USTC - Particle and Nuclear Physics

NPMWorkshop

Quantum Simulation of Fragmentation and Confinement

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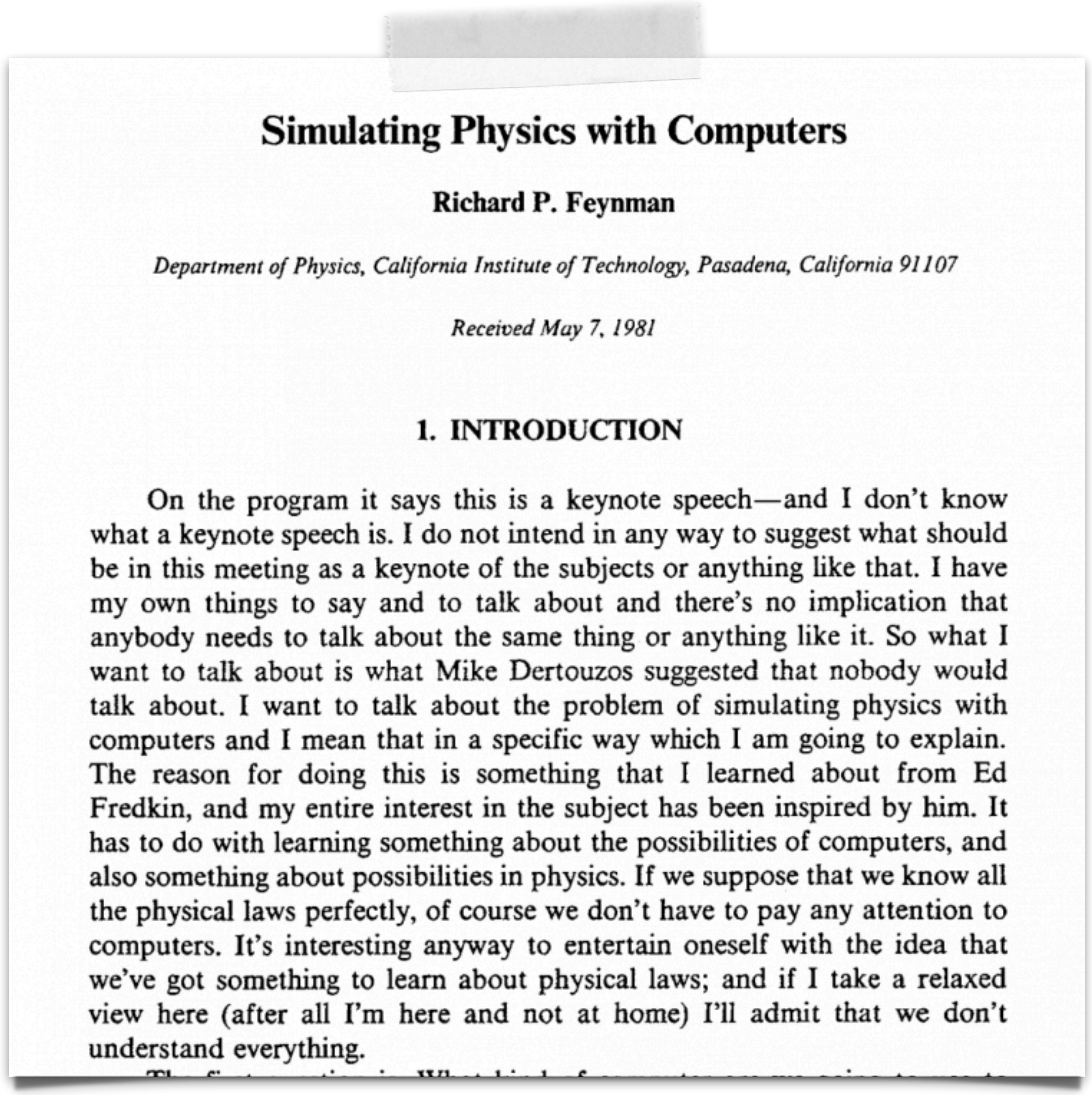
Quantum Computing

- Computing with quantum bits (“qubits”)
  - Hardware: How to build a quantum computer
  - Algorithm: How to “run” a quantum computer
- Exponential acceleration: quantum supremacy

> “... and if you want to make a simulation of nature, you’d better make it quantum mechanical, ...”
>
> —Feynman



Simulating Physics with Computers

Richard P. Feynman

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Received May 7, 1981

1. INTRODUCTION

On the program it says this is a keynote speech—and I don’t know what a keynote speech is. I do not intend in any way to suggest what should be in this meeting as a keynote of the subjects or anything like that. I have my own things to say and to talk about and there’s no implication that anybody needs to talk about the same thing or anything like it. So what I want to talk about is what Mike Dertouzos suggested that nobody would talk about. I want to talk about the problem of simulating physics with computers and I mean that in a specific way which I am going to explain. The reason for doing this is something that I learned about from Ed Fredkin, and my entire interest in the subject has been inspired by him. It has to do with learning something about the possibilities of computers, and also something about possibilities in physics. If we suppose that we know all the physical laws perfectly, of course we don’t have to pay any attention to computers. It’s interesting anyway to entertain oneself with the idea that we’ve got something to learn about physical laws; and if I take a relaxed view here (after all I’m here and not at home) I’ll admit that we don’t understand everything.

