Early Fault-Tolerant Ground State Energy Estimation for Nuclear Systems

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Quantum Computing

Avenue for overcoming computational limitations in Particle Physics, i.e. large combinations of states as possible solutions

Noisy Intermediate-Scale Quantum era: limited system sizes, very prone to errors

On the path towards *Fault-Tolerant Quantum Computing*: lower error rates, prevention of cascading errors

Neutrino Physics

- We're addressing challenges in Neutrino simulations, motivated by :
  - reliance on Event Generators for interpreting experiment outputs
  - increased simulation precision required by upcoming experiments (Hyper-Kamiokande, DUNE, JUNO)
  - Neutrino experiments utilize nuclei, so we need to model nuclear physics effects

arXiv:2209.06786, 2307.03236, 1510.05494

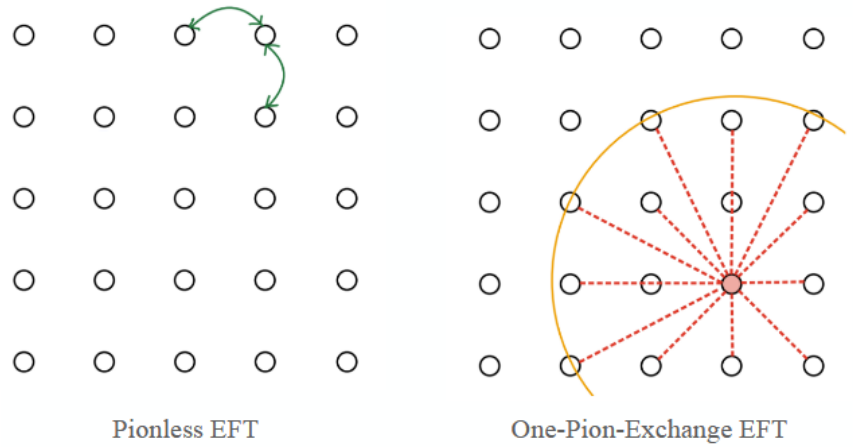
Neutrino-Nucleus Interactions

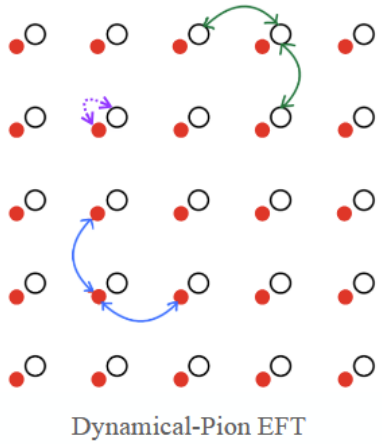
Nuclear EFTs on a lattice: protons and neutrons as non-relativistic fermions

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 ($\simeq 140\ \mathrm{MeV}$)

arXiv:2312.05344, 1906.12122

Kinetic hopping term

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

$$+ \frac{1}{2}C_0\sum_{f\neq f'}^{N_f}\sum_{i=1}^{M} n_{i,f}n_{i,f'}$$

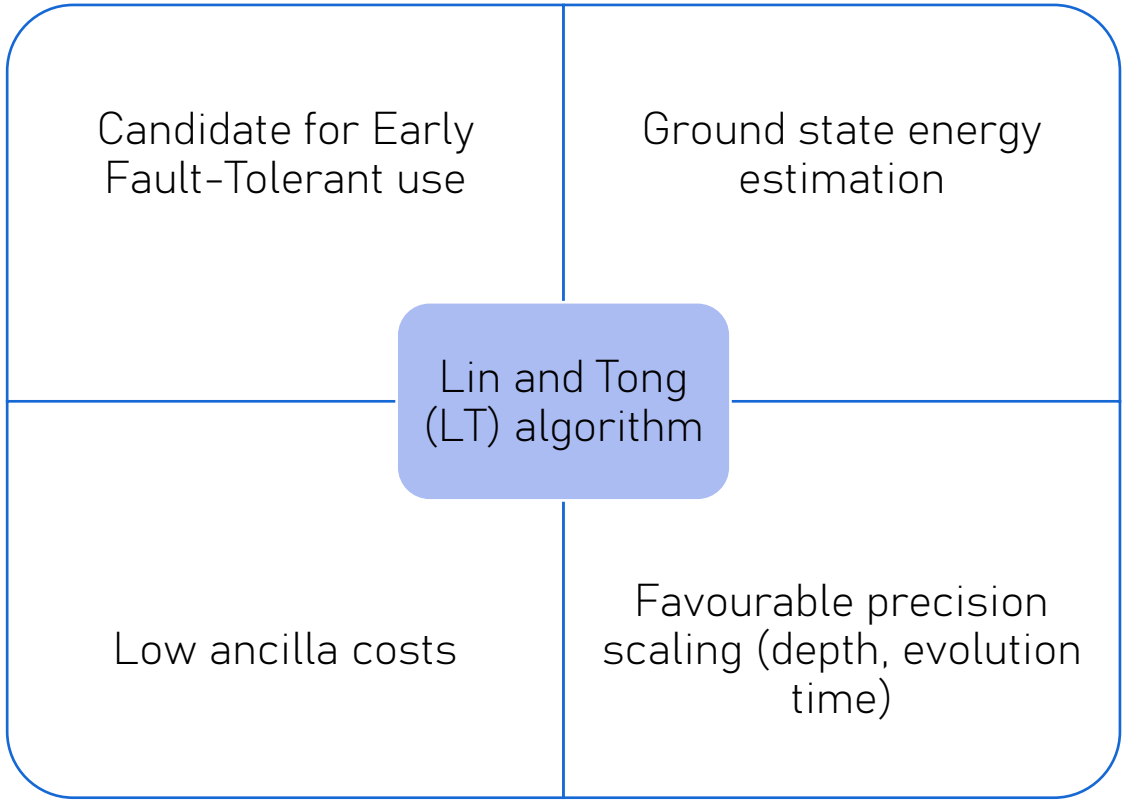
Two–nucleon interaction

$$+ \frac{D_0}{6}\sum_{f\neq f'\neq f''}^{N_f}\sum_{i=1}^{M} n_{i,f}n_{i,f'}n_{i,f''}\ ,$$

