





Funded by the European Union

## Simulating Physics with Quantum Computing

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**The Idea:** "Nature isn't classical, dammit, and if you want to make a simulation of nature, you'd better make it quantum mechanical"

#### **Simulating Physics with Computers**

#### **Richard P. Feynman**

Department of Physics, California Institute of Technology, Pasadena, California 91107

Received May 7, 1981



Quantum computing (QC) is a rapidly-emerging technology that harnesses the laws of quantum mechanics to solve problems.

After 40+ years, we are almost there with various emerging QC technology...

#### Analog quantum computer

Basic idea: Mimic with physical systems using continuous variables



Successfully for optimization problems, ~5000 quantum bits (qubits)

#### Not a universal approach



Argüello-Luengo et al, 1807.09228 ultracold atoms in optical lattices + cavity QED

#### Schematic: D-Wave

### Digital quantum computer

Basic idea: Spin chain = qubits (lines) + unitary gates (operators)



Conceptually clean for universal simulation

Noisy, intermediate-scale (NISQ) era, ~100 qubits

Qubits = Digitalization 0) 
$$\begin{split} |\Psi\rangle &= \alpha |0\rangle + \beta |1\rangle \\ |\alpha|^2 + |\beta|^2 &= 1 \end{split}$$
θ τ Φ |1>

#### Tensor network (classical)

Basic idea: Efficient local representation of Hilbert space obeying the area-law



Many-body Hilbert space Id Area-law states D = 100  $D = 10^{N/40}$  $D = 10^{N/20}$ 

 $S \sim \log D$ 

Very suitable for 1+1 problems

Fail for long time simulation or high entanglement

Here, we focus on the universal, digital quantum computing.

Classical computing

- classical bit: 0, 1
- classical gates: logic gates
- deterministic



Quantum computing

- quantum bit (qubit):

$$|0
angle = inom{1}{0}, \, |1
angle = inom{0}{1}$$

- quantum gates: **unitary operators**
- probabilistic (entanglement & superposition)



$$\begin{split} |\Psi\rangle &= \alpha |0\rangle + \beta |1\rangle \\ |\alpha|^2 + |\beta|^2 &= 1 \end{split}$$

#### QC really outclass CC in multiple qubit states due to entanglement!



D.o.f. for n qubits:

 $2^{n}$ (variables) ×2(complex) -1(normalization constraint) =  $2^{n+1}$ -1 >> 3n

We have really come a long way in past 40 years since Feynman! Feynman, "Simulating Physics with Computers" (1981)

**State-of-the-art:** Noisy intermediate-scale quantum (NISQ) era = substantially imperfect and insufficient qubits. However, this can change fast!



### Quantum supremacy

Quantum supremacy = **anything** with a quantum device "cannot" be performed classically

Specific evidence for supremacy are found in sampling distributions!



random circuit 53 qubits, Google Quantum, 1910.11333



GBS 76 qubits, UTSC, 2012.01625 Schematic: Pennylane

**S** 

Quantum advantage = **sth useful** involving a quantum device "cannot" be performed classically

#### Simply a matter of time before QC revolutionizes the modern research (sth useful)



#### Schematic: De Jong

2. Quantum computing in physics [brief highlights of several directions taking for HEP and NP]

#### ... 13

#### **Proof of principles**

Roadmap: Bauer et al, 2204.03381; Meglio et al, 2307.03236

Variational Approaches: Quantum Eigensolver, Hadronic spectrum, Partonic structure functions, Quantum Machine Learning
 Peruzzo et al. 130





Wiesner, 9603028 (1996); Zalka, 9603026; JLP, 1111.3633 De Jong et al, 2010.03571 & 2106.08394 Czajka et al, 2112.03944 & 2210.03062 Bañuls et al, 2409.16996 WQ et al., 2411.09762, 2307.01792, 2208.06750

Wei et al, 1908.08949; Delgado & Thaler, 2205.02814

Williams et al, 2109.13975, 2207.10694

• Quantum Search Approaches: Grover search, Amplitude estimation, Quantum walk



Image: Miessen (2022)



Applications in HEP/NP

Peruzzo et al, 1304.3061 (2013) Kreshchuk et al, 2011.13443 WQ et al, 2112.01927 Li et al, 2106.03865 & 2301.04179

...

