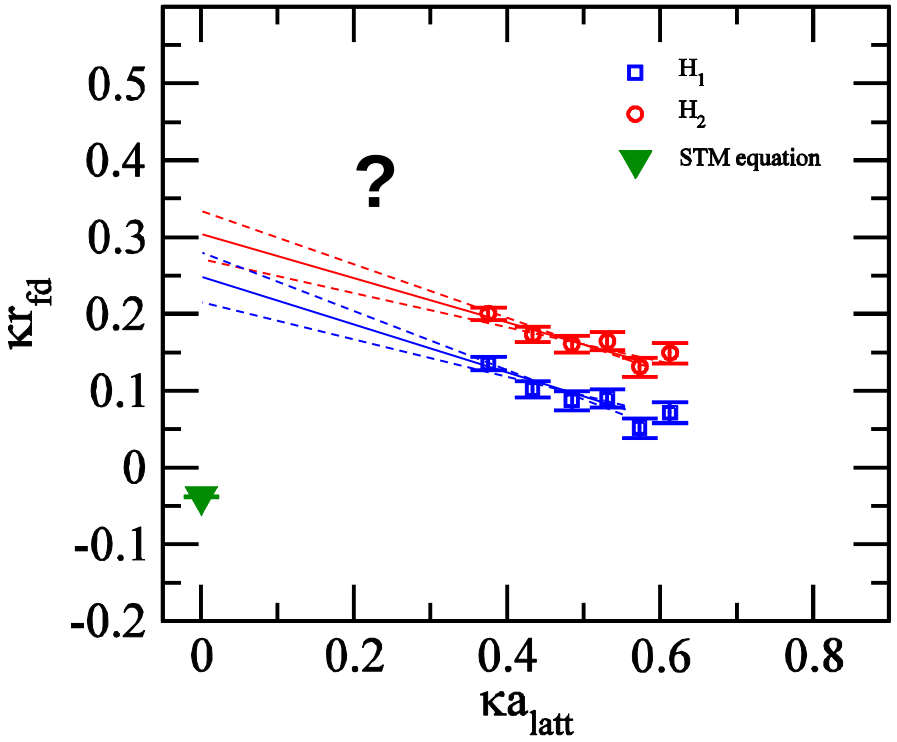
Figure adapted from Gabbiani, Bedaque, Griesshammer, NPA (2000) 675, 601

S. Elhatisari, D. L., in preparation

Using Lüscher's formula: Note of caution

Straightforward application of Lüscher's formula for fermion-dimer scattering for zero range interactions for two-component fermions. We show two different lattice Hamiltonians H_1, H_2 with the same continuum limit.

