Progress towards nuclear scattering and reactions on the lattice

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Nuclear Reactions from Lattice QCD
Institute for Nuclear Theory Workshop
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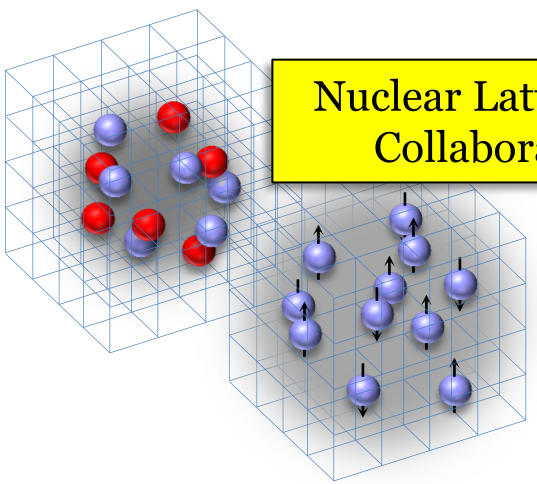


Nuclear Lattice EFT Collaboration

Outline

Bound state scattering at finite volume

What is lattice effective field theory?

Lattice interactions and scattering

Euclidean time projection and auxiliary fields

Structure and rotations of the Hoyle state

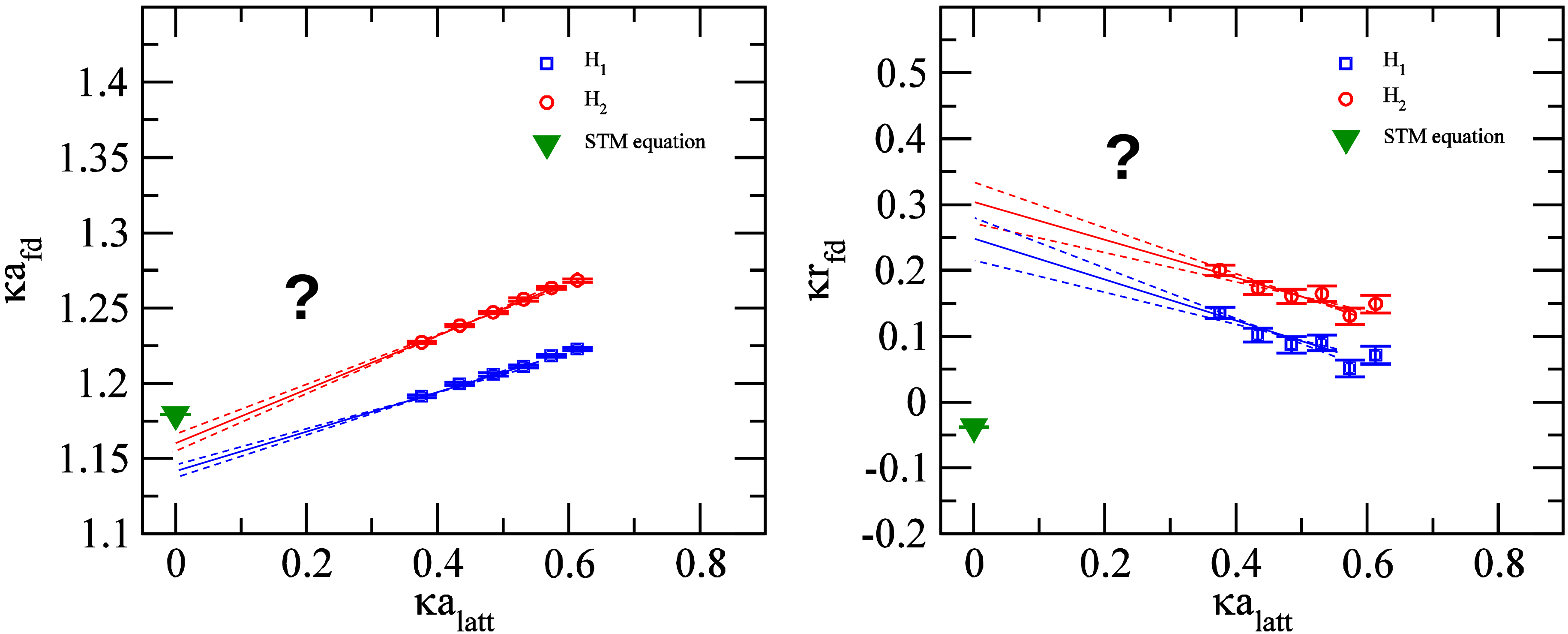
Light quark mass dependence of helium burning

Scattering and reactions on the lattice

Summary and future directions

Fermion-dimer scattering

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

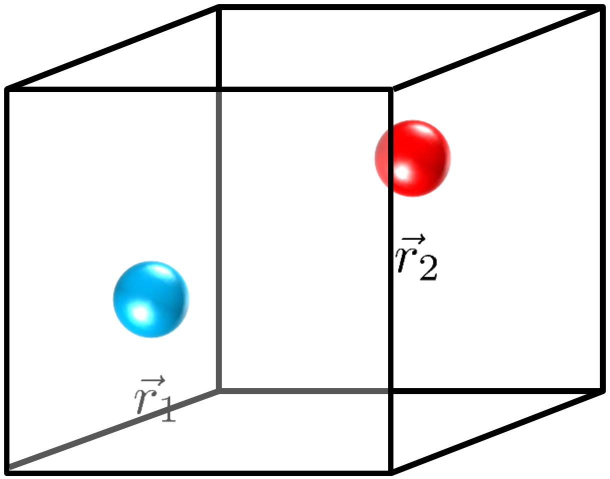


Bour, König, D.L., Hammer, Meißner, PRD 84:091503(R) (2011)

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

Bound states in moving frames at finite volume

Consider a two-body bound state with total momentum **P** in a periodic cube with length L



$$\Psi(\vec{r}_1, \vec{r}_2) = e^{i\vec{P}\cdot\vec{R}}\psi(\vec{r})$$

$$\vec{r} = \vec{r}_1 - \vec{r}_2$$

$$\vec{R} = \alpha\vec{r}_1 + (1-\alpha)\vec{r}_2$$

$$\alpha = \frac{m_1}{m_1 + m_2}$$

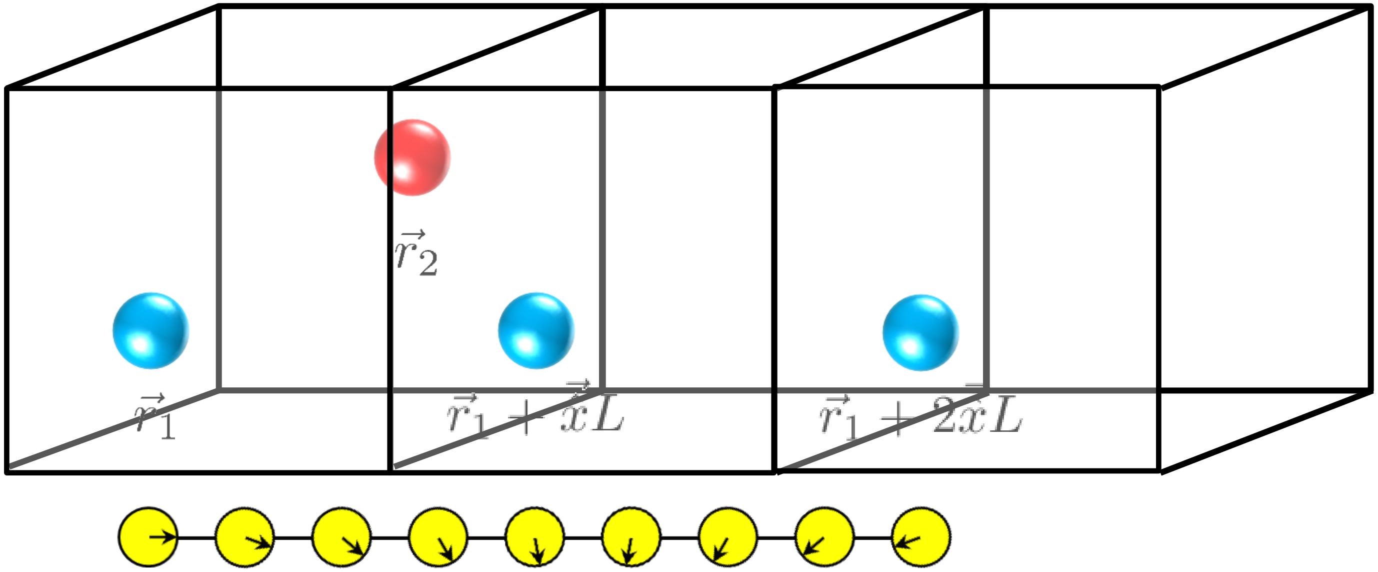
Periodicity requires that the full wavefunction is periodic under translations of length L

$$\Psi(\vec{r}_1, \vec{r}_2) = e^{i\vec{P}\cdot\vec{R}}\psi(\vec{r})$$

$$\Psi(\vec{r}_1, \vec{r}_2) = \Psi(\vec{r}_1 + \vec{n}L, \vec{r}_2) = e^{i\vec{P}\cdot\vec{R}}e^{i\alpha\vec{P}\cdot\vec{n}L}\psi(\vec{r} + \vec{n}L)$$

So relative wavefunction satisfies twisted boundary conditions

$$\psi(\vec{r} + \vec{n}L) = e^{-i\alpha\vec{P}\cdot\vec{n}L}\psi(\vec{r})$$



Energy shift for twisted boundary conditions

We consider finite range interactions

$$V(\vec{r}, \vec{r}\,')$$

and make a periodic extension of the interactions

$$V(\vec{r}, \vec{r}\,') \rightarrow V_L(\vec{r}, \vec{r}\,') = \sum_{\vec{n} \in \mathbf{Z}} V(\vec{r} + \vec{n}L, \vec{r}\,' + \vec{n}L)$$

We use periodic interactions to define our finite-volume Hamiltonian

$$\hat{H} \rightarrow \hat{H}_L$$

We now consider twisted boundary conditions

$$\psi(\vec{r} + \vec{n}L) = e^{-i\vec{\theta}\cdot\vec{n}}\psi(\vec{r}),\ \vec{\theta} = \alpha\vec{P}L$$

Label the Hamiltonians and bound states at infinite volume and finite volume as

$$\hat{H}\,|\psi_B\rangle = E_B(\infty)\,|\psi_B\rangle$$

$$\hat{H}_L\,|\psi\rangle = E_B(L)\,|\psi\rangle$$

We make an ansatz for the finite-volume wavefunction,

$$\psi_0(\vec{r}) = \sum_{\vec{n}\in\mathbf{Z}} \psi_B(\vec{r}+\vec{n}L)e^{i\vec{\theta}\cdot\vec{n}}$$

This gives

$$\hat{H}_L\,|\psi_0\rangle = E_B(\infty)\,|\psi_0\rangle + |\eta\rangle$$

where

$$\eta(\vec{r}) = \sum_{\vec{n}\neq\vec{n}'} \int d^3r'\; V(\vec{r}+\vec{n}L, \vec{r}\,'+\vec{n}L)\psi_B(\vec{r}\,'+\vec{n}'L)e^{i\vec{\theta}\cdot\vec{n}'}$$

The overlap with the exact finite-volume wavefunction gives

$$\langle\psi|\,\hat{H}_L\,|\psi_0\rangle = E_B(L)\,\langle\psi|\,\psi_0\rangle = E_B(\infty)\,\langle\psi|\,\psi_0\rangle + \langle\psi|\,\eta\rangle$$

We solve for the finite volume energy correction,

$$\Delta E_B(L) = E_B(L) - E_B(\infty) = \frac{\langle\psi|\,\eta\rangle}{\langle\psi|\,\psi_0\rangle}$$

$$= \sum_{|\vec{n}|=1} \int d^3r d^3r'\; \psi_B^*(\vec{r})V(\vec{r},\vec{r}\,')\psi_B(\vec{r}\,' + \vec{n}L)e^{i\vec{\theta}\cdot\vec{n}} + O(e^{-\sqrt{2}\kappa L})$$

From the Schrödinger equation

$$\Delta E_B(L) =$$

$$\sum_{|\vec{n}|=1} \int d^3r'\; \frac{1}{2\mu}\left[\Delta_{r'} - \kappa^2\right]\psi_B^*(\vec{r}\,')\psi_B(\vec{r}\,' + \vec{n}L)e^{i\vec{\theta}\cdot\vec{n}} + O(e^{-\sqrt{2}\kappa L})$$

At large distances, the S-wave bound state wavefunction has the form

$$\psi_B(\vec{r}) \to \frac{\gamma e^{-\kappa r}}{r\sqrt{4\pi}}$$

so that

$$\Delta E_B(L) = -|\gamma|^2 \frac{e^{-\kappa L}}{\mu L} \sum_{\vec{n}=\hat{x},\hat{y},\hat{z}} \cos(\vec{\theta}\cdot\vec{n}) + O(e^{-\sqrt{2}\kappa L})$$

Can be extended to bound states with nonzero angular momentum

König, D.L., Hammer, PRL 107 112001 (2012)

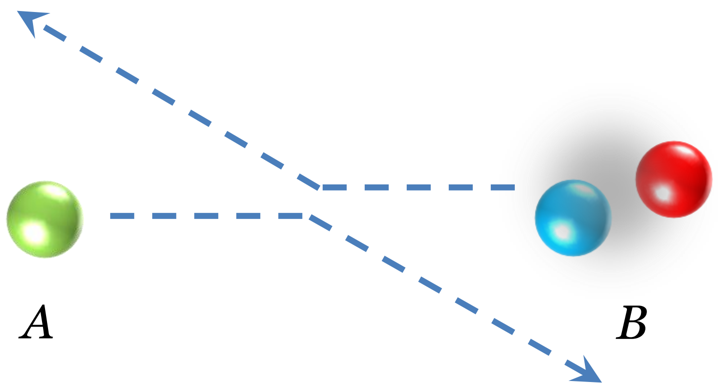
König, D.L., Hammer, Ann. Phys. 327, 1450 (2012)

See also Zohreh's talk at this workshop

Davoudi, Savage, PRD 84 114502 (2011)

Scattering states

Consider scattering of two bodies, A and B, where A is a single particle a B is a two-body bound state.