Grover, 9605043 (1996)

Du & WQ, 2312.16294

### QC for Experimental Physics

Several motivations:

- LHC Physics involves large data processing
- Quantum search algorithm provides theoretical speedup

See recent/comprehensive review:

Delgado et al 2203.08805 Di Meglio et al, 2307.03236



### Tracking particles

Track reconstruction with Quadratic Unconstrained Binary Optimization (QUBO) Zlokapa1 et al, 1908.04475 using quantum annealing to High Luminosity LHC

Quantum speedup to recover charge particle trajectories using quantum search algorithm

Magano et al, 2104.11583



Q-Search principle: Grover, 9605043 (1996) Brassard et al, 0005055 (2000)

### Jet clustering

Digital quantum algorithm to tackle event reconstruction and jet clustering

Jet algorithm for thrust via

- QUBO formulation (quantum annealing)
- Grover search (digital)

$$T(\hat{n}) = \frac{\sum_{i=1}^{N} |\hat{n} \cdot \vec{p_i}|}{\sum_{i=1}^{N} |\vec{p_i}|}$$



Wei et al, 1908.08949; Delgado, Thaler, 2205.02814

#### Quantum k-means Pires et al, 2101.05618





#### Quantum machine learning

Extending classical ML with quantum data encoding

Anomaly detection with parameterized circuits (PQC) and autoencoder

Alvi, Bauer, Nachman, 2206.08391 Ngairangbam, Spannowsky, Takeuchi, 2112.04958

Quantum Generative Adversarial Networks

Chang et al, 2101.11132

B-jet charge tagging in LHCb simulation

Gianelle et al, 2202.13943

$$\epsilon_{\rm tag} = \epsilon_{\rm eff} (2a-1)^2$$





### QC for Theories & Phenomenologies

Several motivations:

- Classical simulation encounters inherent problems and high problem complexity
- Quantum simulation algorithm provides an ultimate path to simulate quantum field theory



See recent/comprehensive review:

Bauer et al, 2204.03381 Di Meglio et al, 2307.03236

### Prototypical task

Quantum simulation of quantum field theory = perform "ideal experiments" on quantum computer

• Prepare initial state in quantum computer

Jordan, Lee, & Preskill, 1111.3633, 1401.7115, 1703.00454

- Evolve state forward in time using Hamiltonian, for some specified time interval
- Measure observables by simulating measurement performed in idealized lab



### Extracting partonic functions

Quark parton distribution function (PDF) evaluated from flavored hadronic states

Mueller, Tarasov, Venugopalan, 1908.07051 Li et al, 2106.03865, 2207.13258, 2406.05683 Banuls et al, 2409.16996

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



Hadron state preparation using Variational approaches (VQE) Other methods include Adiabatic and Tensor Networks





### Simulating parton showers

Quantum algorithm for HEP simulation of parton shower to include quantum interference

Nachman et al, 1904.03196

 $\mathcal{L} = \bar{f}_1 (i\partial \!\!\!/ + m_1) f_1 + \bar{f}_2 (i\partial \!\!\!/ + m_2) f_2 + (\partial_\mu \phi)^2$  $+ g_1 \bar{f}_1 f_1 \phi + g_2 \bar{f}_2 f_2 \phi + g_{12} \left[ \bar{f}_1 f_2 + \bar{f}_2 f_1 \right] \phi$ 



#### Simulating soft functions from EFT Bauer et al, 2102.05044

$$\sigma = H \otimes J_1 \otimes \ldots \otimes J_n \otimes S.$$



#### Quantum walk approach to simulate parton showers





Williams et al, 2109.13975, 2207.10694

#### Pair production and more



Martinez et al, 1605.04570

#### QCD string breaking and external source modification



Hebenstreit, Berges, Gelfand, 1307.4619 Kasper et al, 1506.01238 Florio et al, 2301.11991



Hadron state preparation and evolution on 112 qubits Farrell et al, 2401.08044

### Non-equilibrium dynamics at finite temperature

Simulating hard probes in QGP as open system via Lindblad equation De Jong et al, 2010.03571, 2106.08394