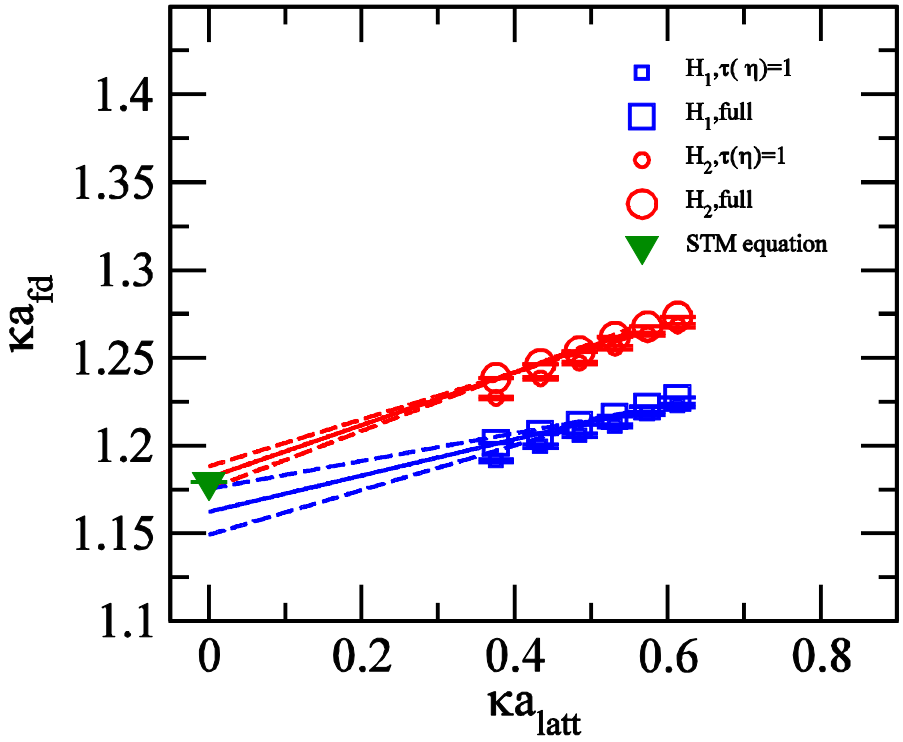


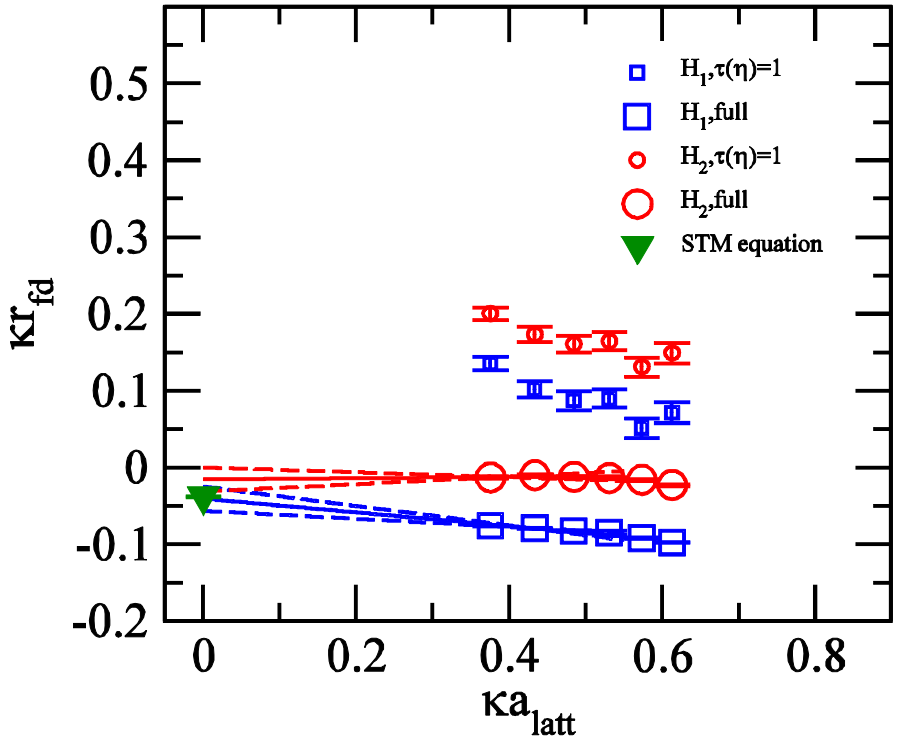


Bour, König, D.L., Hammer, Meißner, PRD 84:091503(R) (2011)

Bour, Hammer, D.L., Meißner, PRC 86, 034003 (2012)

Lüscher's formula is very sensitive to small corrections in the energies. In small volumes, finite volume corrections to the dimer energy must also be considered. This turns out to have an interesting topological character depending on dimer momentum. Here are the lattice results for fermion-dimer scattering for zero range interactions for two-component fermions with these corrections taken into account.