Basic Elements of Quantum Computing

- Operator: unitary
  - Single qubit: X(σ_x), Y(σ_y), Z(σ_z), Rx(θ)($e^{i\theta\sigma_x}$), ...
  - $X_n = I \otimes I \otimes \cdots \otimes X \otimes \cdots$
  - Two(Multi) qubits: CNOT($\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$)
- Measurements: Hermitian
  - X, Y, Z
- The Hamiltonian should be expressed in XYZs!

Quantum Computing in Physics

- Challenges
  - Space complexity
    - Limited number of qubits
    - Classical simulations: exponentially difficult
  - Time complexity
    - Noises
  - Gauge field
    - Analog simulation
    - Digital simulation
  - …

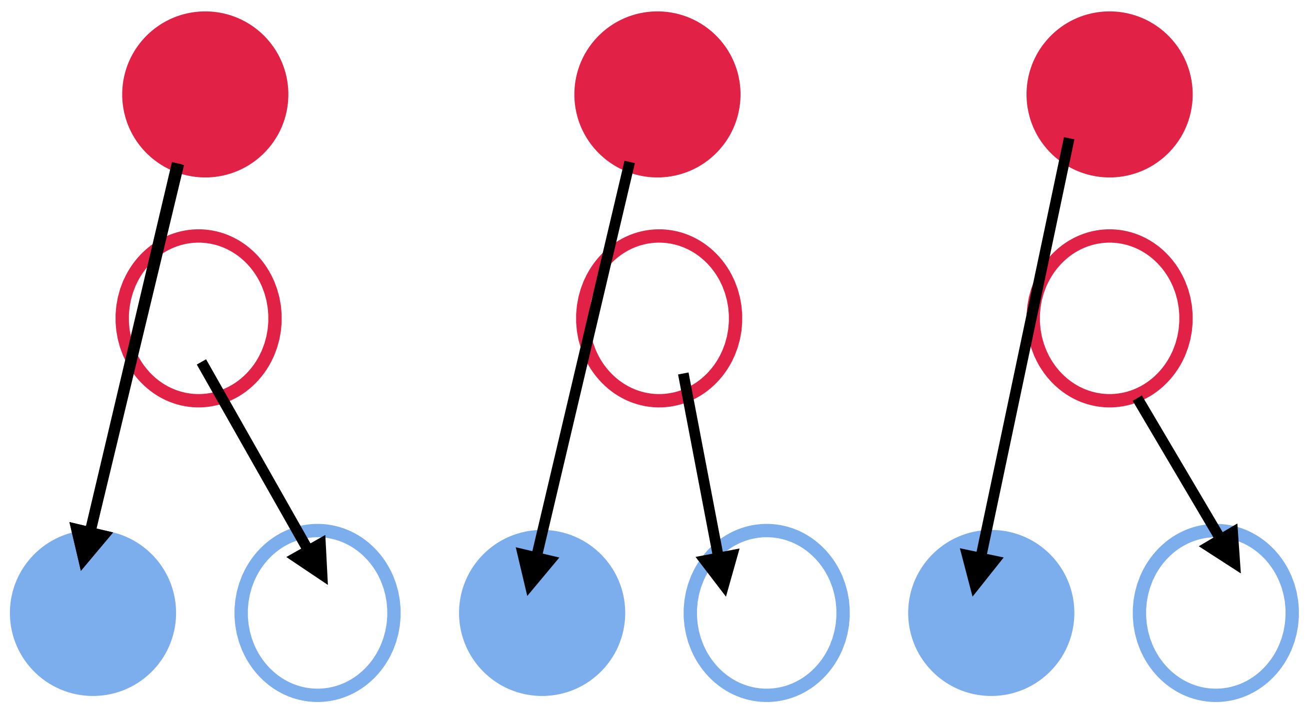
1+1D NJL Model

- Lagrangian:

$$\mathscr{L} = \bar{\psi}_\alpha(i\gamma^\mu\partial_\mu - m_\alpha)\psi_\alpha + g(\bar{\psi}_\alpha\psi_\alpha)^2$$