Three–nucleon interaction

arXiv:1911.06368

Quantum Simulation



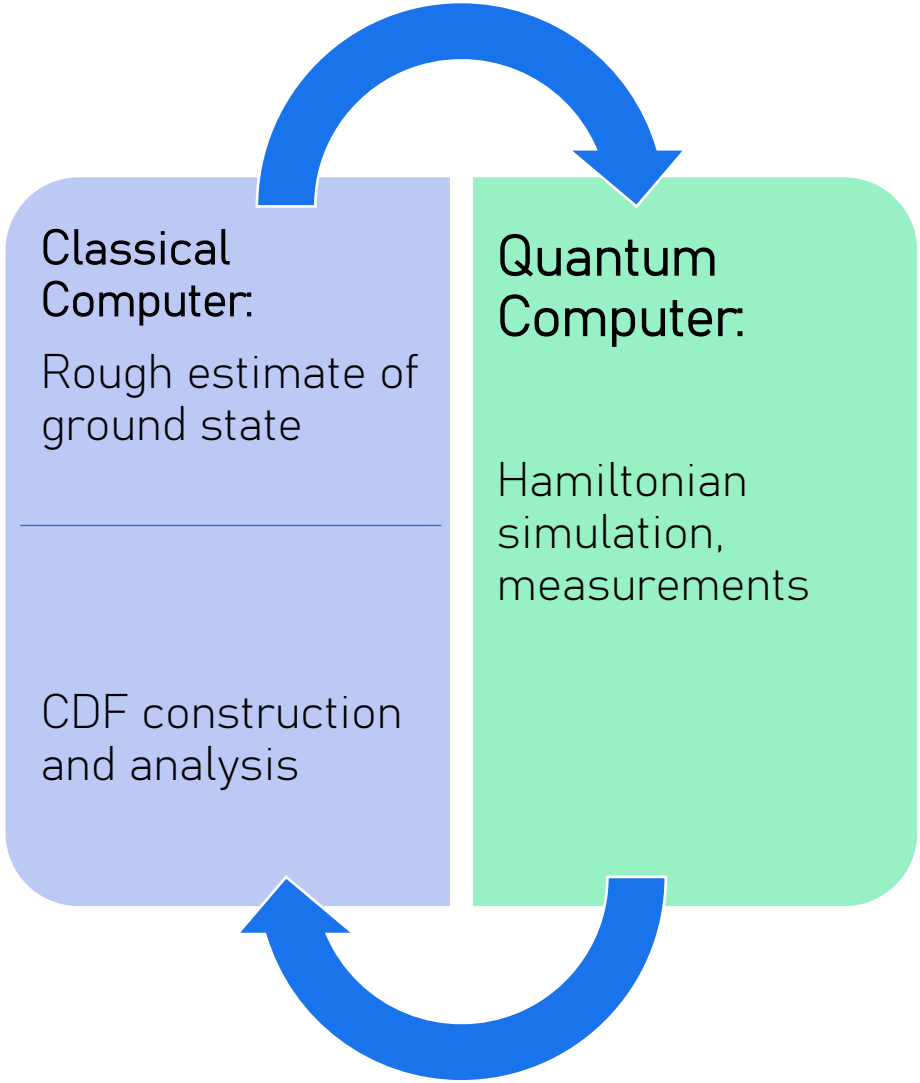
arXiv:2102.11340

LT algorithm

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

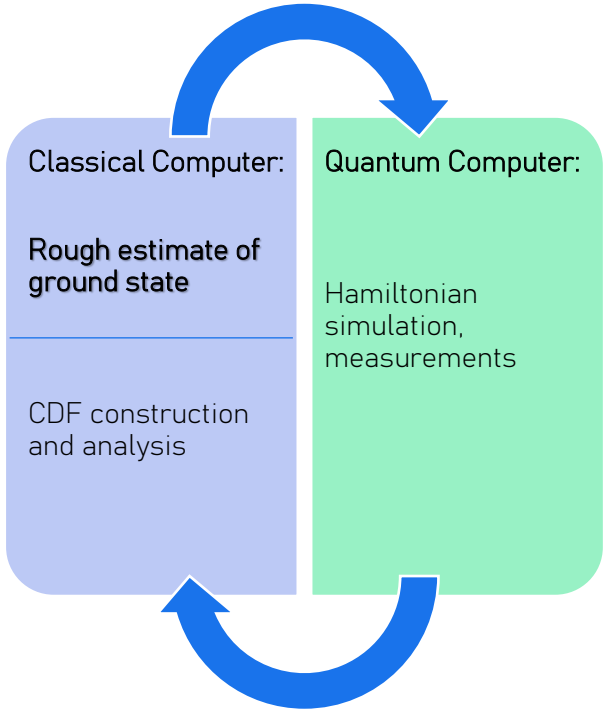
The circuit samples are used to construct a Fourier approximation of the Cumulative Distribution Function (CDF)