Bour, König, D.L., Hammer, Meißner, PRD 84:091503(R) (2011)

Bour, Hammer, D.L., Meißner, PRC 86, 034003 (2012)

Example: Test of coupled channel reactions

Four component fermions in 3D with equal masses and zero-range pair conversion

$$\mathcal{H}_{\rm int} = c\psi_1^\dagger\psi_2^\dagger\psi_3\psi_4 + c\psi_3^\dagger\psi_4^\dagger\psi_1\psi_2$$

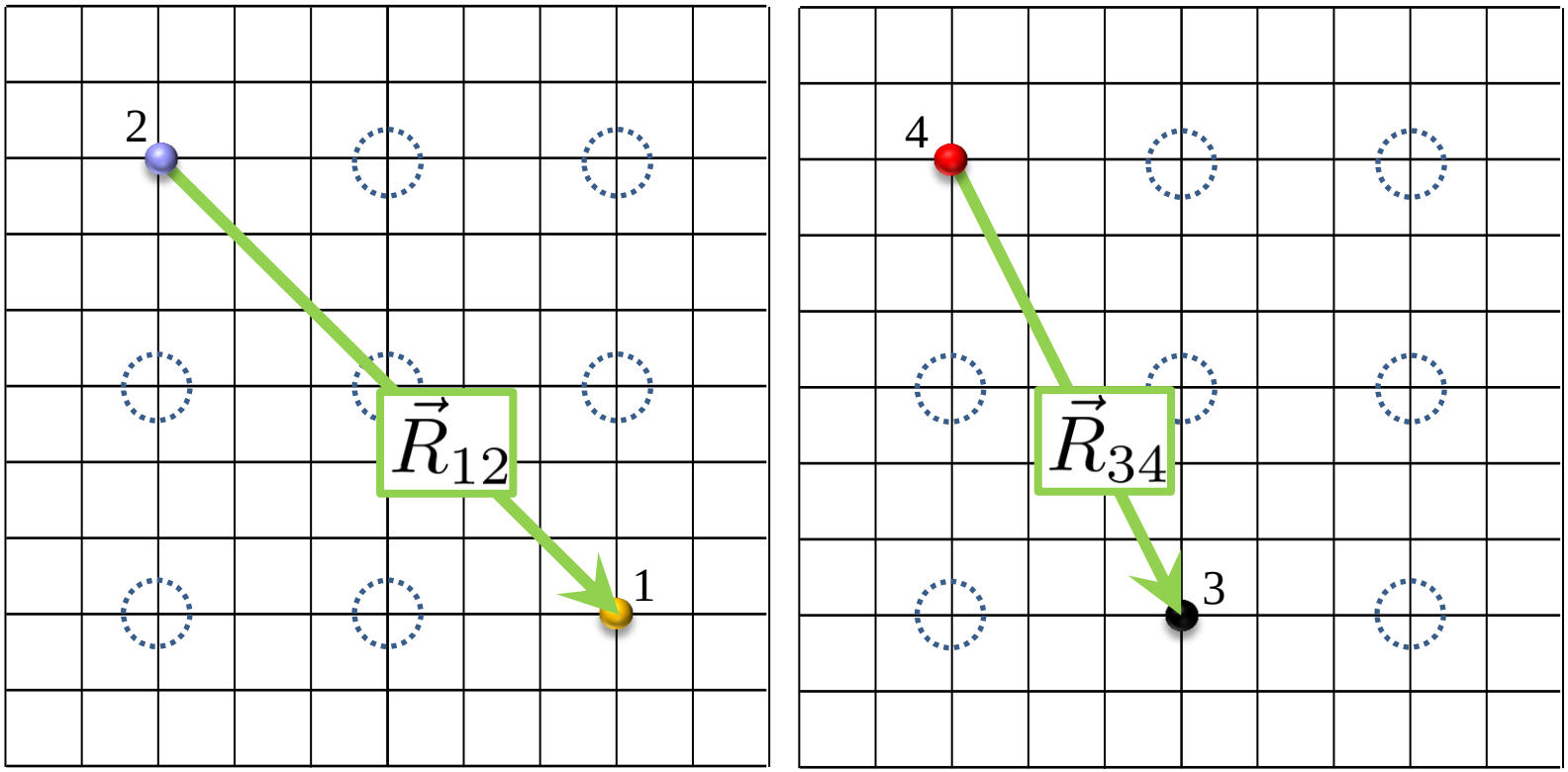
In the continuum limit, the *T* matrix elements with renormalized coupling prescribed via dimensional regularization is

