Perturbation calculations in Nuclear Lattice EFT

Yuanzhuo Ma[1,2]

Nuclear Lattice EFT Collaboration

[1]Facility for Rare Isotope Beams, Michigan State University
[2]Institute of quantum matter, South China Normal University

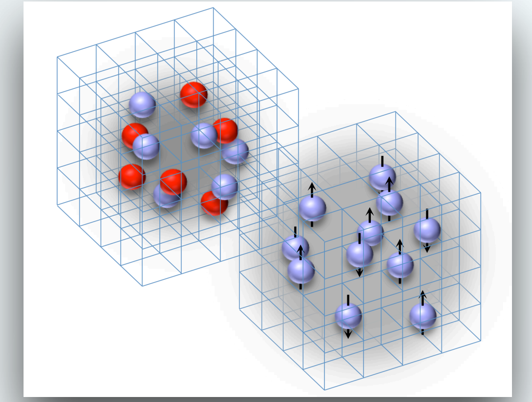
17 May 2023

FRIB

MICHIGAN STATE UNIVERSITY

Outline

- Brief introduction to Nuclear Lattice EFT
  - “Sign problem” & SU(4) symmetry
- Perturbation on Lattice:
  - Wave function matching Hamiltonian (Dean’s talk)
  - 1st order perturbation to wave function
  - Rank-One operator method
- Recent progress I: Neutron matter structure factors
- Recent progress II: Charge Radii (ongoing)
- Summary & Outlook



Nuclear Lattice EFT

= Chiral Effective Field Theory + Quantum Monte Calo on Lattice

QCD and Nuclear physics can be linked by Chiral EFT

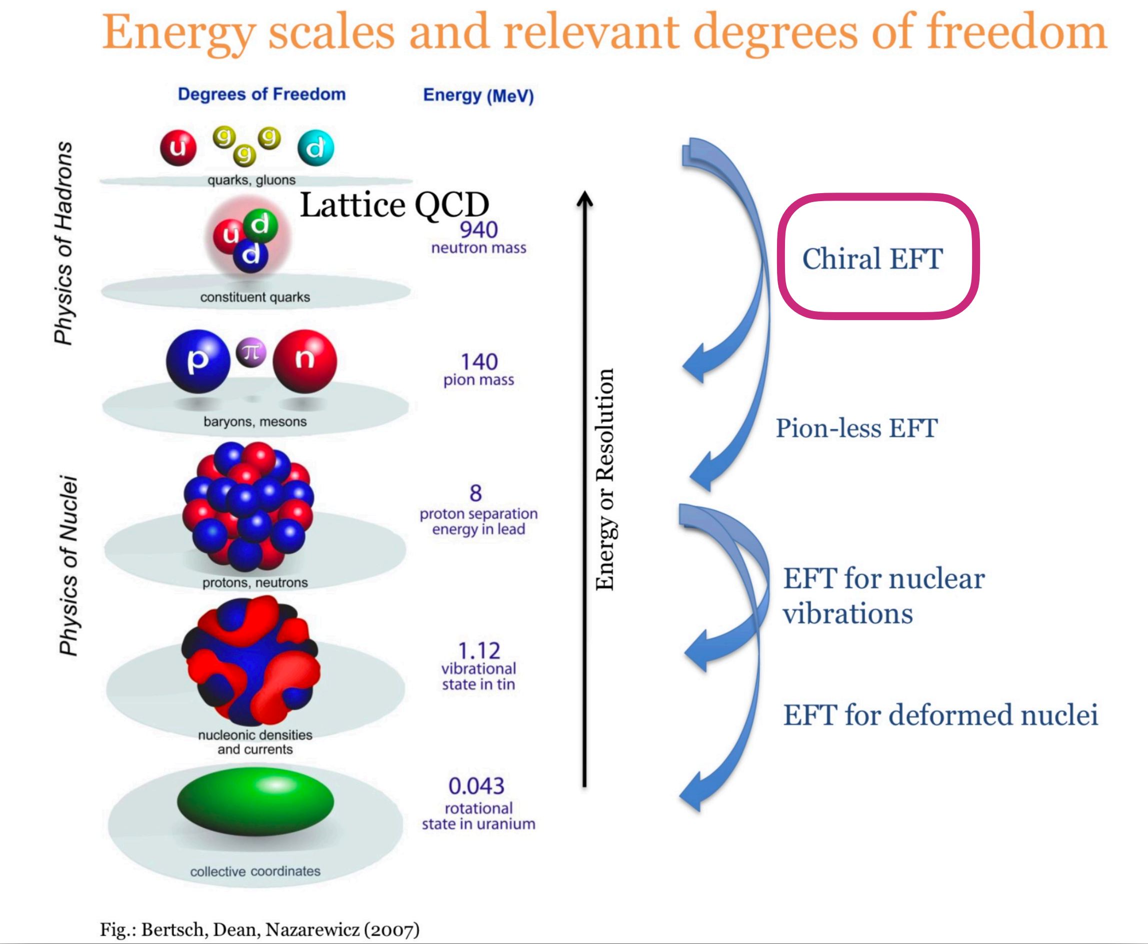
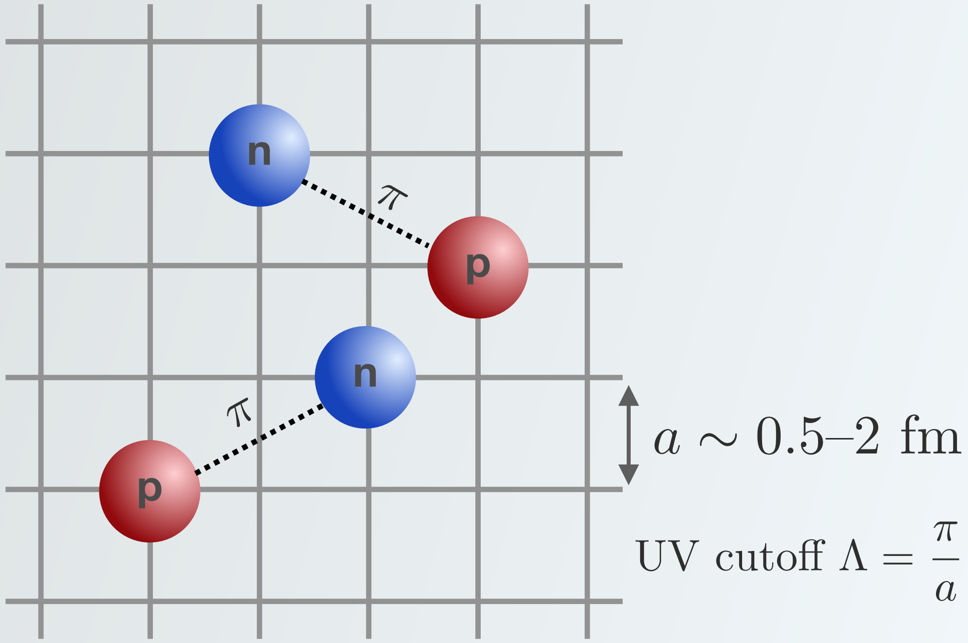


Fig.: Bertsch, Dean, Nazarewicz (2007)



In principle, an **exact** solution for quantum many-body problem

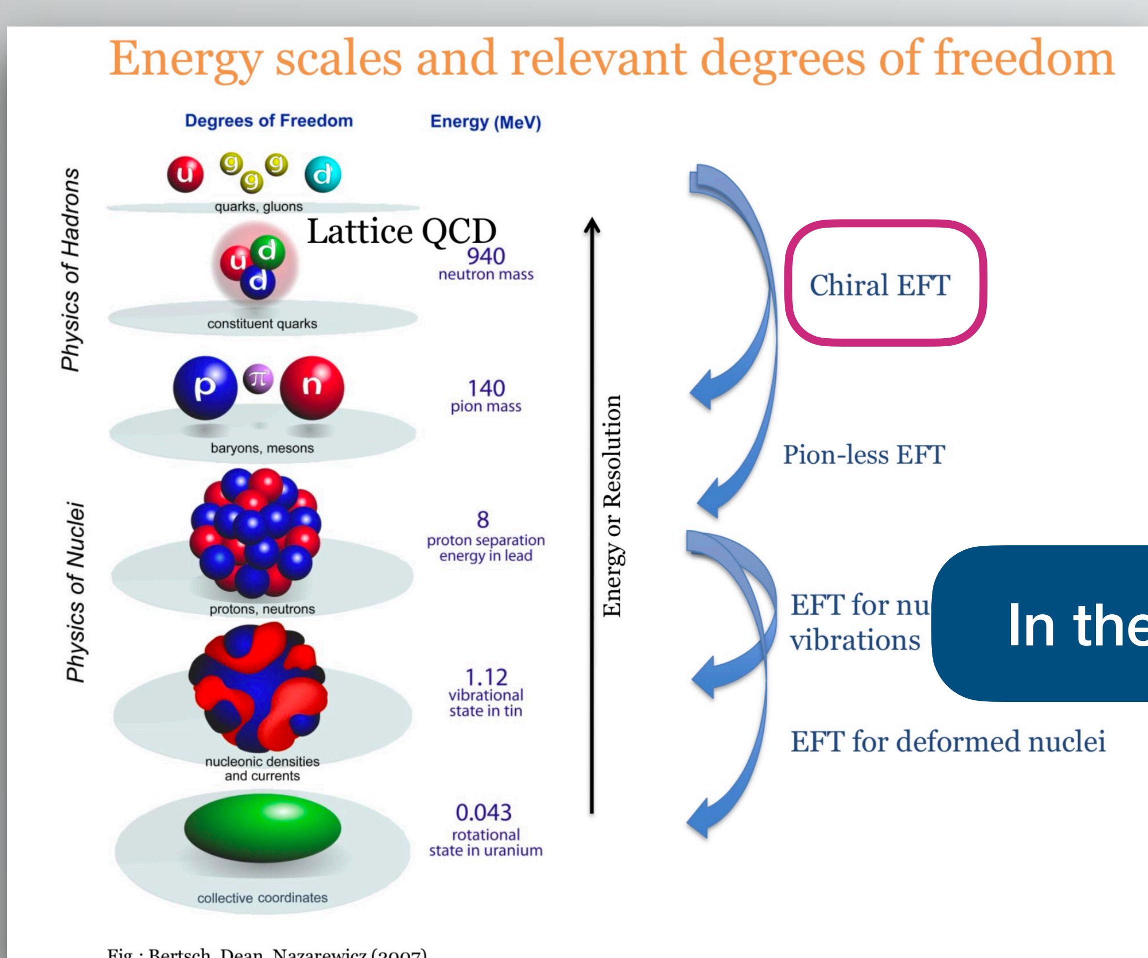
Polynomial scaling ($\sim A^2$)

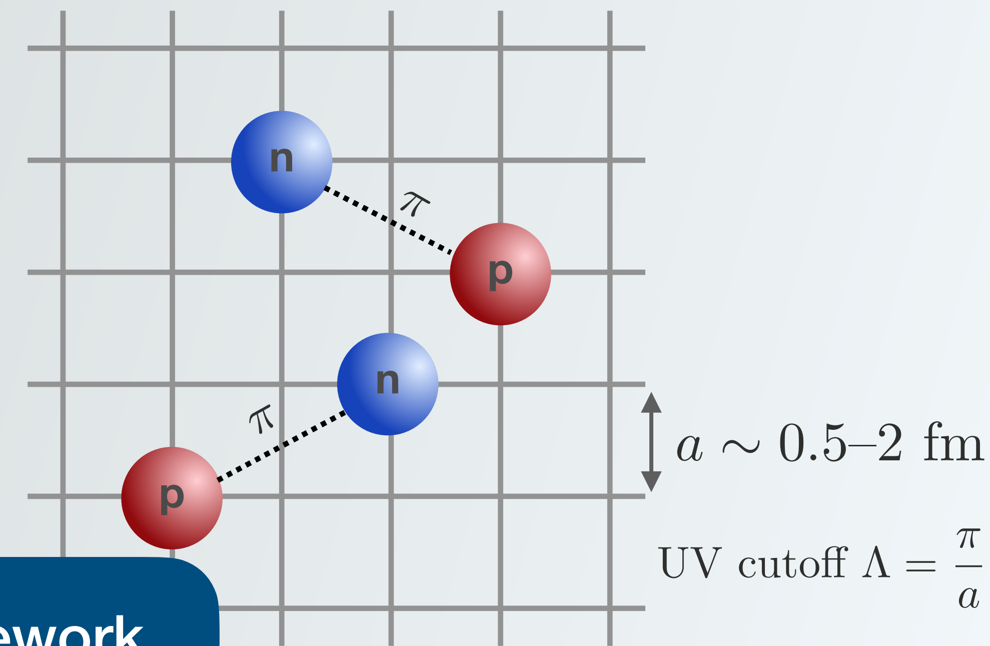
Review: Dean Lee, Prog. Part. Nucl. Phys. 63, 117 (2009),
Lähde, Meißner, "Nuclear Lattice Effective Field Theory", Springer (2019)

Nuclear Lattice EFT

= Chiral Effective Field Theory + Quantum Monte Calo on Lattice

QCD and Nuclear physics can be linked by Chiral EFT





In the same framework

In principle, an **exact** solution for quantum many-body problem

Polynomial scaling (~A^2)

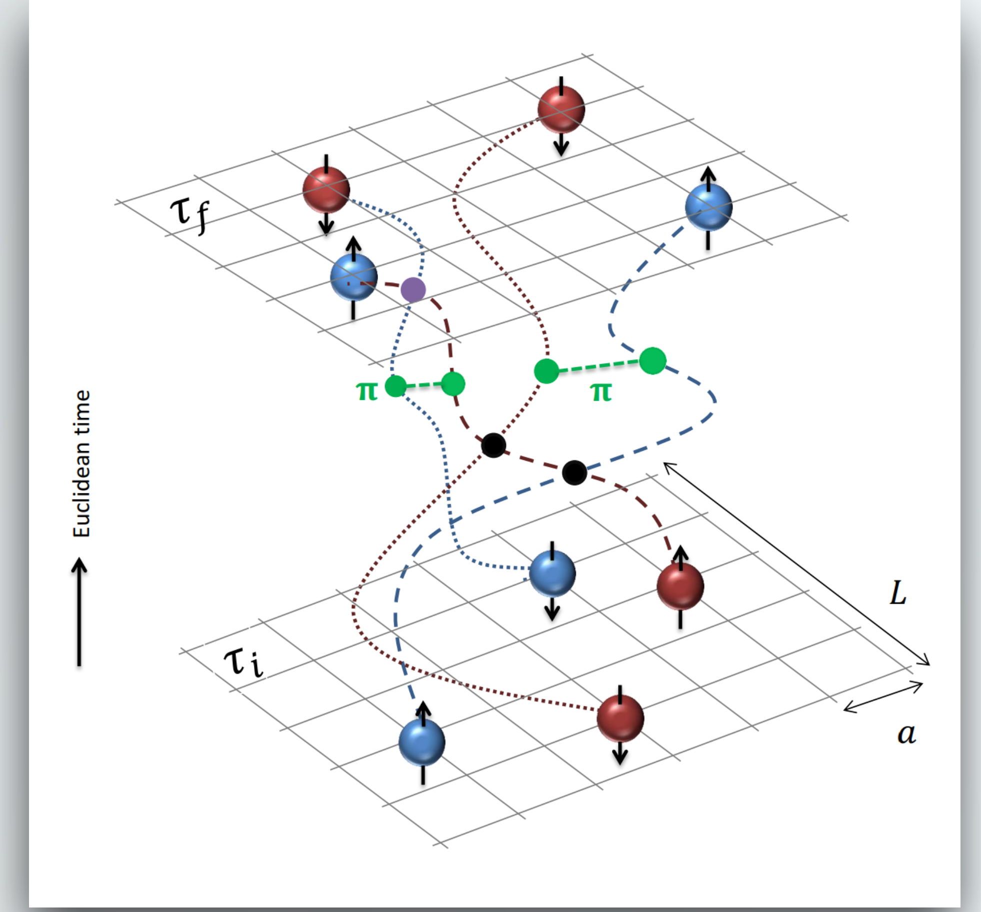
Review: Dean Lee, Prog. Part. Nucl. Phys. 63, 117 (2009),
Lähde, Meißner, "Nuclear Lattice Effective Field Theory", Springer (2019)