- Discretization: staggered fermion

$$\psi_\alpha(x) = \begin{pmatrix} \psi_{\alpha,1}(x) \\ \psi_{\alpha,2}(x) \end{pmatrix} \equiv \begin{pmatrix} \phi_{\alpha,2n} \\ \phi_{\alpha,2n+1} \end{pmatrix}$$



- Hamiltonian:

$$H = \sum_{\alpha,n} [-\frac{i}{2a}(\phi^\dagger_{\alpha,n}\phi_{\alpha,n+1} - h.c) + (-1)^n m_\alpha \phi^\dagger_{\alpha,n}\phi_{\alpha,n}]$$
$$-g \sum_{\alpha,n=even} [\phi^\dagger_{\alpha,n}\phi_{\alpha,n} + \phi^\dagger_{\alpha,n+1}\phi_{\alpha,n+1} - 2\phi^\dagger_{\alpha,n}\phi_{\alpha,n}\phi^\dagger_{\alpha,n+1}\phi_{\alpha,n+1}]$$

Jordan-Wigner Transformation

$$\phi_{\alpha,n} = \prod_{\beta=1}^{\alpha-1} \tilde{\sigma}^z_{\beta,\frac{N}{2}} \tilde{\sigma}^z_{\alpha,n} \sigma^+_{\alpha,n} \equiv \Xi^z_{\alpha,n} \sigma^+_{\alpha,n} ,$$

$$\sigma^{\pm}_{\alpha,n} = \frac{1}{2}(\sigma^x_{\alpha,n} \pm i\sigma^y_{\alpha,n})$$

$$\tilde{\sigma}^z_{\alpha,n} \equiv \prod_{i<n} \sigma^z_{\alpha,i}$$

- Keeps the anti-commuting relation of ϕ.

Calculation of Correlation Functions

- Definition:

$$f_{q/h} = \int \frac{dz}{4\pi} e^{-ixM_h z} \langle h \,|\, \bar{\psi}(z, -z)\gamma^{+}\psi(0k0) \,|\, h \rangle$$

$$= \int \frac{dz}{4\pi} e^{-ixM_h z} \langle h \,|\, e^{iHz}\bar{\psi}(0, -z)e^{-iHz}\gamma^{+}\psi(0,0) \,|\, h \rangle$$

- where $\gamma^{+} = \gamma^{0} + \gamma^{1}$.
- Relevant dimension: 1+1 D
- Prepare the hadronic state
- Calculate the (dynamical) correlation function

Fragmentation Function

- Definition: (collinear quark ff)

$$D_q^h(z) = z^{d-3} \int \frac{dy^-}{4\pi} e^{-iy^-p^+/z} \mathrm{Tr}\left\{ \langle \Omega \,|\, \psi(y^-) \mathscr{H} \bar{\psi}(0) \,|\, \Omega \rangle \right\}$$

$$\mathscr{H} = \sum_X |\, h, X \rangle \langle h, X \,|$$

- One can not prepare all the $|\, h, X\rangle$ states!

Preparation of states

- Find the unitary transformation U from computational basis to energy eigenbasis

$$U|0101\cdots0101\rangle = |\Omega\rangle$$

$$U(|1001\cdots0101\rangle + |0110\cdots0101\rangle + \cdots + |0101\cdots0110\rangle) = |h_1(p=0)\rangle$$

$$\cdots$$

- Equivalently,

$$U|1001\cdots0101\rangle = |h_1^1\rangle$$

$$U|0110\cdots0101\rangle = |h_1^2\rangle$$

Preparation of Multi-particle States

- Separate total space into M parts, each parts encoded by K qubits

$$|I\rangle = \prod_{i=0}^{M-1} \otimes |I_i^{a_i}\rangle$$

- Each part can have at most one particle

$$U|I_i^{\Omega}\rangle = |\Omega_i\rangle$$

$$U|I_i^{q}\rangle = |q_i\rangle$$

$$U|I_i^{h}\rangle = |h_i\rangle$$

$$\dots$$

Preparation of Multi-particle States

- Completeness condition:

$$\sum_a |I_i^a\rangle\langle I_i^a| = \mathrm{Id}_i,$$

where Id is the identical matrix

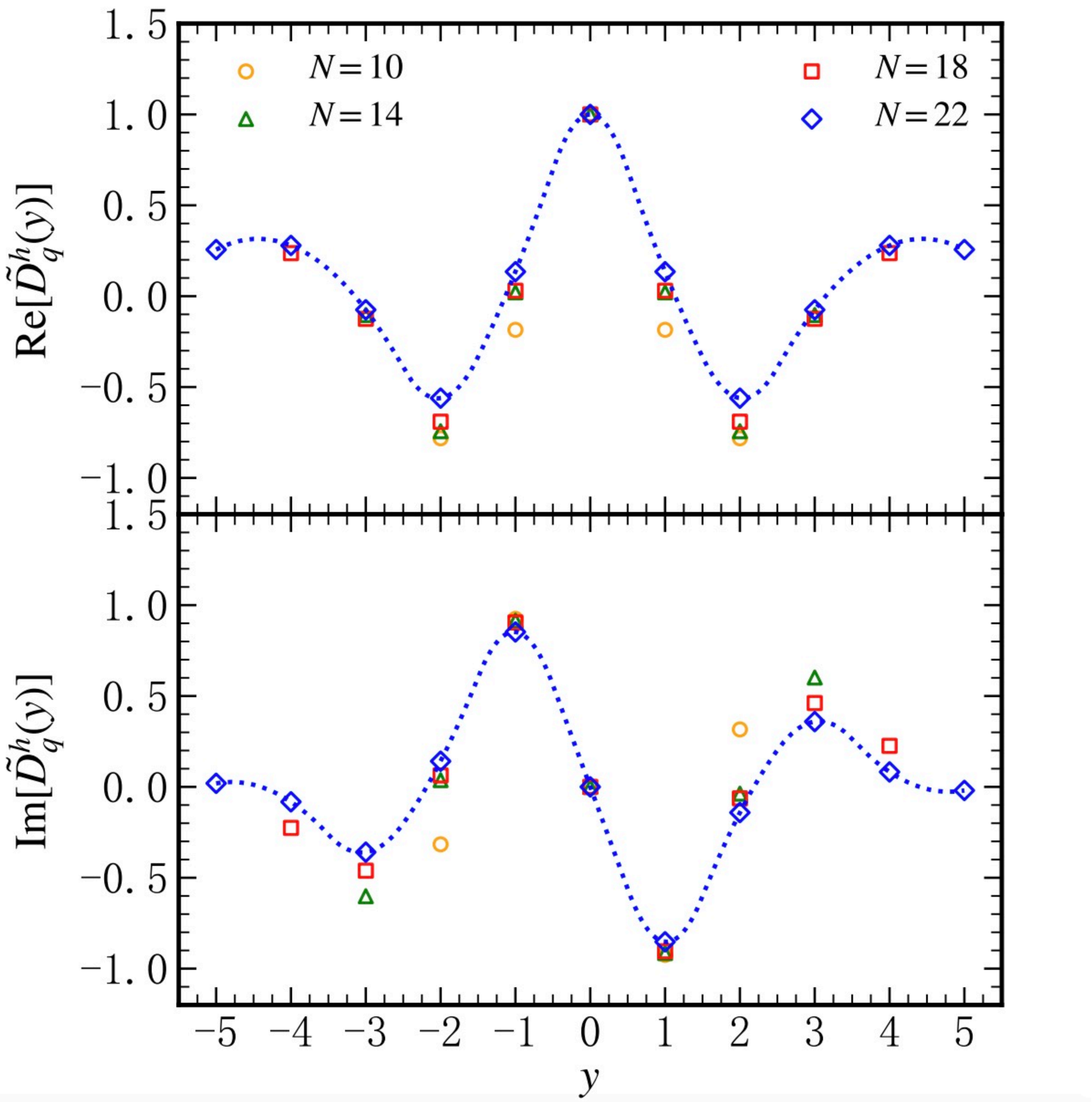
- Therefore

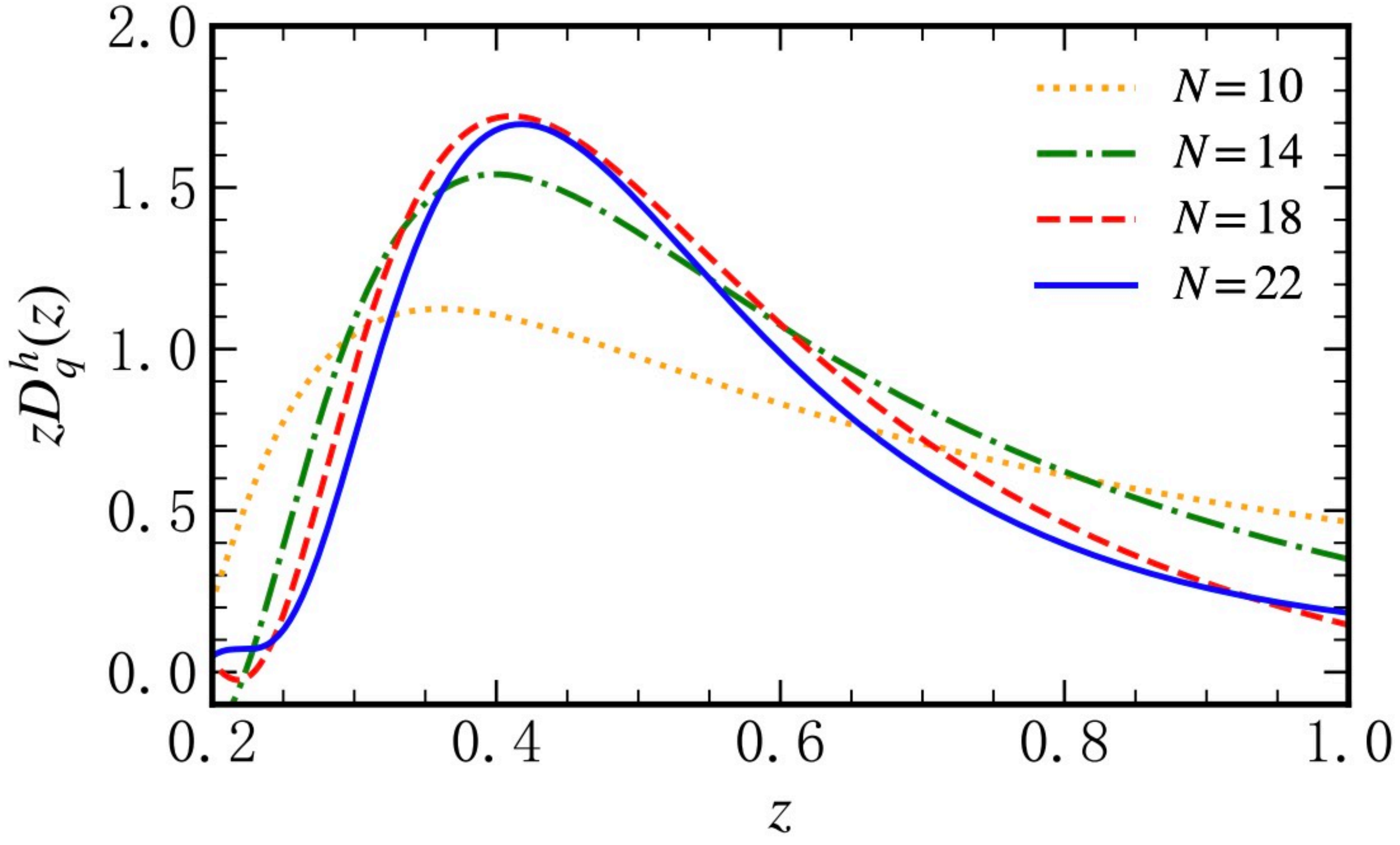
$$\sum_X |h_i, X\rangle\langle h_i, X| = U \sum_{j\neq i} \sum_a |I_i^h, I_j^a\rangle\langle I_i^h, I_j^a| U^\dagger = U \left(|I_i^h\rangle\langle I_i^h| \prod_{j\neq i} \otimes \mathrm{Id}_j \right) U^\dagger$$

$$\mathcal{H} \sim \sum_{i=0}^{M-1} U |I_i^h\rangle\langle I_i^h| U^\dagger$$

- But notice now U must be accurate for all single-particle states

Results





- Converges with N
- Qualitatively agrees with other results
- Finite size effect at large z

Noise in QC

- After each step, there is a probability p of error, the density matrix becomes

$$\epsilon(\rho) = (1-p)\rho + \frac{p}{3}(\sigma^x \rho \sigma^x + \sigma^y \rho \sigma^y + \sigma^z \rho \sigma^z)$$

- Noise error is accumulated along the quantum circuit
- If the number of gates $N \sim \dfrac{1}{p}$, noise may be dominant!
- Error mitigation:
  - Postselection
  - Noise extrapoation