$$2T_{1+2\to1+2} = \frac{c/(2\pi)^3}{1-\frac{\mu c}{2\pi}\sqrt{-p^2-2i\mu\epsilon}} + \frac{-c/(2\pi)^3}{1+\frac{\mu c}{2\pi}\sqrt{-p^2-2i\mu\epsilon}}$$

$$2T_{1+2\to3+4} = \frac{c/(2\pi)^3}{1-\frac{\mu c}{2\pi}\sqrt{-p^2-2i\mu\epsilon}} - \frac{-c/(2\pi)^3}{1+\frac{\mu c}{2\pi}\sqrt{-p^2-2i\mu\epsilon}}$$

We apply the adiabatic projection method to this system.

S. Elhatisari, M. Pine, A. Rokash, H. Krebs, E. Epelbaum, D. L., in preparation



In this case we don't have clusters. But the adiabatic projection method works the same way, and the net effect can be viewed as a "block-spin" renormalization group flow to longer distance scales.

We compute the adiabatic Hamiltonian

$$\langle H \rangle_{\rm adiab} = \langle N \rangle_t^{-1/2} \langle H \rangle_t \langle N \rangle_t^{-1/2}$$

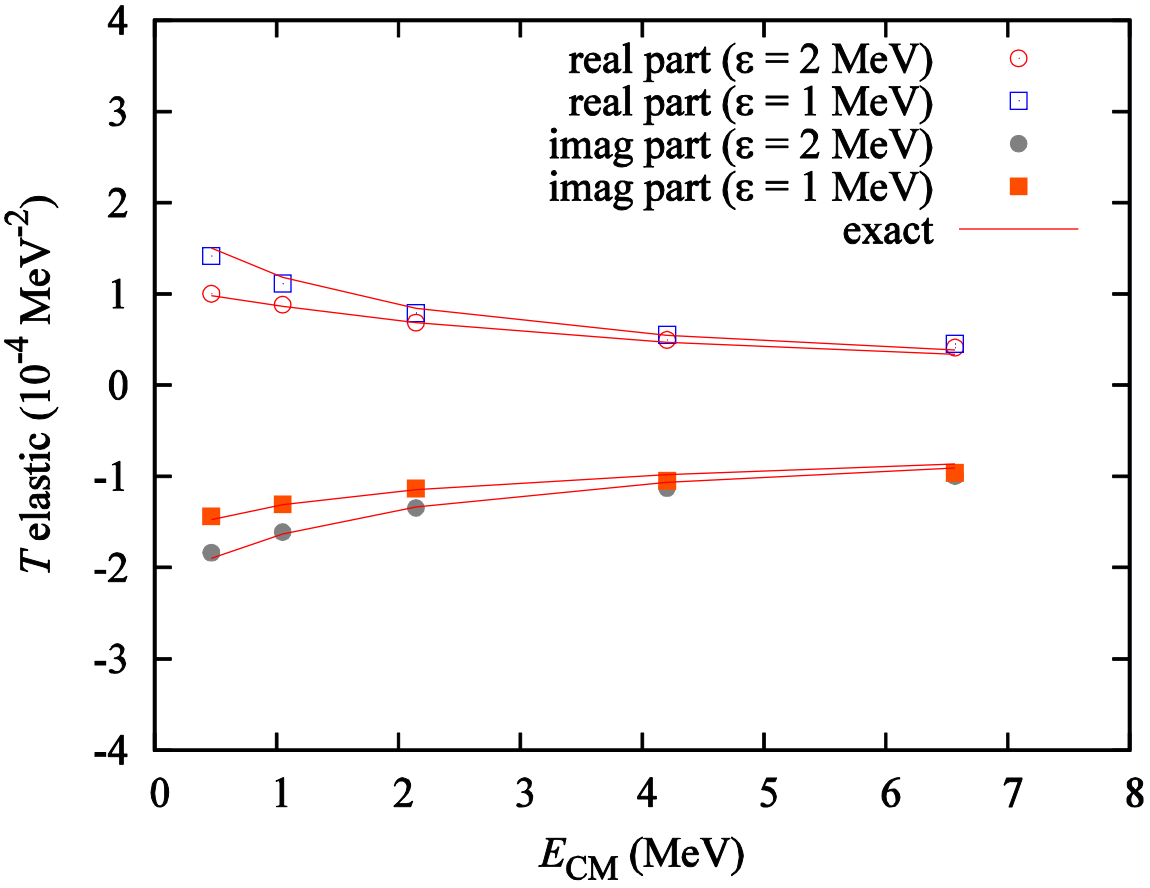
and then treat it as an effective Hamiltonian for clusters to compute *T*-matrix elements. For example, one approach we demonstrate here is the complex energy method.

