Early Fault-Tolerant Ground State Energy Estimation for Nuclear Systems

MARINA MANEYRO

IN COLLABORATION WITH:

- GABRIEL N. PERDUE (FNAL)
- DOĞA MURAT KÜRKÇÜOĞLU (FNAL)
- ALESSANDRO ROGGERO (TRENTO)
- SAM GODWOOD (LIVERPOOL)

Motivation

On the path towards *Fault-Tolerant Quantum Computing*

Early Fault-Tolerant focus: What can we achieve in the medium term, as error rates decrease but system sizes are still limited?

Ground state estimation and preparation are key multipurpose applications of quantum computing, but scalability is a challenge

arXiv:2209.06786, 2307.03236, 1510.05494

Neutrino Physics

- Motivated by addressing challenges in Neutrino simulations: improved descriptions of nuclei
  - Component of Event Generators used in relating experimentally observed final states and underlying kinematics
  - Increased simulation precision requirements from upcoming large experiments (Hyper-Kamiokande, DUNE, JUNO)

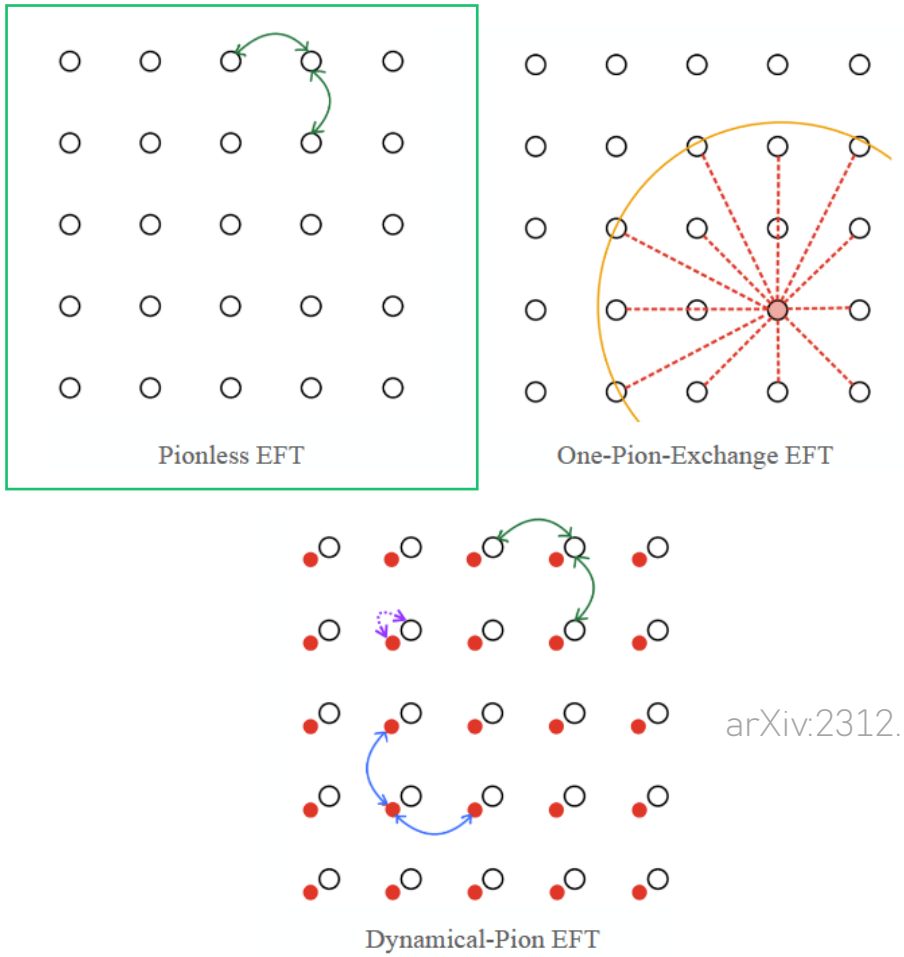
Neutrino-Nucleus Interactions

Nuclear EFTs on a lattice: protons and neutrons as non-relativistic fermions

Pionless: Strong interactions mediated by pion exchanges are not included explicitly. Short range interactions

One-Pion-Exchange: Long range interactions, truncated as rapidly decaying

Dynamical-Pion: Explicit inclusion of bosonic pion field



arXiv:2312.05344

Pionless EFT

- Well understood and suitable for light nuclei
- Prior studies confirm time evolution to be lest costly to implement in a quantum computer, relative to EFTs with explicit pion degrees of freedom
- Low significance of pion exchange contributions for momenta below pion mass ($\simeq 140\ \mathrm{MeV}$)
- Into qubit operations via Jordan-Wigner transform

Kinetic hopping term

$$H = 2DtA - t\sum_{\mathcal{J}=1}^{N_{\mathcal{J}}}\sum_{\langle i,j\rangle}^{M}\left[c_{i,\mathcal{J}}^{\dagger}c_{j,\mathcal{J}} + c_{i,\mathcal{J}}^{\dagger}c_{j,\mathcal{J}}\right]$$

$$+\frac{1}{2}C_0\sum_{\mathcal{J}\neq\mathcal{J}'}^{N_{\mathcal{J}}}\sum_{i=1}^{M} n_{i,\mathcal{J}}n_{i,\mathcal{J}'}$$