Nuclear Lattice EFT

g. s. wave function from Euclidean time projection:

$$|\Psi_{g.s.}\rangle \propto \lim_{\tau\to\infty} \exp(-\tau H)\,|\Psi_A\rangle$$

with $|\Psi_A\rangle$ is an A-body trial wave function

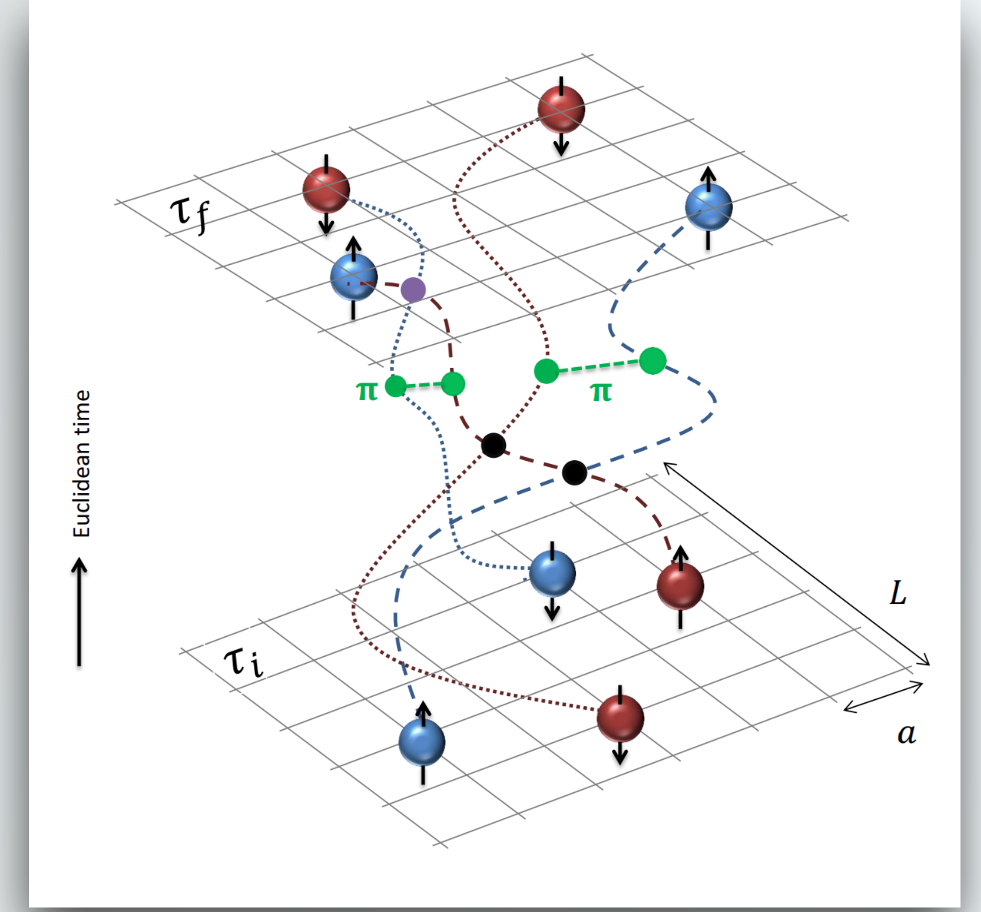


Nuclear Lattice EFT

g. s. wave function from Euclidean time projection:

$$|\Psi_{g.s.}\rangle \propto \lim_{\tau\to\infty} \exp(-\tau H)\,|\Psi_A\rangle$$

with $|\Psi_A\rangle$ is an A-body trial wave function



Expectation value of operators:

$$\langle \mathcal{O} \rangle = \lim_{\tau\to\infty} \frac{\langle \Psi_A \left| e^{-\tau H/2} \mathcal{O} e^{-\tau H/2} \right| \Psi_A \rangle}{\langle \Psi_A \left| e^{-\tau H} \right| \Psi_A \rangle}$$

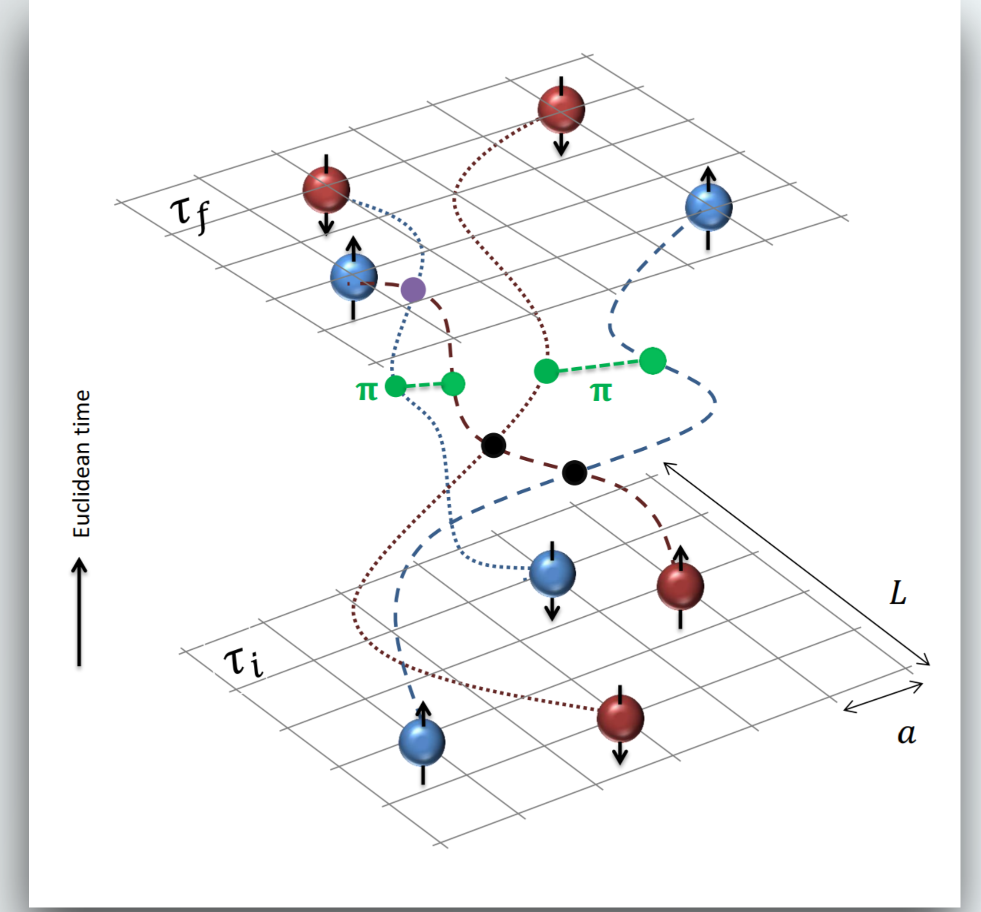
Amplitudes

Nuclear Lattice EFT

g. s. wave function from Euclidean time projection:

$$|\Psi_{g.s.}\rangle \propto \lim_{\tau\to\infty} \exp(-\tau H)\,|\Psi_A\rangle$$

with $|\Psi_A\rangle$ is an A-body trial wave function



Expectation value of operators:

$$\langle \mathcal{O}\rangle = \lim_{\tau\to\infty} \frac{\langle \Psi_A \,| e^{-\tau H/2}\mathcal{O} e^{-\tau H/2} |\, \Psi_A\rangle}{\langle \Psi_A \,| e^{-\tau H} |\, \Psi_A\rangle}$$

Amplitudes

Euclidean time τ is discretized into time slices:

$$\exp(-\tau H) \simeq \left[: \exp\left(-\frac{\tau}{L_t} H\right) : \right]^{L_t}$$

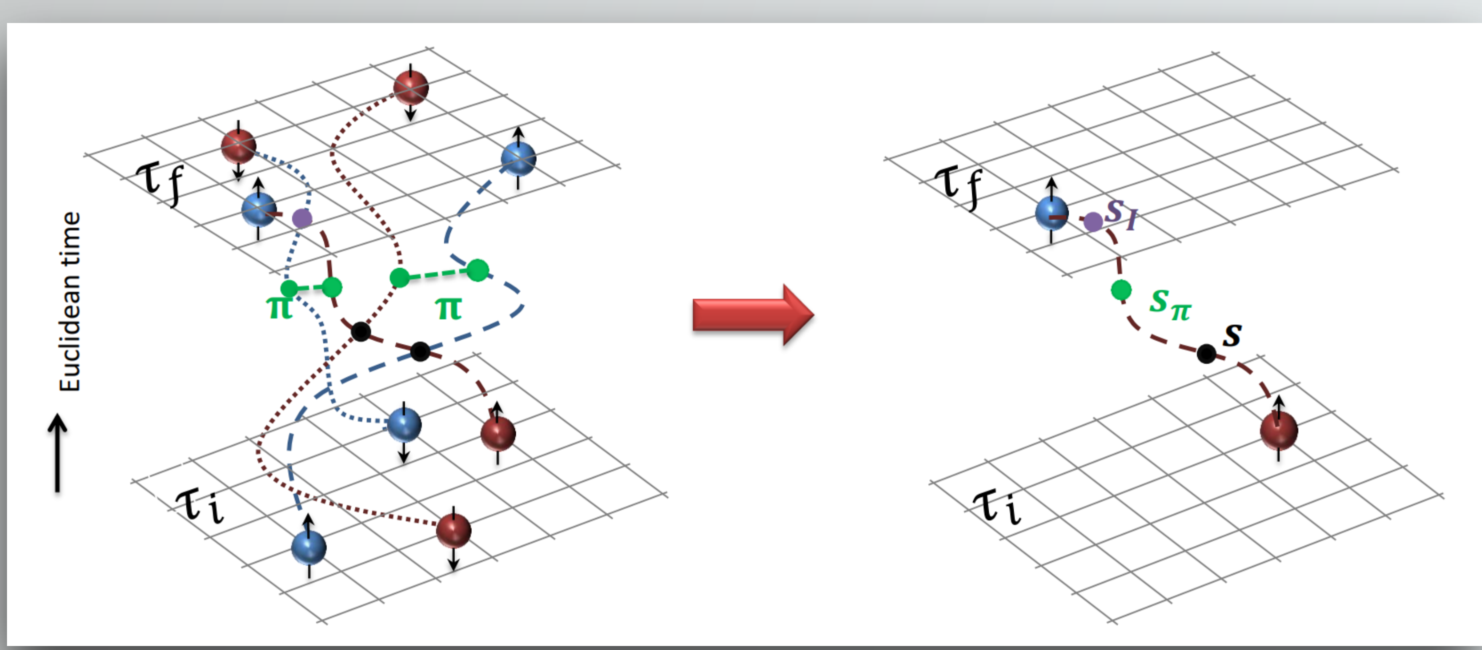
Nuclear Lattice EFT

Auxiliary field Quantum Monte Carlo

Hubbard–Stratonovich transformation

Example: $$H = \sum_{nn'} -\psi_n^\dagger \frac{\nabla^2_{nn'}}{2M}\psi_{n'} + C\sum_n : \left(\psi_n^\dagger \psi_n\right)^2 :$$

$$: \exp\left(-a_t H\right) := \int \prod_n ds_n : \exp\left[\sum_n \left(-\frac{s_n^2}{2} + a_t \psi_n^\dagger \sum_{n'} \frac{\nabla^2_{nn'}}{2M}\psi_{n'} + \sqrt{-a_t C}\, s_n \psi_n^\dagger \psi_n\right)\right] :$$



two-body interaction —> single particle in background fields

Auxiliary field Quantum Monte Carlo

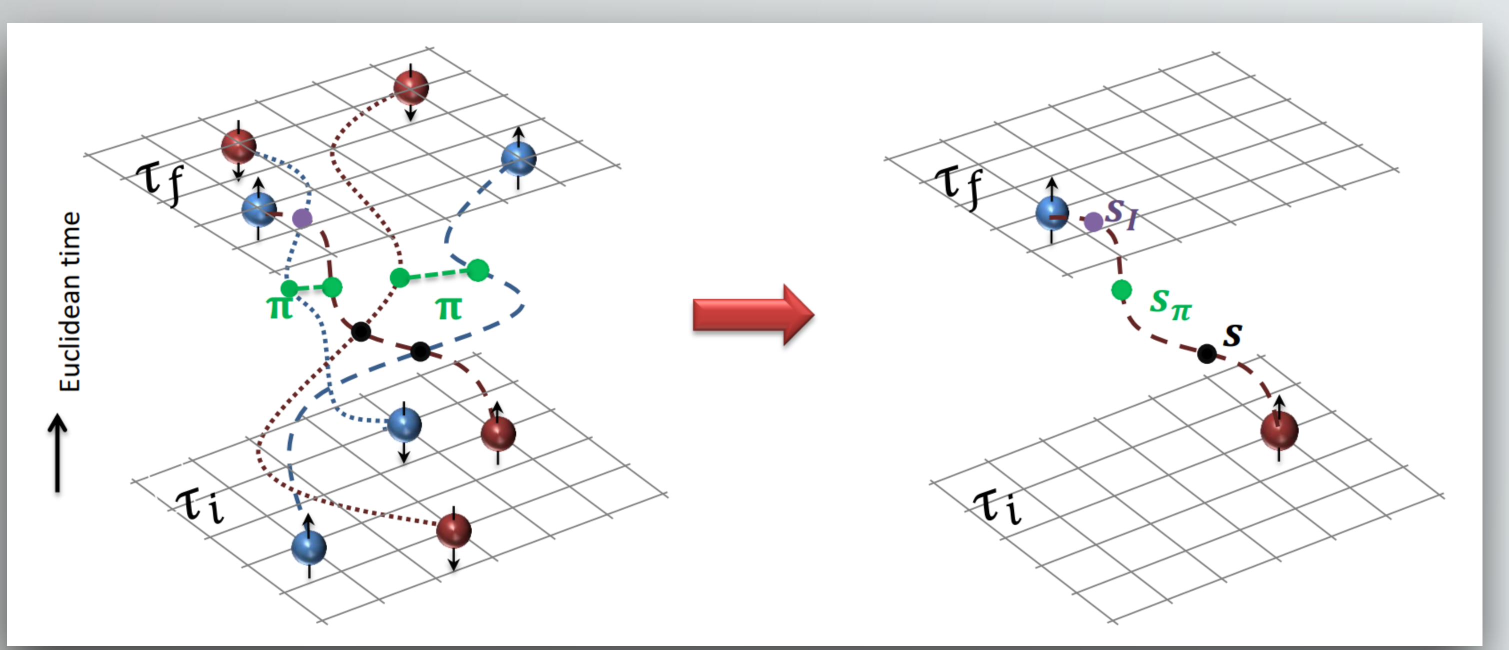
Hubbard–Stratonovich transformation

Example: $$H = \sum_{nn'} -\psi_n^\dagger \frac{\nabla^2_{nn'}}{2M}\psi_{n'} + C\sum_n : \left(\psi_n^\dagger \psi_n\right)^2 :$$

