Many-Body Nuclear Physics With Quantum Monte Carlo Methods And Chiral EFT

Workshop of Recent Developments in QCD and Quantum Field Theories - National Taiwan University







European Research Council Established by the European Cominission

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Motivation





Extending The Nuclear Landscape

Cutting-edge experimental results

Rare-isotope facilities



adapted from A. B. Balentekin et al., Mod. Phys. Lett. A **29**, 1430010 (2014)

Neutron-star mergers



adapted from M. McLaughlin, APS Physics Viewpoint, October 16, (2017)

Nuclear theory has experienced a renaissance in the past few decades thanks (in part) to two developments.

- 1. Advances in *ab initio* many-body methods.
- 2. Chiral effective field theory (EFT) for nuclear interactions.



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work with protons + neutrons & controlled approximations



Reach Of Ab Initio Methods

- <u>1980s & 1990s:</u>
 Exact methods (exponential scaling) e.g. *Green's Function Monte Carlo Method* (*GFMC*), No-Core
 Shell Model. Limited by
 Moore's law A < 10, 12
- <u>2000s and beyond</u>: New methods (polynomial scaling) e.g. Coupled cluster, auxiliary-field diffusion Monte Carlo (AFDMC). Closed-shell nuclei around up to A = 40.



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Quantum Monte Carlo (QMC) methods with chiral effective field theory (xEFT) interactions is a compelling piece of the puzzle!



Outline

- Quantum Monte
 Carlo Methods
- Chiral EFT
 - Locality
 - 3N Interaction



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- Short-range correlations and the EMC effect
- Summary & Outlook



Quantum Monte Carlo (QMC) Methods

- 1. Start with a trial wave function Ψ_T and generate a random position: $\mathbf{R} = \mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_A$.
- 2. Metropolis algorithm: Generate new positions \mathbf{R}' based on the probability $P = \frac{|\Psi_T(\mathbf{R}')|^2}{|\Psi_T(\mathbf{R})|^2}$. $\longrightarrow \{\mathbf{k}\}$
- 3. Invoke the variational principle: $E_T = \frac{\langle \Psi_T | H | \Psi_T \rangle}{\langle \Psi_T | \Psi_T \rangle} > E_0$.

QMC Methods - Diffusion Monte Carlo Method

- The wave function is imperfect: $|\Psi_T\rangle = \sum_{i=0}^{\infty} \alpha_i |\Psi_i\rangle$.
- Propagate in imaginary time to project out the ground state $|\Psi_0\rangle$.

$$\begin{split} |\Psi(\tau)\rangle &= \mathrm{e}^{-(H-E_{T})\tau} |\Psi_{T}\rangle \\ &= \mathrm{e}^{-(E_{0}-E_{T})\tau} [\alpha_{0} |\Psi_{0}\rangle + \sum_{i\neq 0} \alpha_{i} \mathrm{e}^{-(E_{i}-E_{0})\tau} |\Psi_{i}\rangle]. \end{split}$$

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QMC Methods - An Example

$$H = \frac{p^2}{2} + \frac{1}{2}\omega^2 x^2$$
$$\psi_0(x) = \left(\frac{\omega}{\pi}\right)^{1/4} e^{-\omega x^2/2}$$

Trial wave function; e.g.

$$\Psi_T(x) = \sqrt{30}x(1-x).$$











 $\tau = 1.00$



T = 1.25



 $\tau = 1.50$



T = 1.75



 $\tau = 2.00$



T = 2.25



 $\tau = 2.50$


Imaginary-time evolution:

 $\tau = 2.75$



Imaginary-time evolution:

 $\tau = 3.00$



Imaginary-time evolution:

 $\tau = 3.00$



QMC Methods - Compare/Contrast GFMC & AFDMC

Green's function Monte	Auxiliary-field diffusion
Carlo (GFMC)	Monte Carlo (AFDMC)
 Ψ_T) ~ 3A coordinates & 2^A (^A_Z) complex amplitudes: Exponential scaling. 	 Ψ_T) ~ 3A coordinates & 4A complex amplitudes (n↑), n↓), p↑), p↓)): Polynomial scaling.

Chiral Effective Field Theory (EFT)



- If probed at high energies, substructure is resolved.
- At low energies, details are not resolved.
- Can replace fine structure by something simpler (think of multipole expansion): low-energy observables unchanged.





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Weinberg, van Kolck, Kaplan, Savage, Wise, Bernard, Epelbaum, Kaiser, Machleidt, Meißner,... Chiral EFT: Expand in powers of Q/Λ_b . $Q \sim m_{\pi} \sim 100$ MeV $\Lambda_b \sim 500$ MeV

- Long-range physics: π exchanges.
- Short-range physics: Contacts × LECs.
- Many-body forces & currents enter systematically.



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Local construction possible¹ up to N²LO.