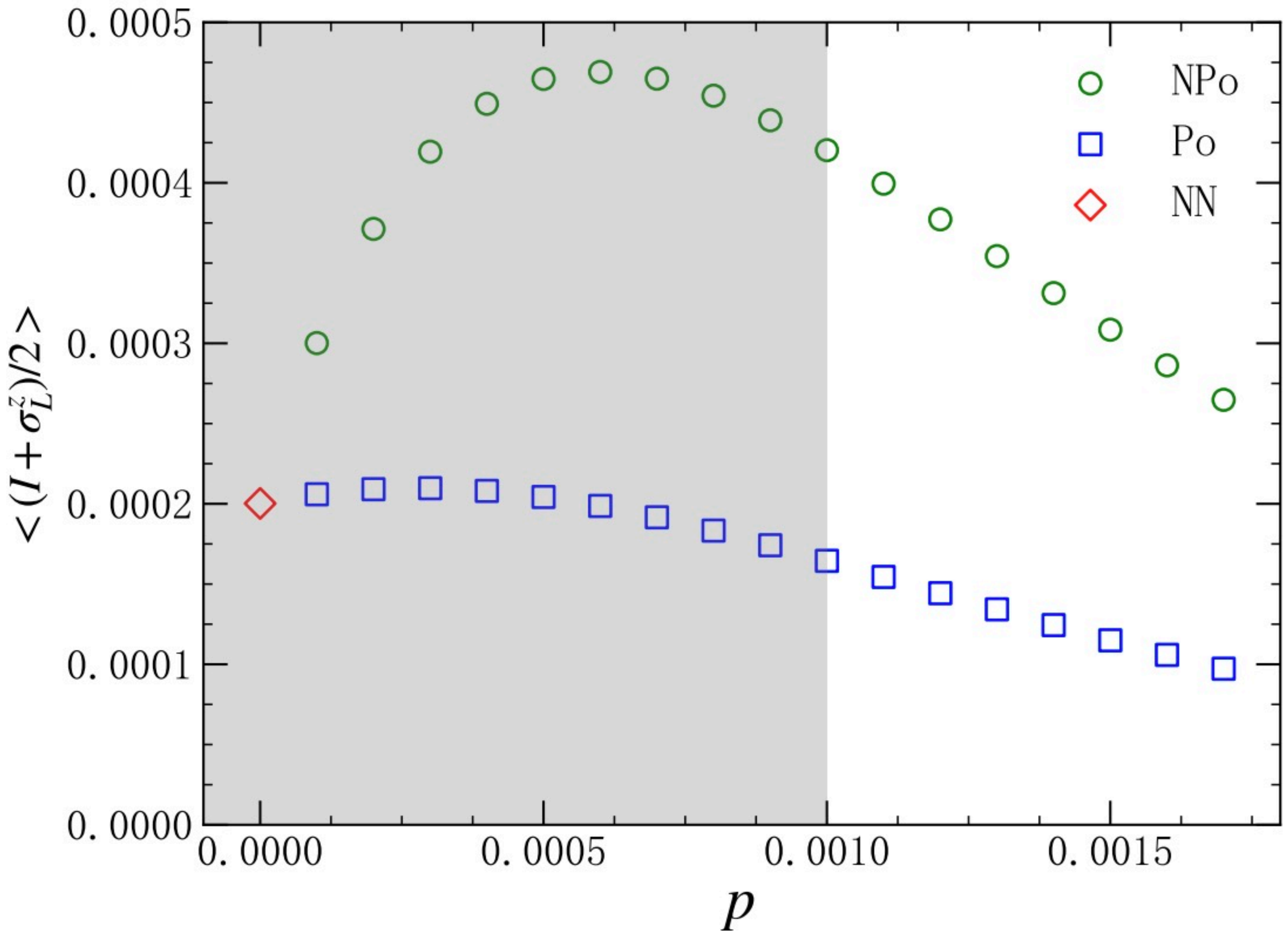
Postselection

$$\epsilon(\rho) = (1-p)\rho + \frac{p}{3}(\sigma^x\rho\sigma^x + \sigma^y\rho\sigma^y + \sigma^z\rho\sigma^z)$$

- Physical states have fixed quantum numbers, such as particle number.
- If these quantities changed, it must be due to noise.
- So results with inaccurate quantum numbers are excluded.
- Effectively, only even number of x and y flips are allowed.

Postselection

- Current NISQ can only works outside shadowed region
- Postslection gives much better results



Noise extrapolation

- Any final measurement can be viewed as a function of noise probability

$$O = O(p)$$

- By measuring at different p and choosing a proper extrapolation method, theoretically one can get $O(0)$