Two-nucleon interaction

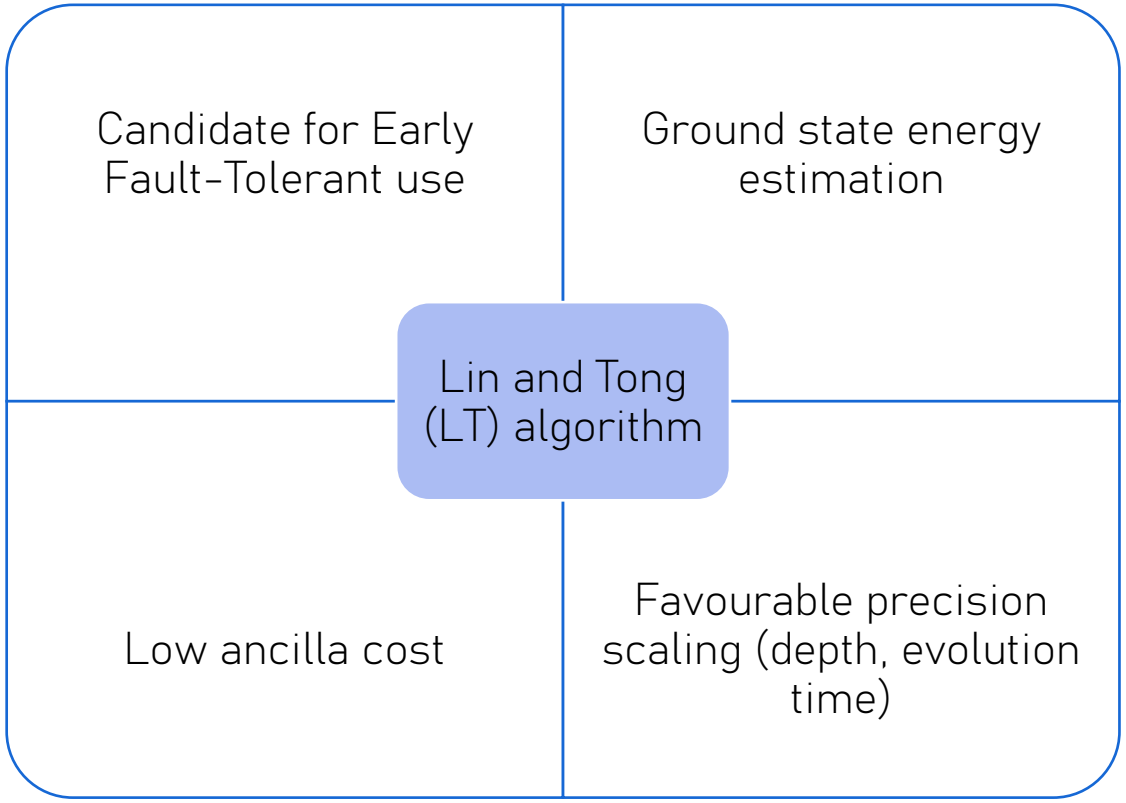
$$+\frac{D_0}{6}\sum_{\mathcal{J}\neq\mathcal{J}'\neq\mathcal{J}''}^{N_{\mathcal{J}}}\sum_{i=1}^{M} n_{i,\mathcal{J}}n_{i,\mathcal{J}'}n_{i,\mathcal{J}''}\ ,$$

Three-nucleon interaction

arXiv:1911.06368

arXiv:2312.05344, 1906.12122

Algorithmic Approach



- Provide spectral information with $1/\varepsilon$ precision scaling
- Avoid pitfalls that make Quantum Phase Estimation unsuitable for Early Fault-Tolerant hardware (ancilla reqs., runtime)
- Relative to heuristic methods (i.e. Variational Quantum Eigensolver)
  - improved scaling, performance guarantees, no reliance on classical optimization

arXiv:2102.11340

LT algorithm

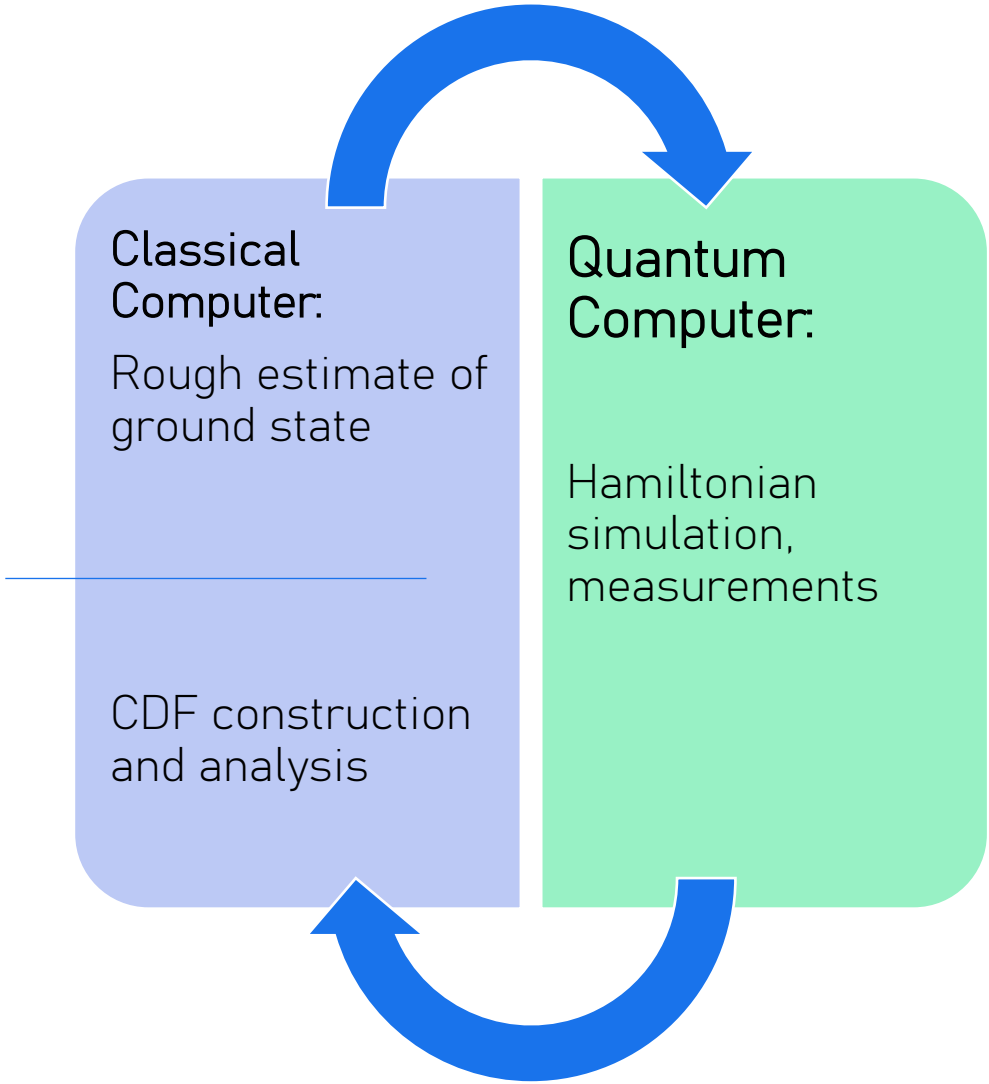
By sampling from a Quantum Computer, it provides spectral information for a given Hamiltonian

The circuit samples are used to construct a Fourier approximation of the Cumulative Distribution Function (CDF)