Definitions. q = p - p', k = p + p'

Regulator: $f(p,p') = e^{-(p/\Lambda)^n} e^{-(p'/\Lambda)^n}$

Contacts: $\propto q$ and k

¹A. Gezerlis et al, PRL **111** 032501 (2013); JEL et al, PRL **113** 192501 (2014); A. Gezerlis et al, PRC **90** 054323 (2014)

Local construction possible¹ up to N²LO.

Definitions. q = p - p', k = p + p'

Regulator:

$$f(p,p') = e^{-(p/A)^n} e^{-(p'/A)^n}$$

$$\rightarrow f_{long}(r) = 1 - e^{-(r/R_0)^4} : R_0 = 1.0, 1.1, 1.2 \text{ fm.}$$
Contacts:
$$\propto \mathbf{q} \text{ and } \mathbf{k}$$

$$\rightarrow \text{Choose contacts} \propto \mathbf{q} \text{ (As much as possible!)}$$

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$$V_{\text{cont}}^{(0)} = \alpha_1 + \alpha_2(\sigma_1 \cdot \sigma_2) + \alpha_3(\tau_1 \cdot \tau_2) + \alpha_4(\sigma_1 \cdot \sigma_2)(\tau_1 \cdot \tau_2)$$

Pauli Exclusion Principle→ Only two independent contacts!

$$V_{\rm cont}^{(0)} = C_{\rm S} + C_{\rm T}(\sigma_1 \cdot \sigma_2)$$





$$V_{\text{cont}}^{(2)} = \gamma_1 q^2 + \gamma_2 q^2 (\sigma_1 \cdot \sigma_2) + \gamma_3 q^2 (\tau_1 \cdot \tau_2) + \gamma_4 q^2 (\sigma_1 \cdot \sigma_2) (\tau_1 \cdot \tau_2) + \gamma_5 k^2 + \gamma_6 k^2 (\sigma_1 \cdot \sigma_2) + \gamma_7 k^2 (\tau_1 \cdot \tau_2) + \gamma_8 k^2 (\sigma_1 \cdot \sigma_2) (\tau_1 \cdot \tau_2) + (\sigma_1 + \sigma_2) (\mathbf{q} \times \mathbf{k}) (\gamma_9 + \gamma_{10} (\tau_1 \cdot \tau_2)) + (\sigma_1 \cdot \mathbf{q}) (\sigma_2 \cdot \mathbf{q}) (\gamma_{11} + \gamma_{12} (\tau_1 \cdot \tau_2)) + (\sigma_1 \cdot \mathbf{k}) (\sigma_2 \cdot \mathbf{k}) (\gamma_{13} + \gamma_{14} (\tau_1 \cdot \tau_2))$$









Choosing Observables

What to fit c_D and c_E to?

- Uncorrelated observables.
- Probe properties of light nuclei: ⁴He E_B.
- Probe T = 3/2 physics: $n-\alpha$ scattering phase shifts.



JEL et al, PRL **116**, 062501 (2016)

QMC Methods + Chiral EFT Interactions - The Rug



First Results



JEL et al, PRL **116**, 062501 (2016)

First Results



JEL et al, PRL **116**, 062501 (2016)

First Results



JEL et al, PRL **116**, 062501 (2016)

Energies and charge radii of selected nuclei up to ¹⁶O well reproduced.



D. Lonardoni, J. Carlson, S. Gandolfi, JEL, K. E. Schmidt, A. Schwenk, X. Wang, arXiv:1709.09143 [nucl-th] (2017)

Short-Range Correlations (SRCs) & EMC Effect

Deep inelastic scattering (DIS) cross section for EM interactions of charged leptons with nuclear targets:

$$\frac{\mathrm{d}^2\sigma}{\mathrm{d}Q^2\mathrm{d}x} \propto \frac{4\pi\alpha^2}{Q^4} \frac{F_2^A(x,Q^2)}{x}$$

Bjorken $x = Q^2/(2p \cdot q)$, and $Q^2 = -q^2$ are defined in terms of the target four-momentum p and the momentum transfer from the lepton to the target, q.

The ratio
$$R_{EMC}(A, x) = \frac{2F_2^A(x, Q^2)}{AF_2^d(x, Q^2)} \sim \frac{2\sigma^A}{A\sigma^d}$$
 plays an important role.

One-picture/One-sentence summary



J. J. Aubert et al. (EMC), Phys. Lett. B. **123**, 275

"We are not aware of any published detailed prediction presently available which can explain the behaviour of these data." The strength of the EMC effect is given in terms of the slope:

 $dR_{EMC}(A, x)/dx|_{0.35 < x < 0.7} \sim d(\sigma^{A}/\sigma^{d})/dx|_{0.35 < x < 0.7}$



Short-Range Correlations And The EMC Effect

SRC scaling factor
$$a_2(A, x) \equiv \frac{2\sigma^A}{A\sigma^d}|_{1.5 < x < 2}$$
.