Scattering wavefunction outside the interacting region

$$\langle \vec{r} | \Psi_p \rangle = c \sum_{\vec{k}} \frac{e^{i2\pi\vec{k}\cdot\vec{r}/L}}{(2\pi\vec{k}/L)^2 - \vec{p}^2}$$

Energy of scattering state at finite volume

$$E_{AB}(p,L) = \frac{\langle \Psi_p | \hat{H}_L | \Psi_p \rangle}{\langle \Psi_p | \Psi_p \rangle}$$

$$\Delta E^A_{\vec{k}}(L) = E^A_{\vec{k}}(L) - E^A_{\vec{k}}(\infty) = 0$$

$$\Delta E^B_{\vec{k}}(L) = -|\gamma|^2 \frac{e^{-\kappa L}}{\mu L} \sum_{l=1,2,3} \cos(2\pi\alpha_B k_l)$$

$$E_{AB}(p,L) - E_{AB}(p,\infty) = \tau_A(\eta)\Delta E^A_{\vec{0}}(L) + \tau_B(\eta)\Delta E^B_{\vec{0}}(L)$$

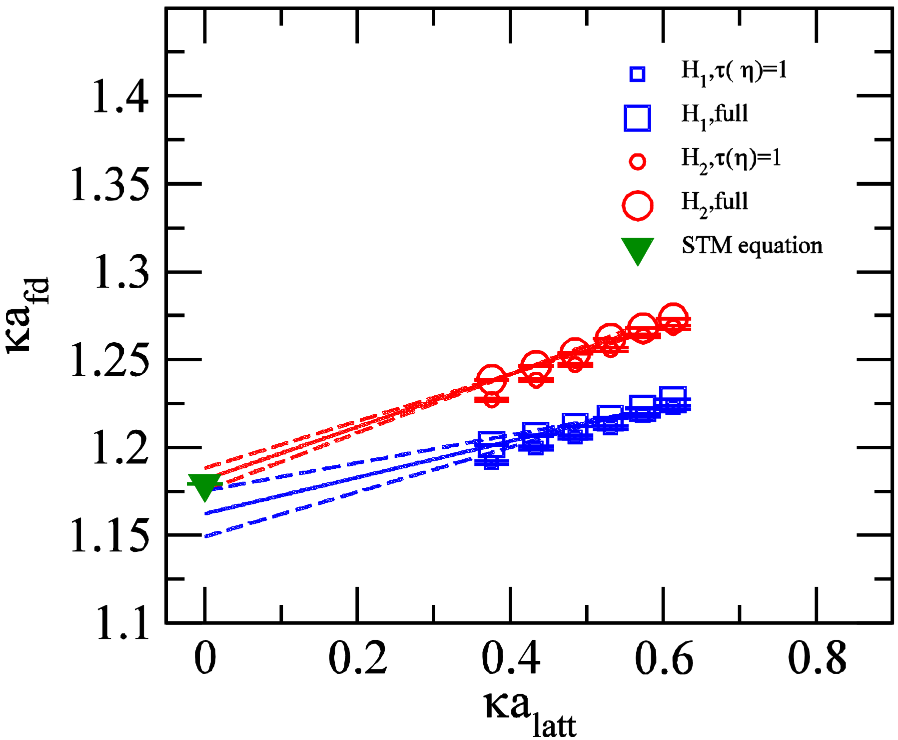
Topological volume factor

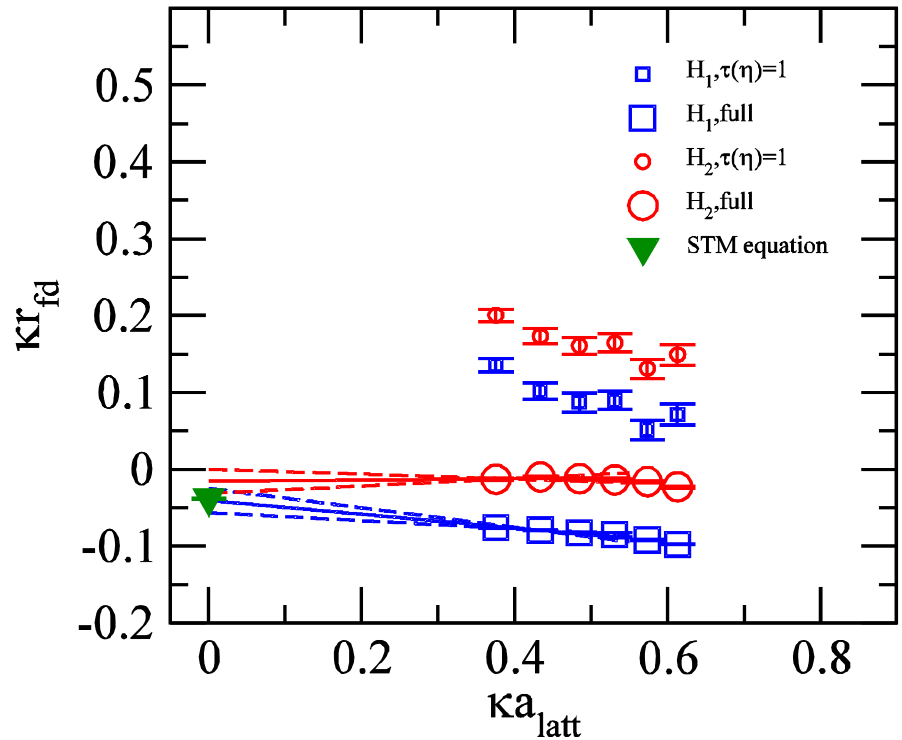
$$\tau(\eta) = \frac{1}{N}\sum_{\vec{k}} \frac{\sum_{l=1,2,3}\cos(2\pi\alpha_B k_l)}{3(\vec{k}^2-\eta)^2}, \quad N = \sum_{\vec{k}} \frac{1}{(\vec{k}^2-\eta)^2}$$

$$\eta = \left(\frac{Lp}{2\pi}\right)^2$$

Results for fermion-dimer scattering

Lattice results for fermion-dimer scattering for zero range interactions for two-component fermions including topological volume correction.