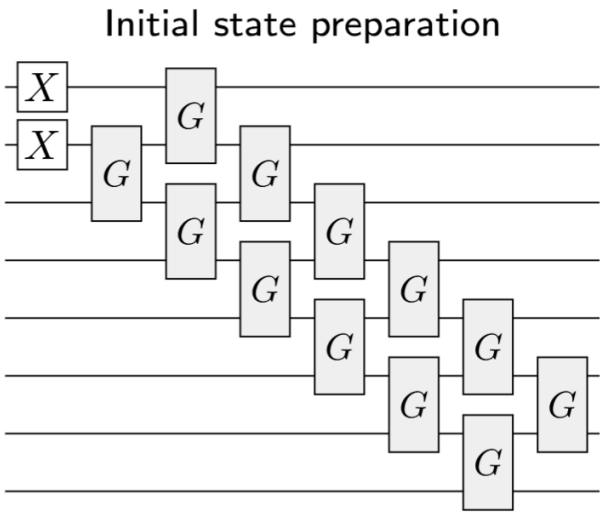
Classical post processing used to identify ground state energy from CDF



LT algorithm

Hartree-Fock Method	Widely used in chemistry and nuclear physics
	Iteratively solving a self consistent equation to estimate ground state
	Can provide a cheap but rough initial guess (mean-field approximate, but still computable for larger systems)
	Efficient quantum state preparation via Givens rotations



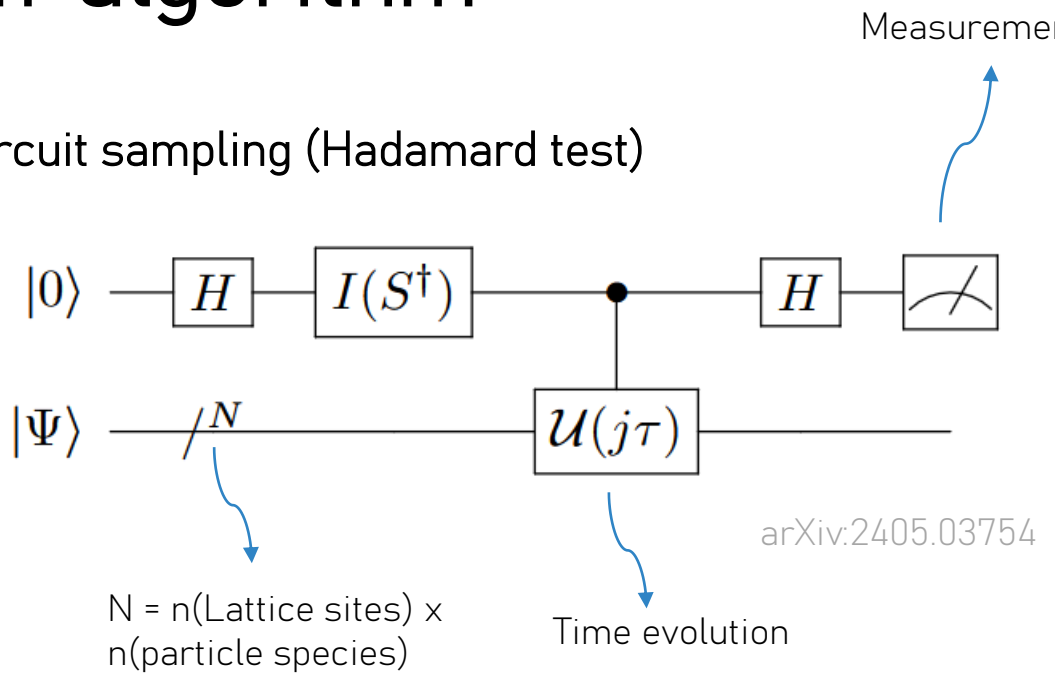


$$G = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos\theta & -\sin\theta & 0 \\ 0 & \sin\theta & \cos\theta & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

arXiv:2010.07965

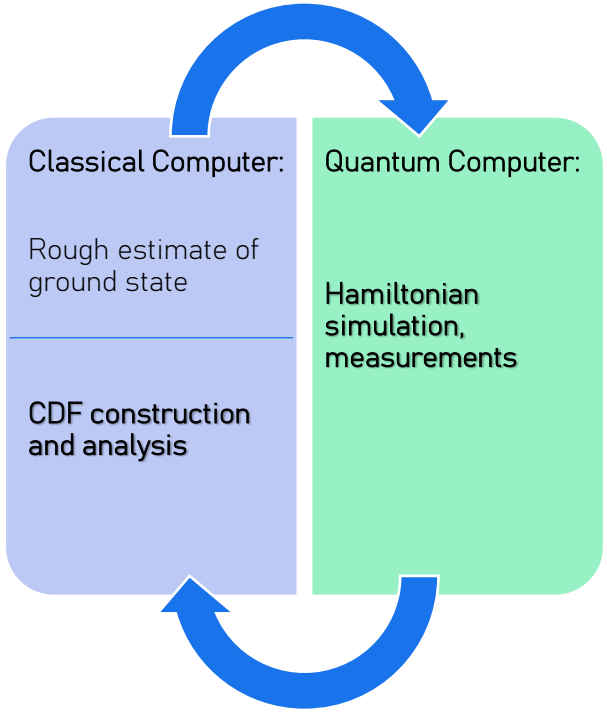
LT algorithm

Circuit sampling (Hadamard test)