Classical post processing used to identify ground state energy from CDF

$$C(x) = \sum_{i:\, \lambda_i \leq x} p_i$$

$$p_i = |\langle E_i | \Psi \rangle|^2$$



LT algorithm

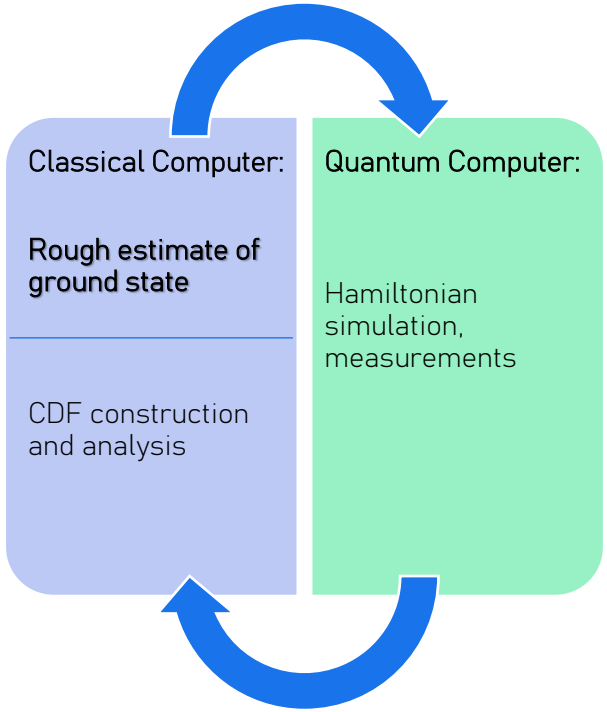
Hartree-Fock Method

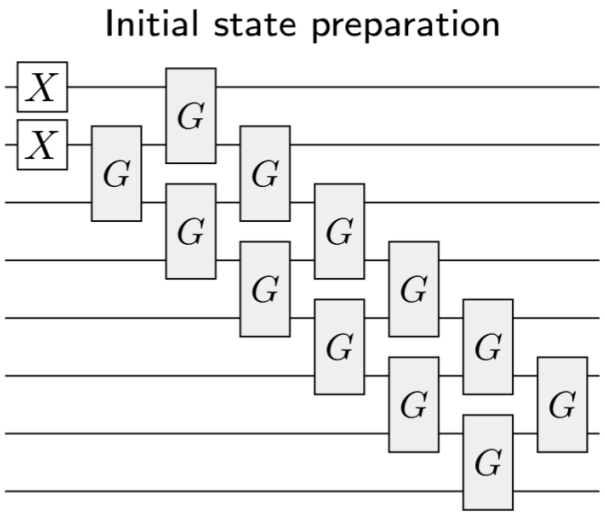
Widely used in chemistry and nuclear physics

Can provide a cheap but rough initial guess (computable for larger systems)

The goal is to provide a big enough initial overlap with the ground state, guaranteeing performance

Efficient quantum state preparation via Givens rotations



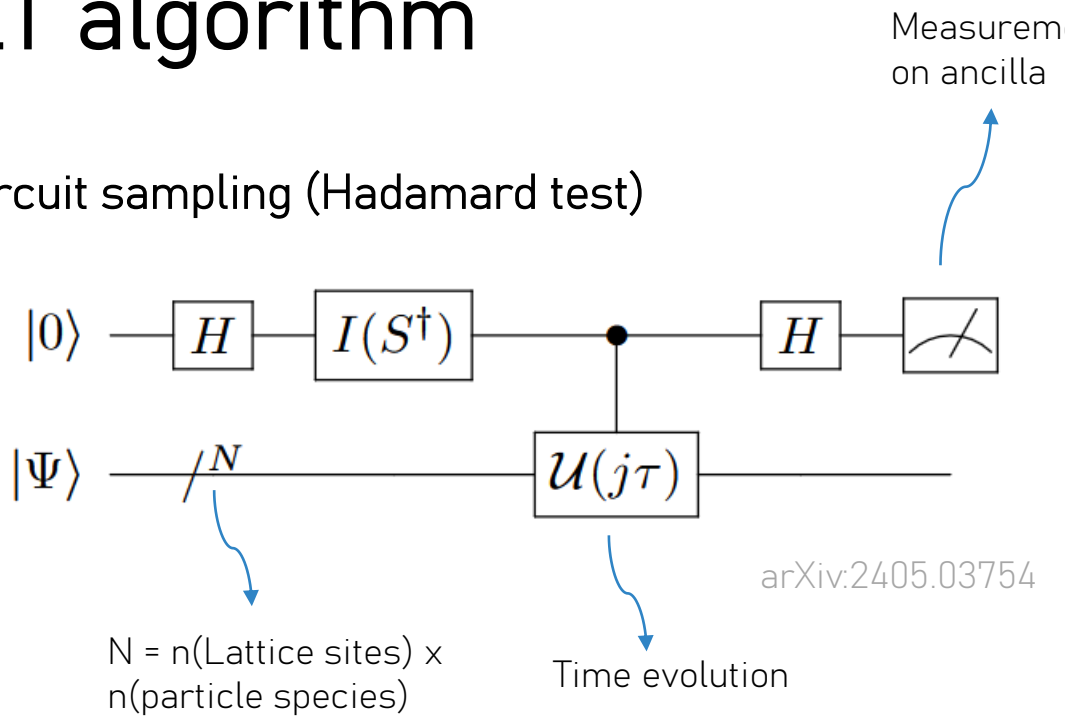


$$G = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos\theta & -\sin\theta & 0 \\ 0 & \sin\theta & \cos\theta & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

arXiv:2010.07965

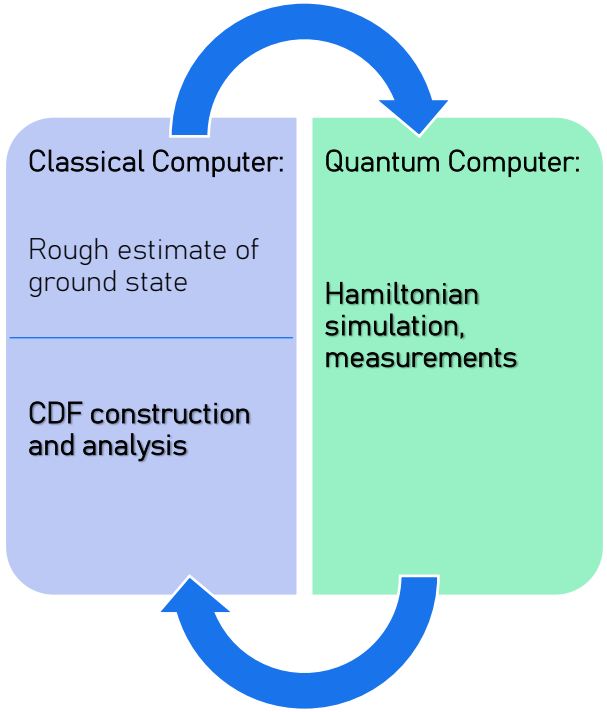
LT algorithm

Circuit sampling (Hadamard test)