Open quantum system formulation for quarkonia, jets, etc

Blaizot & Escobedo, 1711.10812, 1803.07996

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho_{S}(t) = -i\left[H_{S1}(t) + H_{L}, \rho_{S}(t)\right] + \sum_{j=1}^{m} \left(L_{j}\rho_{S}(t)L_{j}^{\dagger} - \frac{1}{2}\left\{L_{j}^{\dagger}L_{j}, \rho_{S}(t)\right\}\right)$$



#### 3. Quantum simulation of hadron structures [from 3+1 effective theory to 1+1 field theory in continuum]

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WQ, Jia, Li, Vary, Phys..Rev.C, 2005.13806 WQ, Basili, Pal, Luecke, Vary; Phys.Rev.Research, 2112.01927 Kang, Moran, Nguyen, WQ (to appear)

#### Effective Hamiltonian for hadron

One may also consider effective (3+1)d Hamiltonian on the light front. Valence  $|q\bar{q}\rangle$  for light mesons



For given set of basis states, the Hamiltonian operator can be written in creation and annihilation operators for those modes:  $\hat{\mu} = \hat{\mu} + \hat{\mu}$ 

$$\hat{H} = \hat{H}_1 + \hat{H}_2 + \dots = \sum_{ij} h_{ij} \hat{a}_i^{\dagger} \hat{a}_j + \frac{1}{4} \sum_{ijkl} h_{ijkl} \hat{a}_i^{\dagger} \hat{a}_j^{\dagger} \hat{a}_k \hat{a}_l + \dots$$

Qubit encoding: One-hot encoding and Binary encoding  $(N, N) = (2^n, 2^n) \rightarrow H_q = \sum_{\alpha} c_{\alpha} P_{\alpha}$ O(N)  $O(\log N)$ 

Jordan & Wigner (1928); Kreshchuk et al, 2002.04016

Variational approaches are used to solve the hadronic mass spectrum

Based on variational principle, build parameterized wave functions  $\langle \psi(\theta) | H | \psi(\theta) \rangle \ge \langle E_0 \rangle = \langle \psi_0 | H | \psi_0 \rangle$ 



#### Hadronic spectrum

WQ, Basili, Pal, Luecke, Vary; 2112.01927



Qubit representation (density matrix) for lowest two states:  $D_{ij} = |\psi_i\rangle \langle \psi_j|$ 





😫 Qiskit 27

Collins (2011)

Difficulty of simulating Wilson line is

 $\pi/\rho$  (exact)

π (qasm)

 $\rho$  (qasm)

¥

0.2 0.4 0.6 0.8 1.0

Using light-front wave functions (LFWF) on qubits to compute various observables with projection ops

$$\begin{split} q(x;\mu) &= \frac{1}{x(1-x)} \sum_{s\bar{s}} \int \frac{\mathrm{d}^2 \mathbf{k}_{\perp}}{2(2\pi)^3} |\psi_{s\bar{s}}^{(m_j=0)}(x,\mathbf{k}_{\perp})|^2 \\ &\equiv \frac{1}{4\pi} \sum_{s\bar{s}} \sum_{nm} \sum_{l\bar{l}} \tilde{\psi}_{s\bar{s}}^{*(m_j=0)}(n,m,\bar{l}) \tilde{\psi}_{s\bar{s}}^{(m_j=0)}(n,m,l) \chi_l(x) \chi_{\bar{l}}(x) \\ f_{\mathrm{P,V}} &= 2\sqrt{2N_c} \int_0^1 \frac{\mathrm{d}x}{2\sqrt{x(1-x)}} \int \frac{\mathrm{d}^2 \mathbf{k}_{\perp}}{(2\pi)^3} \psi_{\uparrow\downarrow\mp\downarrow\uparrow}^{(m_j=0)}(x,\mathbf{k}_{\perp}) \\ &\equiv \frac{\kappa\sqrt{N_c}}{\pi} \sum_{nl} (-1)^n C_l(m_q,\kappa) \left( \tilde{\psi}_{\uparrow\downarrow}^{(m_j=0)}(n,0,l) \mp \tilde{\psi}_{\downarrow\uparrow}^{(m_j=0)}(n,0,l) \right) \end{split}$$
 lifted for using light-cone gauge Kreshchuk et al, 2002.04016 \\ q(x) &= \sum\_{s\bar{s}} \sum\_{nm} \sum\_{l\bar{l}} \langle \psi(\vec{\theta}) | \hat{O}\_{\mathrm{pdf}}(x) | \psi(\vec{\theta}) \rangle \\ f\_{\mathrm{P,V}} &\propto | \langle \nu\_{\mathrm{P,V}} | \psi(\vec{\theta}) \rangle | \end{split}