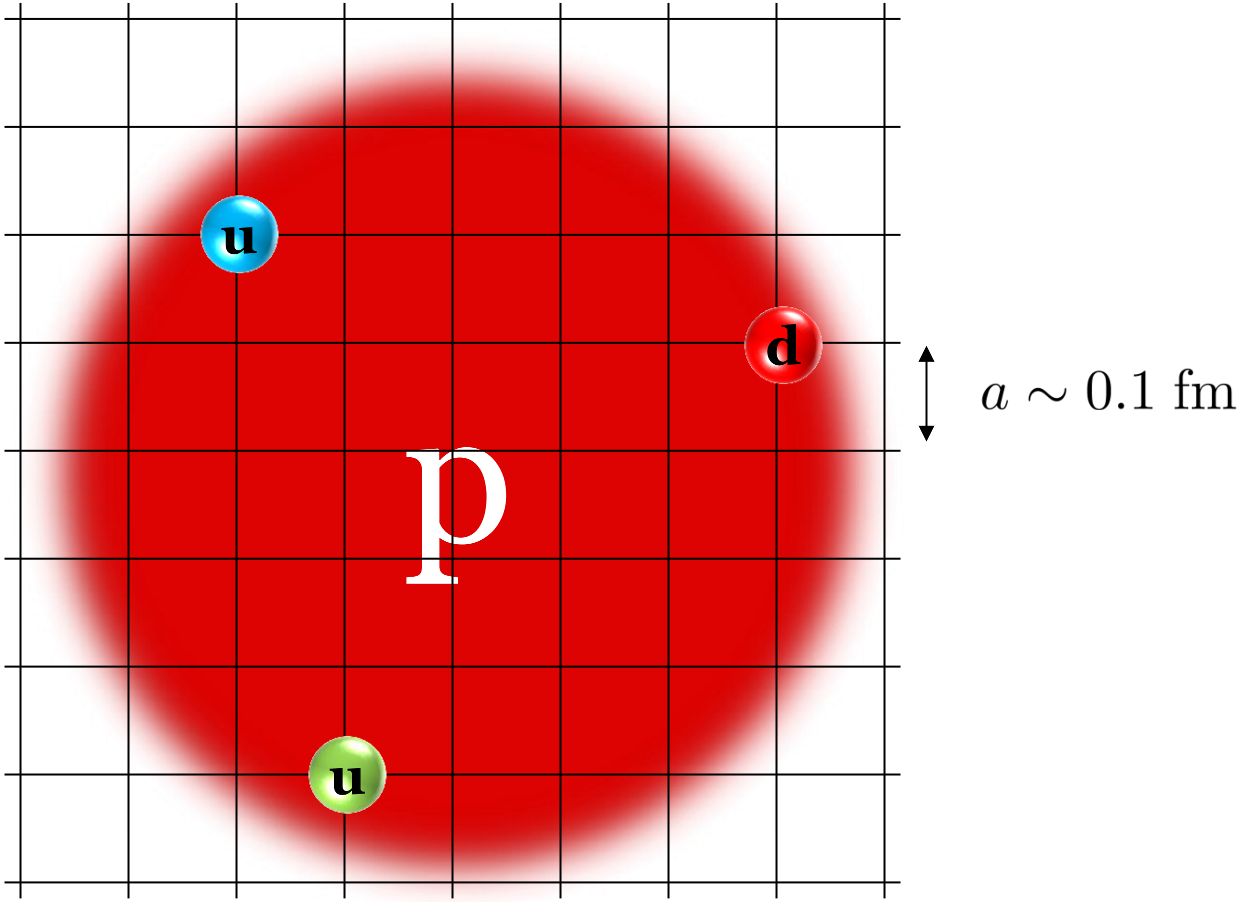




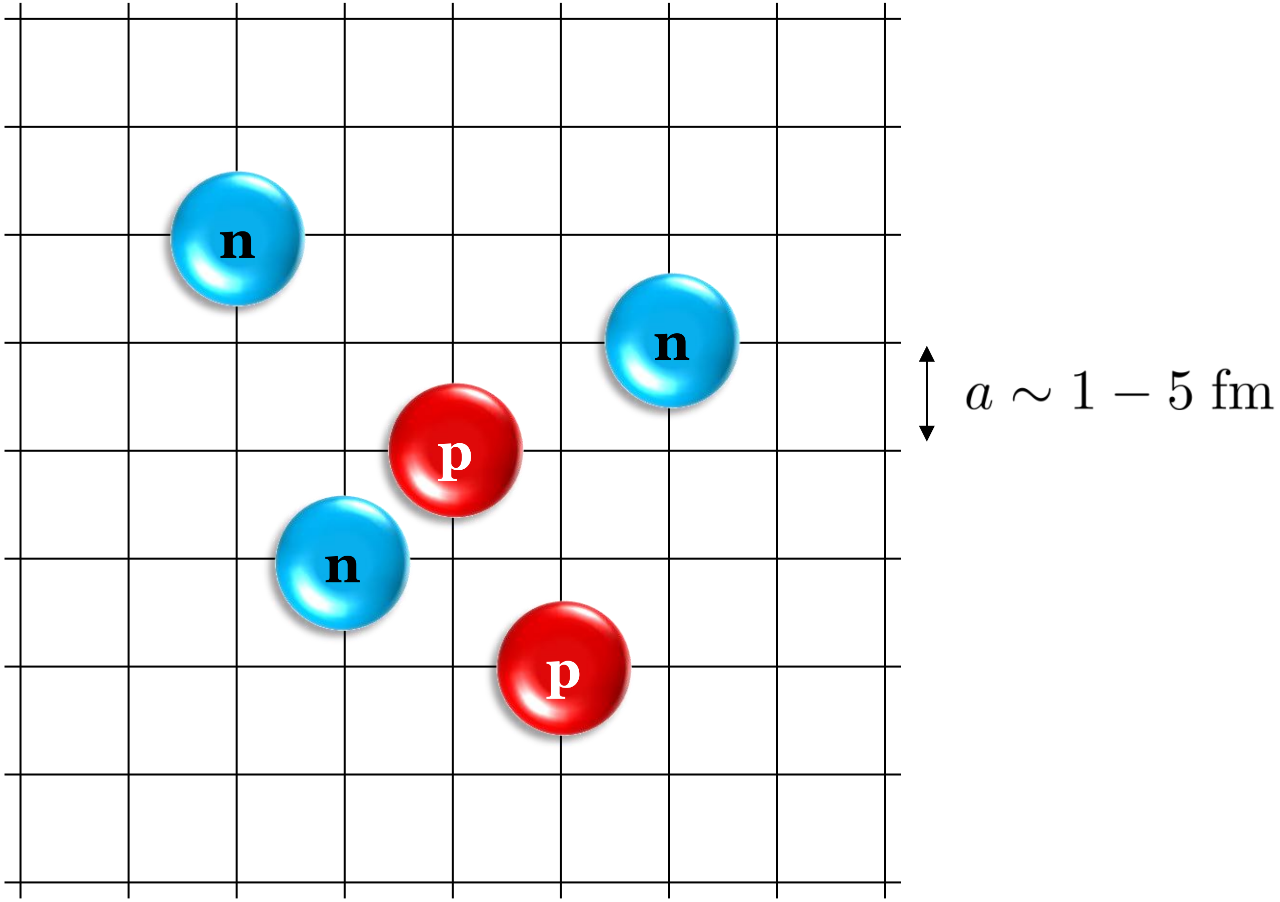
Bour, König, D.L., Hammer, Meißner, PRD 84:091503(R) (2011)

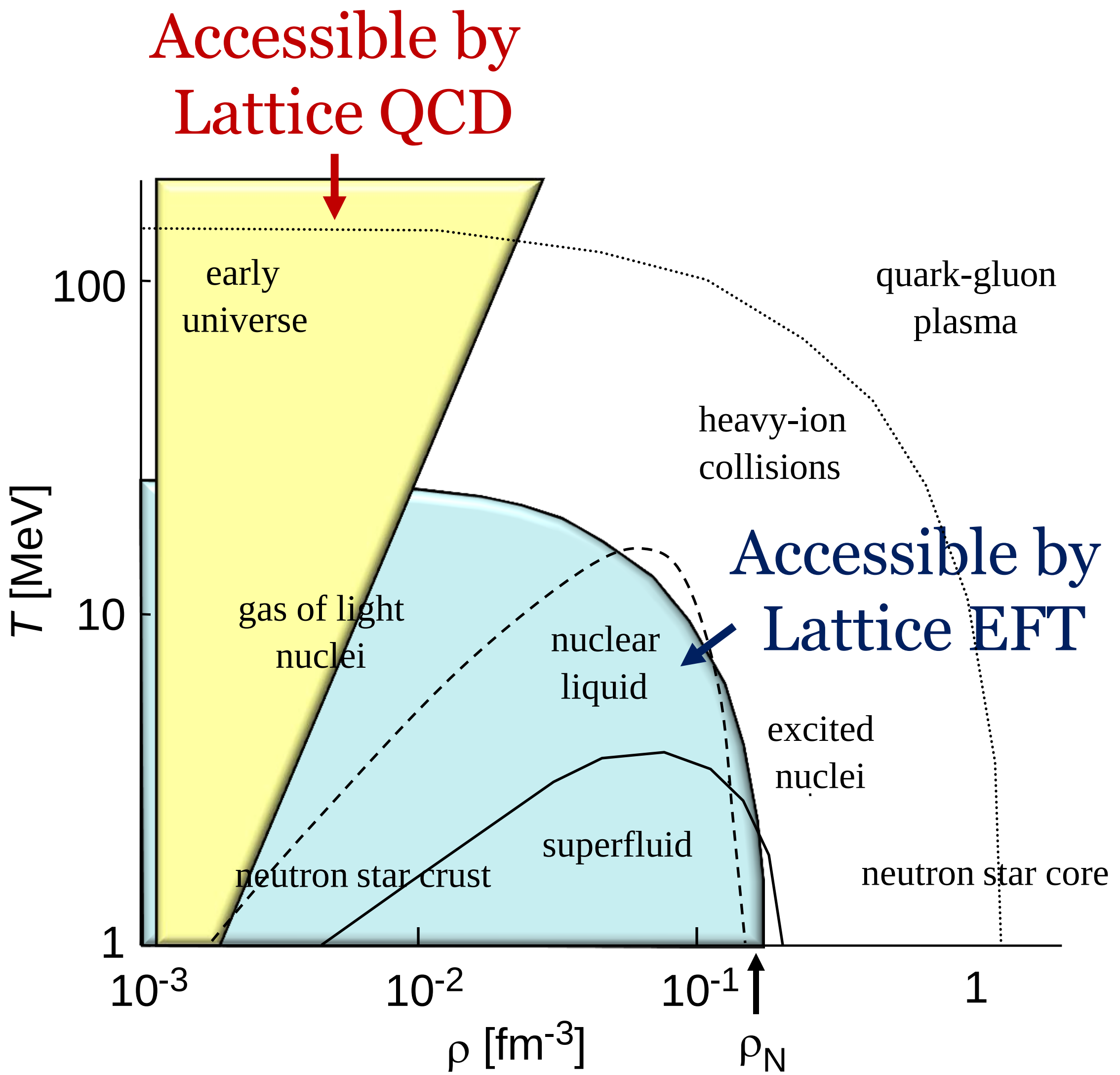
Bour, Hammer, D.L., Meißner, PRC 86, 034003 (2012)

Lattice quantum chromodynamics



Lattice effective field theory

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neutron star crust
neutron star core
10^{-3}
10^{-2}
10^{-1}
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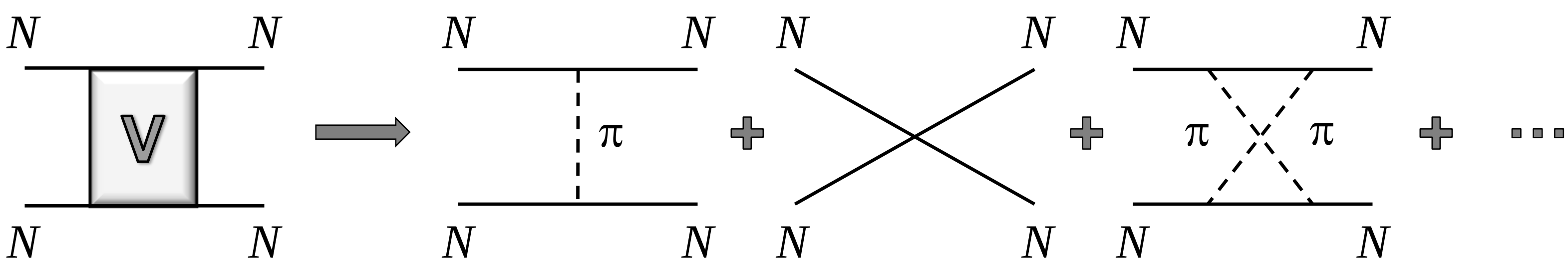
ρ [fm^{-3}]
ρ_N

Low energy nucleons: Chiral effective field theory

Weinberg, PLB 251 (1990) 288; NPB 363 (1991) 3

Construct the effective potential order by order



V^{OPEP}

Contact interactions

$1,\ \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2$

V^{TPEP}

Leading order (LO)

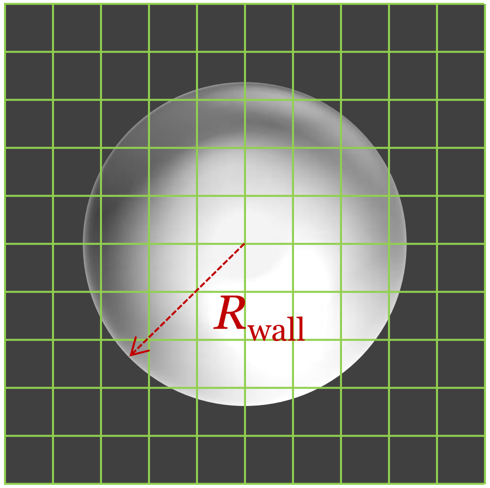
Next-to-leading order (NLO)

Physical scattering data → Unknown operator coefficients

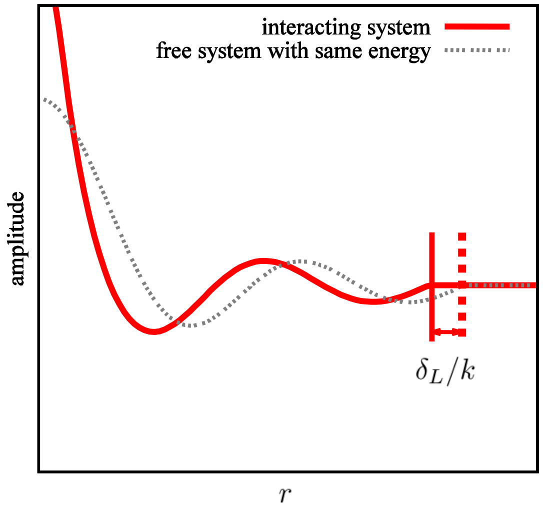
Spherical wall method

Borasoy, Epelbaum, Krebs, D.L., Meißner, EPJA 34 (2007) 185

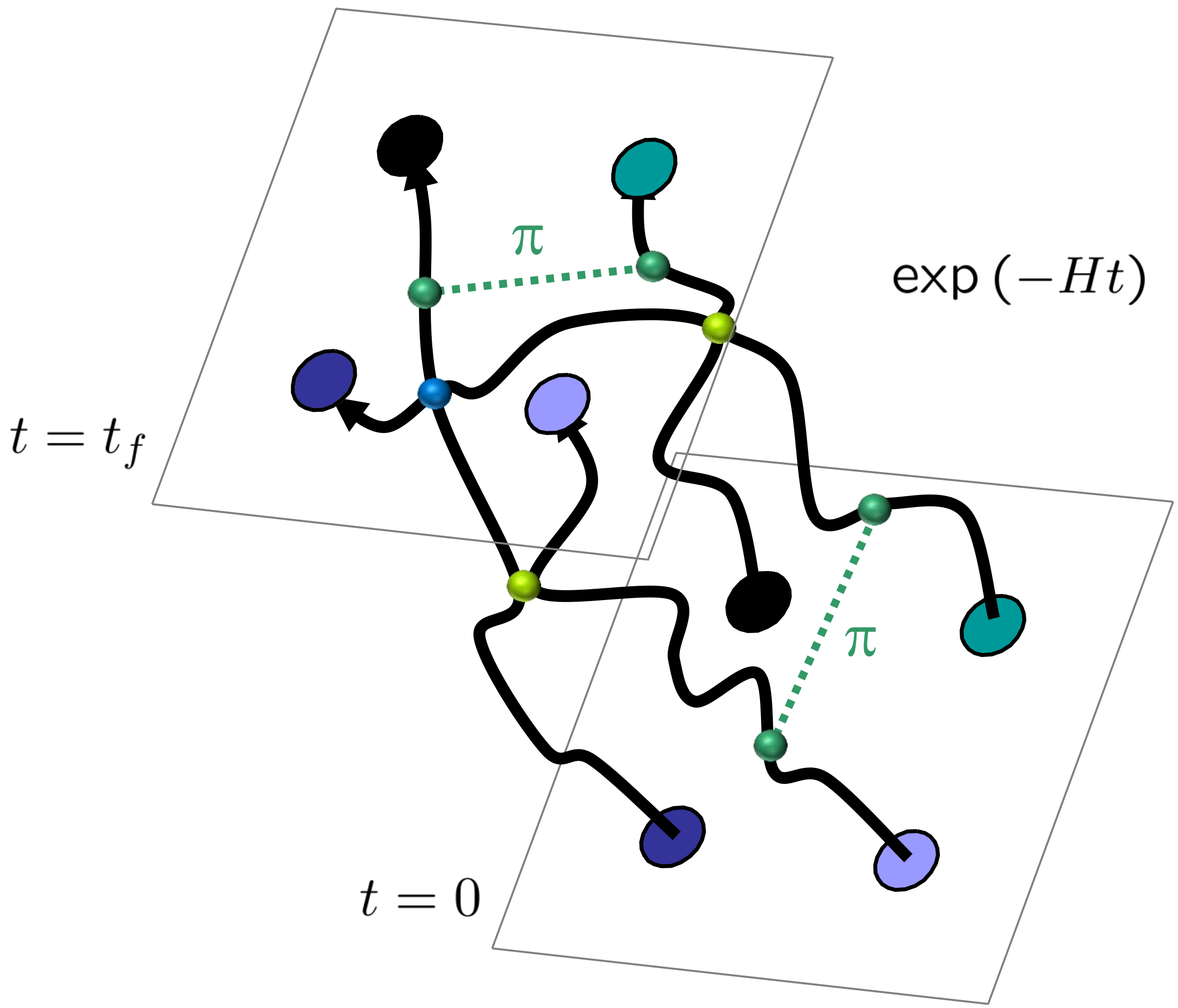
Spherical wall imposed in the center of mass frame