Repeated samples provide expectation values of real and imaginary parts of Fourier momenta

$g_k = \langle\Psi|\mathcal{U}(j\tau)|\Psi\rangle$



CDF construction

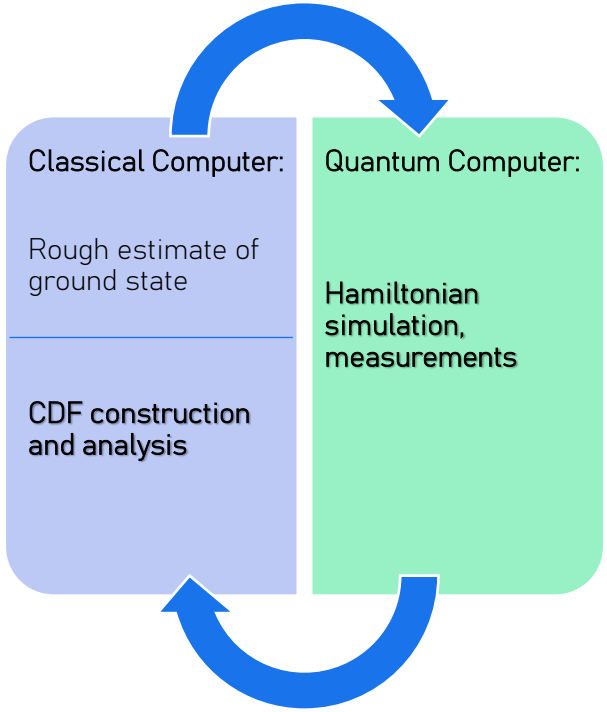
$$\tilde{C}(x) = \frac{1}{2} + 2\sum_{k=1}^{d} |F_j|\big(\mathrm{Re}[g_j]\sin jx + \mathrm{Im}[g_j]\cos jx\big)$$

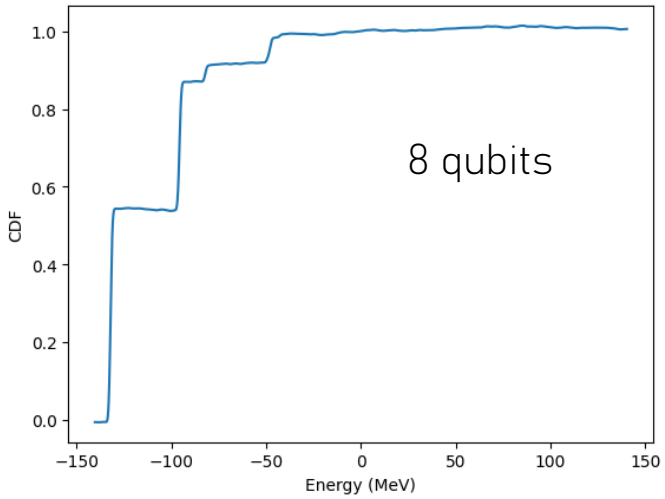
$$j \equiv 2k+1$$

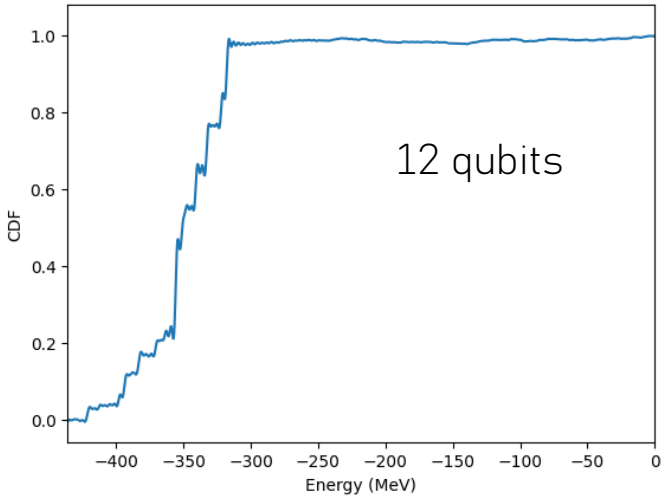
LT algorithm

CDF analysis

In smaller systems, it's straightforward to see where the jumps in the CDF occur. For larger systems, a higher number of eigenstates smooths the CDF. Hartree-Fock solutions also have lower accuracy, and it becomes harder to pinpoint eigenstate locations