$N_{\rm max}$	$L_{\max}$	Decay constants	Exact result (MeV)	qasm sim (MeV)
1	1	$f_{\pi}$	178.18	$178.17\pm1.97$
		$f_ ho$	178.18	$178.17\pm1.97$
4	1	$f_{\pi}$	193.71	$194.28\pm15.49$
		$f_ ho$	231.00	$225.72\pm13.44$





#### Go beyond classical results

WQ, Jia, Li, Vary, 2005.13806

0.8

-1

 $-2 \\ -3$ 

• E791 data

0.6

0.4

0.2

0.6

0.8

Meson spectrum



**Recent applications:** Anisotropic flow, Li, WQ, Wu, Zhang, 2304.06557



0.6

0.5

0.4

(x) 4<sup>(x)</sup>

0.2

×



1.0 29

#### Parton structure functions

Parton distribution functions (PDF) is highly relevant to the core QCD programs.

Direct computation of the PDFs remains difficult as they are non-perturbative quantities defined as real-time correlators of quark and gluon fields.

$$f_{\psi}\left(\xi\right) = \int_{-\infty}^{\infty} \frac{dt}{4\pi} e^{-it\,\xi\,\vec{n}\cdot\vec{P}} \left\langle P\left|\overline{\psi}(t\vec{n})W(t\vec{n}\leftarrow\vec{0})\vec{n}\cdot\vec{\gamma}\psi(\vec{0})\right|P\right\rangle_{c}$$

Two main difficulties

- Hadron state preparation
- Wilson line

Similarly for the light-cone distribution amplitude, etc

Density Matrix Renormalization Group Algorithm (DMRG) White, 1992



Banuls, Cichy, Lin, Schneider, 2409.16996

Schienbein, CTEQ-MCnet 2021

Hadronic tensor (HT) is another important non-perturbative quantity. It is responsible for computing the cross section.

$$W^{\mu
u}(P,q) = rac{1}{4\pi} \int d^2y e^{iq\cdot y} \langle \Psi(P) | J^\mu(y) J^
u(0) | \Psi(P) 
angle \,,$$

Its calculation directly relates long/trans structure function

We are currently working on PDA, LCDA, HT in the same setting with tensor network + quantum computing.



#### Tensor network simulation results

Simulation results on PDA and LCDA in the same setting with tensor network on 102 qubits.



Exploratory calculation in 1+1 Nambu–Jona-Lasinio with **ALL** Fock sectors

Ongoing work with Zhongbo, Peter, Noah

### 4. Quantum simulation of jets in heavy-ion collisions [using (3+1) light-front Hamiltonian formalism]

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Barata, Du, Li, WQ, Salgado, Phys.Rev.D, 2208.06750 Barata, Du, Li, WQ, Salgado, Phys.Rev.D, 2307.01792 WQ, Li, Kreshchuk, Salgado, 2411.09762

#### Quantum jet simulation: Big picture





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### Quantum jet simulation: Method

Light-front QCD Hamiltonian + Classical background field

- First-principle method formulated in the front form
- Hamiltonian is used to study hadron structure and time evolution alike

**Natural** to extend from classical simulation to quantum simulation

#### **Classical simulation**

Electron in laser field Zhao et al, 1303.3273

Ultrarelativistic guark-nucleus scattering Li et al. 2002.09757

Scattering and gluon emission in a color field

Li, Lappi, Zhao, 2107.02225 Li et al, 2305.12490

Jet in Glasma field

Ongoing work by Avramescu et al

# front form

 $r^+ \triangleq r^0 + r^3$ 

#### Quantum simulation

Nuclear inelastic scattering

Du et al, 2006.01369

Strategy to Jet quenching parameter

Barata, Salgado, 2104.04661

Medium-induced QCD jet

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Barata et al. 2208.06750, 2307.01792 Yao, 2205.07902 Wu et al. 2404.00819 WQ et al, 2411.09762