Representation	J_z	Example
A_1	$0 \bmod 4$	$Y_{0,0}$
T_1	$0, 1, 3 \bmod 4$	$\{Y_{1,0}, Y_{1,1}, Y_{1,-1}\}$
E	$0, 2 \bmod 4$	$\left\{Y_{2,0}, \frac{Y_{2,-2}+Y_{2,2}}{\sqrt{2}}\right\}$
T_2	$1, 2, 3 \bmod 4$	$\left\{Y_{2,1}, \frac{Y_{2,-2}-Y_{2,2}}{\sqrt{2}}, Y_{2,-1}\right\}$
A_2	$2 \bmod 4$	$\frac{Y_{3,2}-Y_{3,-2}}{\sqrt{2}}$



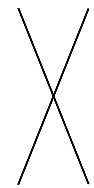
Euclidean time projection



Auxiliary field method

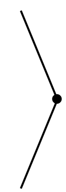
We can write exponentials of the interaction using a Gaussian integral identity

$$\exp\left[-\frac{C}{2}(N^{\dagger}N)^2\right]$$



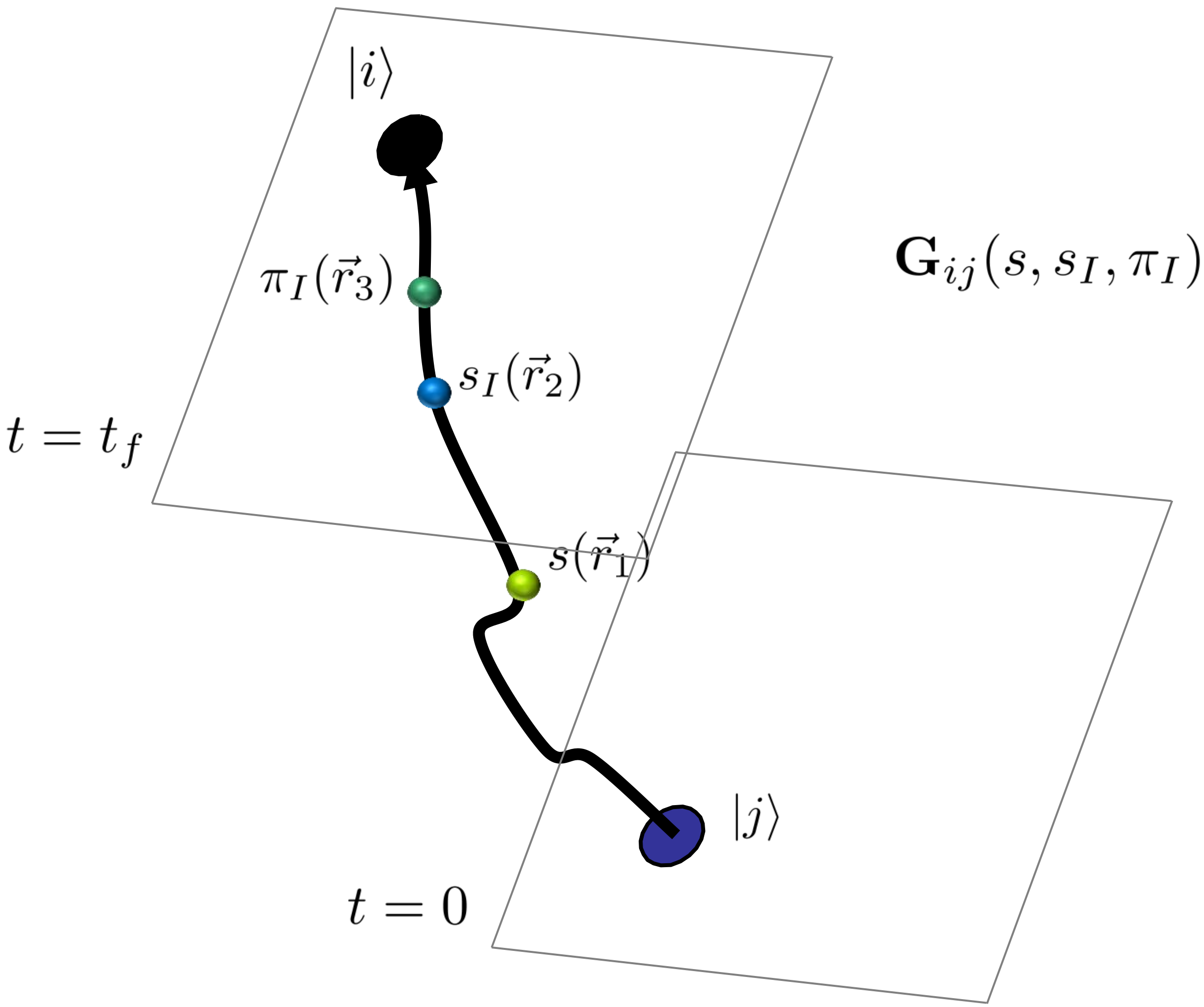
$(N^{\dagger}N)^2$

$$=\sqrt{\frac{1}{2\pi}}\int_{-\infty}^{\infty} ds \exp\left[-\frac{1}{2}s^2+\sqrt{-C}\, s(N^{\dagger}N)\right]$$

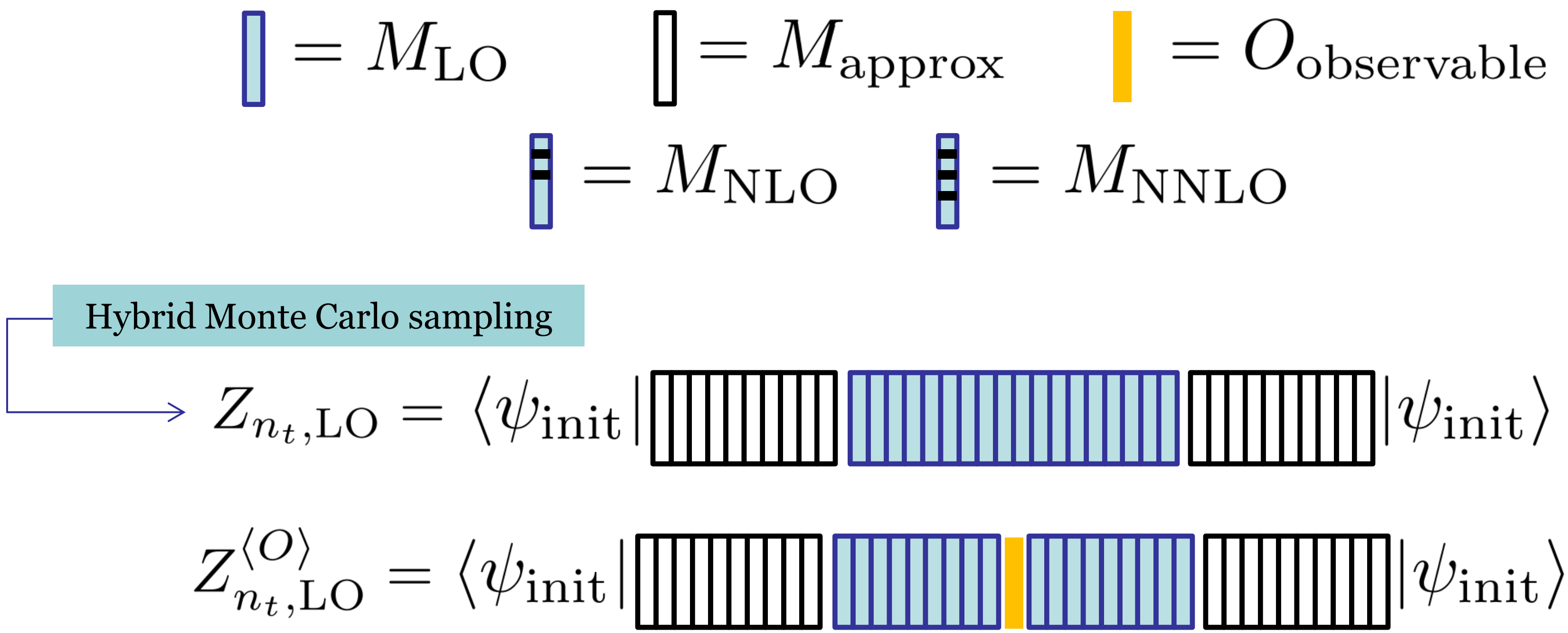


$sN^{\dagger}N$

We remove the interaction between nucleons and replace it with the interactions of each nucleon with a background field.


$|i\rangle$
$\mathbf{G}_{ij}(s, s_I, \pi_I)$
$\pi_I(\vec{r}_3)$
$s_I(\vec{r}_2)$
$t = t_f$
$s(\vec{r}_1)$
$|j\rangle$
$t = 0$

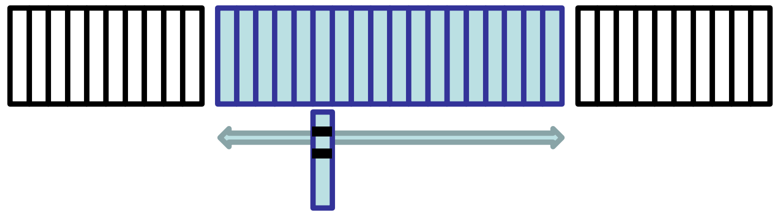
Schematic of lattice Monte Carlo calculation



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

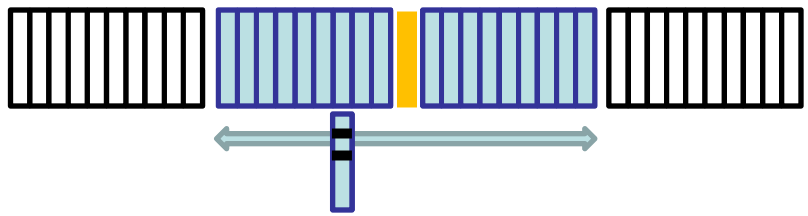
$$\langle O \rangle_{0,\mathrm{LO}} = \lim_{n_t \to \infty} Z^{\langle O \rangle}_{n_t,\mathrm{LO}} / Z_{n_t,\mathrm{LO}}$$

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



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

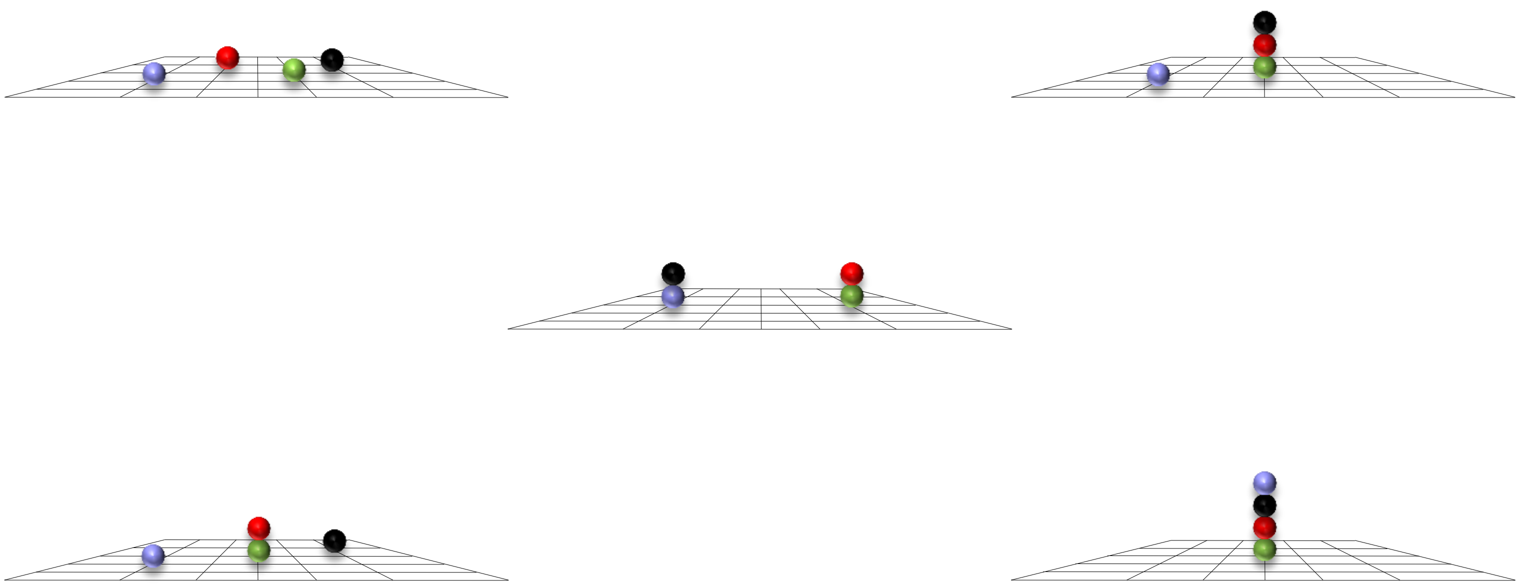
$$Z^{\langle O \rangle}_{n_t,\mathrm{NLO}} = \langle \psi_{\mathrm{init}} |$$