$$: \exp\left(-a_t H\right) := \int \prod_n ds_n : \exp\left[\sum_n \left(-\frac{s_n^2}{2} + a_t \psi_n^\dagger \sum_{n'} \frac{\nabla^2_{nn'}}{2M}\psi_{n'} + \sqrt{-a_t C}\, s_n \psi_n^\dagger \psi_n\right)\right] :$$

or Gaussian integral (Exact)

$$e^{\frac{b^2}{4a}+c} = \sqrt{\frac{a}{\pi}}\int_{-\infty}^{\infty} e^{-ax^2+bx+c}\,dx$$



two-body interaction —> single particle in background fields

Auxiliary field Quantum Monte Carlo

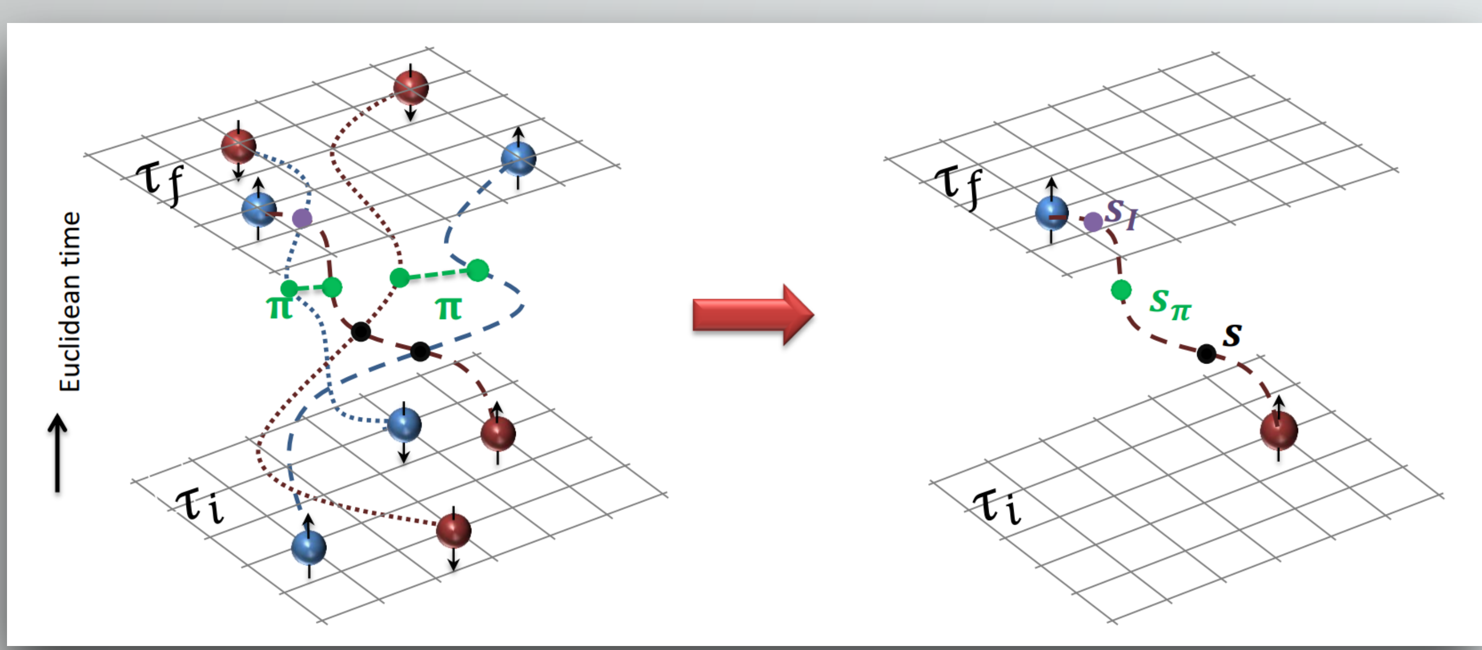
Hubbard–Stratonovich transformation

Example: $H = \sum_{nn'} -\psi_n^\dagger \frac{\nabla^2_{nn'}}{2M}\psi_{n'} + C\sum_n :\left(\psi_n^\dagger\psi_n\right)^2:$

$$:\exp(-a_t H) := \int \prod_n ds_n :\exp\left[\sum_n\left(-\frac{s_n^2}{2} + a_t\psi_n^\dagger\sum_{n'}\frac{\nabla^2_{nn'}}{2M}\psi_{n'} + \sqrt{-a_t C}\,s_n\psi_n^\dagger\psi_n\right)\right]:$$

or Gaussian integral (Exact)

$$e^{\frac{b^2}{4a}+c} = \sqrt{\frac{a}{\pi}}\int_{-\infty}^{\infty} e^{-ax^2+bx+c}\,dx$$



two-body interaction —> single particle in background fields

Antisymmetry from the **determinant of correlation matrix** $\langle \Psi_A | e^{-\tau H} | \Psi_A \rangle$

$$\det\begin{bmatrix} a_{11} & a_{12} & \cdots \\ a_{21} & \ddots & \\ \vdots & & a_{AA} \end{bmatrix}$$

single particle amplitude $a_{ij} = \langle \phi_i | e^{-\tau H} | \phi_j \rangle$

Nuclear Lattice EFT

$$:\exp\left(-a_t H\right) := \int \prod_n ds_n :\exp\left[\sum_n \left(-\frac{s_n^2}{2} + a_t \psi_n^\dagger \sum_{n'} \frac{\nabla_{nn'}^2}{2M} \psi_{n'} + \sqrt{-a_t C}\, s_n \psi_n^\dagger \psi_n\right)\right]:$$

Nuclear Lattice EFT

$$: \exp\left(-a_t H\right) := \int \prod_n ds_n : \exp\left[\sum_n \left(-\frac{s_n^2}{2} + a_t \psi_n^\dagger \sum_{n'} \frac{\nabla^2_{nn'}}{2M} \psi_{n'} + \underline{\sqrt{-a_t C} s_n} \psi_n^\dagger \psi_n\right)\right] :$$

If *C* is (-) attractive: real Good!

Nuclear Lattice EFT

$$:\exp\left(-a_t H\right) := \int \prod_n ds_n :\exp\left[\sum_n \left(-\frac{s_n^2}{2} + a_t \psi_n^\dagger \sum_{n'} \frac{\nabla^2_{nn'}}{2M}\psi_{n'} + \sqrt{-a_t C}\, s_n \psi_n^\dagger \psi_n\right)\right]:$$

If C is (-) attractive: real Good!

If C is (+) repulsive: complex phase —> cancellation in $\langle \mathcal{O} \rangle = \dfrac{\int \mathcal{D}s \, |\det \mathcal{M}_s(\mathcal{O})| \exp(i\theta[s])}{\int \mathcal{D}s \, |\det \mathcal{M}_s| \exp(i\theta[s])}$

Nuclear Lattice EFT

$$:\exp\left(-a_t H\right) := \int \prod_n ds_n :\exp\left[\sum_n \left(-\frac{s_n^2}{2} + a_t \psi_n^\dagger \sum_{n'} \frac{\nabla^2_{nn'}}{2M} \psi_{n'} + \sqrt{-a_t C}\, s_n \psi_n^\dagger \psi_n\right)\right]:$$

Sign problem

If C is (-) attractive: real Good!

If C is (+) repulsive: complex phase —> cancellation in $\langle \mathcal{O} \rangle = \dfrac{\int \mathcal{D}s\, |\det \mathcal{M}_s(\mathcal{O})| \exp(i\theta[s])}{\int \mathcal{D}s\, |\det \mathcal{M}_s| \exp(i\theta[s])}$

Nuclear Lattice EFT

$$:\exp\left(-a_t H\right) := \int \prod_n ds_n :\exp\left[\sum_n \left(-\frac{s_n^2}{2} + a_t \psi_n^\dagger \sum_{n'} \frac{\nabla^2_{nn'}}{2M}\psi_{n'} + \sqrt{-a_t C}\, s_n \psi_n^\dagger \psi_n\right)\right]:$$

Sign problem

If C is (-) attractive: real Good!

If C is (+) repulsive: complex phase —> cancellation in $\langle \mathcal{O} \rangle = \frac{\int \mathcal{D}s\, |\det \mathcal{M}_s(\mathcal{O})| \exp(i\theta[s])}{\int \mathcal{D}s\, |\det \mathcal{M}_s| \exp(i\theta[s])}$

But, if a Hamiltonian has Wigner's SU(4) symmetry:

Nuclear Lattice EFT

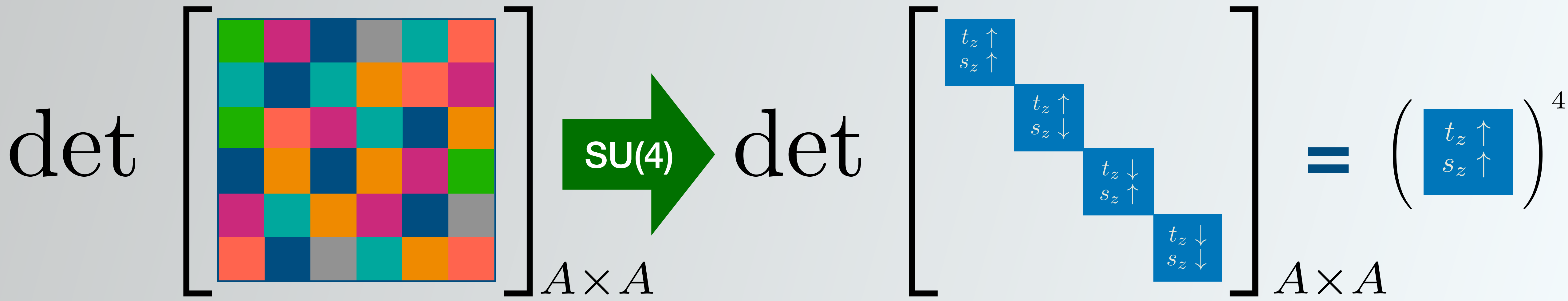
$$: \exp\left(-a_t H\right) := \int \prod_n ds_n : \exp\left[\sum_n \left(-\frac{s_n^2}{2} + a_t \psi_n^\dagger \sum_{n'} \frac{\nabla^2_{nn'}}{2M}\psi_{n'} + \sqrt{-a_t C}\, s_n \psi_n^\dagger \psi_n\right)\right] :$$

Sign problem

If C is (-) attractive: real Good!

If C is (+) repulsive: complex phase —> cancellation in $\langle \mathcal{O} \rangle = \dfrac{\int \mathcal{D}s\, |\det \mathcal{M}_s(\mathcal{O})| \exp(i\theta[s])}{\int \mathcal{D}s\, |\det \mathcal{M}_s| \exp(i\theta[s])}$

But, if a Hamiltonian has Wigner's SU(4) symmetry:



Dean Lee, PRL 98, 182501 (2007)

Nuclear Lattice EFT

$$: \exp\left(-a_t H\right) := \int \prod_n ds_n : \exp\left[\sum_n \left(-\frac{s_n^2}{2} + a_t \psi_n^\dagger \sum_{n'} \frac{\nabla^2_{nn'}}{2M}\psi_{n'} + \sqrt{-a_t C}\, s_n \psi_n^\dagger \psi_n \right)\right] :$$

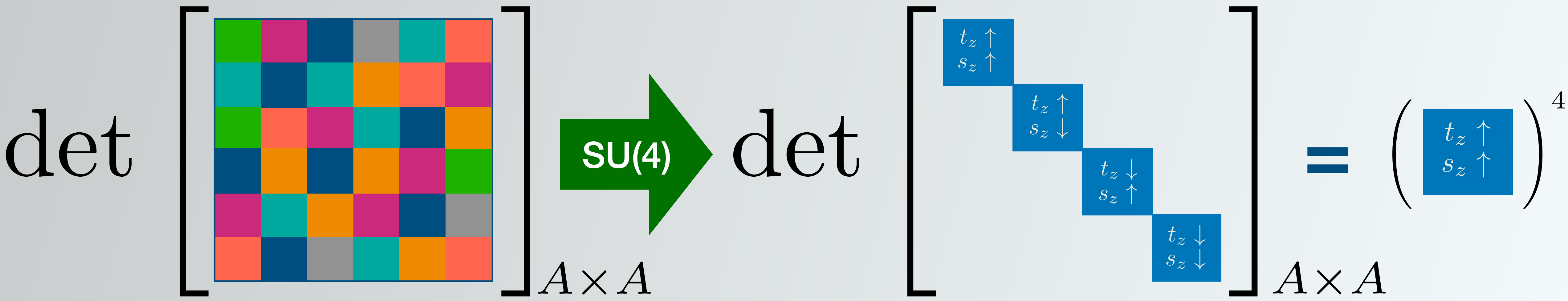
Sign problem

If C is (-) attractive: real Good!

If C is (+) repulsive: complex phase —> cancellation in $\langle \mathcal{O} \rangle = \dfrac{\int \mathcal{D}s \, |\det \mathcal{M}_s(\mathcal{O})| \exp(i\theta[s])}{\int \mathcal{D}s \, |\det \mathcal{M}_s| \exp(i\theta[s])}$

But, if a Hamiltonian has Wigner's SU(4) symmetry:

No sign problem !



Dean Lee, PRL 98, 182501 (2007)

Nuclear Lattice EFT

$$:\exp\left(-a_t H\right) := \int \prod_n ds_n :\exp\left[\sum_n \left(-\frac{s_n^2}{2} + a_t \psi_n^\dagger \sum_{n'} \frac{\nabla^2_{nn'}}{2M}\psi_{n'} + \sqrt{-a_t C}\, s_n \psi_n^\dagger \psi_n\right)\right]:$$

Sign problem

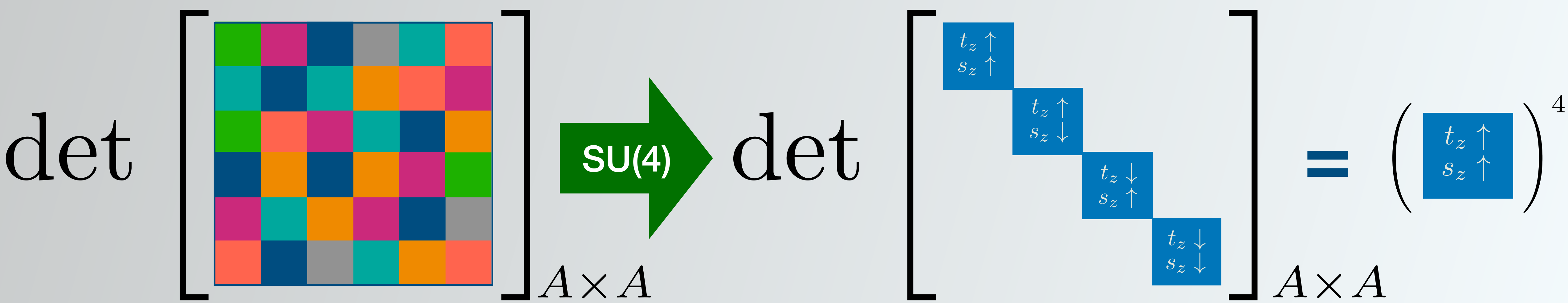
If C is (-) attractive: real Good!

If C is (+) repulsive: complex phase —> cancellation in $\langle \mathcal{O} \rangle = \frac{\int \mathcal{D}s\, |\det \mathcal{M}_s(\mathcal{O})| \exp(i\theta[s])}{\int \mathcal{D}s\, |\det \mathcal{M}_s| \exp(i\theta[s])}$

Real word is complex! realistic nuclear potential can cause severe sign problem

But, if a Hamiltonian has Wigner's SU(4) symmetry:

No sign problem !