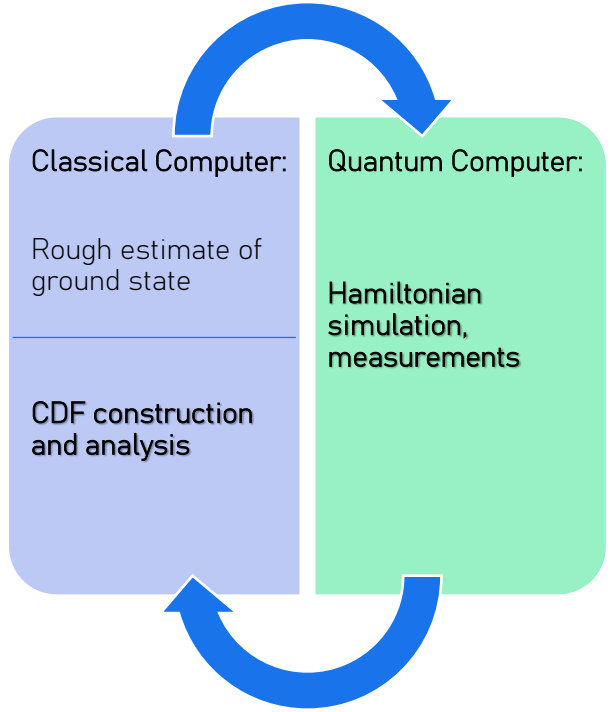


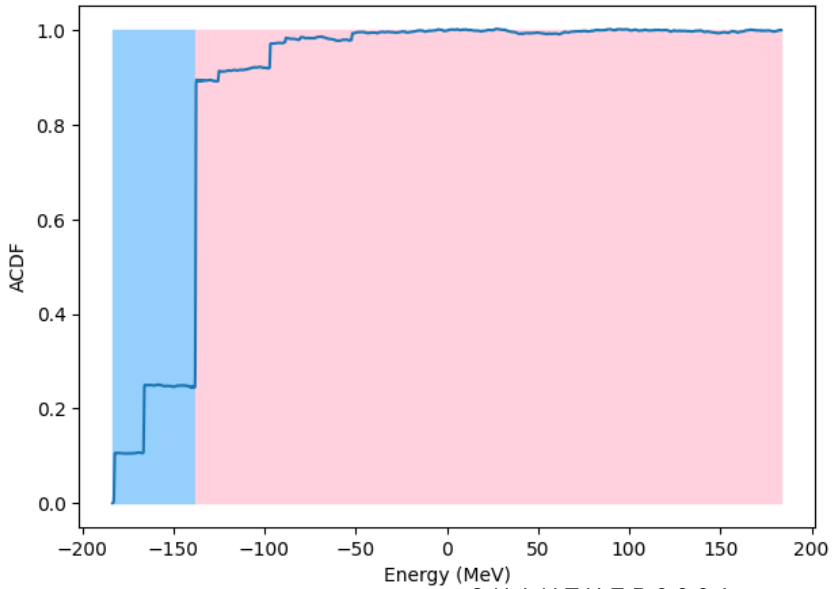


LT algorithm

CDF analysis

- Find change point (*ruptures* library for Python)
- Validate: statistical test, comparison to statistical noise
- Discard points to the right of valid jump
- Repeat on left side range (until no further valid points are found)
- Find maximum of CDF derivative on range around leftmost valid change point (precision dependent)





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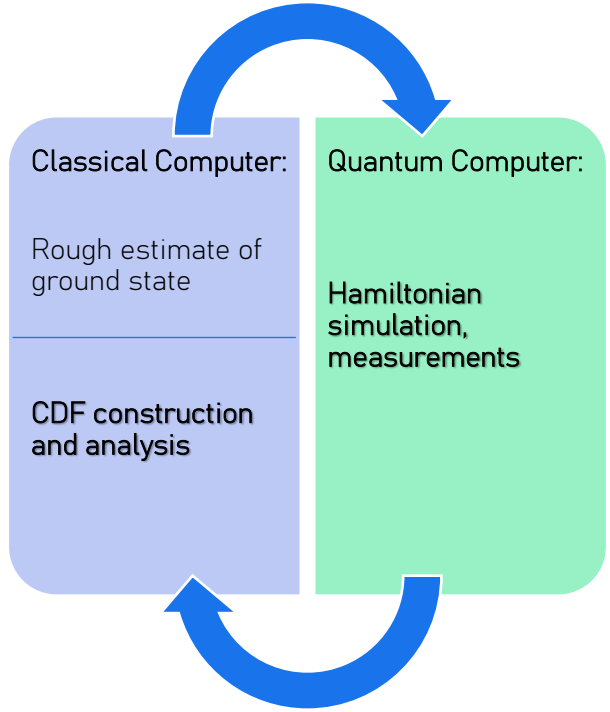