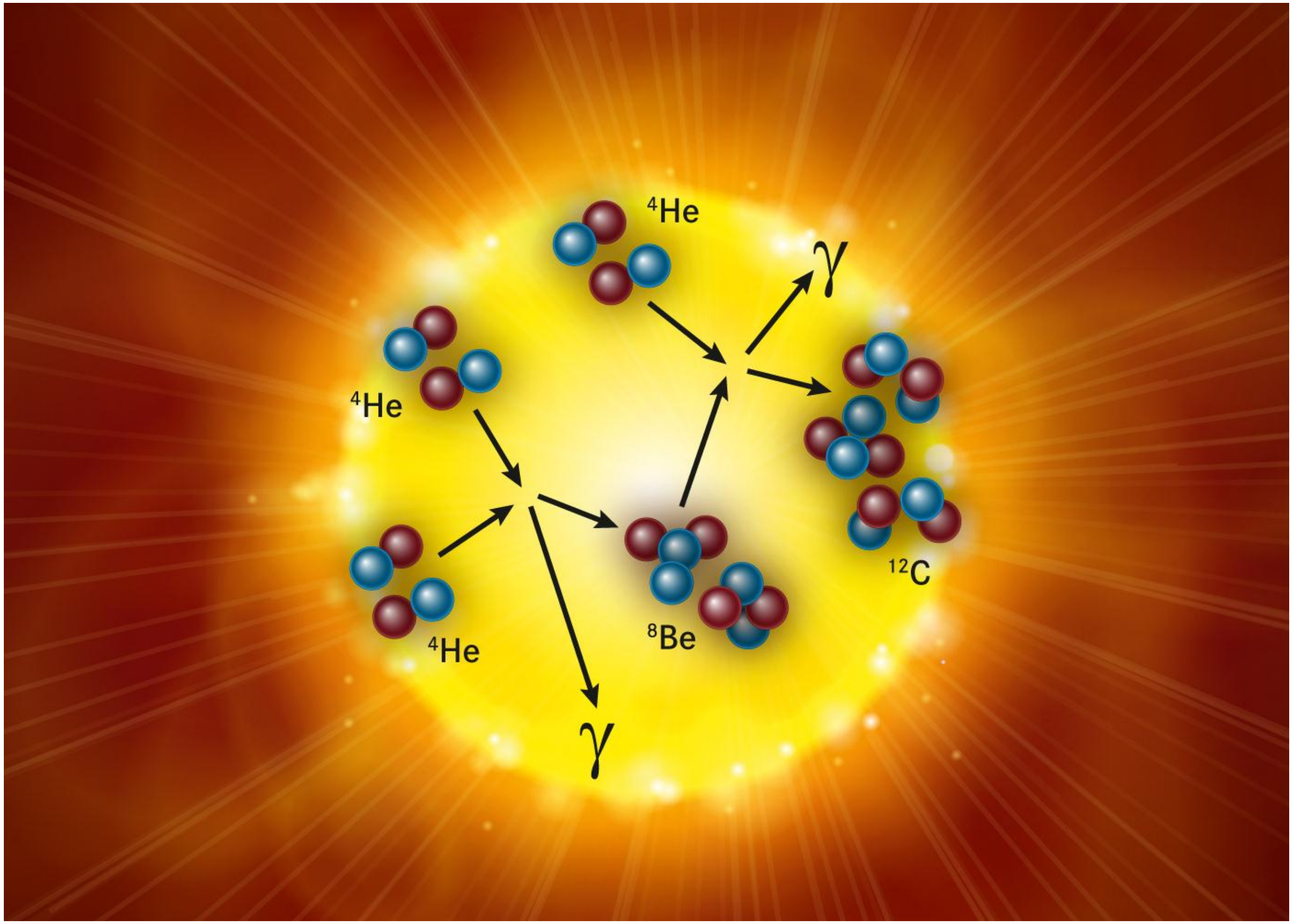
$$| \psi_{\mathrm{init}} \rangle$$

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

Particle clustering included automatically

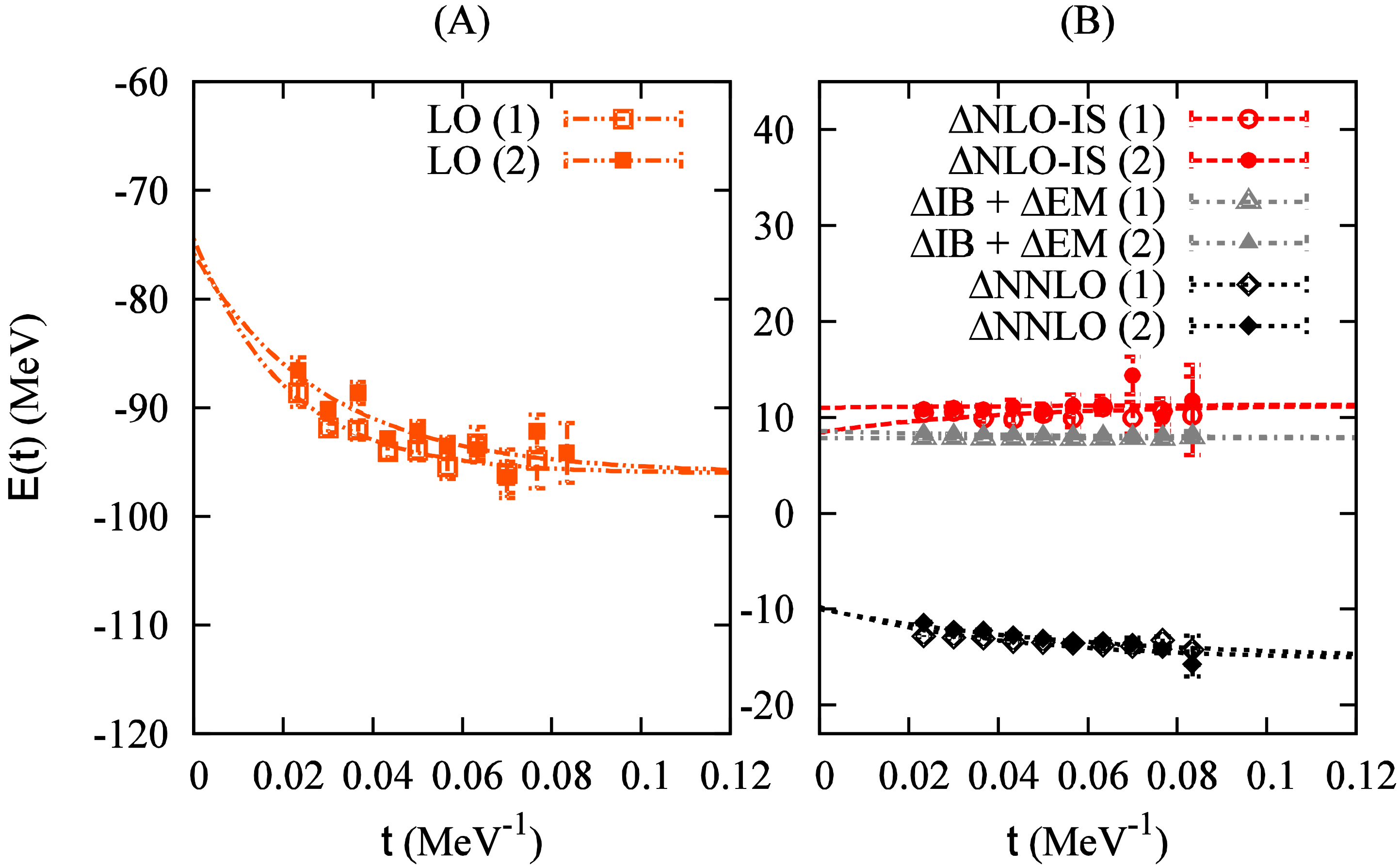


Carbon-12 spectrum and the Hoyle state



Ground state of Carbon-12

$L = 11.8\,\text{fm}$



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

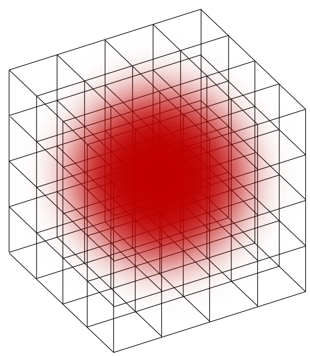
Ground state of Carbon-12

$$L = 11.8\,\mathrm{fm}$$

LO ($O(Q^0)$)	-96(2) MeV
NLO ($O(Q^2)$)	-77(3) MeV
NNLO ($O(Q^3)$)	-92(3) MeV
Experiment	-92.2 MeV

c_1, c_3, c_4 three-nucleon	-2.5(5) MeV
c_D three-nucleon	-6(1) MeV
c_E three-nucleon	-6(2) MeV

Simulations using general initial/final state wavefunctions



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

Construct states with well-defined momentum using all possible translations.

$$L^{-3/2} \sum_{\vec{m}} \psi_j(\vec{n}+\vec{m})\, e^{i\vec{P}\cdot\vec{m}} \quad j = 1, \cdots A$$

Shell model wavefunctions

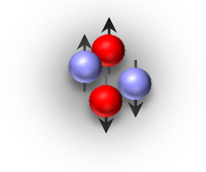
$$\psi_j(\vec{n}) = \exp(-c\vec{n}^2)$$
$$\psi'_j(\vec{n}) = n_x \exp(-c\vec{n}^2)$$
$$\psi''_j(\vec{n}) = n_y \exp(-c\vec{n}^2)$$
$$\psi'''_j(\vec{n}) = n_z \exp(-c\vec{n}^2)$$
$$\vdots$$

Alpha cluster wavefunctions

$$\psi_j(\vec{n}) = \exp[-c(\vec{n} - \vec{m})^2]$$
$$\psi'_j(\vec{n}) = \exp[-c(\vec{n} - \vec{m}')^2]$$
$$\psi''_j(\vec{n}) = \exp[-c(\vec{n} - \vec{m}'')^2]$$
$$\vdots$$

