# Quantum Algorithms for Quantum Many-Body Systems

Dean Lee Facility for Rare Isotope Beams Michigan State University

NP-AMO QIS Workshop University of Massachusetts Boston January 13, 2024







# Outline

Nuclear lattice effective field theory What problems are beyond classical computing? Rodeo algorithm Controlled reversal gates Multi-state rodeo algorithm Fusion method Quantum evaporative cooling Wavefunction matching Adiabatic perturbation theory Nuclear lattice simulations on quantum computers Summary

### Lattice effective field theory



D.L, Prog. Part. Nucl. Phys. 63 117-154 (2009); D.L., arXiv:2501.03303 Lähde, Meißner, Nuclear Lattice Effective Field Theory (2019), Springer



### Chiral effective field theory

Construct the effective potential order by order



#### $a = 1.315 \,\mathrm{fm}$



Li, Elhatisari, Epelbaum, D.L., Lu, Meißner, PRC 98, 044002 (2018)

### **Binding energies**



Elhatisari, Bovermann, Ma, Epelbaum, Frame, Hildenbrand, Krebs, Lähde, D.L., Li, Lu, M. Kim, Y. Kim, Meißner, Rupak, Shen, Song, Stellin, Nature 630, 59 (2024)

#### Charge radii



Elhatisari, Bovermann, Ma, Epelbaum, Frame, Hildenbrand, Krebs, Lähde, D.L., Li, Lu, M. Kim, Y. Kim, Meißner, Rupak, Shen, Song, Stellin, Nature 630, 59 (2024)

### <u>Emergent geometry and duality of <sup>12</sup>C</u>



Shen, Elhatisari, Lähde, D.L., Lu, Meißner, Nature Commun. 14, 2777 (2023)



Liquid-vapor critical point

$$
T_c = 15.80(0.32)(1.60) \text{ MeV}
$$

$$
\rho_c = 0.089(04)(18) \text{ fm}^{-3}
$$

$$
\mu_c = -22.20(0.44)(2.20) \text{ MeV}
$$

$$
P_c = 0.260(05)(30) \text{ MeV fm}^{-3}
$$

Lu, Li, Elhatisari, D.L., Drut, Lähde, Epelbaum, Meißner, Phys. Rev. Lett. 125, 192502 (2020)

# What problems are beyond classical computing?

 $\exp(-iHt) \rightarrow \exp(-H\tau)$ 



# Rodeo algorithm



Choi, D.L., Bonitati, Qian, Watkins, PRL 127, 040505 (2021)

Consider a single qubit and a Hadamard gate

$$
U = \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}}\\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{bmatrix} = U^{\dagger} = U^{-1}
$$

Consider another unitary operation that is a diagonal phase rotation

$$
R(E_{\text{obj}}, E, t) = \begin{bmatrix} 1 & 0\\ 0 & e^{-it(E_{\text{obj}} - E)} \end{bmatrix}
$$

We then have

$$
U^{\dagger}R(E_{\text{obj}}, E, t)U = \begin{bmatrix} \frac{1}{2} + \frac{1}{2}e^{-it(E_{\text{obj}} - E)} & \frac{1}{2} - \frac{1}{2}e^{-it(E_{\text{obj}} - E)}\\ \frac{1}{2} - \frac{1}{2}e^{-it(E_{\text{obj}} - E)} & \frac{1}{2} + \frac{1}{2}e^{-it(E_{\text{obj}} - E)} \end{bmatrix}
$$

Let us now start in the  $\begin{bmatrix} 0 \\ 1 \end{bmatrix}$  state and perform these unitary operations

$$
U^{\dagger}R(E_{\text{obj}}, E, t)U\begin{bmatrix}0\\1\end{bmatrix} = \begin{bmatrix} \frac{1}{2} - \frac{1}{2}e^{-it(E_{\text{obj}} - E)}\\ \frac{1}{2} + \frac{1}{2}e^{-it(E_{\text{obj}} - E)} \end{bmatrix}
$$

and then project back to the  $\begin{bmatrix} 0 \\ 1 \end{bmatrix}$  state

$$
\begin{bmatrix} 0 & 0 \ 0 & 1 \end{bmatrix} U^{\dagger} R(E_{\text{obj}}, E, t) U \begin{bmatrix} 0 \ 1 \end{bmatrix} = \begin{bmatrix} 0 \\ \frac{1}{2} + \frac{1}{2} e^{-it(E_{\text{obj}} - E)} \end{bmatrix}
$$