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

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

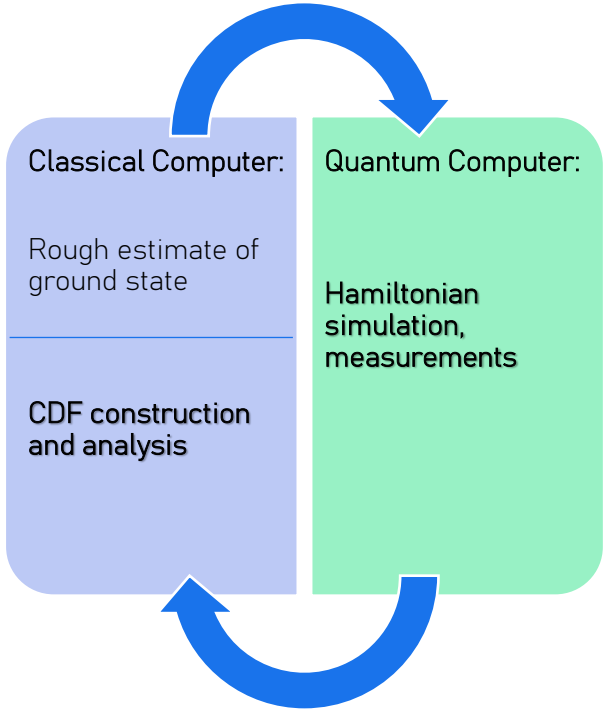


CDF construction

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

$$j \equiv 2k+1$$

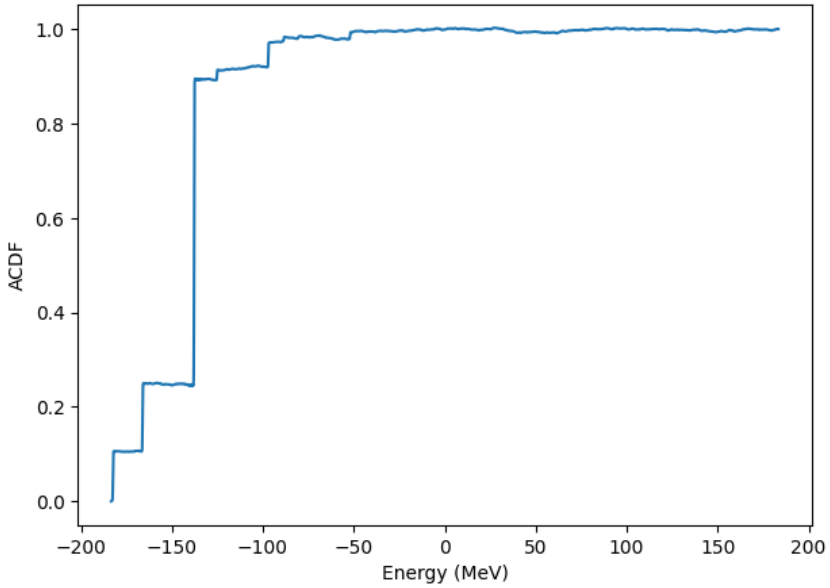
LT algorithm



CDF analysis

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

- 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



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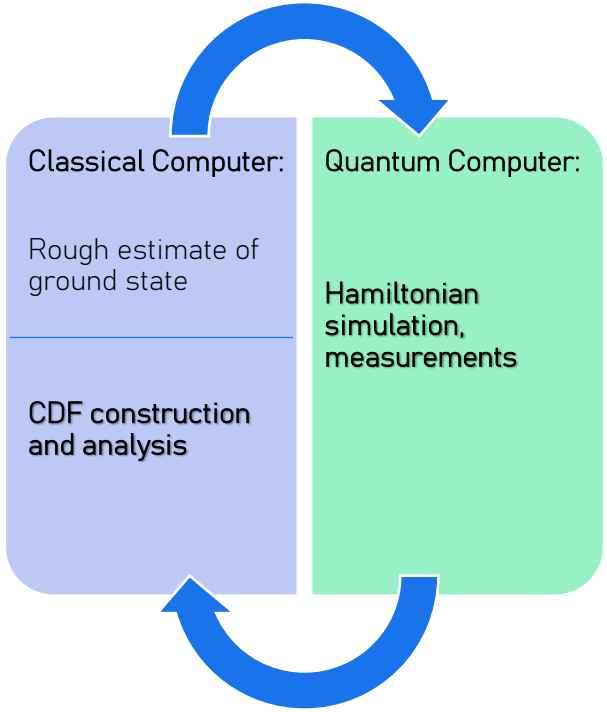