Shell model wavefunctions do not have enough local four nucleon correlations

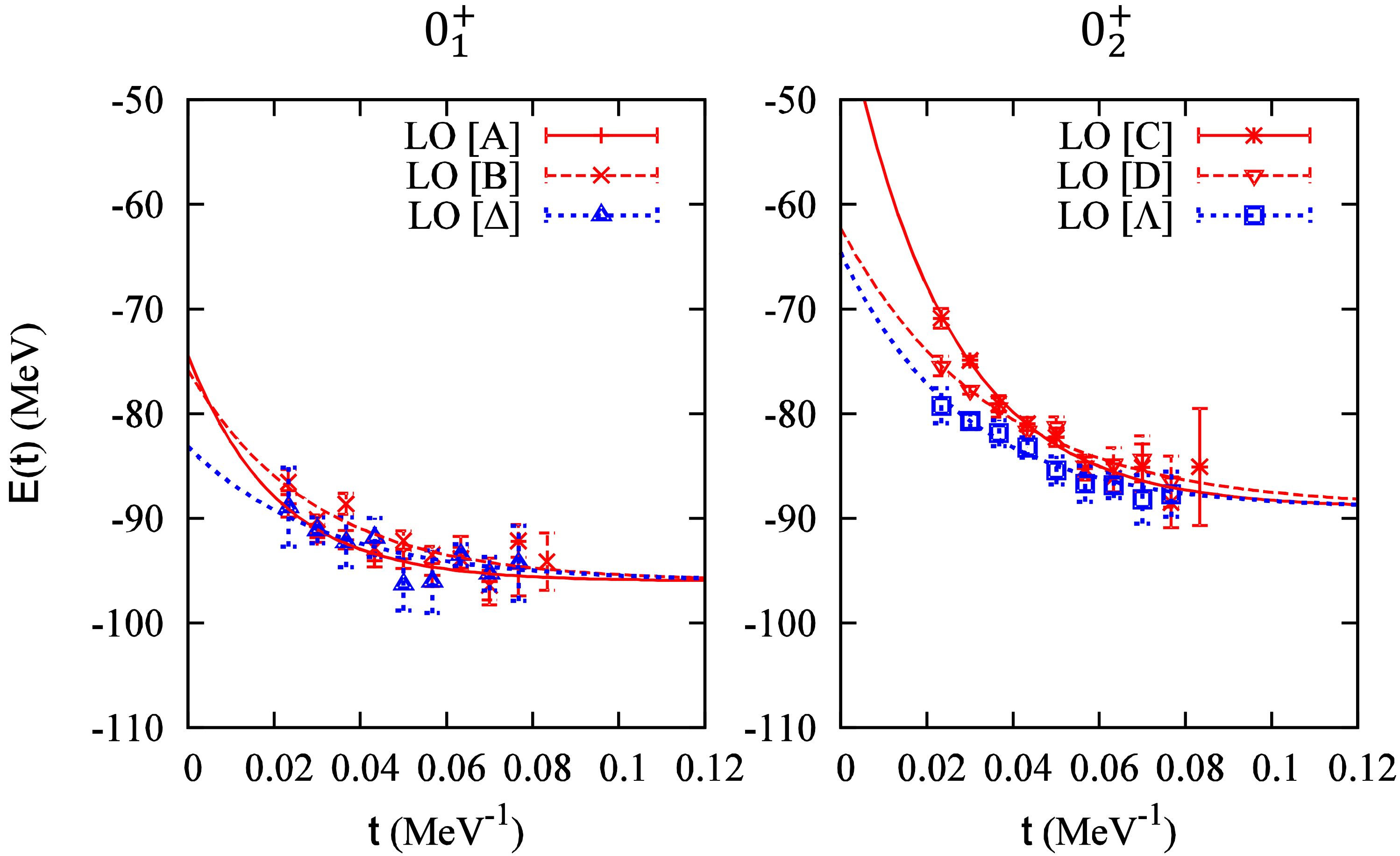
$$\propto < (N^\dagger N)^4 >$$



Needs to develop the four nucleon correlations after significant amount of Euclidean time projection.

$$e^{-Ht}|\Psi >$$

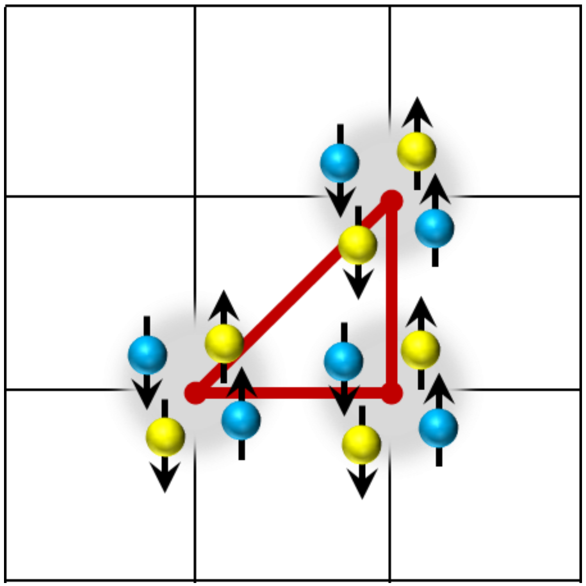
We can obtain good results more directly starting from alpha cluster wavefunctions [Δ and Λ in plots on next slide].



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

Structure of ground state and first 2^+

Strong overlap with compact triangle configuration

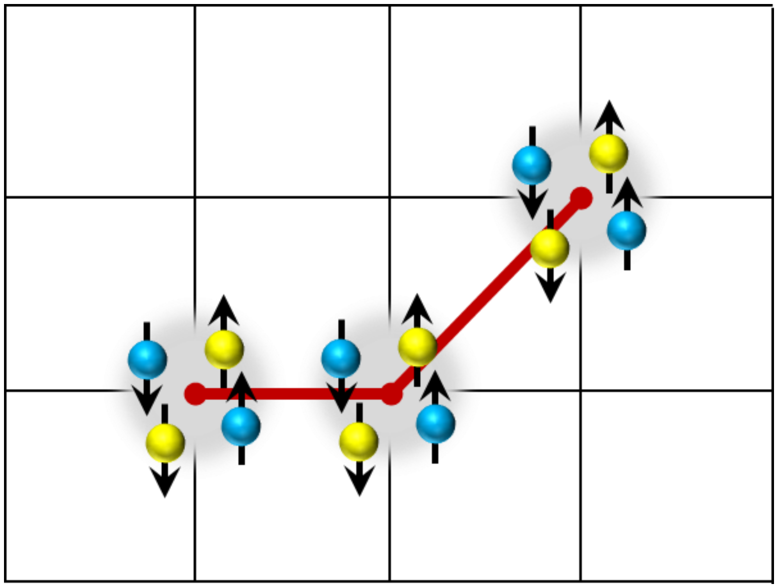


12 rotational orientations

$a = 1.97 \text{ fm}$

Structure of Hoyle state and second 2^+

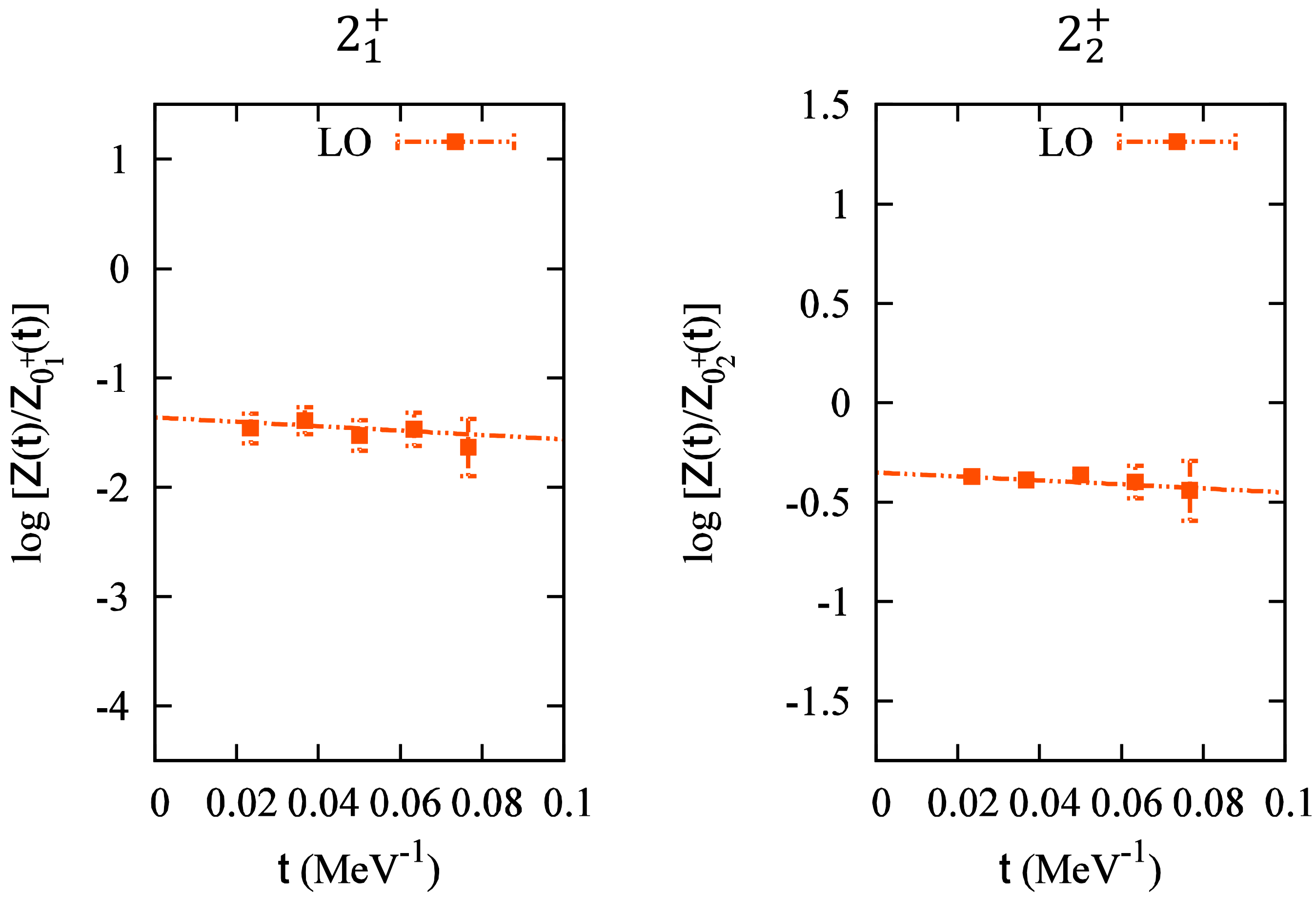
Strong overlap with bent arm configuration



24 rotational orientations

$a = 1.97$ fm

Rotational excitations – 2_1^+, 2_2^+



Excited state spectrum of carbon-12 (even parity)

	2_1^+	0_2^+	2_2^+
LO ($O(Q^0)$)	-94(2) MeV	-89(2) MeV	-88(2) MeV
NLO ($O(Q^2)$)	-74(3) MeV	-72(3) MeV	-70(3) MeV
NNLO ($O(Q^3)$)	-89(3) MeV	-85(3) MeV	-83(3) MeV
Experiment	-87.72 MeV	-84.51 MeV	-82.6(1) MeV (*A*,*B*) -81.1(3) MeV (*C*) -82.13(11) MeV (*D*)

A – Freer et al., PRC 80 (2009) 041303

B – Zimmerman et al., PRC 84 (2011) 027304

C – Hyldegaard et al., PRC 81 (2010) 024303

D – Itoh et al., PRC 84 (2011) 054308

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

RMS charge radius

bound states at leading order

	LO	Experiment
$r_{0_1^+}$ [fm]	2.2(2)	2.47(2)
$r_{2_1^+}$ [fm]	2.2(2)	-
$r_{0_2^+}$ [fm]	2.4(2)	-
$r_{2_2^+}$ [fm]	2.4(2)	-

Schaller, et al.
NPA 379 (1982) 523

Quadrupole moment

	LO	Experiment
$Q_{2_1^+}$ [e fm^2]	6(2)	6(3)
$Q_{2_2^+}$ [e fm^2]	-7(2)	-

Vermeer, et al.
PLB 122 (1983) 23

Electromagnetic transition strengths

	LO	Experiment	
$B(E2, 2_1^+ \to 0_1^+)$ $[e^2\ \mathrm{fm}^4]$	5(2)	7.6(4)	*Ajzenberg-Selove, NPA 506 (1990) 1*
$B(E2, 2_1^+ \to 0_2^+)$ $[e^2\ \mathrm{fm}^4]$	1.5(7)	2.6(4)	*ibid.*
$B(E2, 2_2^+ \to 0_1^+)$ $[e^2\ \mathrm{fm}^4]$	2(1)	0.73(13)	*Weller, INT Workshop 8/2012*
$B(E2, 2_2^+ \to 0_2^+)$ $[e^2\ \mathrm{fm}^4]$	6(2)	-	
$m(E0, 0_2^+ \to 0_1^+)$ $[e\ \mathrm{fm}^2]$	3(1)	5.5(1)	*Chernykh, et al., PRL 105 (2010) 022501*