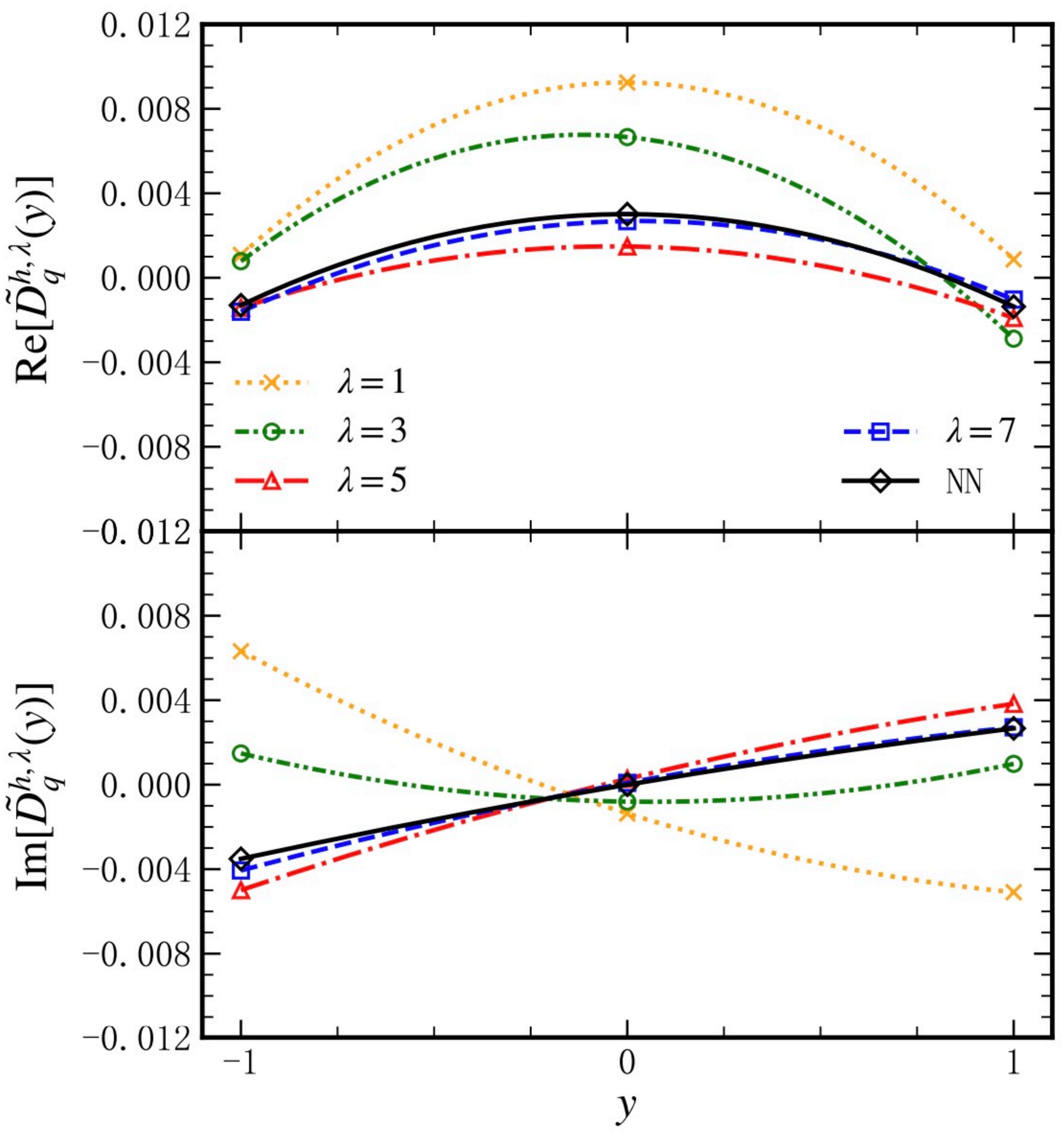
- Richardson zero noise extrapolation of λ order:

$$O^{\lambda} = \sum_{j=0}^{\lambda} \gamma_j O(c_j p)$$

$$\gamma_j = \prod_{m \neq j} c_m (c_j - c_m)^{-1}$$

Results

- Poststlection plus error extrapolation can effectively eliminate errors.



Thermal States

- Gibbs state:

$$\rho = \frac{e^{-H/T}}{\mathrm{Tr}e^{-H/T}}$$

- Thermal states are mixed states, which are difficult for quantum computing
  - Time complexity: measure repeatedly on different states
  - Space complexity: purification into a pure state with more qubits

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Variational Algorithm

- Gibbs state is the state with minimal free energy.
- So we can use variational algorithm again!
- But how to parametrize the density matrix?
- Especially: how to measure the entropy?

Variational Algorithm

- Parametrization:

$$\rho(\phi, \theta) = U(\phi)\rho_0(\theta)U^\dagger(\phi)$$

$$\rho_0(\theta) = \prod_{i=0}^{N-1} \otimes \rho_i(\theta_i)$$

$$\rho_i(\theta_i) = \cos^2\theta_i |0\rangle\langle 0|_i + \sin^2\theta_i |1\rangle\langle 1|_i$$

- Purification:

$$\cos\theta|00\rangle\langle 00| + \sin\theta|11\rangle\langle 11| \rightarrow \cos^2\theta|0\rangle\langle 0| + \sin^2\theta|1\rangle\langle 1|$$

Variational Algorithm

- The entropy of such a density matrix is analytical:

$$F(\phi,\theta) = \mathrm{Tr}[\rho(\phi,\theta)H] - \frac{1}{T}S(\theta)$$

$$S(\theta) = -\sum_{i=0}^{N-1}\left[\sin^2\theta_i \log(\sin^2\theta_i) + \cos^2\theta_i \log(\cos^2\theta_i)\right]$$