Dean Lee, PRL 98, 182501 (2007)

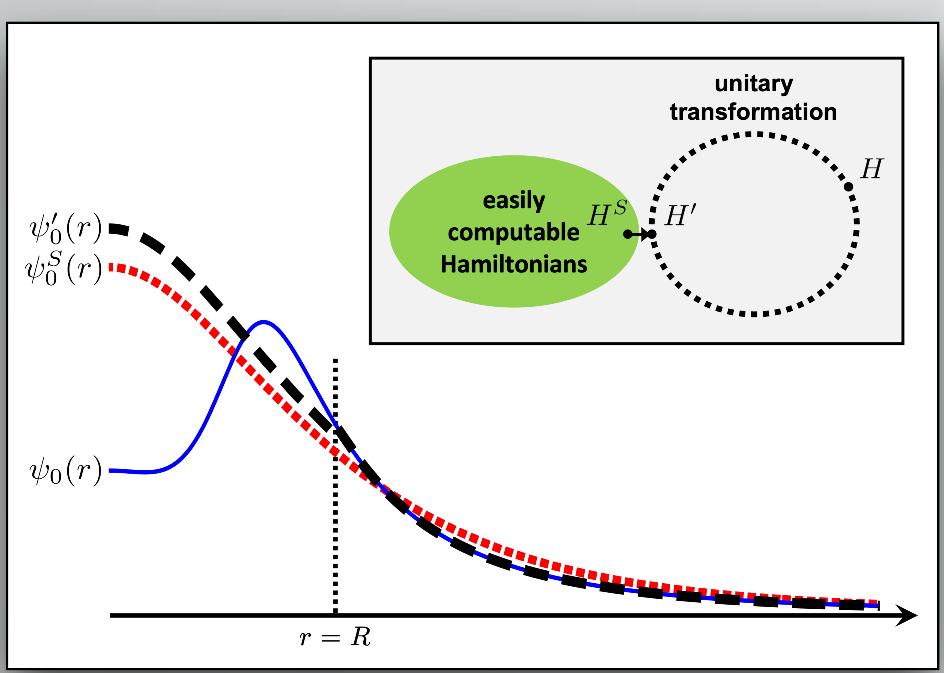
Perturbation Hamiltonian

Can we build a χEFT Hamiltonian which is close to a SU(4) Hamiltonian?

Perturbation Hamiltonian

Can we build a χEFT Hamiltonian which is close to a SU(4) Hamiltonian?

Yes! Wave function Matching (Dean's Talk)

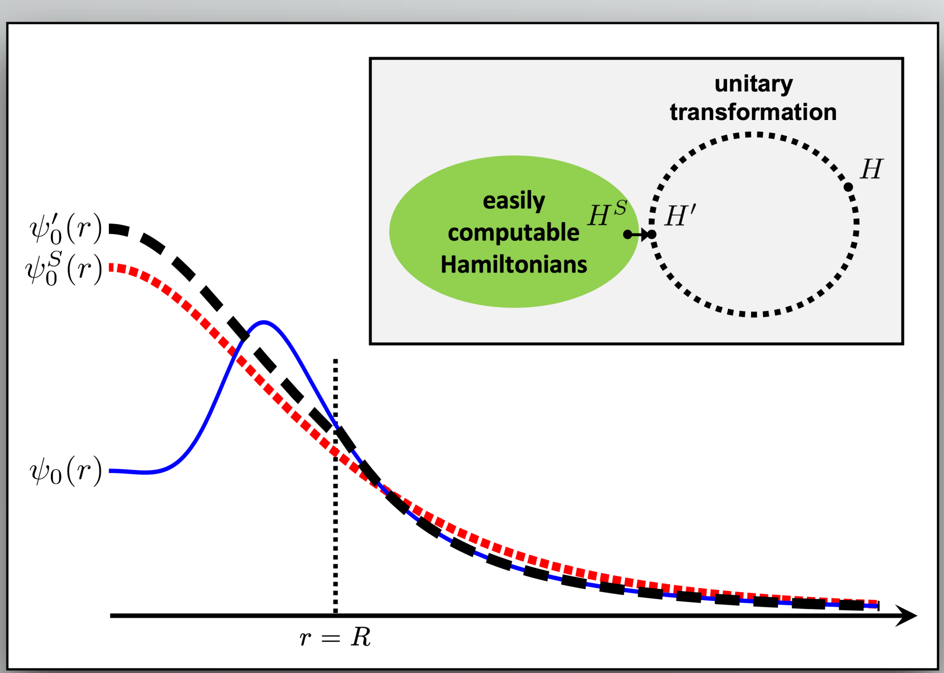


arXiv:2210.17488

Perturbation Hamiltonian

Can we build a χEFT Hamiltonian which is close to a SU(4) Hamiltonian?

Yes! Wave function Matching (Dean's Talk)



Unitary transformation

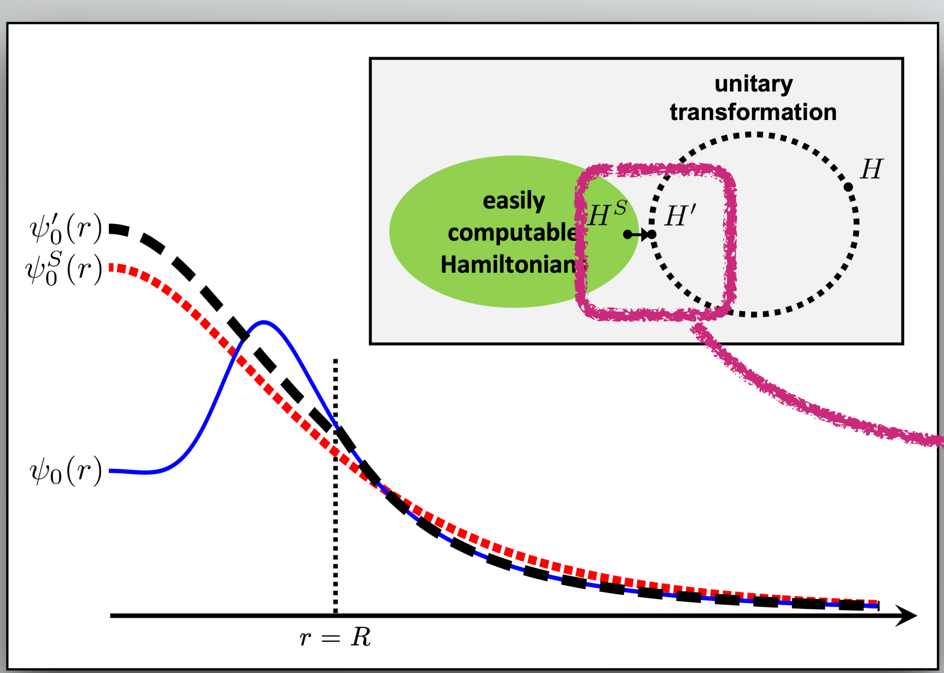
$$H'_{\mathrm{N3LO}} \longleftrightarrow H_{\mathrm{N3LO}}$$

arXiv:2210.17488

Perturbation Hamiltonian

Can we build a χEFT Hamiltonian which is close to a SU(4) Hamiltonian?

Yes! Wave function Matching (Dean's Talk)



Unitary transformation

$$H'_{\rm N3LO} \longleftrightarrow H_{\rm N3LO}$$

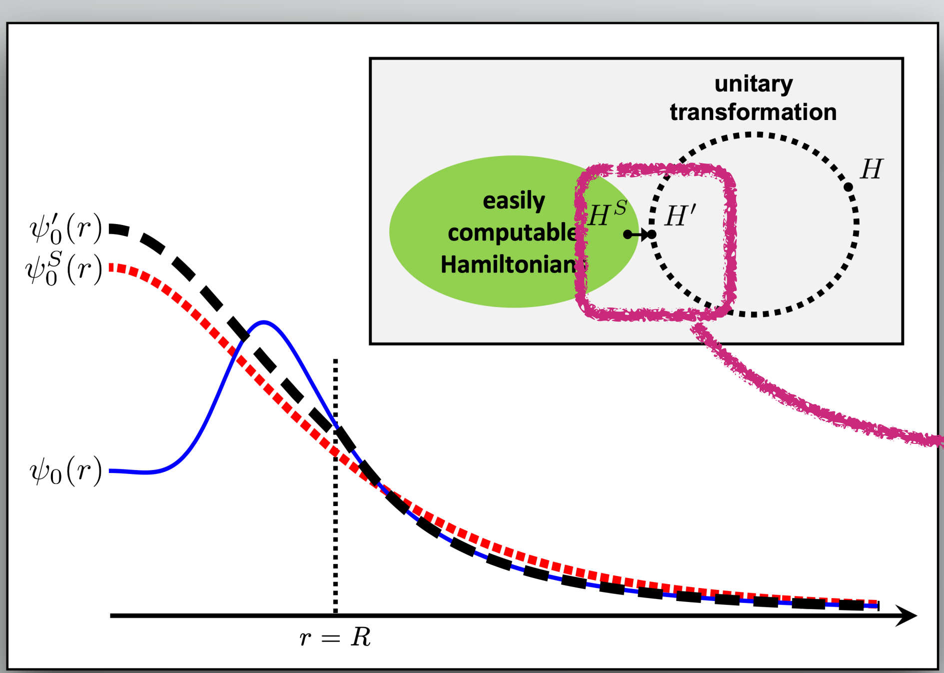
$H_1 = H'_{\rm N3LO} - H_{\rm SU(4)}$ **is small**

arXiv:2210.17488

Perturbation Hamiltonian

Can we build a χEFT Hamiltonian which is close to a SU(4) Hamiltonian?

Yes! Wave function Matching (Dean's Talk)



Unitary transformation

$$H'_{\mathrm{N3LO}} \longleftrightarrow H_{\mathrm{N3LO}}$$

$$H_1 = H'_{\mathrm{N3LO}} - H_{\mathrm{SU(4)}}$$ **is small**

arXiv:2210.17488

Perturbation Hamiltonian: $$H_{\mathrm{N3LO}} \to H_{\mathrm{SU(4)}} + H_1$$

$$E^{\mathrm{1st}}_{\mathrm{N3LO}} = \frac{\langle \Psi_{\mathrm{SU(4)}} | H_{\mathrm{SU(4)}} + H_1 | \Psi_{\mathrm{SU(4)}} \rangle}{\langle \Psi_{\mathrm{SU(4)}} | \Psi_{\mathrm{SU(4)}} \rangle}$$

Perturbation for wave function

How about perturbation corrections to wave functions? $|\Psi\rangle = |\Psi\rangle^{(0)} + |\Psi\rangle^{(1)} + \cdots$

Perturbation for wave function

How about perturbation corrections to wave functions? $|\Psi\rangle = |\Psi\rangle^{(0)} + |\Psi\rangle^{(1)} + \cdots$

On lattice: $\det \mathcal{M} = \langle \Psi_0| \cdots : e^{-\Delta\tau(H_0+H_1)} : \cdots : e^{-\Delta\tau(H_0+H_1)} : \cdots |\Psi_0\rangle$

Perturbation for wave function

How about perturbation corrections to wave functions? $|\Psi\rangle = |\Psi\rangle^{(0)} + |\Psi\rangle^{(1)} + \cdots$

On lattice: $\det \mathcal{M} = \langle \Psi_0 | \cdots : e^{-\Delta\tau(H_0+H_1)} : \cdots : e^{-\Delta\tau(H_0+H_1)} : \cdots | \Psi_0 \rangle$

At 1st order level:

$$\langle \Psi_0 | : e^{-\Delta\tau H_0} : \cdots : e^{-\Delta\tau H_0} :: -\Delta\tau H_1 : | \Psi_0 \rangle$$

$$\langle \Psi_0 | : e^{-\Delta\tau H_0} : \cdots : -\Delta\tau H_1 :: e^{-\Delta\tau H_0} : | \Psi_0 \rangle$$

$$\vdots$$

$$\langle \Psi_0 | : -\Delta\tau H_1 :: e^{-\Delta\tau H_0} : \cdots : e^{-\Delta\tau H_0} : | \Psi_0 \rangle$$

Bing-nan, Ning, Serdar, Yuan-zhuo, Dean, Ulf. PRL. 128, 242501 (2022)

Perturbation for operators

Operators with perturbation corrections from wave functions

$$\langle \mathcal{O} \rangle = \frac{\langle \Psi | \mathcal{O} | \Psi \rangle}{\langle \Psi | \Psi \rangle} = \frac{\langle \Psi^{(0)} + \Psi^{(1)} + \cdots | \mathcal{O} | \Psi^{(0)} + \Psi^{(1)} + \cdots \rangle}{\langle \Psi^{(0)} + \Psi^{(1)} + \cdots | \Psi^{(0)} + \Psi^{(1)} + \cdots \rangle}$$

Perturbation for operators

Operators with perturbation corrections from wave functions

$$\langle \mathcal{O} \rangle = \frac{\langle \Psi | \mathcal{O} | \Psi \rangle}{\langle \Psi | \Psi \rangle} = \frac{\langle \Psi^{(0)} + \Psi^{(1)} + \cdots | \mathcal{O} | \Psi^{(0)} + \Psi^{(1)} + \cdots \rangle}{\langle \Psi^{(0)} + \Psi^{(1)} + \cdots | \Psi^{(0)} + \Psi^{(1)} + \cdots \rangle}$$

On Lattice:

$$\langle \mathcal{O} \rangle = \frac{\det \mathcal{M}_o^{(0)} + \det \mathcal{M}_o^{(1)}}{\det \mathcal{M}^{(0)} + \det \mathcal{M}^{(1)}} = \underbrace{\frac{\det \mathcal{M}_o^{(0)}}{\det \mathcal{M}^{(0)}}}_{\text{zeroth}} + \underbrace{\left(\frac{\det \mathcal{M}_o^{(1)}}{\det \mathcal{M}^{(0)}} - \frac{\det \mathcal{M}_o^{(0)} \det \mathcal{M}^{(1)}}{\det \mathcal{M}^{(0)} \det \mathcal{M}^{(0)}} \right)}_{\text{1st order correction}} + \cdots$$

Perturbation for operators

Operators with perturbation corrections from wave functions

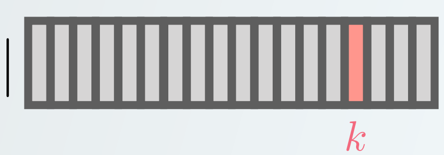
$$\langle \mathcal{O} \rangle = \frac{\langle \Psi | \mathcal{O} | \Psi \rangle}{\langle \Psi | \Psi \rangle} = \frac{\langle \Psi^{(0)} + \Psi^{(1)} + \cdots | \mathcal{O} | \Psi^{(0)} + \Psi^{(1)} + \cdots \rangle}{\langle \Psi^{(0)} + \Psi^{(1)} + \cdots | \Psi^{(0)} + \Psi^{(1)} + \cdots \rangle}$$

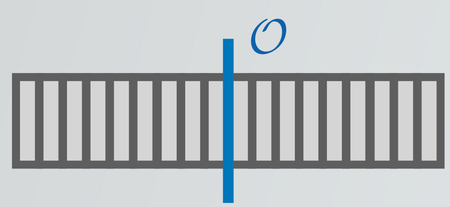
On Lattice:

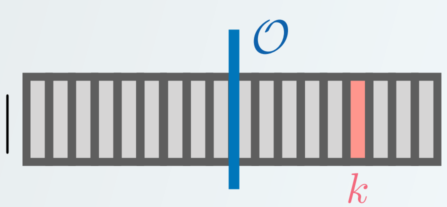
$$\langle \mathcal{O} \rangle = \frac{\det \mathcal{M}_o^{(0)} + \det \mathcal{M}_o^{(1)}}{\det \mathcal{M}^{(0)} + \det \mathcal{M}^{(1)}} = \underbrace{\frac{\det \mathcal{M}_o^{(0)}}{\det \mathcal{M}^{(0)}}}_{\text{zeroth}} + \underbrace{\left(\frac{\det \mathcal{M}_o^{(1)}}{\det \mathcal{M}^{(0)}} - \frac{\det \mathcal{M}_o^{(0)} \det \mathcal{M}^{(1)}}{\det \mathcal{M}^{(0)} \det \mathcal{M}^{(0)}} \right)}_{\text{1st order correction}} + \cdots$$

Four types of amplitudes:

A: $\det \mathcal{M}^{(0)} = \langle \Psi_0 |$  $| \Psi_0 \rangle$

C: $\det \mathcal{M}^{(1)} = 2 \sum_{k=0}^{L_t/2} \langle \Psi_0 |$  $| \Psi_0 \rangle$

B: $\det \mathcal{M}_o^{(0)} = \langle \Psi_0 |$  $| \Psi_0 \rangle$

D: $\det \mathcal{M}_o^{(1)} = 2 \sum_{k=0}^{L_t/2} \langle \Psi_0 |$  $| \Psi_0 \rangle$

Perturbation for operators

Operators with perturbation corrections from wave functions

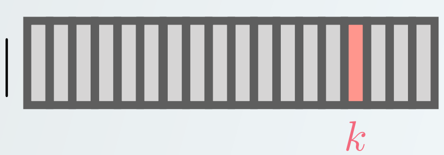
$$\langle \mathcal{O} \rangle = \frac{\langle \Psi | \mathcal{O} | \Psi \rangle}{\langle \Psi | \Psi \rangle} = \frac{\langle \Psi^{(0)} + \Psi^{(1)} + \cdots | \mathcal{O} | \Psi^{(0)} + \Psi^{(1)} + \cdots \rangle}{\langle \Psi^{(0)} + \Psi^{(1)} + \cdots | \Psi^{(0)} + \Psi^{(1)} + \cdots \rangle}$$

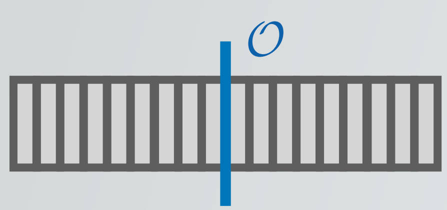
On Lattice:

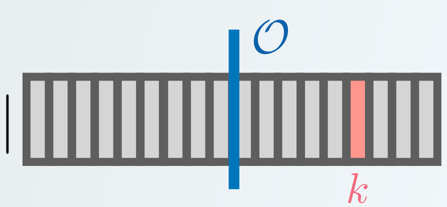
$$\langle \mathcal{O} \rangle = \frac{\det \mathcal{M}_o^{(0)} + \det \mathcal{M}_o^{(1)}}{\det \mathcal{M}^{(0)} + \det \mathcal{M}^{(1)}} = \underbrace{\frac{\det \mathcal{M}_o^{(0)}}{\det \mathcal{M}^{(0)}}}_{\text{zeroth}} + \underbrace{\left(\frac{\det \mathcal{M}_o^{(1)}}{\det \mathcal{M}^{(0)}} - \frac{\det \mathcal{M}_o^{(0)} \det \mathcal{M}^{(1)}}{\det \mathcal{M}^{(0)} \det \mathcal{M}^{(0)}} \right)}_{\text{1st order correction}} + \cdots$$

Four types of amplitudes:

A: $\det \mathcal{M}^{(0)} = \langle \Psi_0 |$  $| \Psi_0 \rangle$

C: $\det \mathcal{M}^{(1)} = 2 \sum_{k=0}^{L_t/2} \langle \Psi_0 |$  $| \Psi_0 \rangle$

B: $\det \mathcal{M}_o^{(0)} = \langle \Psi_0 |$  $| \Psi_0 \rangle$

D: $\det \mathcal{M}_o^{(1)} = 2 \sum_{k=0}^{L_t/2} \langle \Psi_0 |$  $| \Psi_0 \rangle$

Jacobi formula

Perturbation for operators

Operators with perturbation corrections from wave functions

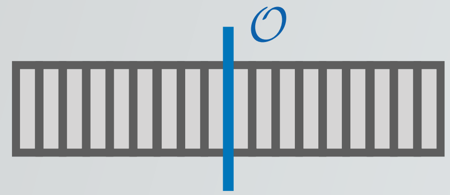
$$\langle \mathcal{O} \rangle = \frac{\langle \Psi | \mathcal{O} | \Psi \rangle}{\langle \Psi | \Psi \rangle} = \frac{\langle \Psi^{(0)} + \Psi^{(1)} + \cdots | \mathcal{O} | \Psi^{(0)} + \Psi^{(1)} + \cdots \rangle}{\langle \Psi^{(0)} + \Psi^{(1)} + \cdots | \Psi^{(0)} + \Psi^{(1)} + \cdots \rangle}$$

On Lattice:

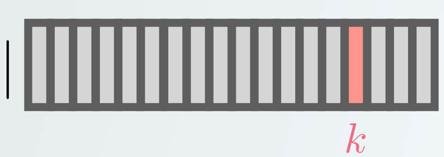
$$\langle \mathcal{O} \rangle = \frac{\det \mathcal{M}_o^{(0)} + \det \mathcal{M}_o^{(1)}}{\det \mathcal{M}^{(0)} + \det \mathcal{M}^{(1)}} = \underbrace{\frac{\det \mathcal{M}_o^{(0)}}{\det \mathcal{M}^{(0)}}}_{\text{zeroth}} + \underbrace{\left(\frac{\det \mathcal{M}_o^{(1)}}{\det \mathcal{M}^{(0)}} - \frac{\det \mathcal{M}_o^{(0)} \det \mathcal{M}^{(1)}}{\det \mathcal{M}^{(0)} \det \mathcal{M}^{(0)}} \right)}_{\text{1st order correction}} + \cdots$$

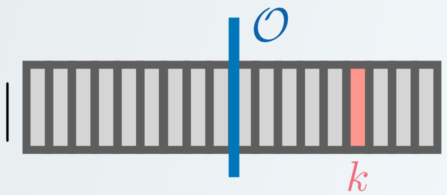
Four types of amplitudes:

A: $\det \mathcal{M}^{(0)} = \langle \Psi_0 |$  $| \Psi_0 \rangle$

B: $\det \mathcal{M}_o^{(0)} = \langle \Psi_0 |$  $| \Psi_0 \rangle$

Jacobi formula

C: $\det \mathcal{M}^{(1)} = 2 \sum_{k=0}^{L_t/2} \langle \Psi_0 |$  $| \Psi_0 \rangle$

D: $\det \mathcal{M}_o^{(1)} = 2 \sum_{k=0}^{L_t/2} \langle \Psi_0 |$  $| \Psi_0 \rangle$

M_0 M_1

Rank-One Operator method

Rank-one operator:

$\mathcal{O}^I_{ij} \equiv F^\dagger_{ij} F_{ij}$ with ij is isospin and spin, and $F^\dagger_{ij} = \sum_{\vec{n}} a^\dagger_{ij}(\vec{n}) f^*_{ij}(\vec{n})$, $F_{ij} = \sum_{\vec{n}} a_{ij}(\vec{n}) f_{ij}(\vec{n})$

a) **When acting on a single particle state, higher rank of $F^\dagger_{ij} F_{ij}$ will vanish** $:e^{cF^\dagger_{ij} F_{ij}}: = :1 + cF^\dagger_{ij} F_{ij}:$

b) **Any operator can be decomposed into Rank-One operator** $\mathcal{O} = \sum_{ij} \mathcal{O}^I_{ij}$

c) **The determinant of correlation matrix has a linear dependence property**

Example:

$$\langle \Psi | :e^{cF^\dagger_\uparrow F_\uparrow}: | \Psi \rangle = \det \begin{array}{c} \begin{bmatrix} c \cdot m_{\uparrow\uparrow} & c \cdot m_{\uparrow\downarrow} \\ m_{\downarrow\uparrow} & m_{\downarrow\downarrow} \end{bmatrix} \begin{array}{c} |\uparrow\rangle \\ |\downarrow\rangle \end{array} \\ \begin{array}{cc} \langle\uparrow| & \langle\downarrow| \end{array} \end{array} = c[m_{\uparrow\uparrow} m_{\downarrow\downarrow} - m_{\uparrow\downarrow} m_{\downarrow\uparrow}]$$

Amplitude with one-body operator:

$$\det \mathcal{M}(\mathcal{O}) = \lim_{c\to\infty} \sum_{i,j=0,1} \left\langle \Psi \middle| :e^{c\cdot\mathcal{O}^I_{ij}}: \middle| \Psi \right\rangle / c$$

can be expanded to many-body operators

Rank-One Operator method

Rank-one operator:

$\mathcal{O}^I_{ij} \equiv F^\dagger_{ij} F_{ij}$ with ij is isospin and spin, and $F^\dagger_{ij} = \sum_{\vec{n}} a^\dagger_{ij}(\vec{n}) f^*_{ij}(\vec{n})$, $F_{ij} = \sum_{\vec{n}} a_{ij}(\vec{n}) f_{ij}(\vec{n})$

a) When acting on a single particle state, higher rank of $F^\dagger_{ij} F_{ij}$ will vanish $: e^{cF^\dagger_{ij}F_{ij}} :=: 1 + cF^\dagger_{ij}F_{ij} :$

b) Any operator can be decomposed into Rank-One operator $\mathcal{O} = \sum_{ij} \mathcal{O}^I_{ij}$

c) The determinant of correlation matrix has a linear dependence property

Example: $\langle \Psi | : e^{cF^\dagger_\uparrow F_\uparrow} : | \Psi \rangle = \det \begin{array}{c} \\ \\ \end{array} \begin{bmatrix} c \cdot m_{\uparrow\uparrow} & c \cdot m_{\uparrow\downarrow} \\ m_{\downarrow\uparrow} & m_{\downarrow\downarrow} \end{bmatrix} \begin{array}{c} |\uparrow\rangle \\ |\downarrow\rangle \end{array} = c[m_{\uparrow\uparrow} m_{\downarrow\downarrow} - m_{\uparrow\downarrow} m_{\downarrow\uparrow}]$

$\qquad\qquad\langle\uparrow| \quad \langle\downarrow|$

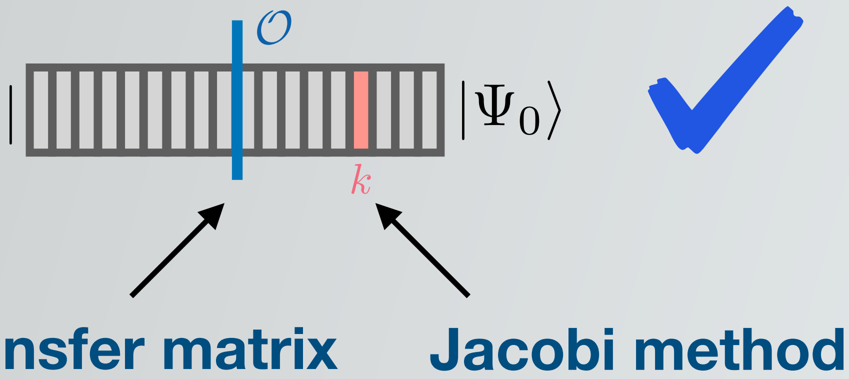
Amplitude with one-body operator:

$$\det \mathcal{M}(\mathcal{O}) = \lim_{c\to\infty} \sum_{i,j=0,1} \left\langle \Psi \middle| : e^{c \cdot \mathcal{O}^I_{ij}} : \middle| \Psi \right\rangle / c$$

can be expanded to many-body operators

Rank-One Operator method

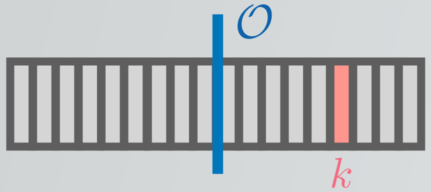
Rank-one operator for perturbation:

D: $\det \mathcal{M}_o^{(1)} = 2 \sum_{k=0}^{L_t/2} \langle \Psi_0 |$  $| \Psi_0 \rangle$

RO transfer matrix $M_{o_{ij}^I} =: e^{c O_{ij}^I} :$

Rank-One Operator method

Rank-one operator for perturbation:

D: $\det \mathcal{M}_o^{(1)} = 2 \sum_{k=0}^{L_t/2} \langle \Psi_0 |$  $| \Psi_0 \rangle$

RO transfer matrix   Jacobi method

RO transfer matrix $M_{o_{ij}^I} =: e^{cO_{ij}^I}:$

Computational challenge:

- **Every perturbation transfer matrix M1 contains all the components of N3LO chiral potential**
- **Perturbation: sum of all k in Lt step**
- **In RO method: sum {i,j}, every O^I_{ij} need propagation from O to k**

Compared to 1st order perturbation to Energy, workload $\times L_t \times 4 \times L^3$ **for one-body operator**

$\times L_t \times 16 \times L^3$ **for two-body operator**

Computational challenge

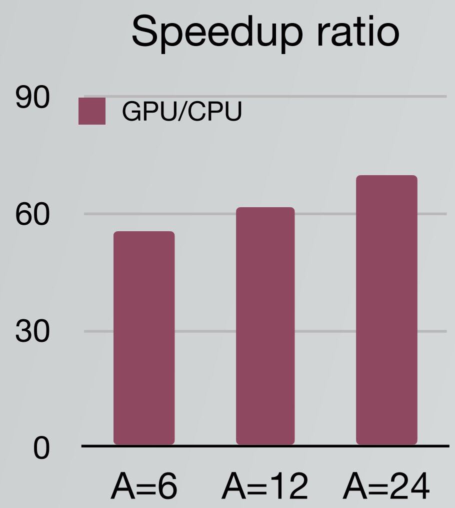
Tools to resolve computational challenge:

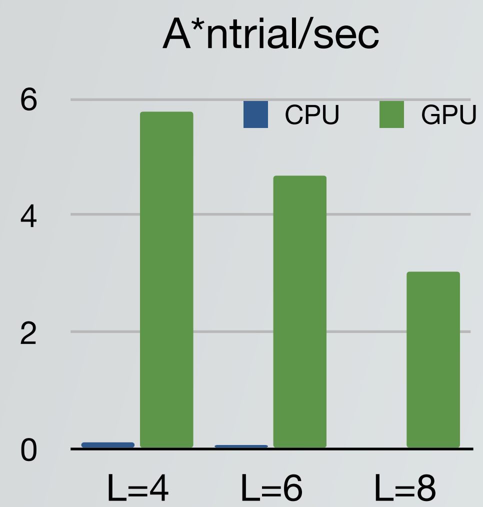
OAK RIDGE National Laboratory | LEADERSHIP COMPUTING FACILITY

1. **Monte Carlo sampling for L_t and L^3**
2. **More powerful devices —— GPU**

Hybrid: MPI(c++) & GPU(cuda)

Amount of *CUDA* kernels ~ 70, GPU usage ~ 80%





One chip comparison

Andes CPU: AMD EPYC ~ 4 tera Flops
Summit GPU: Nvidia Tesla V100 ~ 125 tera Flops
Frontier GPU: AMD MI250X ~ 383 tera Flops