$$\langle \vec{p}\,' | T_{\rm adiab}(E_p + i\epsilon) | \vec{p} \rangle$$
$$= \langle \vec{p}\,' | G_{\rm adiab}(E_p + i\epsilon) | \vec{p} \rangle (i\epsilon)^2 - i\epsilon \delta^3(\vec{p}\,' - \vec{p})$$

Other techniques include *R*-matrix theory and other boundary constraint approaches.

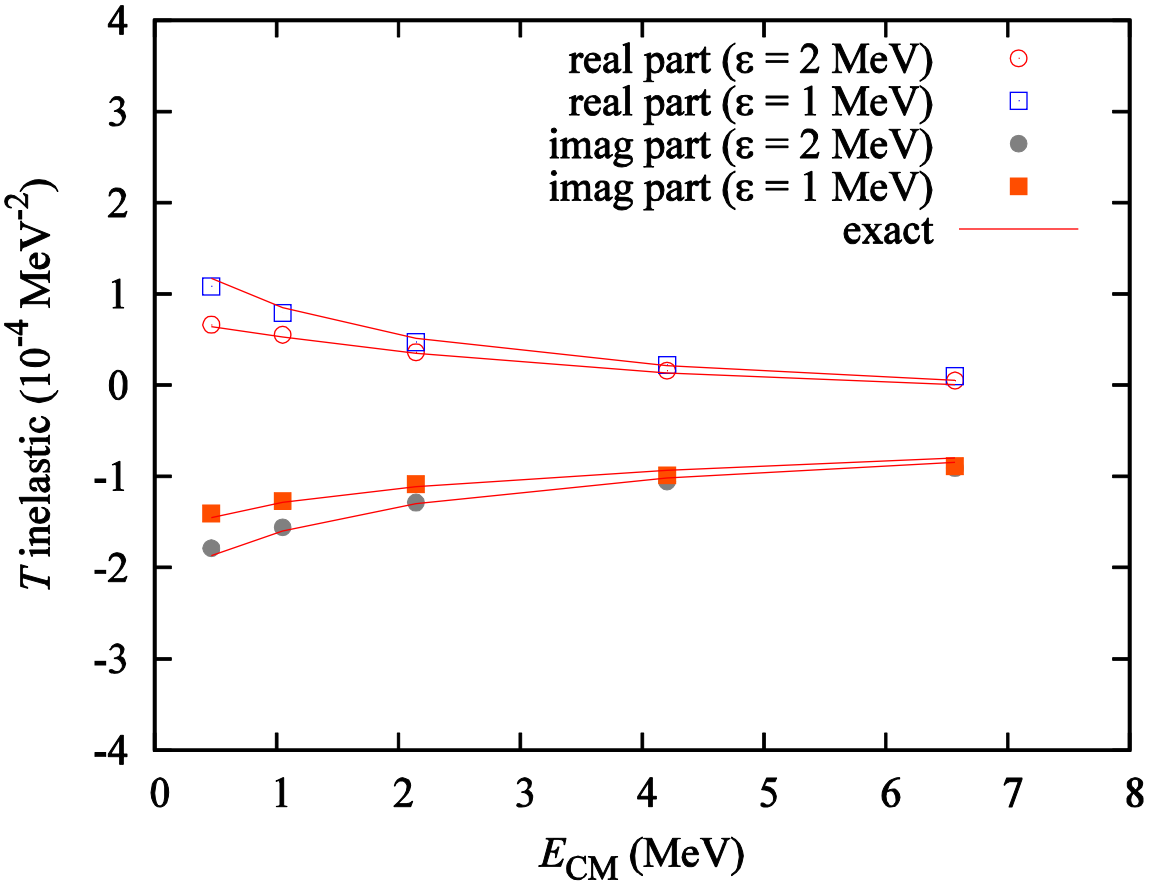
S. Elhatisari, M. Pine, A. Rokash, H. Krebs, E. Epelbaum, D. L., in preparation