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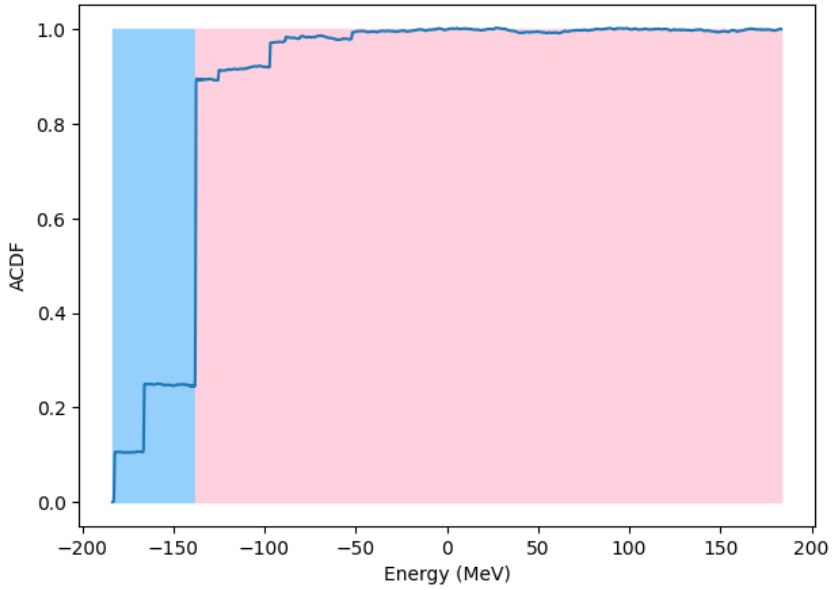

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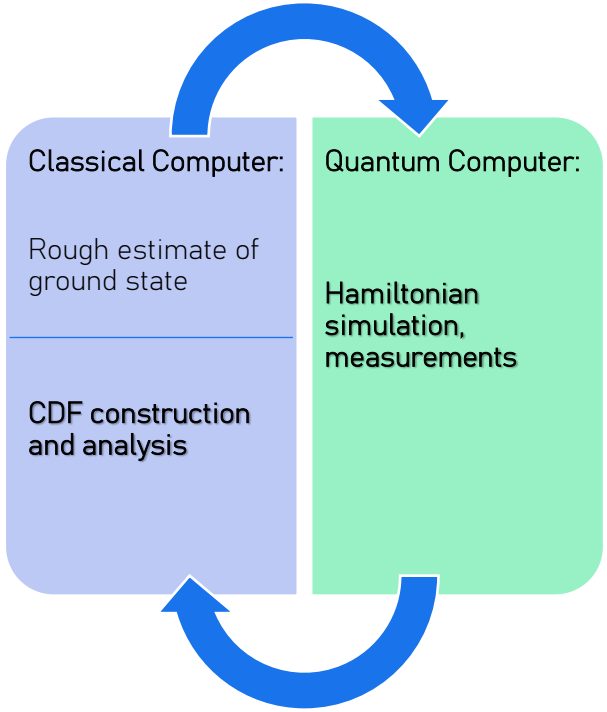

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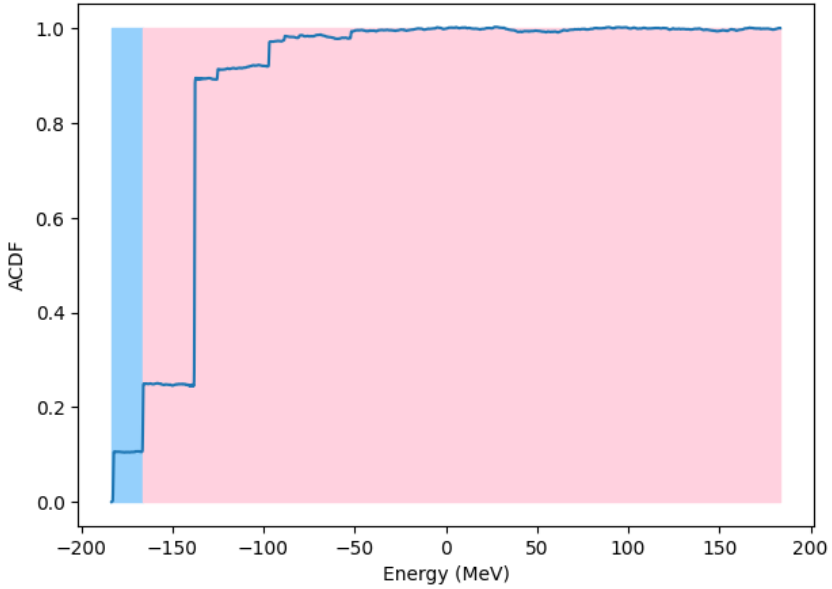

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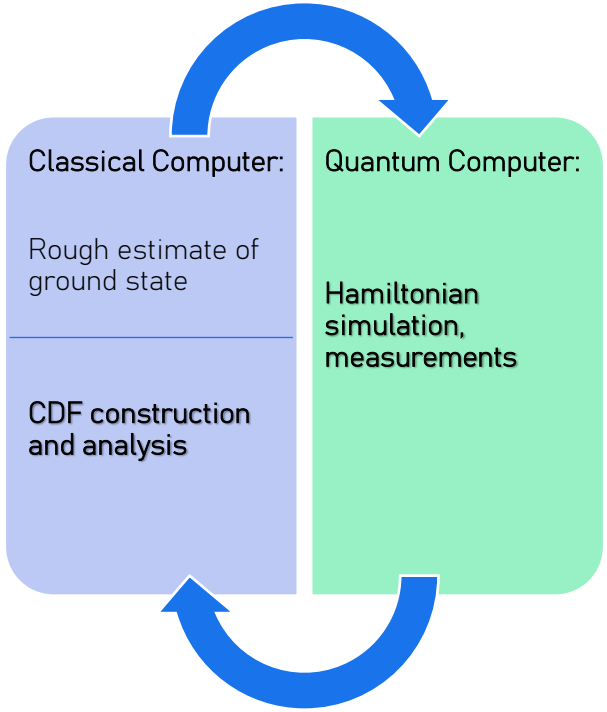