- 2N qubits, N entangled pairs
- Measure on half of the qubits = partial trace the other half

1+1D Schwinger Model

- Confinement and deconfinement in such model
- Hamiltonian

$$H = \frac{1}{2a}\sum_{j=0}^{N-2}[\phi_j^\dagger U_{j,j+1}\phi_{j+1} + h.c.] + m\sum_{j=0}^{N-1}(-1)^{j+1}\phi_j^\dagger\phi_j + \frac{g^2a}{2}\sum_{j=0}^{N-2}L_{j,j+1}^2$$

- Gauss' law

$$L_{j,j+1} - L_{j-1,j} = \phi_j^\dagger\phi_j - \frac{1-(-1)^{j+1}}{2} \rightarrow L_{j,j+1} = \epsilon + \sum_{l=0}^{j}[\phi_j^\dagger\phi_j - \frac{1-(-1)^{j+1}}{2}]$$

- Gauge field can be expressed by fermion field

1+1D Schwinger Model

- Gauge transformation

$$\phi_j \to \prod_{l=0}^{j-1} U_{j,j+1}\phi_j$$

- Simplified Hamiltonian

$$H = \frac{1}{2a}\sum_{j=0}^{N-2}[\phi_j^\dagger \phi_{j+1} + h.c.] + m\sum_{j=0}^{N-1}(-1)^{j+1}\phi_j^\dagger \phi_j$$
$$+\frac{g^2 a}{2}\sum_{j=0}^{N-2}\left\{\epsilon + \sum_{l=0}^{j}[\phi_j^\dagger \phi_j - \frac{1-(-1)^{l+1}}{2}]\right\}^2$$

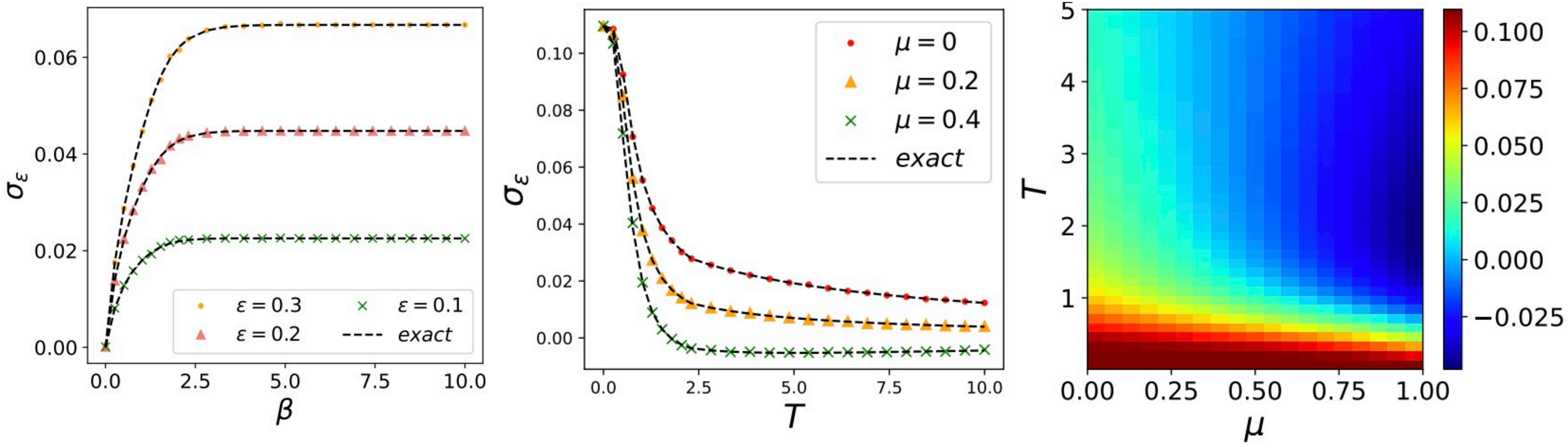
String Tension

- ϵ can be interpreted as a pair of fermion-antifermion with charge ϵg at the two ends of the system
- The "potential" between the fermion-anntifermion pairs:

$$\sigma_\epsilon(\beta) = \frac{1}{Nga}\left(F_\epsilon(\beta) - F_0(\beta) - f_\epsilon\right)$$

$$f_\epsilon = \frac{g^2 a(N-1)}{2}(\epsilon^2 - \frac{\epsilon}{2})$$

Results



- Variational quantum algorithm can effectively simulate thermal states
- Deconfinement behavior can ben seen at high temperature

Summary and Outlook

- We propose quantum algorithms to calculate fragmentation functions and simulate thermal states.
- We calculated FF with 1+1D NJL model and string tension with Schwinger model.
- Quantum algorithms give very promising results.
- More study on thermal states and phase transition ongoing.