$T_{1+2\to 1+2}$



S. Elhatisari, M. Pine, A. Rokash, H. Krebs, E. Epelbaum, D. L., in preparation

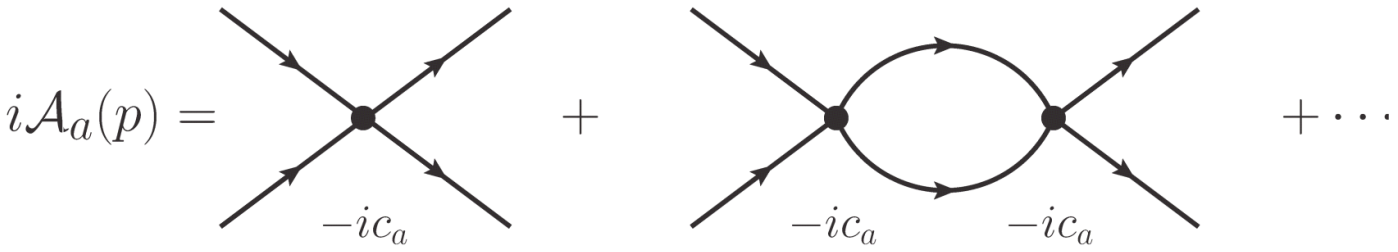
$T_{1+2\to3+4}$



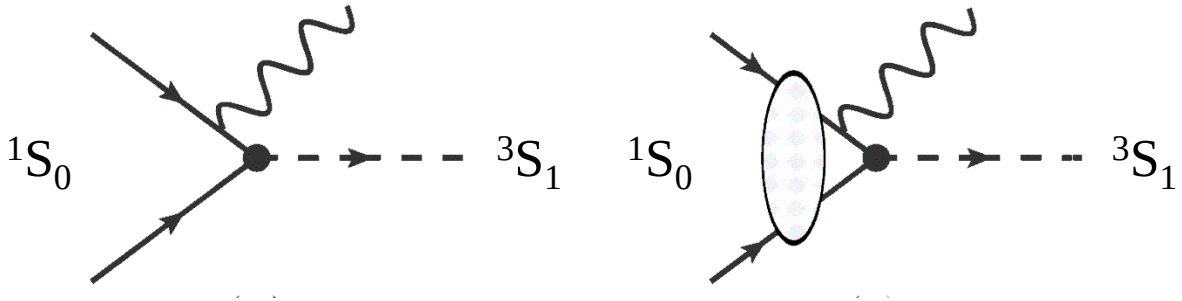
S. Elhatisari, M. Pine, A. Rokash, H. Krebs, E. Epelbaum, D. L., in preparation

Once we have the adiabatic Hamiltonian, we can also do capture reaction calculations. Here is a test of lattice Green's function methods for radiative capture for $n + p \to d + \gamma$ in pionless effective field theory at leading order.

Elastic scattering amplitude ($^1S_0$ and $^3S_1$)