Recent progress

- Brief introduction to Nuclear Lattice EFT
  - "Sign problem" & SU(4) symmetry
- Perturbation on Lattice:
  - Wave function matching Hamiltonian (Dean's talk)
  - 1st order perturbation to wave function
  - Rank-One operator method
- **Recent progress I: Neutron matter static structure factors**
- Recent progress II: Charge Radii (ongoing)
- Summary & perspective

Structure factors of Neutron matter

"As much as 99% of the gravitational binding energy released in core-collapse supernovae escapes the star in the form of neutrinos. This enormous flux, when it interacts with the nuclear matter on its way out of the star, is believed to be an essential ingredient in the explosion of the star." *PRL 126,132701 (2021)*

Supernova explosion, figure from Science News

Neutrino-neutron cross section in medium

$$\frac{1}{N}\frac{d\sigma}{d\Omega} = \frac{G_{\mathrm{F}}^2 E_v^2}{16\pi^2}\left(g_a^2(3-\cos\theta)S_a(q) + (1+\cos\theta)S_v(q)\right)$$

G_F : Fermi coupling constant

E_ν : neutrino energy

PLB 642 (2006) 326-332

Neutron structure factor

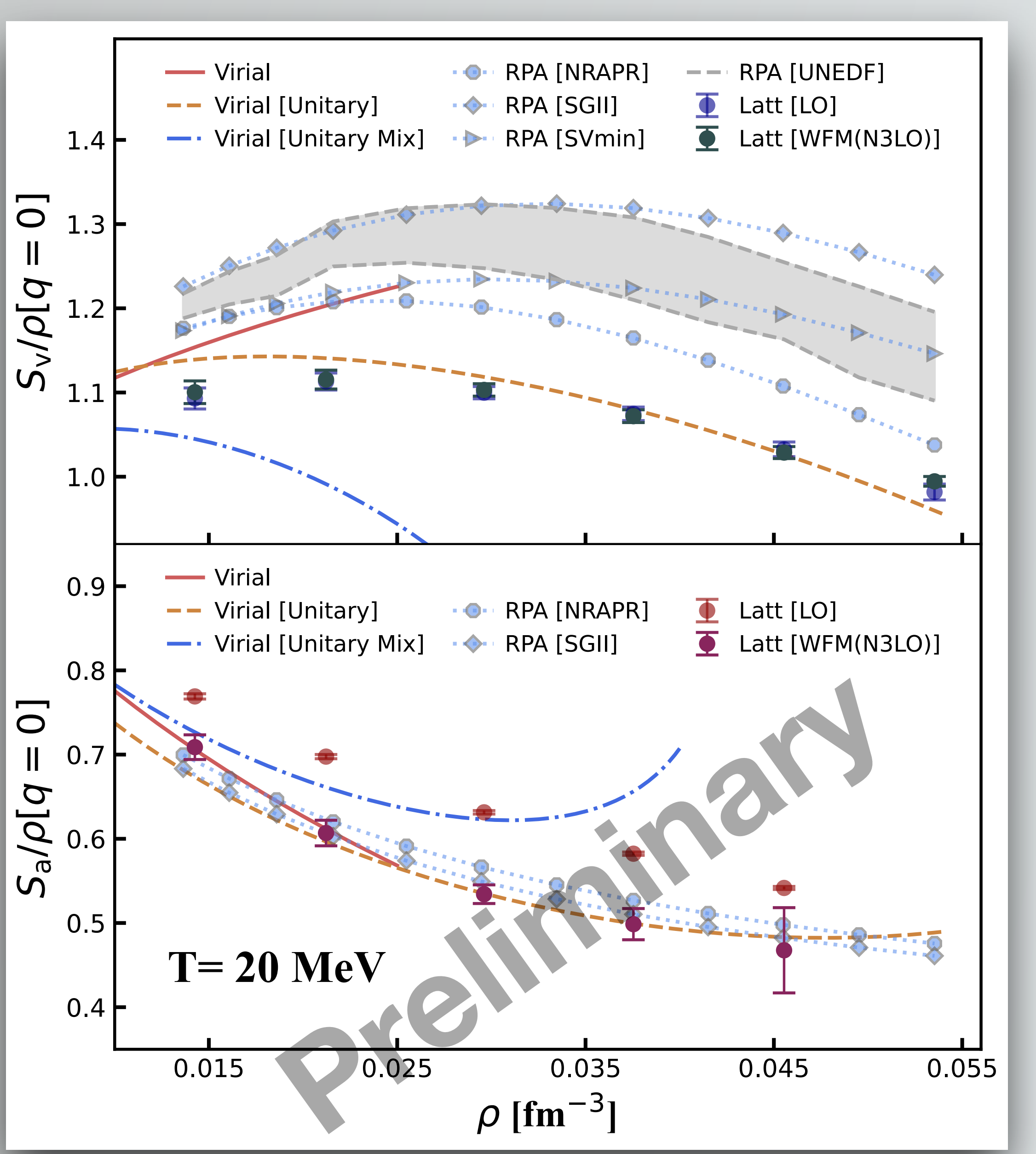
$$S_V(q) = \int d^3\mathbf{r} e^{-i\mathbf{q}\cdot\mathbf{r}} \langle \delta n(0,\mathbf{r})\delta n(0,\mathbf{0})\rangle$$

$$S_A(q) = \int d^3\mathbf{r} e^{-i\mathbf{q}\cdot\mathbf{r}} \langle \delta S_z(0,\mathbf{r})\delta S_z(0,\mathbf{0})\rangle$$

Not yet an *ab initio* calculation

Neutron matter at finite Temperature

Structure factor at long-wave limit



- First *ab initio* calculation of this content
- Overall agreement of the trend
- At low density agree with Virial expansion
- Sv of Lattice calculation is smaller
- N3LO correction to Sa is significant
- Calibrate RPA for supernova simulations

Recent progress

- **Brief introduction to Nuclear Lattice EFT**
  - **"Sign problem" & SU(4) symmetry**
- **Perturbation on Lattice:**
  - **Wave function matching Hamiltonian (Dean's talk)**
  - **1st order perturbation to wave function**
  - **Rank-One operator method**
- **Recent progress I: Neutron matter static structure factors**
- **Recent progress II: Charge Radii (ongoing)**
- **Summary & perspective**

Charge Radii

Experimental measurements

- Electron-scattering experiments, charge form factor $F_c(\mathbf{q})$ and $\rho_c(\boldsymbol{r}) = \frac{1}{(2\pi)^3} \int d^3q e^{-i\boldsymbol{q}\cdot\boldsymbol{r}} F_c(\boldsymbol{q})$

Charge Radii

Experimental measurements

- Electron-scattering experiments, charge form factor $F_c(\mathbf{q})$ and $\rho_c(\boldsymbol{r}) = \frac{1}{(2\pi)^3}\int d^3q e^{-i\boldsymbol{q}\cdot\boldsymbol{r}} F_c(\boldsymbol{q})$

- Laser spectroscopy experiments, hyperfine spectra and isotope shift

$$\delta\nu^{A,A'} = \nu^{A'} - \nu^{A} = k\frac{m_{A'} - m_A}{m_{A'}m_A} + F\delta\left\langle r^2\right\rangle^{A,A'}$$

Miller, A.J., Minamisono, K. *et al.* Nat. Phys. 15, 432–436 (2019)

Charge Radii

Experimental measurements

- Electron-scattering experiments, charge form factor $F_c(\mathbf{q})$ and $\rho_c(\boldsymbol{r}) = \frac{1}{(2\pi)^3}\int d^3q e^{-i\boldsymbol{q}\cdot\boldsymbol{r}} F_c(\boldsymbol{q})$

- Laser spectroscopy experiments, hyperfine spectra and isotope shift

$$\delta\nu^{A,A'} = \nu^{A'} - \nu^{A} = k\frac{m_{A'} - m_A}{m_{A'} m_A} + F\delta\left\langle r^2\right\rangle^{A,A'}$$

Miller, A.J., Minamisono, K. *et al.* Nat. Phys. 15, 432–436 (2019)

Theoretical calculation

$$\left\langle r_{\rm ch}^2\right\rangle = \left\langle r_{\rm pp}^2\right\rangle + R_{\rm p}^2 + \frac{N}{Z}R_{\rm n}^2 + \left\langle r^2\right\rangle^{\rm (rel)}$$

P. Reinhard, W. Nazarewicz. PRC 103, 054310 (2021)

Charge Radii

Experimental measurements

- Electron-scattering experiments, charge form factor $F_c(\mathbf{q})$ and $\rho_c(\boldsymbol{r}) = \frac{1}{(2\pi)^3}\int d^3q e^{-i\boldsymbol{q}\cdot\boldsymbol{r}} F_c(\boldsymbol{q})$

- Laser spectroscopy experiments, hyperfine spectra and isotope shift

$$\delta\nu^{A,A'} = \nu^{A'} - \nu^{A} = k\frac{m_{A'} - m_A}{m_{A'} m_A} + F\delta\left\langle r^2\right\rangle^{A,A'}$$

Miller, A.J., Minamisono, K. *et al.* Nat. Phys. 15, 432–436 (2019)

Theoretical calculation

$$\left\langle r_{\mathrm{ch}}^2\right\rangle = \underline{\left\langle r_{\mathrm{pp}}^2\right\rangle} + R_{\mathrm{p}}^2 + \frac{N}{Z}R_{\mathrm{n}}^2 + \left\langle r^2\right\rangle^{(\mathrm{rel})}$$

P. Reinhard, W. Nazarewicz. PRC 103, 054310 (2021)

$$\hat{r}_{\mathrm{pp}}^2 = \frac{1}{Z}\sum_{i=1}^{Z}(\overrightarrow{r_i} - \overrightarrow{r_0})^2$$

Charge Radii

Experimental measurements

- Electron-scattering experiments, charge form factor $F_c(\mathbf{q})$ and $\rho_c(\boldsymbol{r}) = \frac{1}{(2\pi)^3}\int d^3q e^{-i\boldsymbol{q}\cdot\boldsymbol{r}} F_c(\boldsymbol{q})$

- Laser spectroscopy experiments, hyperfine spectra and isotope shift

$$\delta\nu^{A,A'} = \nu^{A'} - \nu^{A} = k\frac{m_{A'} - m_A}{m_{A'}m_A} + F\delta\left\langle r^2\right\rangle^{A,A'}$$

Miller, A.J., Minamisono, K. *et al.* Nat. Phys. 15, 432–436 (2019)

Theoretical calculation

$$\left\langle r_{\mathrm{ch}}^2\right\rangle = \left\langle r_{\mathrm{pp}}^2\right\rangle + R_{\mathrm{p}}^2 + \frac{N}{Z}R_{\mathrm{n}}^2 + \left\langle r^2\right\rangle^{(\mathrm{rel})}$$

P. Reinhard, W. Nazarewicz. PRC 103, 054310 (2021)

relativistic correction

$$\hat{r}_{\mathrm{pp}}^2 = \frac{1}{Z}\sum_{i=1}^{Z}(\vec{r_i} - \vec{r_0})^2$$

$$\left\langle r^2\right\rangle^{(\mathrm{rel})} = 3\mathcal{D} + \left(\mu_p - \frac{1}{2}\right)\mathcal{D}\langle\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\ell}}\rangle_p + \frac{\mu_n N}{Z}\mathcal{D}\langle\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\ell}}\rangle_n$$ with Darwin-Foldy $\mathcal{D} = \frac{\hbar^2}{4m_{\mathrm{p}}^2c^2}$

Charge Radii

Experimental measurements

- Electron-scattering experiments, charge form factor $F_c(\mathbf{q})$ and $\rho_c(\boldsymbol{r}) = \frac{1}{(2\pi)^3}\int d^3q e^{-i\boldsymbol{q}\cdot\boldsymbol{r}} F_c(\boldsymbol{q})$

- Laser spectroscopy experiments, hyperfine spectra and isotope shift

$$\delta\nu^{A,A'} = \nu^{A'} - \nu^{A} = k\frac{m_{A'} - m_A}{m_{A'}m_A} + F\delta\left\langle r^2\right\rangle^{A,A'}$$

Miller, A.J., Minamisono, K. *et al.* Nat. Phys. 15, 432–436 (2019)

Theoretical calculation

$$\left\langle r^2_{\mathrm{ch}}\right\rangle = \left\langle r^2_{\mathrm{pp}}\right\rangle + R^2_{\mathrm{p}} + \frac{N}{Z}R^2_{\mathrm{n}} + \left\langle r^2\right\rangle^{(\mathrm{rel})}$$

P. Reinhard, W. Nazarewicz. PRC 103, 054310 (2021)

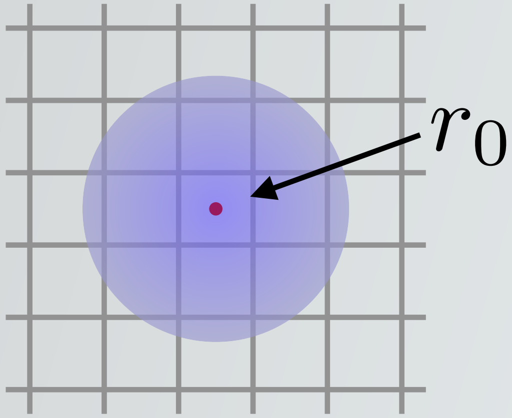
relativistic correction

$$\hat{r}^2_{\mathrm{pp}} = \frac{1}{Z}\sum_{i=1}^{Z}(\vec{r_i} - \vec{r_0})^2$$

$$\left\langle r^2\right\rangle^{(\mathrm{rel})} = 3\mathcal{D} + \left(\mu_p - \frac{1}{2}\right)\mathcal{D}\langle\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\ell}}\rangle_p + \frac{\mu_n N}{Z}\mathcal{D}\langle\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\ell}}\rangle_n \quad \text{with Darwin-Foldy } \mathcal{D} = \frac{\hbar^2}{4m^2_{\mathrm{p}}c^2}$$

On Lattice

$$\hat{r}^2_{\mathrm{pp}} = \frac{1}{Z}\sum_{i=1}^{Z}(\vec{r_i} - \vec{r_0})^2$$



Pinhole ALG

Charge Radii

Experimental measurements

- Electron-scattering experiments, charge form factor $F_c(\mathbf{q})$ and $\rho_c(\boldsymbol{r}) = \frac{1}{(2\pi)^3}\int d^3q e^{-i\boldsymbol{q}\cdot\boldsymbol{r}} F_c(\boldsymbol{q})$
- Laser spectroscopy experiments, hyperfine spectra and isotope shift

$$\delta\nu^{A,A'} = \nu^{A'} - \nu^{A} = k\frac{m_{A'} - m_A}{m_{A'} m_A} + F\delta\left\langle r^2\right\rangle^{A,A'}$$

Miller, A.J., Minamisono, K. *et al.* Nat. Phys. 15, 432–436 (2019)

Theoretical calculation

$$\left\langle r_{\mathrm{ch}}^2\right\rangle = \underline{\left\langle r_{\mathrm{pp}}^2\right\rangle} + R_{\mathrm{p}}^2 + \frac{N}{Z}R_{\mathrm{n}}^2 + \underline{\left\langle r^2\right\rangle^{(\mathrm{rel})}}$$