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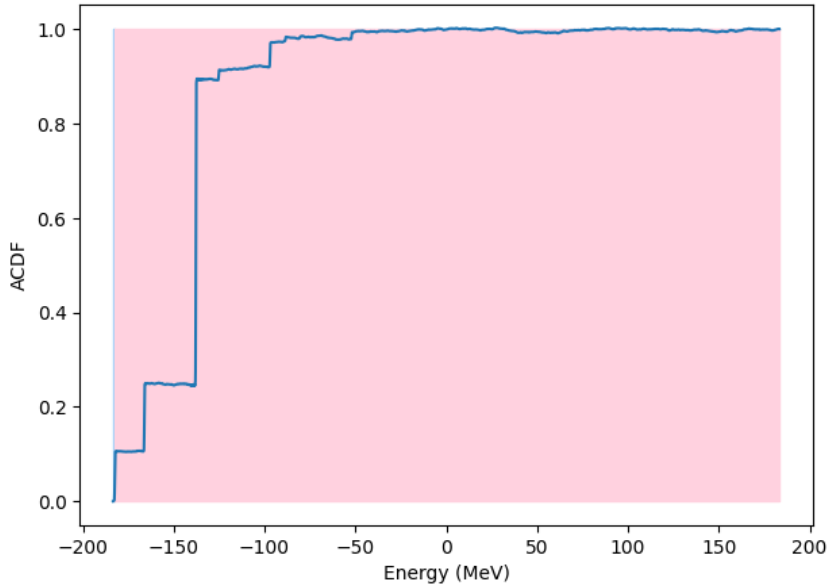
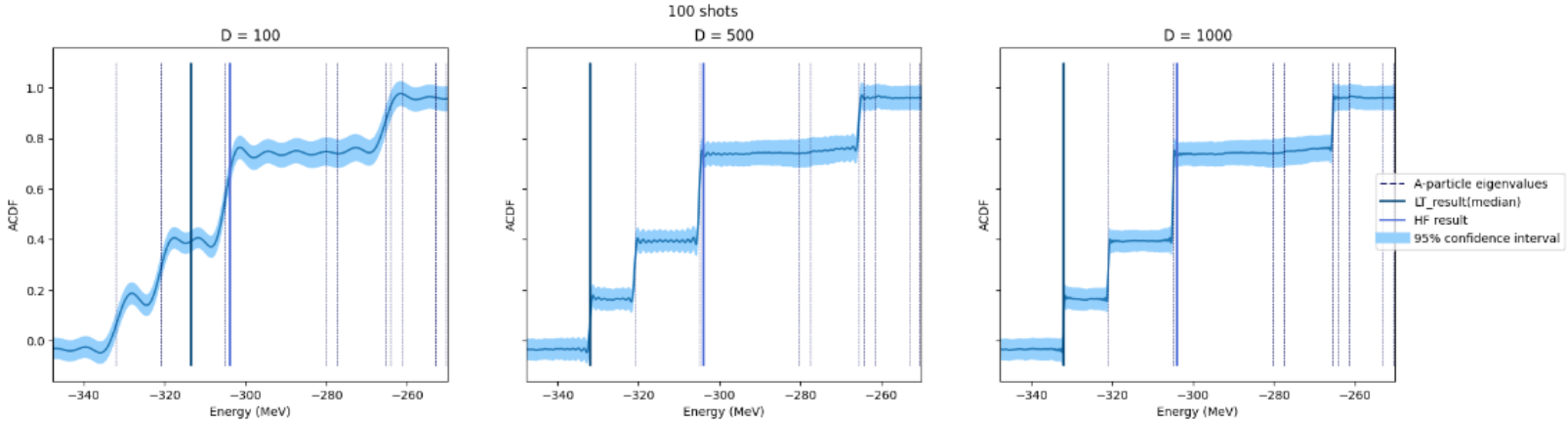
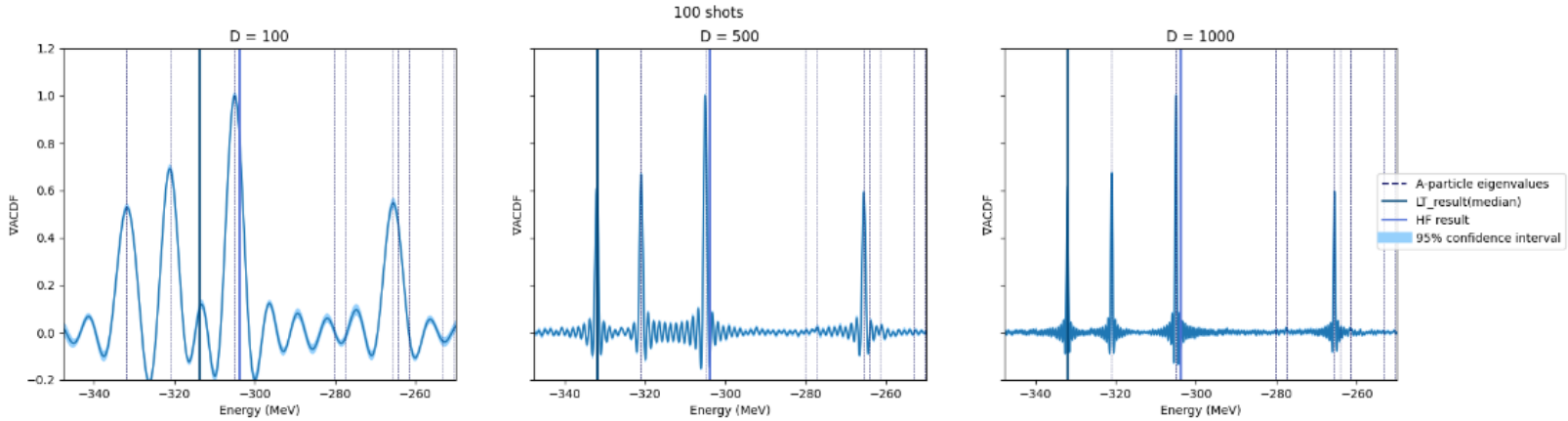