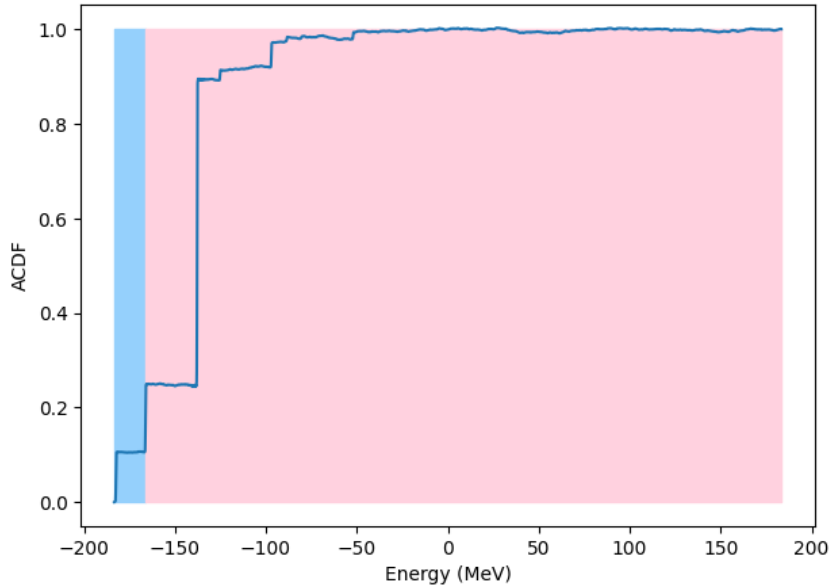

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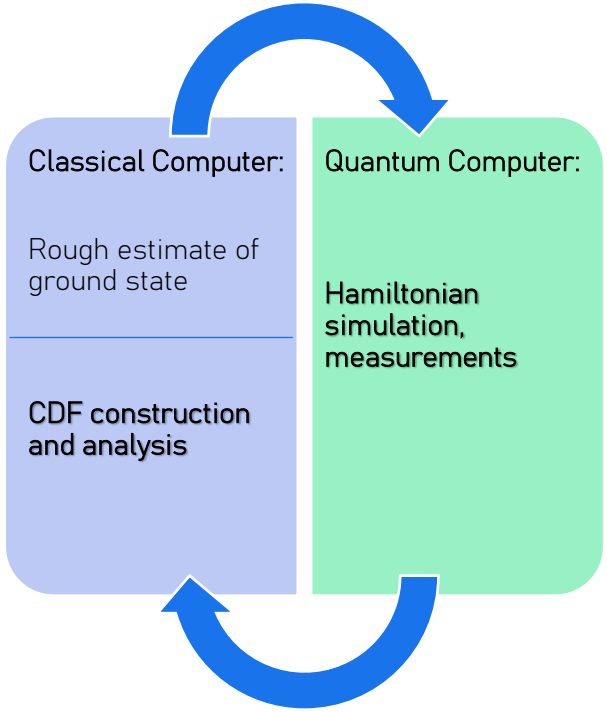
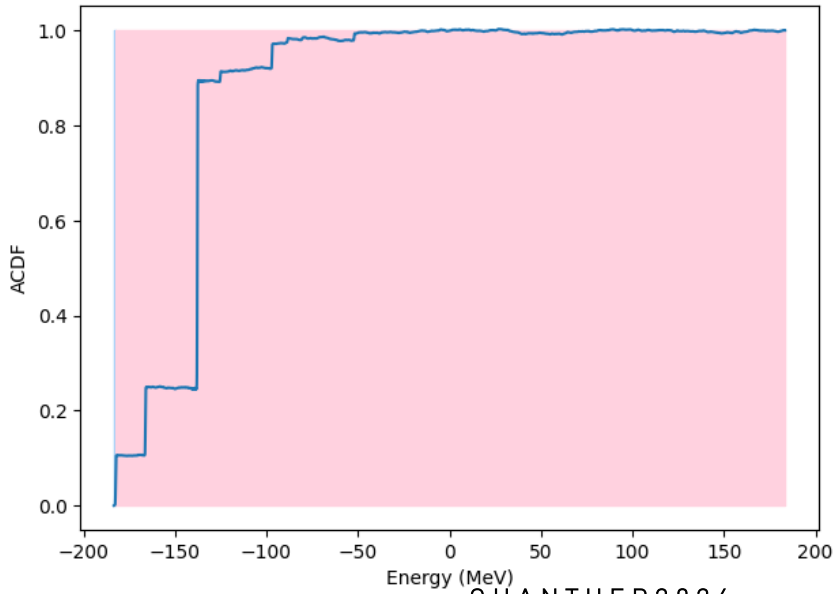
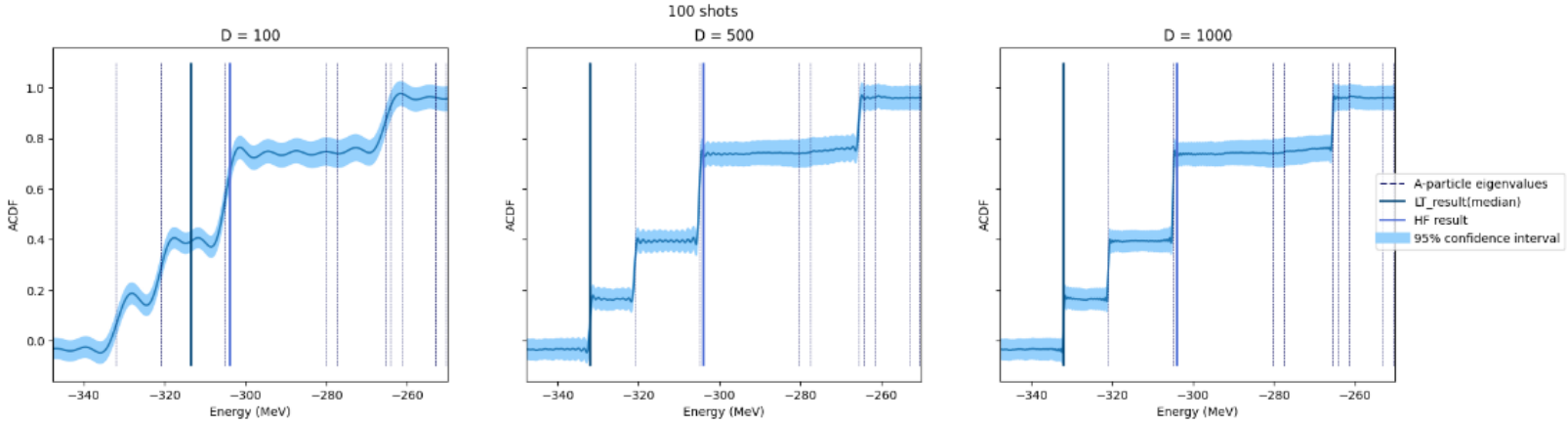


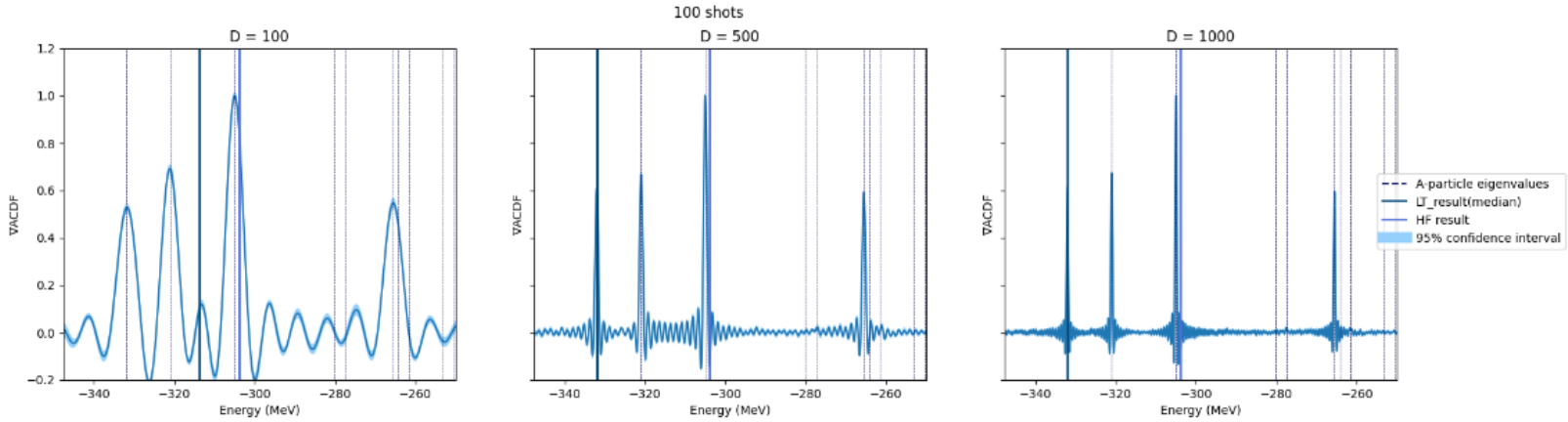


Results (prelim.)

- Testing of the complete approach for small systems in 1D and 2D lattices (up to 12 qubits)
- Assessment of performance of Cirq simulation under different conditions:
  - Infinite statistics
  - Effect of statistical noise
  - Number of terms in CDF approximation
  - Tuning of parameters
- We observe consistent improvements over Hartree-Fock outcomes, and high success rates in approximating the ground state