M1 radiative capture amplitude



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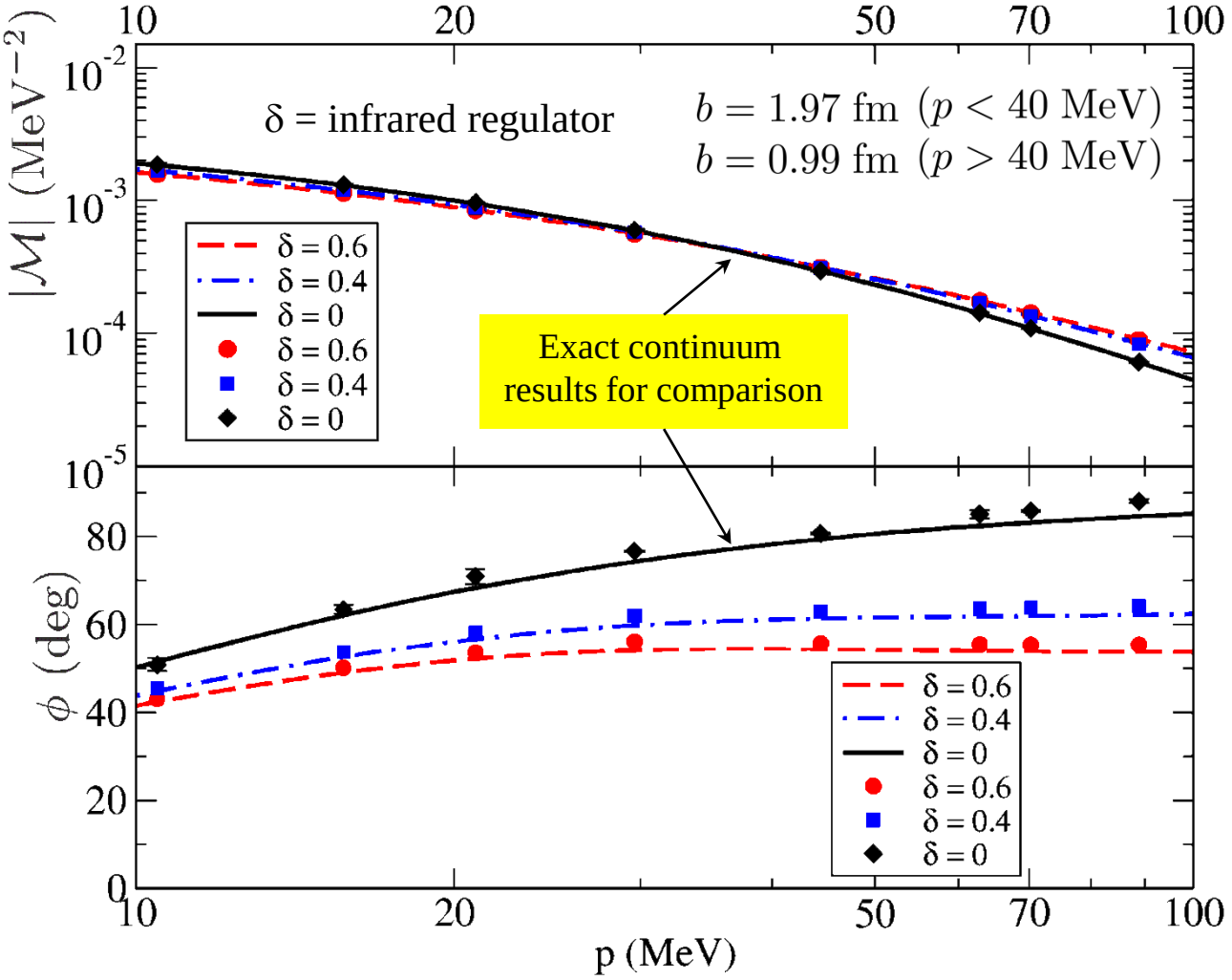
M1 transition amplitude $n + p \rightarrow d + \gamma$



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Summary

A golden age for nuclear theory from first principles. Big science discoveries being made and many more around the corner.

Lattice effective field theory is a relatively new and promising tool that combines the framework of effective field theory and computational lattice methods. May play a significant role in the future of *ab initio* nuclear theory.

Topics being addressed now and in the near future…

Different lattice spacings, decoupling lattice spacing from ultraviolet regulator, sign extrapolations for $N \neq Z$ nuclei, nuclear structure up to $A = 28$, elastic and inelastic reactions, neutron matter equation of state and superfluid transition from *S*-wave to *P*-wave, etc.

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for organizing an excellent program.