Results

- Testing of the complete approach for small systems in 1D and 2D lattices (up to 12 qubits)
- Assessment of performance 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 result



(a) ACDF for 3x1 lattice with three particles



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

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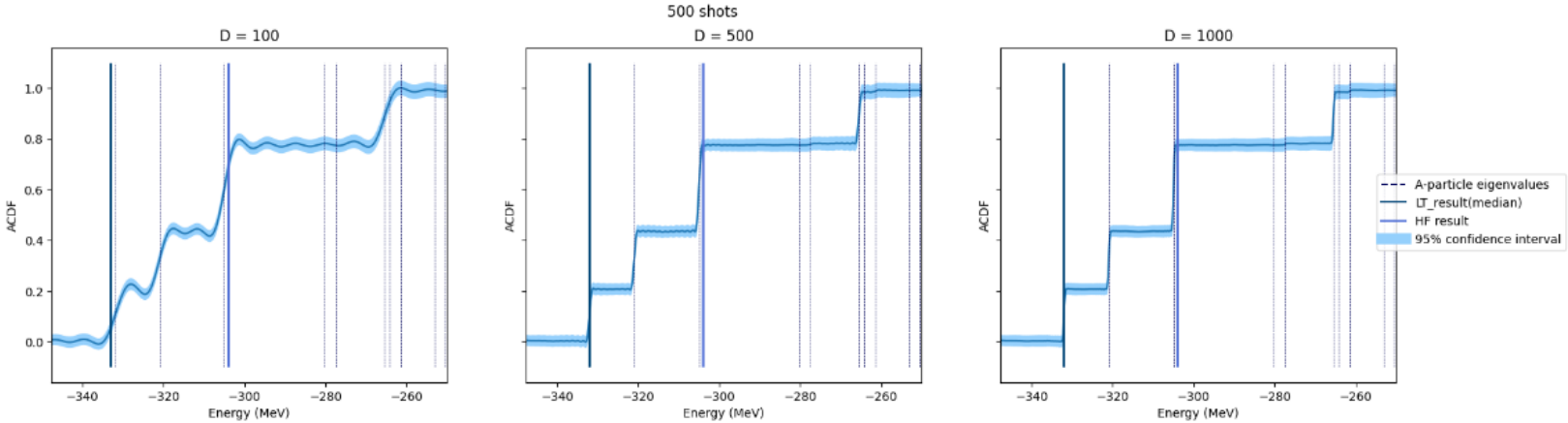

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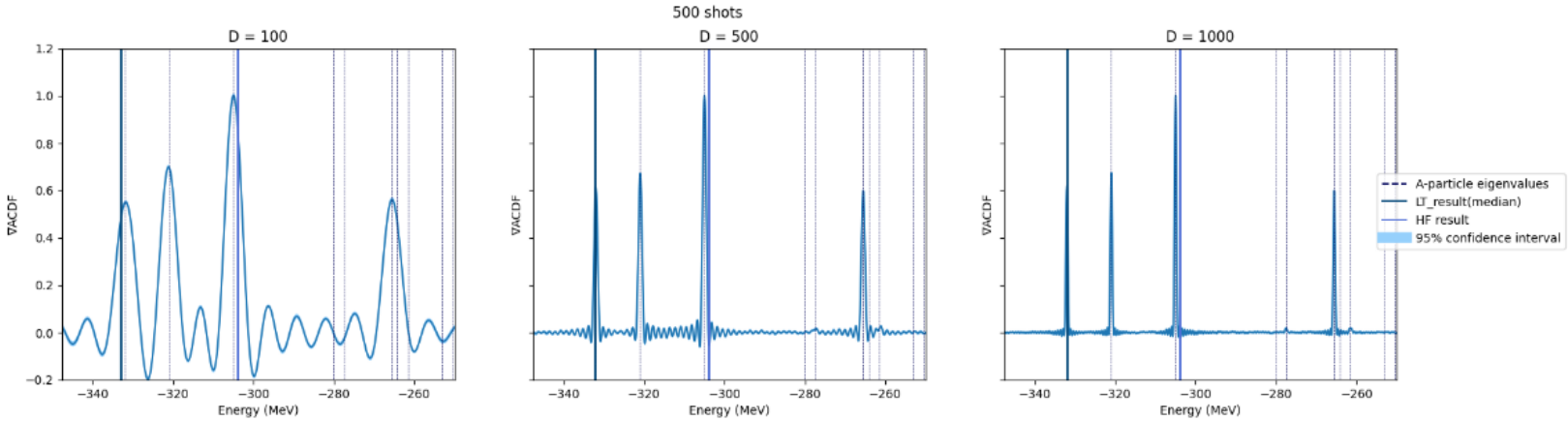