(a) ACDF for 3x1 lattice with three particles



(b) ∇ACDF for 3x1 lattice with three particles

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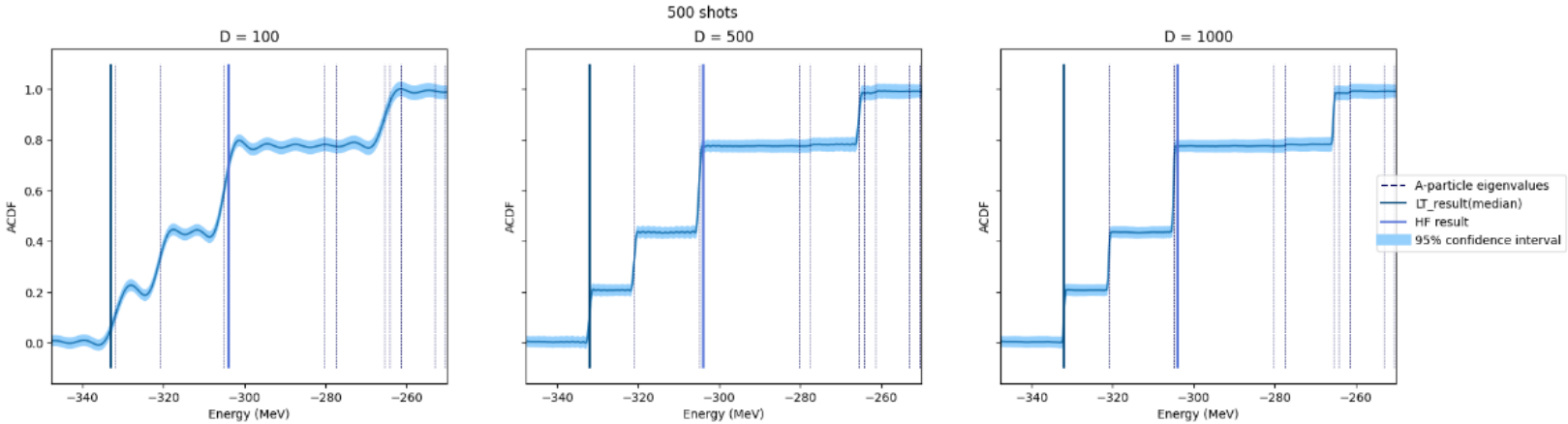

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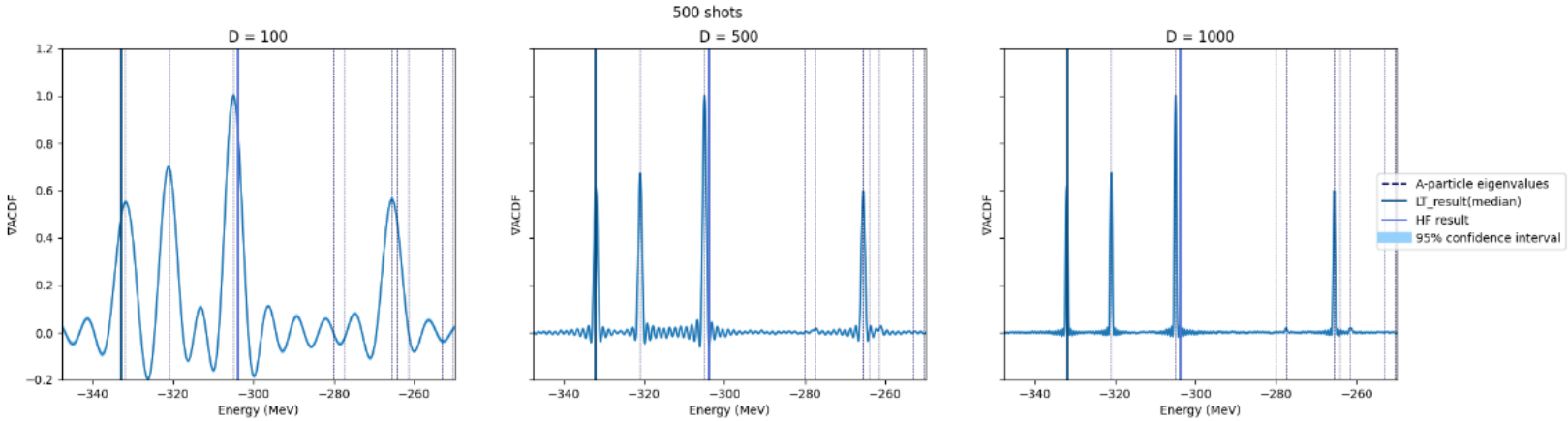

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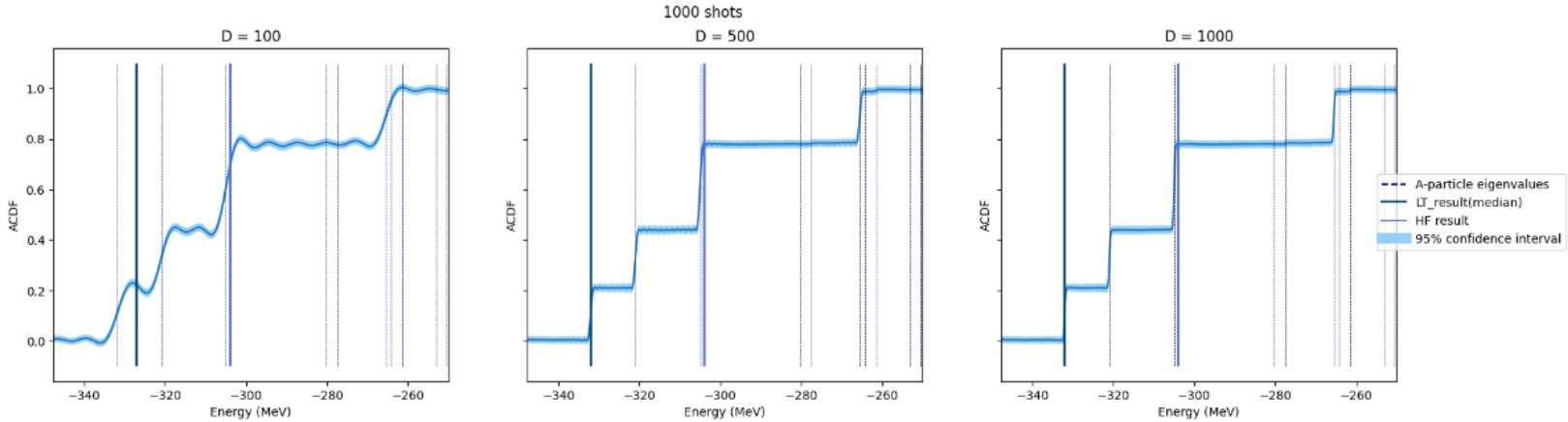