 $dR_{\rm EMC}/dx \propto a_2$



J.-W. Chen & W. Detmold, Phys. Lett. B 625, 165 (2005):

Structure functions factorize: $F_2^A(x)/A = F_2^N(x) + g_2(A, \Lambda)f_2(x, \Lambda)$ $g_2(A, \Lambda) = \frac{1}{A} \langle A | (N^{\dagger}N)^2 | A \rangle_{\Lambda}$

> J.-W. Chen, W. Detmold, JEL, A. Schwenk, arXiv:1607.03065 [hep-ph] (2016) (PRL in press):

$$a_2(A, x > 1) = \frac{g_2(A, \Lambda)}{g_2(2, \Lambda)} \Rightarrow \frac{dR_{EMC}}{dx} \propto a_2.$$

EFT Arguments In Detail

$$F_2^A(x,Q^2) = \sum_i Q_i^2 x q_i^A(x,Q)$$
$$q_i^A(x,Q) \text{ nuclear PDFs}$$

Leading twist (twist-2) expansion of PDFs + Operator product expansion:

$$\langle A; p | \mathcal{O}^{\mu_0 \cdots \mu_n} | A; p \rangle = \langle x^n \rangle_A (Q) p^{(\mu_0} \cdots p^{\mu_n)}$$

$$\langle x^n \rangle_A(Q) = \int_{-A}^{A} dx x^n q_A(x, Q)$$
 Mellin transform

$$\mathcal{O}^{\mu_0\cdots\mu_n}=\bar{q}\gamma^{(\mu_0}\mathrm{i}D^{\mu_1}\cdots\mathrm{i}D^{\mu_n})q$$

Matching QCD operators to hadronic operators.

$$\mathcal{O}^{\mu_0\cdots\mu_n} \to : \langle x^n \rangle_N M^n v^{(\mu_0}\cdots v^{\mu_n)} N^\dagger N [1 + \alpha_n N^\dagger N] \\ + \langle x^n \rangle_\pi \pi^\alpha i \partial^{(\mu_0}\cdots i \partial^{\mu_n)} + \cdots :$$

 $Q \gg \Lambda \gg P$

 $\left\langle x^{n}\right\rangle _{A}\left(Q\right)=\left\langle x^{n}\right\rangle _{N}\left(Q\right)\left[A+\alpha_{n}(\Lambda,Q)\left\langle A|\colon(N^{\dagger}N)^{2}:\left|A\right\rangle _{\Lambda}\right]$

Inverse Mellin transform $q_A(x,Q)/A \simeq q_N(x,Q) + g_2(A,\Lambda)\tilde{q}_2(x,Q,\Lambda)$ $F_2^A(x,Q^2) \simeq F_2^N(x,Q^2) + g_2(A,\Lambda)f_2(x,Q^2,\Lambda)$

For quasielastic kinematics

$$\sigma_A/A \simeq \sigma_N + g_2(A, \Lambda)\sigma_2(\Lambda)$$

$$a_2(A, x > 1) \simeq \frac{g_2(A, \Lambda)}{g_2(2, \Lambda)}$$

$$\frac{\mathrm{d}R_{\mathrm{EMC}}(A,x)}{\mathrm{d}x} \simeq C(x)[a_2(A)-1]$$

Two-Body Distribution Functions (g_2)

$$g_2(A,\Lambda) = \rho_{2,1}(A,r=0)/A, \ \rho_{2,1}(A,r) \equiv \frac{1}{4\pi r^2} \left\langle \Psi_0 \right| \sum_{i < j} \delta(r - r_{ij}) \left| \Psi_0 \right\rangle$$

Scale and scheme dependent


SRC Correlation Factors

$$a_2 \equiv \lim_{r \to 0} \frac{2\rho_{2,1}(A, r)}{A\rho_{2,1}(2, r)}$$

Scale and scheme *independent*!



J.-W Chen, W. Detmold, JEL, A. Schwenk, arXiv:1607.03065 [hep-ph] (2016)

SRC Correlation Factors

$$a_2 \equiv \lim_{r \to 0} \frac{2\rho_{2,1}(A, r)}{A\rho_{2,1}(2, r)}$$

A prediction for a_2 in ${}^{40}Ca$: Saturates as expected.



- An exciting time in nuclear physics thanks to new experiments, many-body methods, and chiral EFT.
- QMC methods with chiral EFT interactions: A powerful set of tools to advance nuclear physics.
- EFT predicts (postdicts) the linear relationship between
- We can make scheme- and scale-independent predictions for SRC scaling factors.
- Our results suggest that EFT can shed light on the existence of a_3 .









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EST 1949



Thank you for your attention!