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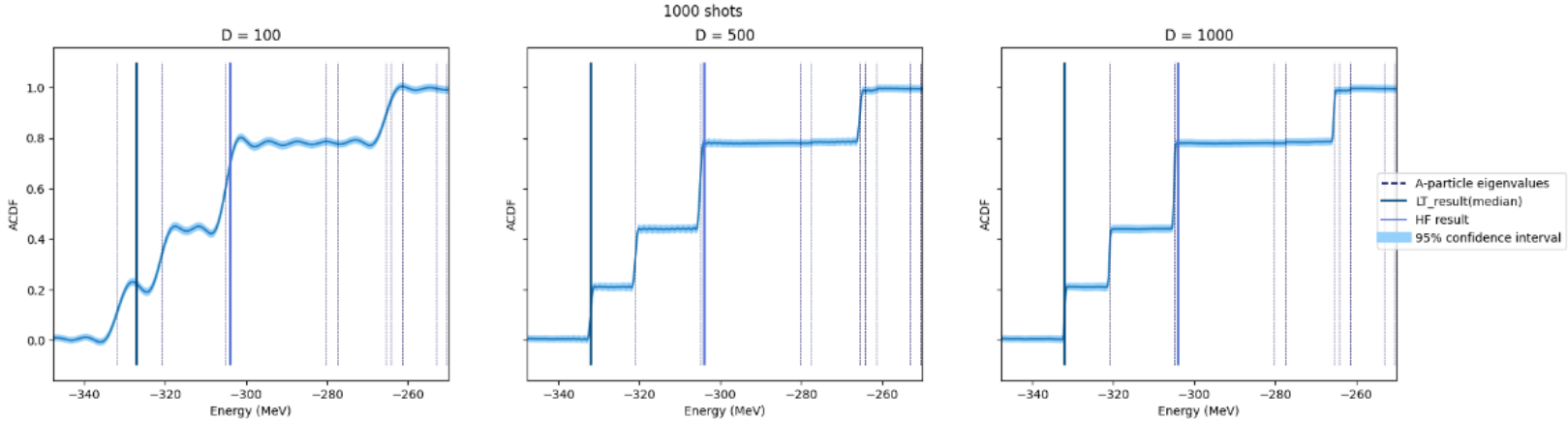

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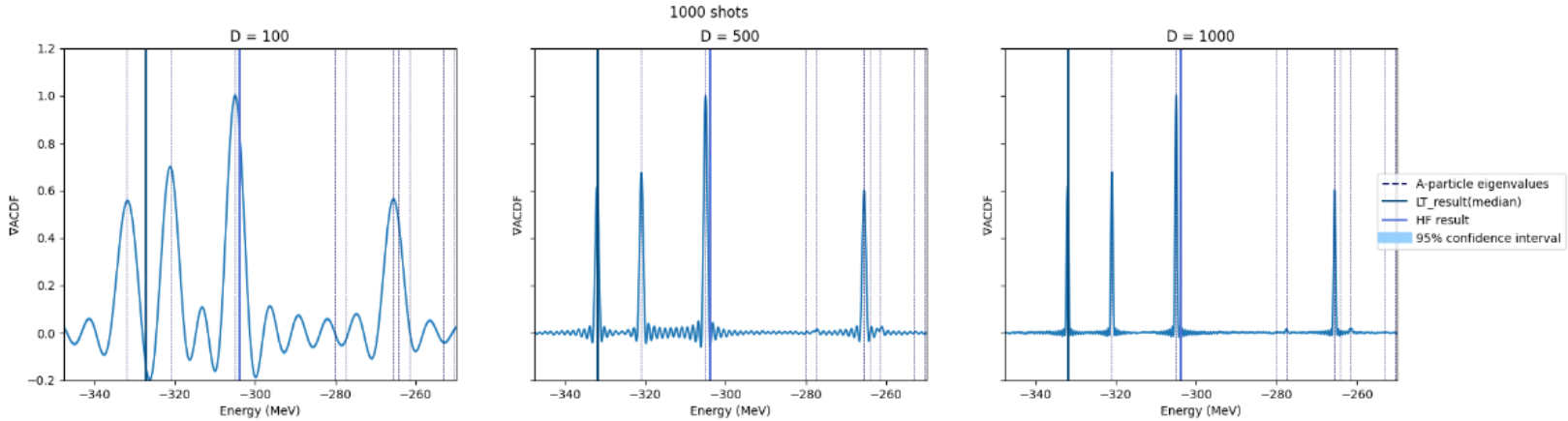
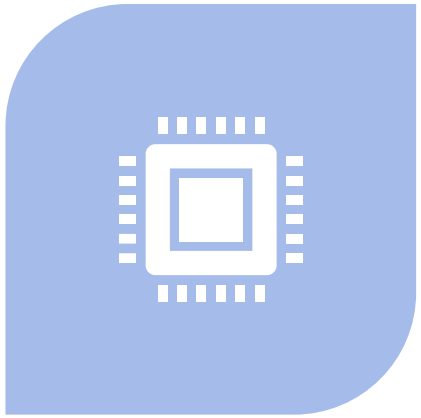


(b) ∇ACDF for 3x1 lattice with three particles

Future Work

EVALUATING TIME EVOLUTION USING PRODUCT FORMULA (TROTTER, IN PROGRESS)



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

CONSIDER FURTHER WORK ON EXPLICIT CIRCUIT CONSTRUCTION, COST REDUCTION