This projection is done via quantum measurement and the success probability is

$$
P(E_{\text{obj}}, E, t) = \left| \frac{1}{2} + \frac{1}{2} e^{-it(E_{\text{obj}} - E)} \right|^2 = \cos^2 \left[ \frac{t(E_{\text{obj}} - E)}{2} \right]
$$



 $P(E_{\text{obj}}, E, 14.2023)$ 







Let us couple this qubit, which we call the "arena" or "ancilla" qubit, to another system that we call the "object". We also promote the 2 x 2 matrices to become 2 x 2 matrices of operators acting on the object.

$$
\begin{bmatrix}\n\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\
\frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}}\n\end{bmatrix}\n\rightarrow\n\begin{bmatrix}\n\frac{\hat{I}}{\sqrt{2}} & \frac{\hat{I}}{\sqrt{2}} \\
\frac{\hat{I}}{\sqrt{2}} & -\frac{\hat{I}}{\sqrt{2}}\n\end{bmatrix}
$$
\n
$$
\begin{bmatrix}\n1 & 0 \\
0 & e^{-it(E_{\text{obj}}-E)}\n\end{bmatrix}\n\rightarrow\n\begin{bmatrix}\n\hat{I} & 0 \\
0 & e^{-it(\hat{H}_{\text{obj}}-E)}\n\end{bmatrix}
$$

We then consider the same combination

$$
\begin{bmatrix}\n\frac{\hat{I}}{\sqrt{2}} & \frac{\hat{I}}{\sqrt{2}} \\
\frac{\hat{I}}{\sqrt{2}} & -\frac{\hat{I}}{\sqrt{2}}\n\end{bmatrix}\n\begin{bmatrix}\n\hat{I} & 0 \\
0 & e^{-it(\hat{H}_{\text{obj}}-E)}\n\end{bmatrix}\n\begin{bmatrix}\n\frac{\hat{I}}{\sqrt{2}} & \frac{\hat{I}}{\sqrt{2}} \\
\frac{\hat{I}}{\sqrt{2}} & -\frac{\hat{I}}{\sqrt{2}}\n\end{bmatrix}
$$

We start from the state  $\begin{bmatrix} 0 \\ |\psi_{\text{init}}\rangle \end{bmatrix}$  and we perform the operations and then measure if the arena qubit is in the  $\begin{bmatrix} 0 \\ 1 \end{bmatrix}$  state

$$
\begin{bmatrix} 0 & 0 \\ 0 & \hat{I} \end{bmatrix} \begin{bmatrix} \frac{\hat{I}}{\sqrt{2}} & \frac{\hat{I}}{\sqrt{2}} \\ \frac{\hat{I}}{\sqrt{2}} & -\frac{\hat{I}}{\sqrt{2}} \end{bmatrix} \begin{bmatrix} \hat{I} & 0 \\ 0 & e^{-it(\hat{H}_{\text{obj}}-E)} \end{bmatrix} \begin{bmatrix} \frac{\hat{I}}{\sqrt{2}} & \frac{\hat{I}}{\sqrt{2}} \\ \frac{\hat{I}}{\sqrt{2}} & -\frac{\hat{I}}{\sqrt{2}} \end{bmatrix} \begin{bmatrix} 0 \\ |\psi_{\text{init}} \rangle \end{bmatrix} = \begin{bmatrix} 0 \\ \left[\frac{1}{2} + \frac{1}{2}e^{-it(\hat{H}_{\text{obj}}-E)}\right] |\psi_{\text{init}} \rangle \end{bmatrix}
$$

By repeated successful measurements with random values of  $t$ , we reduce the spectral weight of eigenvectors with energies that do not match  $E$ .

The convergence is exponential. For  $N$  cycles of the rodeo algorithm, the suppression factor for undesired energy states is  $1/4<sup>N</sup>$ .



FIG. 1. (color online) Circuit diagram for the rodeo algorithm. The object system starts in an arbitrary state  $|\psi_I\rangle$ . Each of the arena qubits are initialized in the state  $|1\rangle$  and operated on by a Hadamard gate H. We use each arena qubit  $n = 1, \dots, N$  for the controlled time evolution of the object Hamiltonian,  $H_{obj}$ , for time  $t_n$ . This is followed by a phase rotation  $P(Et_n)$  on arena qubit *n*, another Hadamard gate H, and then measurement.

Choi, D.L., Bonitati, Qian, Watkins, PRL 127, 040505 (2021)

Initial-state spectral function and state preparation. The example shown below is for a 1D Heisenberg chain with ten sites, antiferromagnetic interactions, and uniform magnetic field.