P. Reinhard, W. Nazarewicz. PRC 103, 054310 (2021)

$$\hat{r}_{\mathrm{pp}}^2 = \frac{1}{Z}\sum_{i=1}^{Z}(\vec{r_i} - \vec{r_0})^2$$

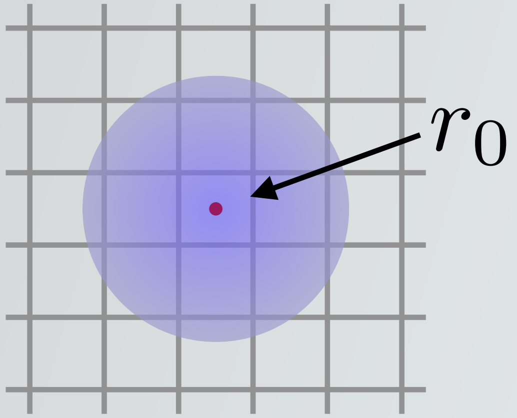
relativistic correction

$$\left\langle r^2\right\rangle^{(\mathrm{rel})} = 3\mathcal{D} + \left(\mu_p - \frac{1}{2}\right)\mathcal{D}\langle\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\ell}}\rangle_p + \frac{\mu_n N}{Z}\mathcal{D}\langle\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\ell}}\rangle_n \quad \text{with Darwin-Foldy } \mathcal{D} = \frac{\hbar^2}{4m_{\mathrm{p}}^2 c^2}$$

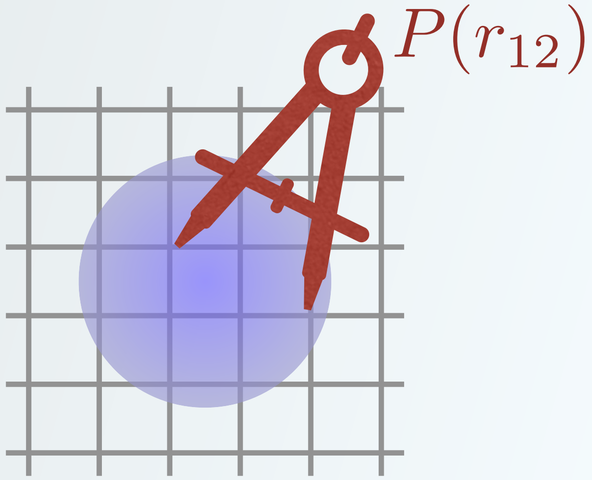
On Lattice

$$\hat{r}_{\mathrm{pp}}^2 = \frac{1}{Z}\sum_{i=1}^{Z}(\vec{r_i} - \vec{r_0})^2$$

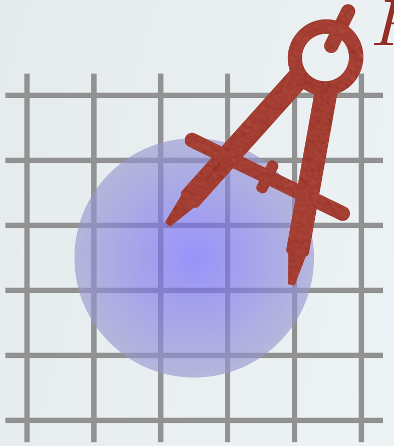
Pinhole ALG



Two-body density correlation function



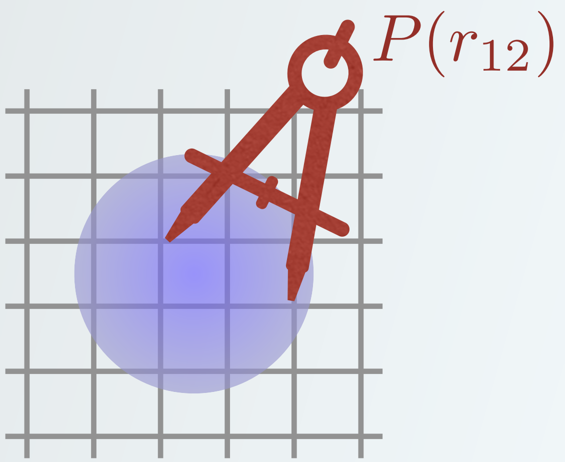
Two-body correlation function



Charge radii from density correlation function

$$\langle r_{pp}^2 \rangle = \frac{1}{ZA}\int d^3r d^3r' \langle \rho_p(\vec{r})(\vec{r}-\vec{r}')^2 \rho(\vec{r}')\rangle - \frac{1}{2A^2}\int d^3r d^3r' \langle \rho(\vec{r})(\vec{r}-\vec{r}')^2 \rho(\vec{r}')\rangle$$

Two-body correlation function



Charge radii from density correlation function

$$\langle r_{pp}^2 \rangle = \frac{1}{ZA}\int d^3r d^3r' \langle \rho_p(\vec{r})(\vec{r}-\vec{r}')^2 \rho(\vec{r}')\rangle - \frac{1}{2A^2}\int d^3r d^3r' \langle \rho(\vec{r})(\vec{r}-\vec{r}')^2 \rho(\vec{r}')\rangle$$

Rank-One operator methods for perturbation of charge radii

Test Hamiltonian: $H_{\mathrm{full}} = T + V$

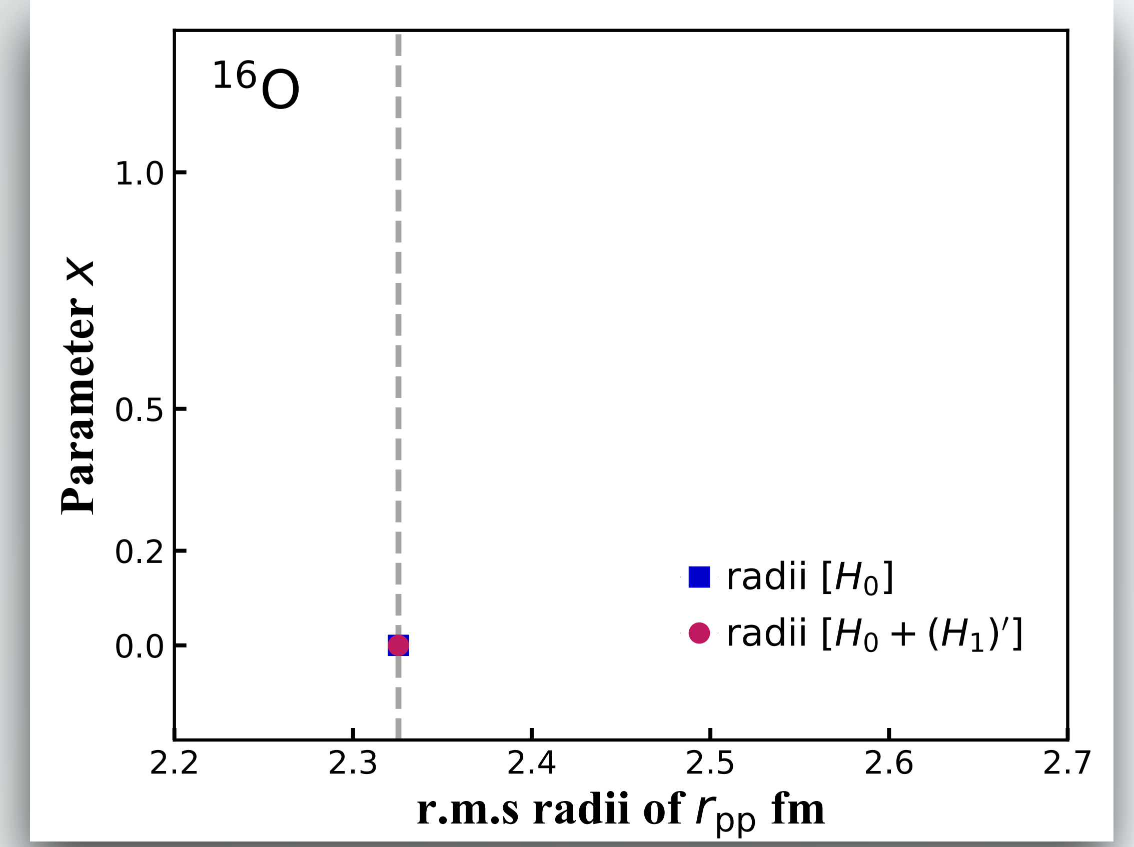
T: kinetic **V: two-body contact**

Perturbation: $H_{\mathrm{pert}} = H_0 + (H_1)'$

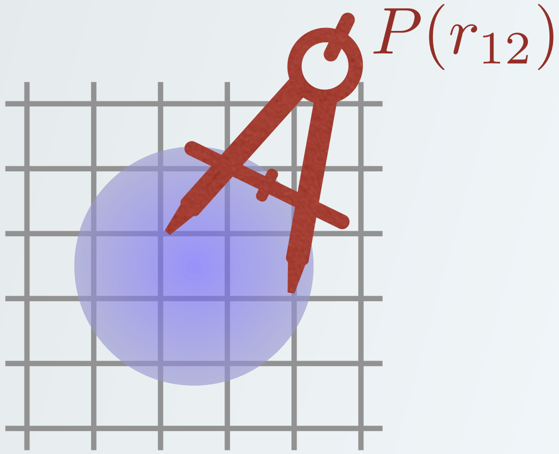
with $H_0 = T + (1-x)V$

and $H_1 = xV$

Setups: L=6, Lt=80, Vcc= -3.9e-07 MeV^-2



Two-body correlation function



Charge radii from density correlation function

$$\langle r_{pp}^2 \rangle = \frac{1}{ZA} \int d^3r d^3r' \langle \rho_p(\vec{r})(\vec{r}-\vec{r}')^2 \rho(\vec{r}') \rangle - \frac{1}{2A^2} \int d^3r d^3r' \langle \rho(\vec{r})(\vec{r}-\vec{r}')^2 \rho(\vec{r}') \rangle$$

Rank-One operator methods for perturbation of charge radii

Test Hamiltonian: $H_{\text{full}} = T + V$

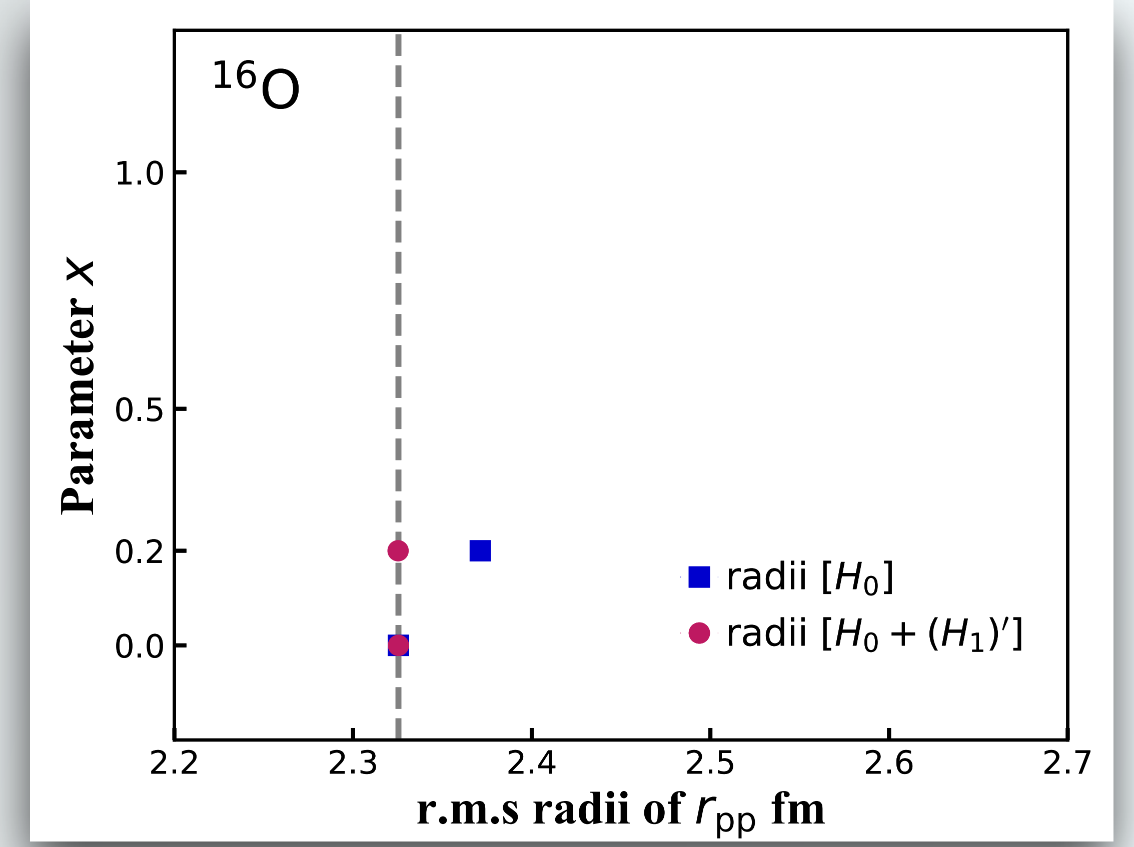
T: kinetic V: two-body contact

Perturbation: $H_{\text{pert}} = H_0 + (H_1)'$

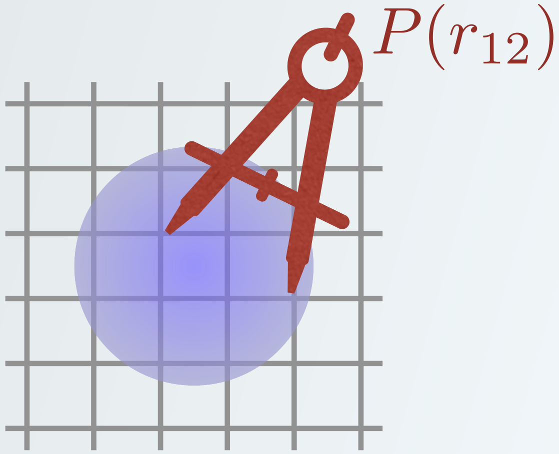
with $H_0 = T + (1-x)V$

and $H_1 = xV$

Setups: L=6, Lt=80, Vcc= -3.9e-07 MeV^-2



Two-body correlation function



Charge radii from density correlation function

$$\langle r_{pp}^2\rangle = \frac{1}{ZA}\int d^3r d^3r' \langle \rho_p(\vec{r})(\vec{r}-\vec{r}')^2\rho(\vec{r}')\rangle - \frac{1}{2A^2}\int d^3r d^3r' \langle \rho(\vec{r})(\vec{r}-\vec{r}')^2\rho(\vec{r}')\rangle$$