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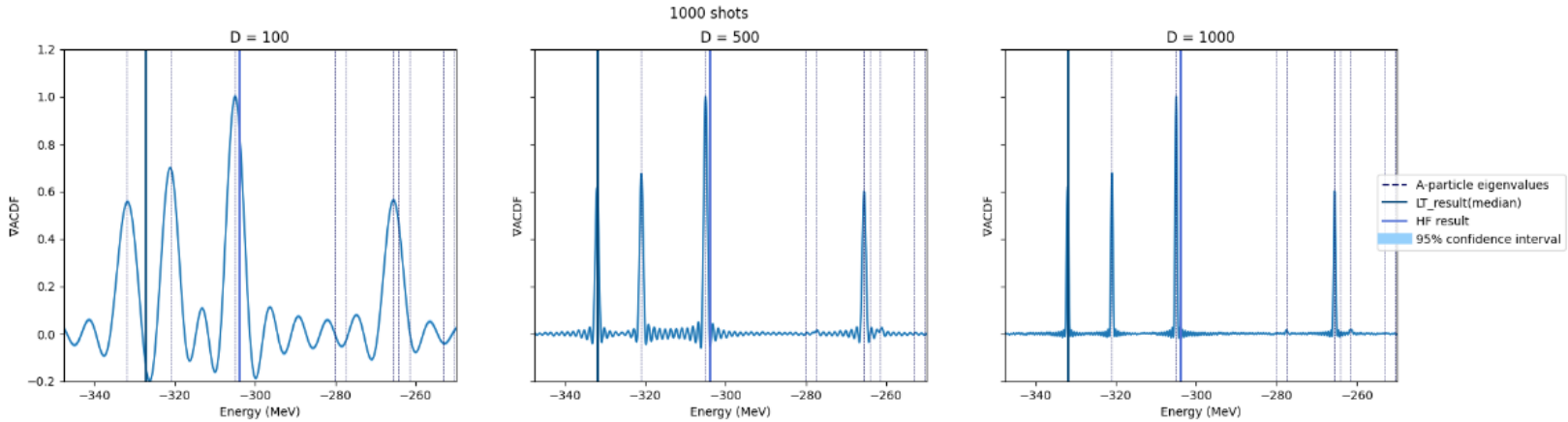
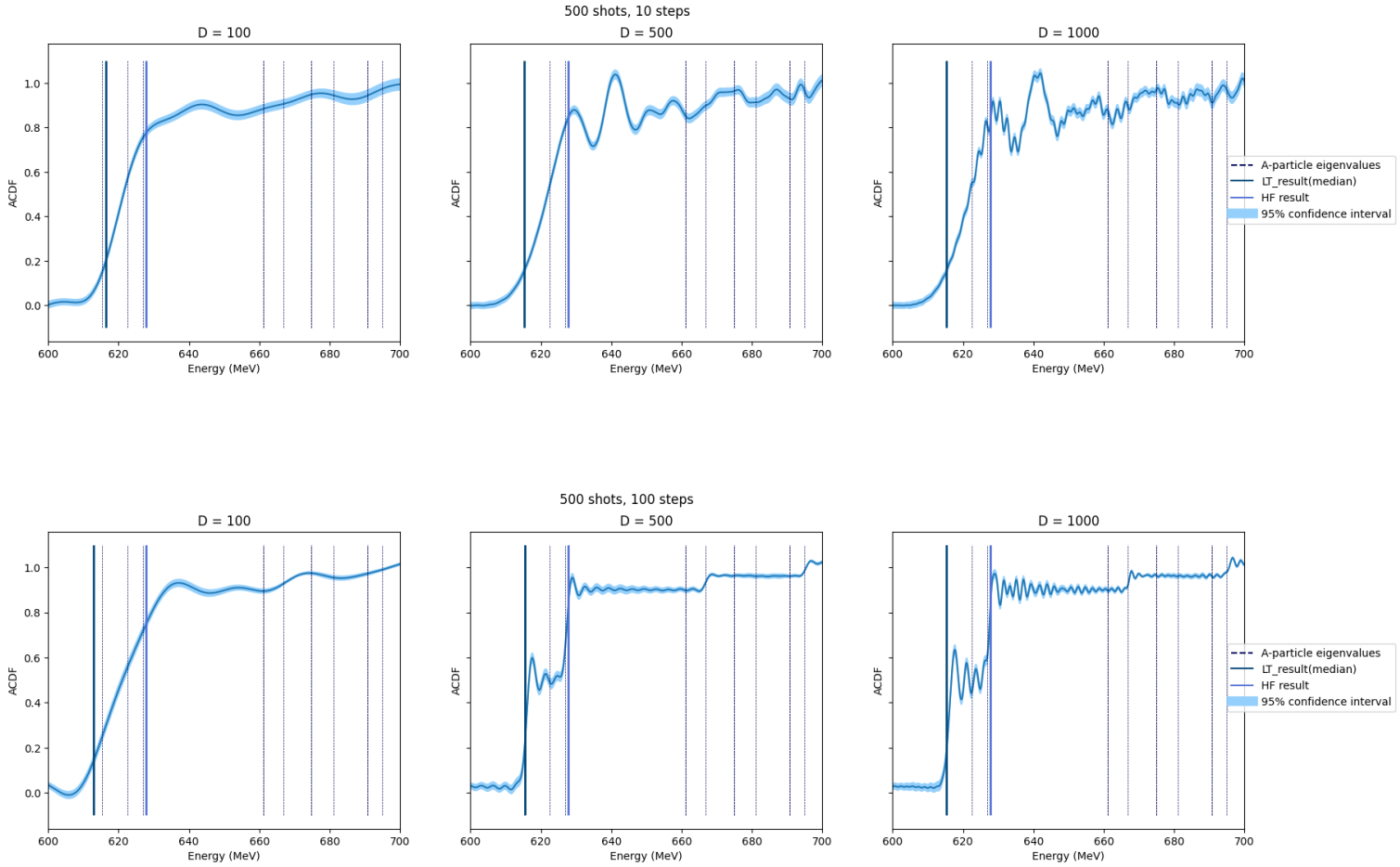


(b) ∇ACDF for 3x1 lattice with three particles

Results (prelim.)

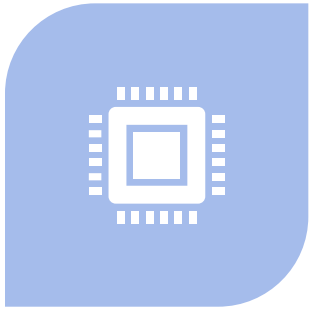
Tested outcomes for different numbers of Trotter steps in the time evolution

- Even for low (~10) step numbers the jump corresponding to the ground state can be identified from the CDF, if the initial state overlap is large enough



In progress

FURTHER EVALUATING RESULTS WITH TIME EVOLUTION USING PRODUCT FORMULA



PREPARING CODE FOR USE IN SPECIALIZED COMPUTING SUITES, TO TEST LARGER SYSTEM SIZES

CONSIDER FURTHER WORK ON EXPLICIT CIRCUIT CONSTRUCTION, COST REDUCTION

PAPER COMING SOON