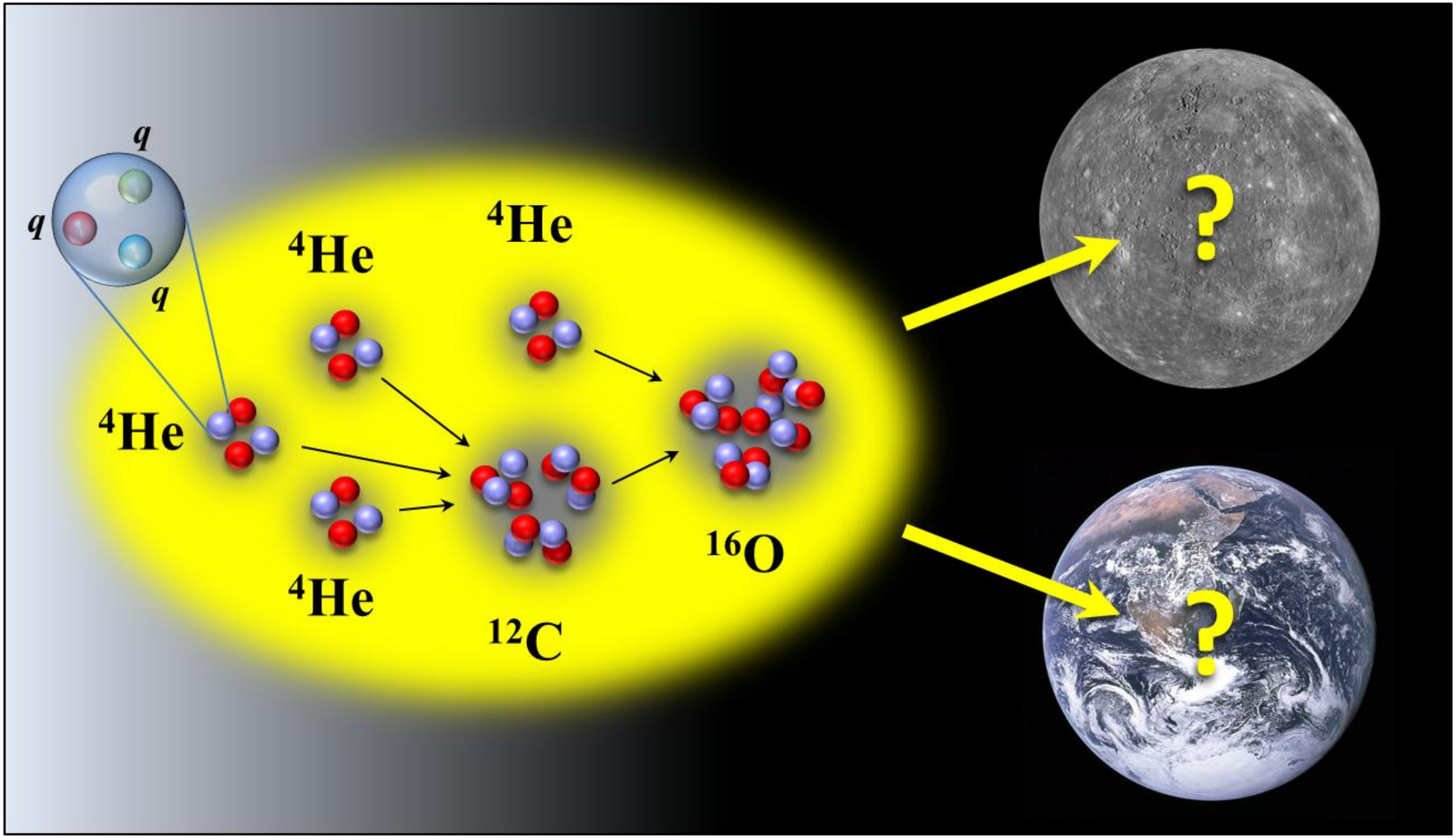
See also other recent calculations using fermionic molecular dynamics

Chernykh, et al., PRL 98 (2007) 032501

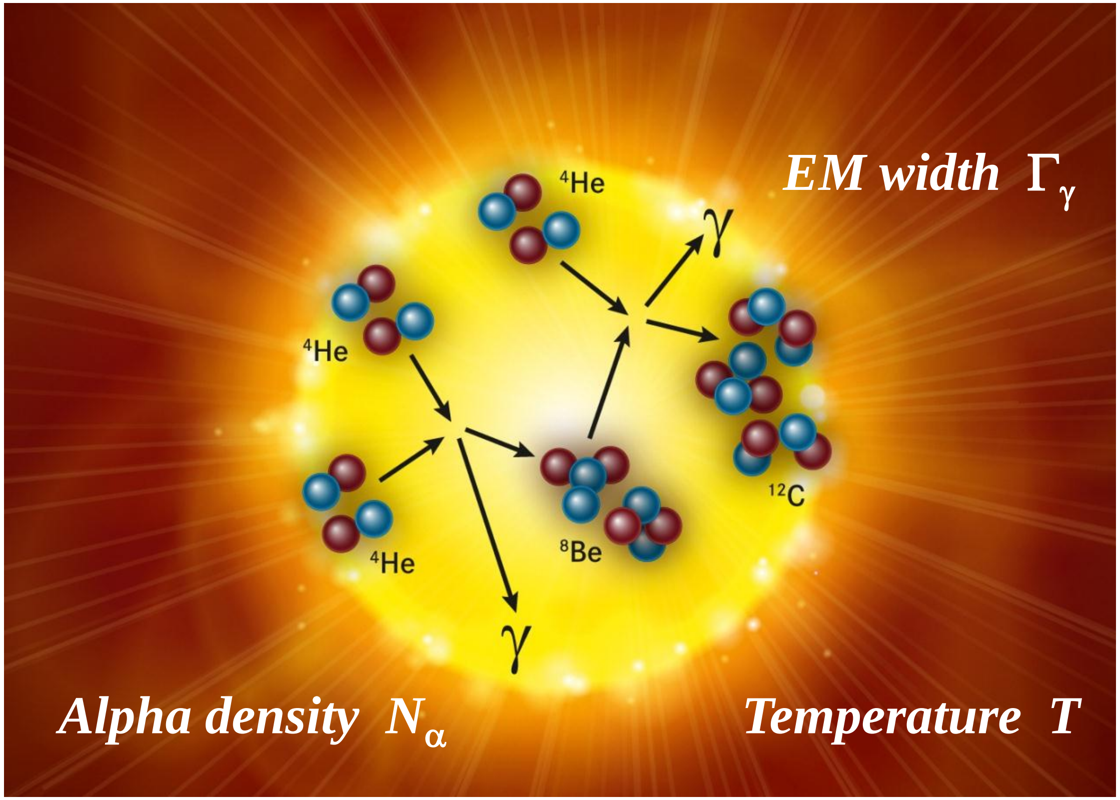
and no-core shell model

Forssen, Roth, Navratil, arXiv:1110.0634v2

Light quark mass dependence of helium burning



Triple alpha reaction rate



$$r_{3\alpha} \propto \Gamma_\gamma \, (N_\alpha / k_B T)^3 \times \exp(-\varepsilon / k_B T)$$

$\varepsilon = E_h - 3E_\alpha$ Hoyle relative to triple-alpha

Is nature fine-tuned?

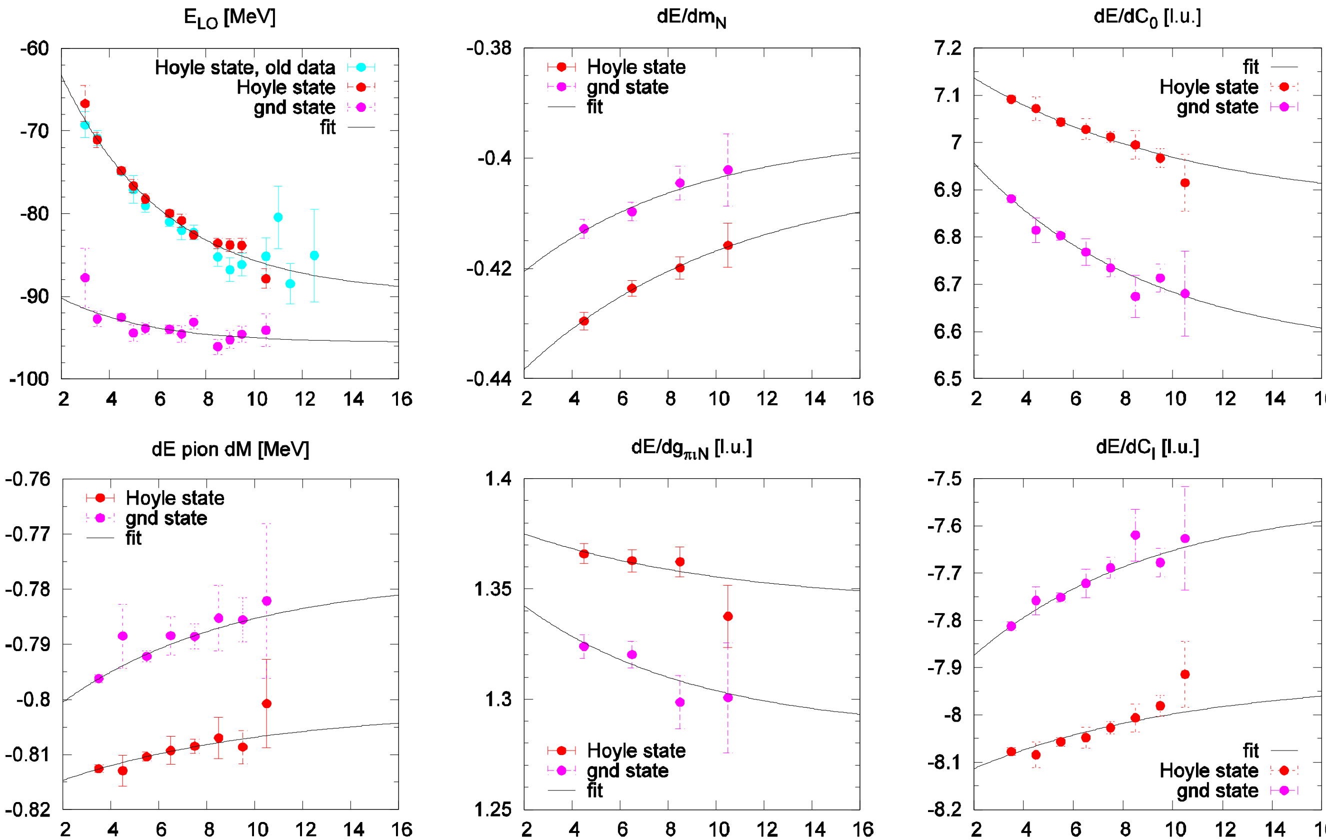
$$\varepsilon = E_h - 3E_\alpha = 379\,\mathrm{keV}$$

$\varepsilon > 479\,\mathrm{keV}$	$\varepsilon < 279\,\mathrm{keV}$
Less resonance enhancement. Rate of carbon production smaller by several orders of magnitude. Low carbon abundance is unfavorable for carbon-based life.	Carbon production occurs at lower stellar temperatures and oxygen production greatly reduced. Low oxygen abundance is unfavorable for carbon-based life.

Schlattl et al., Astrophys. Space Sci., 291, 27–56 (2004)

We investigate the dependence on the fundamental parameters of the standard model such as the light quark masses. Can be parameterized by the pion mass.

Lattice results for pion mass dependence



$\Delta E_h = E_h - E_b - E_\alpha$	Hoyle relative to Be-8-alpha
$\Delta E_b = E_b - 2E_\alpha$	Be-8 relative to alpha-alpha
$\varepsilon = E_h - 3E_\alpha$	Hoyle relative to triple-alpha

$$\left.\frac{\partial \Delta E_h}{\partial M_\pi}\right|_{M_\pi^{\rm ph}} = -0.455(35)\bar{A}_s - 0.744(24)\bar{A}_t + 0.051(19)$$

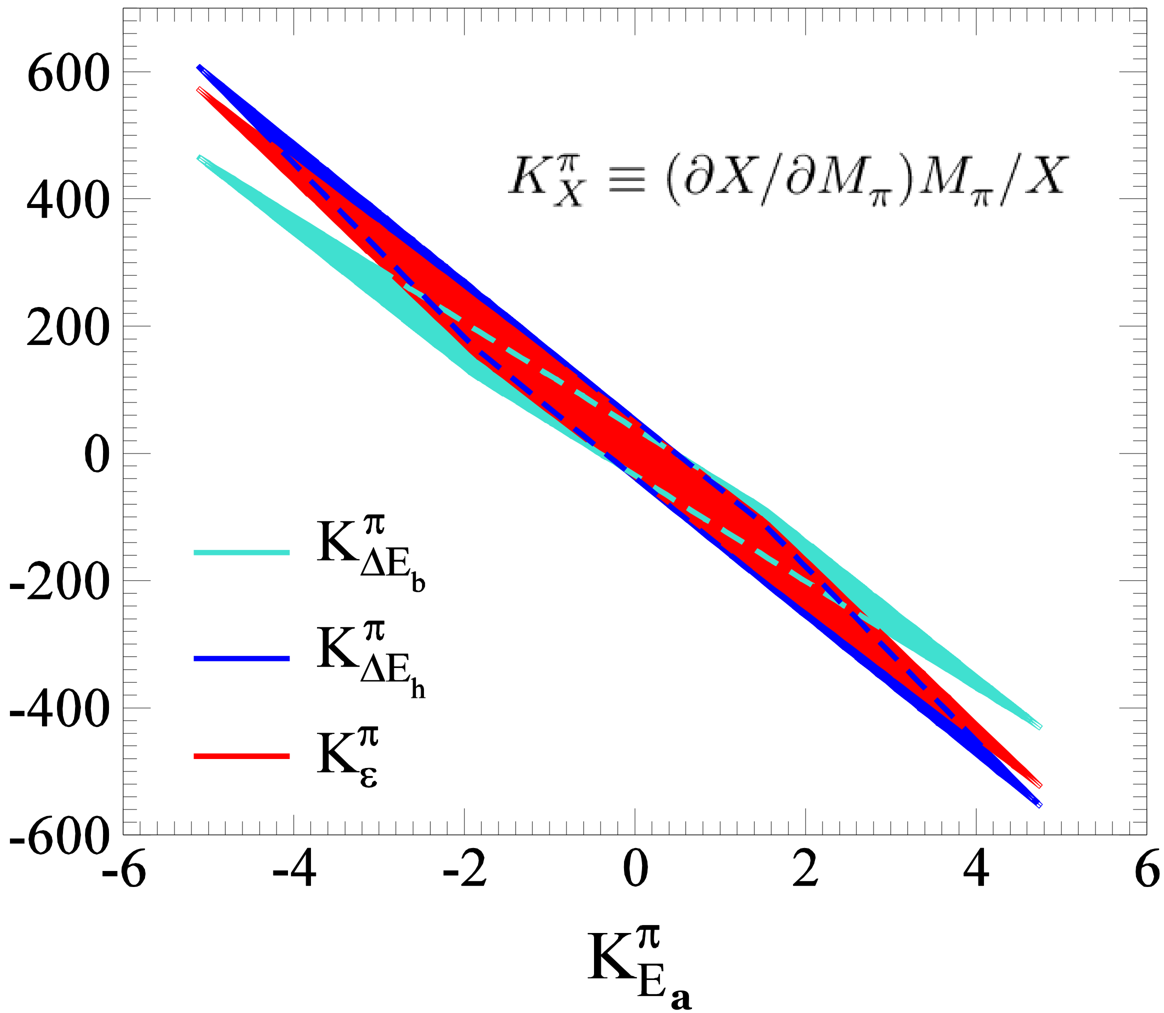
$$\left.\frac{\partial \Delta E_b}{\partial M_\pi}\right|_{M_\pi^{\rm ph}} = -0.117(34)\bar{A}_s - 0.189(24)\bar{A}_t + 0.013(12)$$