FIG. 4. (color online) Initial-state spectral function for the Heisenberg model. We plot the initial-state spectral function using the rodeo algorithm for the Heisenberg spin chain with 3 (thin blue line), 6 (thick green line), and 9 (medium red line) cycles. We have averaged over 20 sets of Gaussian random values for  $t_n$  with  $t_{\rm RMS}$  = 5. For comparison, we also show the exact initial-state spectral function with black open circles.

$$
\ket{\psi_{\mathrm{init}}}=\ket{0101010101}
$$

### Controlled reversal gates

A reversal gate,  $R$ , is a product of single qubit gates that anticommutes with some subset of the terms in a Hamiltonian.

$$
RH=-HR
$$

We note that

$$
Re^{-iHt}R = e^{+iHt}
$$

Let  $C_R$  be the controlled reversal gate that performs R if the ancilla qubit is in the 1 state and does nothing if the ancilla qubit is in the 0 state.

 $C_R$  toggles the flow of time back and forth. With  $C_R$  we can reduce the number of gates needed for state preparation.

Our Hamiltonian has the form

$$
H_{\rm obj} = c_1 X_1 \otimes Z_2 + c_2 Z_1 \otimes X_2
$$
  

$$
c_1 = 2.5, \ c_2 = 1.5
$$

The time evolution of the Hamiltonian can be expressed with this simple circuit



Using controlled reversal gates, one cycle of the rodeo algorithm is implemented as



The controlled reversal gates provide a fivefold reduction in the number of gates. The comparison is made with respect to Qiskit-transpiled code without controlled reversal gates.

Bee-Lindgren, Qian, DeCross, Brown, Gilbreth, Watkins, Zhang, D.L., arXiv:2208.13557





# Multi-state rodeo algorithm

We can prepare an arbitrary linear combination of two eigenvectors with two different energies.



Bee-Lindgren, Qian, et al., work in progress

This allows us to create the general superposition state

$$
\ket{\theta,\phi} = \cos(\theta/2)\ket{E} + e^{i\phi}\sin(\theta/2)\ket{E'}
$$

We can now measure the expectation value of any observable  ${\cal O}$ 

$$
\langle \theta, \phi | O | \theta, \phi \rangle = \cos^{2}(\theta/2) \langle E | O | E \rangle + \sin^{2}(\theta/2) \langle E' | O | E' \rangle
$$

$$
+ \Re[e^{i\phi} \sin(\theta) \langle E | O | E' \rangle]
$$

From this we can extract the transition matrix element

 $\langle E|O|E'\rangle$ 

## Fusion method



Figure by M. Patkowski

Patkowski, Ayyildiz, Hunt, D.L., work in progress

### Quantum evaporative cooling





McRae, Hjorth-Jensen, D.L., work in progress

# Wavefunction matching



Elhatisari, Bovermann, Ma, Epelbaum, Frame, Hildenbrand, Krebs, Lähde, D.L., Li, Lu, M. Kim, Y. Kim, Meißner, Rupak, Shen, Song, Stellin, Nature 630, 59 (2024)

Adiabatic perturbation theory

$$
H = H_0 + H_1
$$
  
\n
$$
H_1(t) = f(t)H_1 \begin{cases} f(0) = 0, f'(0) = 0, \cdots \\ f(t_F) = 1, f'(t_F) = 0, \cdots \end{cases}
$$

$$
T \exp[-i \int_0^{t_F} dt (H_0 + H_1(t))]
$$
  
=  $\sum_k \left[ \int_0^{t_F} dt_1 \cdots \int_{t_{k-1}}^{t_F} dt_k \right] e^{-iH_0(t_F - t_k)} H_1(t_k) e^{-iH_0(t_k - t_{k-1})} \cdots H_1(t_1) e^{-iH_0 t_1}$ 

Cariello, Given, Hjorth-Jensen, D.L., work in progress

# Nuclear lattice simulations on quantum computers



### Summary

We introduced nuclear lattice effective field theory and discussed the possibility of future calculations of spectral functions and real time dynamics on quantum computers. We then discussed the rodeo algorithm and introduced the concept of controlled reversal gates for reducing circuit depth. We showed some applications of the rodeo algorithm on real quantum devices and considered the multi-state rodeo algorithm for preparing arbitrary linear combinations of energy eigenstates in order to compute transition matrix elements. We briefly introduced the fusion method, quantum evaporative cooling, wavefunction matching, and adiabatic perturbation theory. We concluded with an outlook on future prospects for nuclear lattice simulations on quantum computers.