Rank-One operator methods for perturbation of charge radii

Test Hamiltonian: $H_{\text{full}} = T + V$

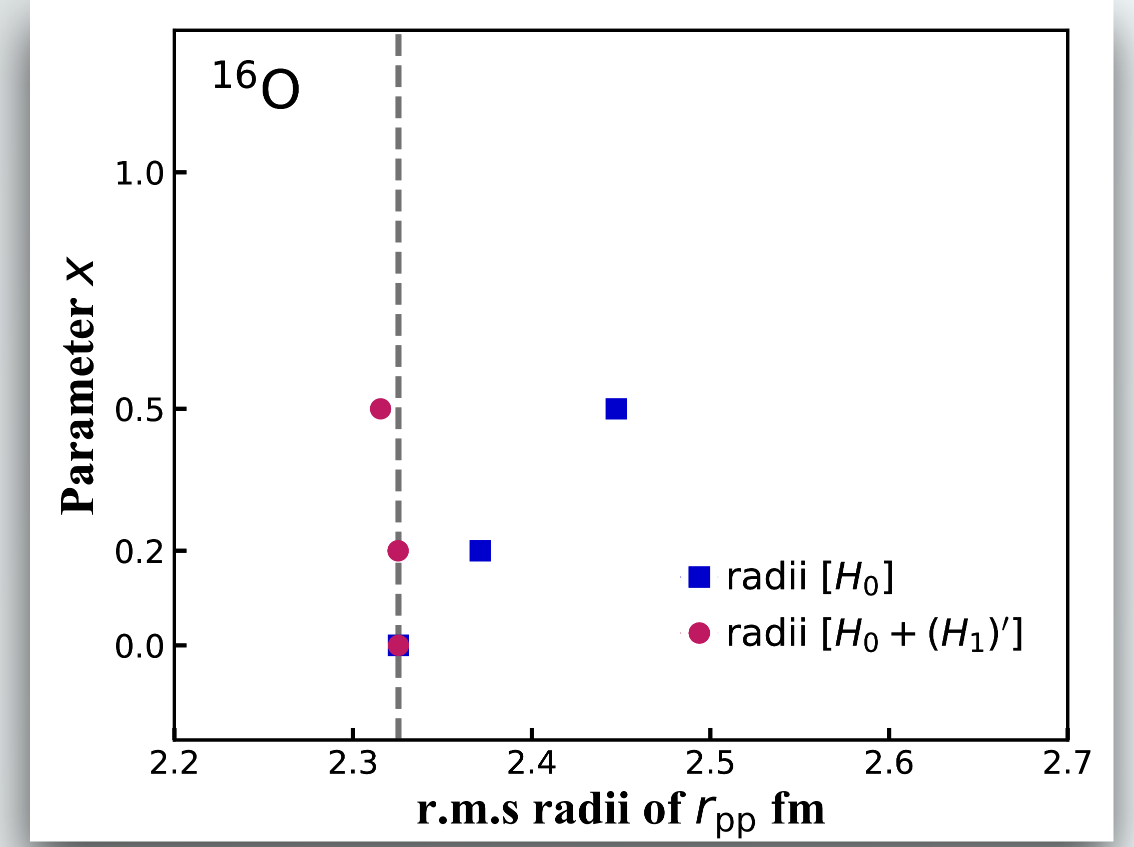
T: kinetic **V: two-body contact**

Perturbation: $H_{\text{pert}} = H_0 + (H_1)'$

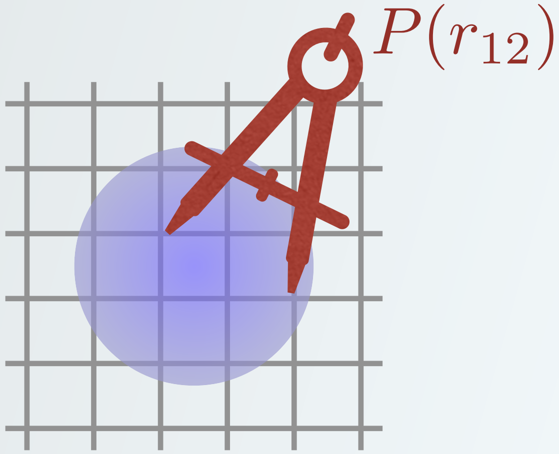
with $H_0 = T + (1-x)V$

and $H_1 = xV$

Setups: L=6, Lt=80, Vcc= -3.9e-07 MeV^-2



Two-body correlation function



Charge radii from density correlation function

$$\langle r_{pp}^2 \rangle = \frac{1}{ZA}\int d^3r d^3r' \langle \rho_p(\vec{r})(\vec{r}-\vec{r}')^2 \rho(\vec{r}')\rangle - \frac{1}{2A^2}\int d^3r d^3r' \langle \rho(\vec{r})(\vec{r}-\vec{r}')^2 \rho(\vec{r}')\rangle$$

Rank-One operator methods for perturbation of charge radii

Test Hamiltonian: $H_{\text{full}} = T + V$

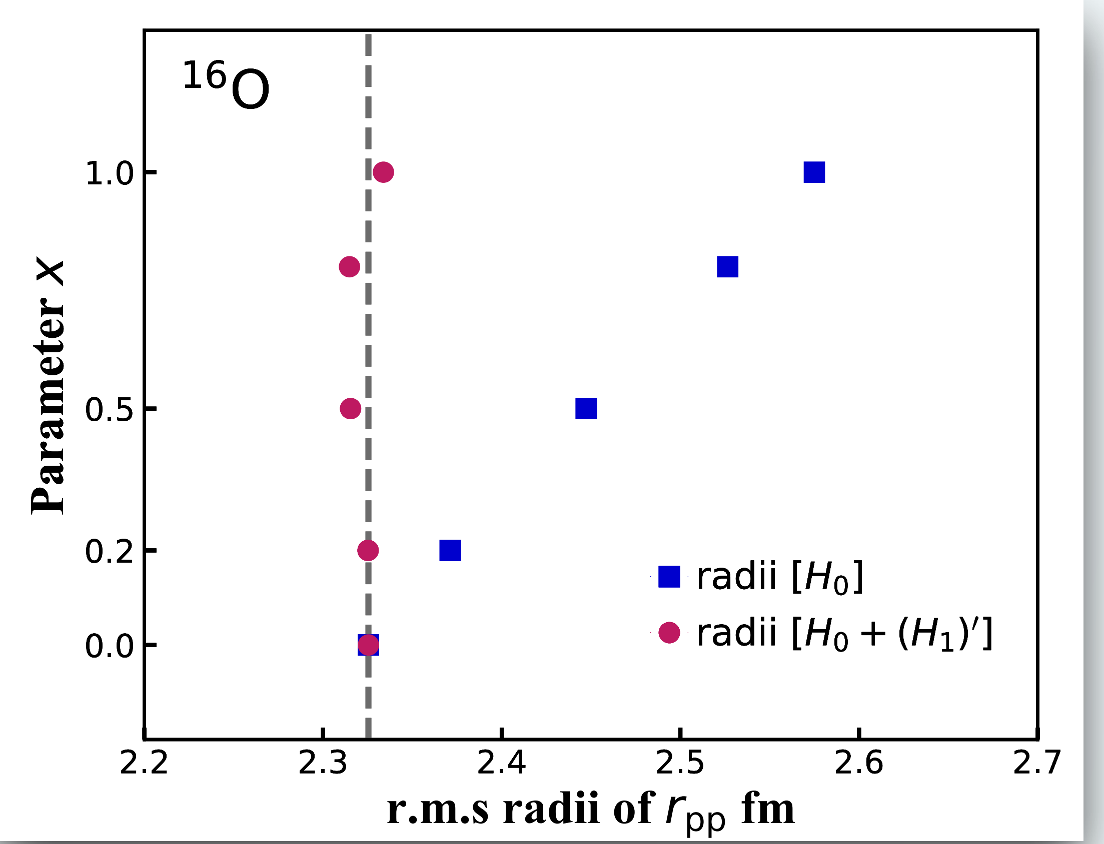
T: kinetic **V: two-body contact**

Perturbation: $H_{\text{pert}} = H_0 + (H_1)'$

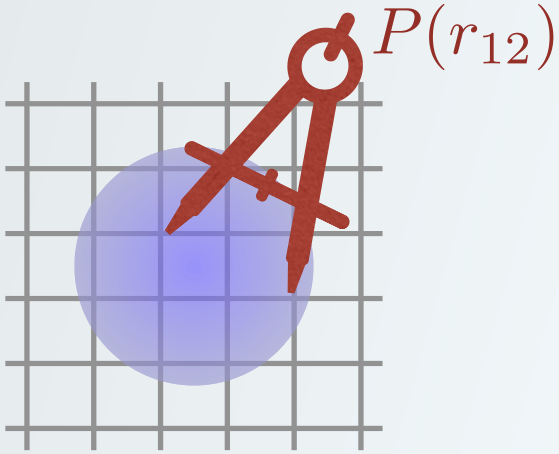
with $H_0 = T + (1-x)V$

and $H_1 = xV$

Setups: L=6, Lt=80, Vcc= -3.9e-07 MeV^-2



Two-body correlation function



Charge radii from density correlation function

$$\langle r_{pp}^2 \rangle = \frac{1}{ZA} \int d^3r d^3r' \langle \rho_p(\vec{r})(\vec{r}-\vec{r}')^2 \rho(\vec{r}') \rangle - \frac{1}{2A^2} \int d^3r d^3r' \langle \rho(\vec{r})(\vec{r}-\vec{r}')^2 \rho(\vec{r}') \rangle$$

Rank-One operator methods for perturbation of charge radii

Test Hamiltonian: $H_{\text{full}} = T + V$

T: kinetic V: two-body co

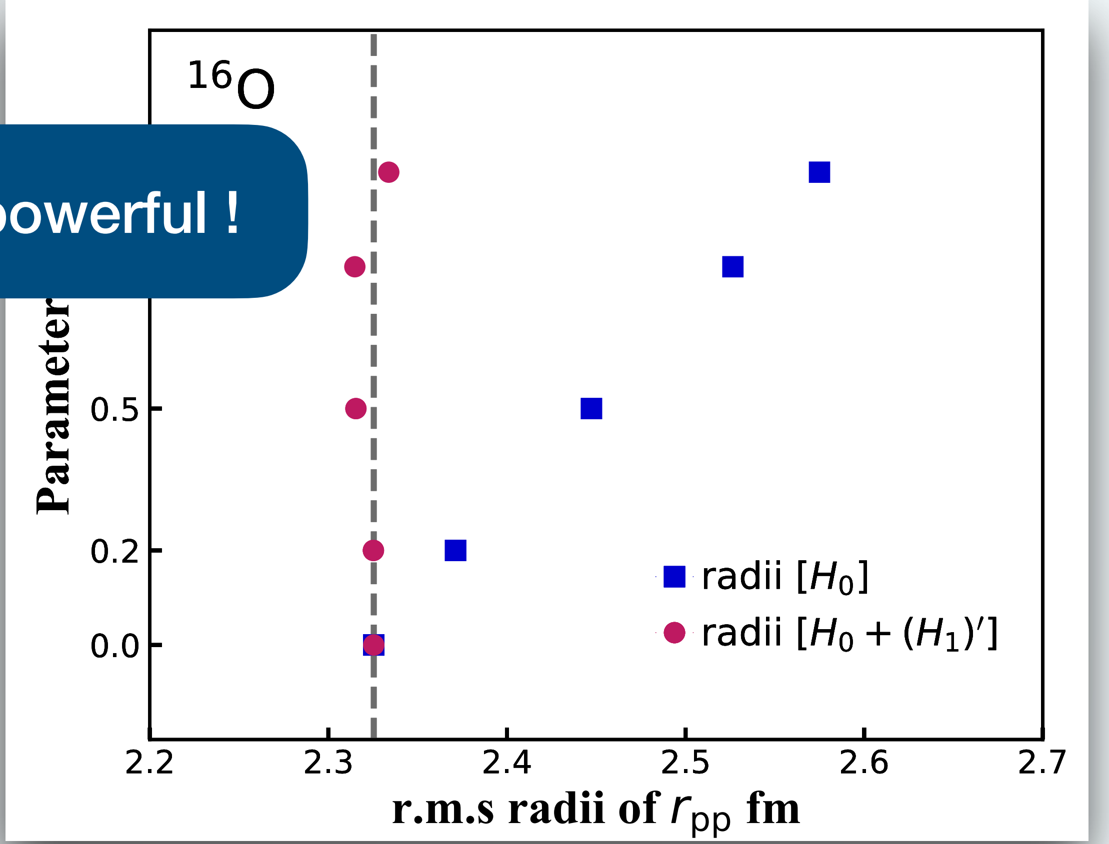
Perturbation is powerful !

Perturbation: $H_{\text{pert}} = H_0 + (H_1)'$

with $H_0 = T + (1-x)V$

and $H_1 = xV$

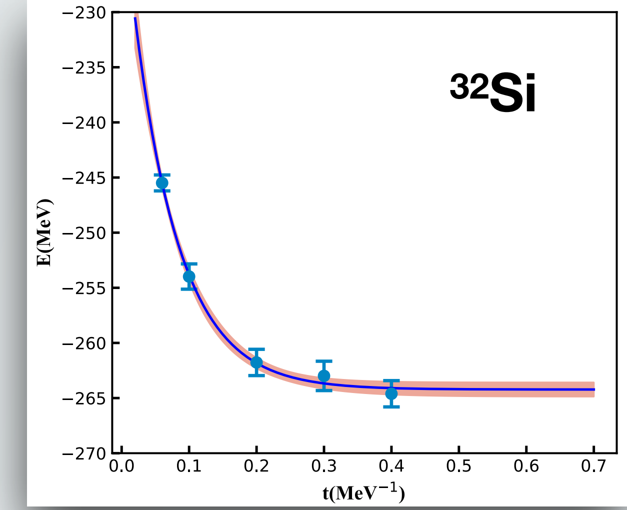
Setups: L=6, Lt=80, Vcc= -3.9e-07 MeV^-2



Charge Radii of Silicon isotopes

Experiments measurement of charge radii difference: < 1%

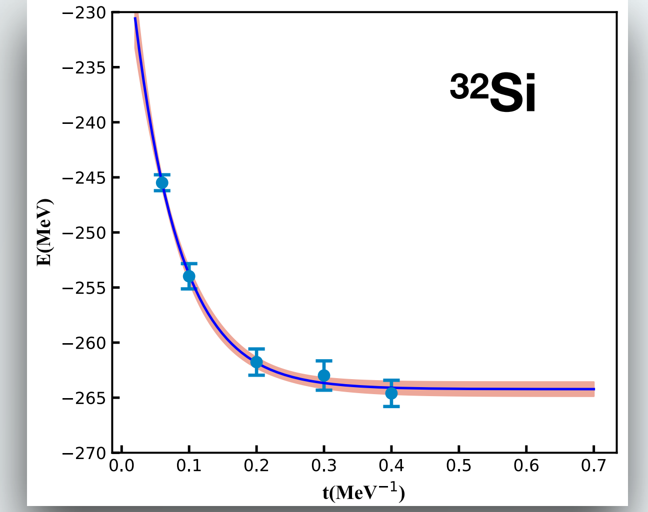
E (MeV)	Exp	Latt (N3LO)	different
28Si	-236.536	-235.06 (92)	~ 0.6%
32Si	-271.407	-263.46 (82)	~ 3%



Charge Radii of Silicon isotopes

Experiments measurement of charge radii difference: < 1%

E (MeV)	Exp	Latt (N3LO)	different
28Si	-236.536	-235.06 (92)	~ 0.6%
32Si	-271.407	-263.46 (82)	~ 3%



High precision calculation needs highly efficient methods and huge computational resources

$\langle r_{ch}^2 \rangle$	Exp	Latt (LO)	Latt (N3LO)
28Si	9.749	10.126 (8)	9.258 (228)
32Si	-	10.273 (8)	9.553 (521)

Preliminary

Only Lt = 60
More works need to be done

Summary & Outlook

- **Chiral EFT** and **Many-body correlation** are treated within the same framework of **NLEFT**
- "**Sign problem**" can be resolved by ***Wave function matching*** and ***Perturbation theory***
- ***Rank-one operator*** method pave the way to accurate observable calculations on lattice
- As applications, **neutron matter structure factors** and **charge radii** are discussed

- **Efficient methods** and **large-scale calculation** are needed for **high precision** charge radii
- More observables: **Electric and Magnetic transitions**, $0\nu\beta\beta$, **EDM**, …
- Advanced lattice algorithm and efficient code …

Thanks for your attention!

Nuclear Lattice EFT Collaboration

Dean Lee, Ulf-G. Meißner, Timo A. Lähde, Evgeny Epelbaum, Serdar Elhatisari, Bingnan Lu, Myungkuk Kim, Young-Ho Song, Shihang Shen, Zhengxue Ren, Fabian Hildenbrand, Avik Sarkar, Lukas Bovermann, Gianluca Stellin,…….