$$\left.\frac{\partial \varepsilon}{\partial M_\pi}\right|_{M_\pi^{\rm ph}} = -0.572(19)\bar{A}_s - 0.933(15)\bar{A}_t + 0.064(16)$$

$$\bar{A}_s \equiv \partial a_s^{-1}/\partial M_\pi\big|_{M_\pi^{\rm ph}} \qquad \bar{A}_t \equiv \partial a_t^{-1}/\partial M_\pi\big|_{M_\pi^{\rm ph}}$$

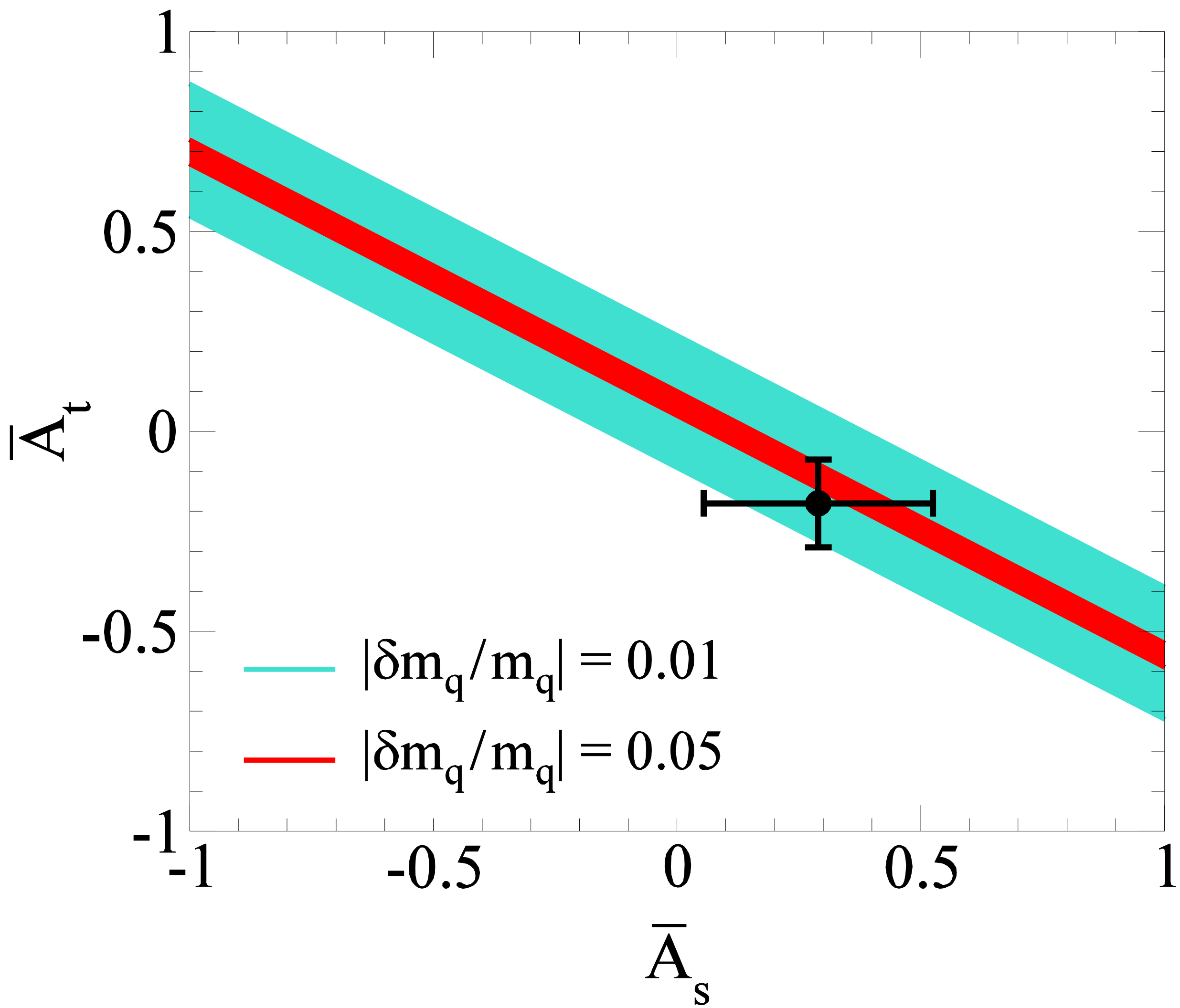
Epelbaum, Krebs, Lähde, D.L, Meißner, arXiv:1212.4181 [nucl-th], PRL in press

Evidence for correlation with alpha binding energy



Epelbaum, Krebs, Lähde, D.L, Meißner, arXiv:1212.4181 [nucl-th], PRL in press

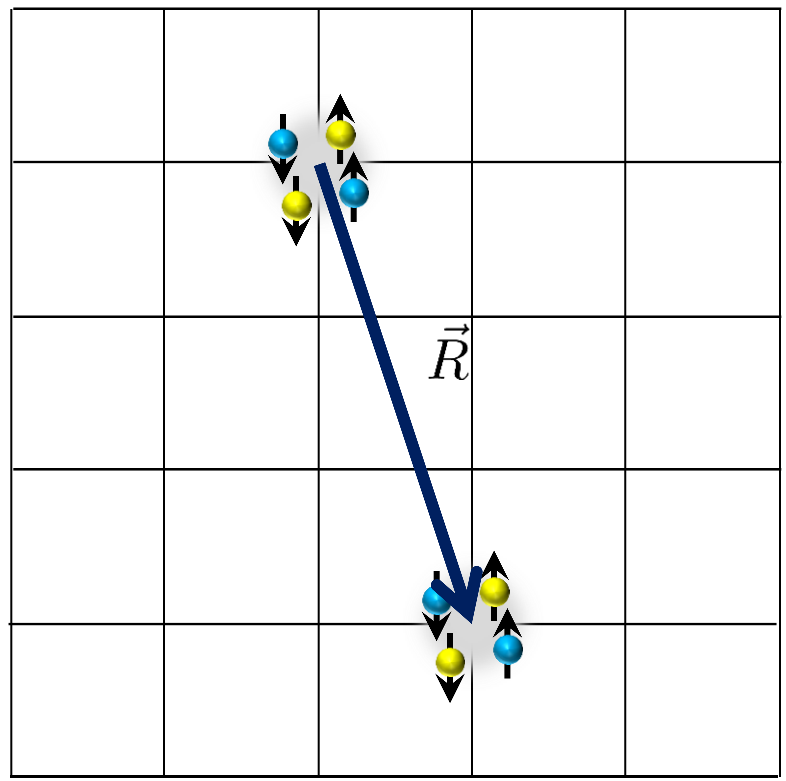
“End of the world” plot



Epelbaum, Krebs, Lähde, D.L, Meißner, arXiv:1212.4181 [nucl-th], PRL in press

Nucleus scattering and reactions on the lattice

Projected adiabatic matrix method

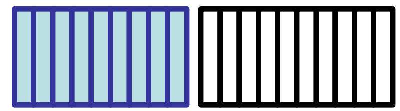


Using cluster wavefunctions for continuum scattering states

initial state $|\vec{R}>$

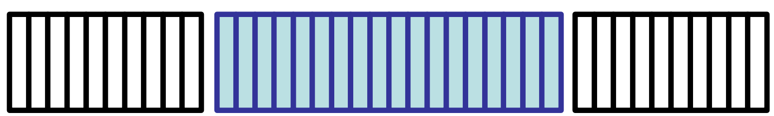
Use projection Monte Carlo to propagate cluster wavefunctions in Euclidean time

$$|\vec{R}>_t = e^{-Ht}|\vec{R}>$$

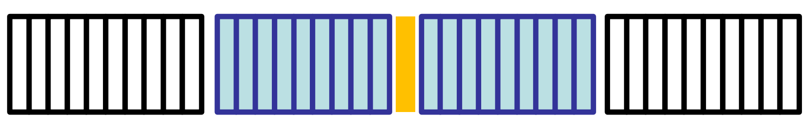
$|\vec{R}>_t =$  $|\vec{R}>$

Construct a norm matrix and matrix of expectation values

$$<N>_t = {}_t\!<\vec{R}'|\vec{R}>_t =$$

$<\vec{R}'|$  $|\vec{R}>$

$$<O>_t = {}_t\!<\vec{R}'|O|\vec{R}>_t =$$

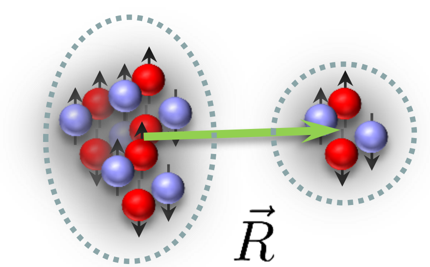
$<\vec{R}'|$  $|\vec{R}>$

Compute the projected adiabatic matrix.

$$< O >_{\text{adiab}} =< N >_t^{-1/2} < O >_t < N >_t^{-1/2}$$

Projected adiabatic Hamiltonian is now an effective two-body Hamiltonian. Similar in spirit to no-core shell model with resonating group method. See Petr's talk in this workshop.

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



Example: Elastic dimer-fermion scattering in periodic cube

H_{adiab} energies (MeV) t = 0.1 MeV^{-1}	H_{adiab} energies (MeV) t = 0.2 MeV^{-1}	**Exact *H* energies (MeV)**
-0.77277	-0.87779	**-0.88204991**
3.99476	3.65905	**3.64407898**
3.99476	3.65905	**3.64407898**
3.99476	3.65905	**3.64407898**
5.30360	5.04521	**5.02101284**
5.30360	5.04521	**5.02101284**
7.34249	7.23189	**7.21346675**
10.68645	10.53473	**10.4947553**
10.68645	10.53473	**10.4947553**
10.68645	10.53473	**10.4947553**

Allow for several coupled channels to calculate capture reactions, exchange processes, and break up processes

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

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

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

Rupak, D.L., arXiv:1302.4158 [nucl-th]

See Gautam's talk in this workshop. Several projects in progress.

Pine, D. L., Rupak work in progress

Elhatisari, D.L., Rupak, work in progress

Rokash, Epelbaum, Krebs, D.L., work in progress

Summary and future directions

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 to be addressed in the near future…

Different lattice spacings, alpha-alpha scattering, structure and rotations of oxygen-16, adiabatic Hamiltonians for scattering and reactions, alpha clustering in nuclei, transition from S-wave to P-wave pairing in superfluid neutron matter, weak matrix elements, etc.

How to do reactions in lattice QCD?

Probably a bit early to set out specific benchmarks

Which methods can give inclusive and exclusive reaction cross-sections?

Error tolerance. Can the method work with the typical stochastic and systematic errors produced in the lattice simulations?

Try implementing the projected adiabatic matrix method with lattice QCD sources. Fairly intensive. Need amplitudes for all initial and final cluster states.