### QCD Lagrangian

We start with the QCD lagrangian, with an external field

$$\mathcal{L} = -\frac{1}{4} F^{\mu\nu}{}_{a} F^{a}_{\mu\nu} + \overline{\Psi} (i\gamma^{\mu} D_{\mu} - m_{q}) \Psi$$
$$D^{\mu} \equiv \partial_{\mu} + ig(A^{\mu} + \mathcal{A}^{\mu})$$



The light-front Hamiltonian is obtained by the canonical light-front quantization via the standard Legendre transformation, For review: Brodsky, Pauli, Pinsky (1997)


#### Physical setup



High-energy quark jet moving close to the light cone scattering on a dense nucleus medium

For example, light-front Hamiltonian in |q
angle+|qg
angle Fock space

$$P^{-}(x^{+}) = P_{\rm KE}^{-} + V(x^{+}) = P_{\rm KE}^{-} + \left\{ V_{qg} + V_{\mathcal{A}}(x^{+}) \right\}$$



Medium

## Medium and Evolution

Classical stochastic background field (to reduce problem complexity)

$$\langle\!\langle \rho_a(x^+, \boldsymbol{x}) \rho_b(y^+, \boldsymbol{y}) \rangle\!\rangle = g^2 \mu^2 \delta_{ab} \delta^{(2)}(\boldsymbol{x} - \boldsymbol{y}) \delta(x^+ - y^+)$$

$$(m_g^2 - \nabla_\perp^2) \mathcal{A}_a^-(x^+, \mathbf{x}) = \rho_a(x^+, \mathbf{x}) \qquad \qquad Q_s^2 \equiv \frac{C_F g^4 \mu^2 L_\eta}{2\pi} \quad \text{sature}$$



McLerran and Venugopalan, 9309289 (1993)

 $\tau^{--}$ 

 $\delta x^+$ 

Jet probe evolution, decomposed as sequence of unitary operators

$$\begin{split} |\psi_{L_{\eta}}\rangle = &U(L_{\eta};0) |\psi_{0}\rangle \equiv \mathcal{T}_{+}e^{-i\int_{0}^{L_{\eta}} \mathrm{d}x^{+} P^{-}(x^{+})} |\psi_{0}\rangle \\ U(L_{\eta};0) = \prod_{k=1}^{N_{t}} U(x_{k}^{+};x_{k-1}^{+}) \quad \text{non-perturbative} \end{split}$$

1 0

Universal framework to simulate (3+1)-d QCD jet probe evolution in medium in real-time!

### Quantum simulation algorithm



FT allows efficient/sparse simulation in the respective basis

# Extracting quenching parameter

#### **First quenching parameter** calculation on QC

Barata, Du, Li, WQ, Salgado, 2208.06750



Similarly done for momentum broadening at finite p+

simulator, 10-12 gubits

🛱 Qiskit

40

# Gluon production and entropy growth

#### Gluon production in mediums (error from stochastic medium)



Entropy expansion linear in Fock |q> and power-law in Fock |q> + |qg> with radiation

Verified in leading |q> with classical calc, Barata et al, 2305.10476



## Towards efficient simulation of many more particles

Go far beyond classical computations. But current setup is still expensive with increasing particle.

Our new solution: Direct encoding on the particle operators

- No need to evaluate Hamiltonian matrix to Pauli operators (instantly)
- Shallow + sparse quantum circuits
- Particle exchange symmetry automatically satisfied



#### Aspuru-Guzik et al, 0604193

total modes  $N_{
m tot}$  gluon occupancy  $n_{
m max}$ 



## Qubit encoding of quantized operators, "Direct encoding"



- QCD vertices encoded into bosonic (a) and fermonic (b) creation/annihilation operators
- Operator encoding: Aspuru-Guzik et al, 0604193 Sawaya et al, 1909.12847



Vertex coefficients are instantly computed

## Efficient quantum simulation of quark/gluon jet



WQ, Li, Kreshchuk, Salgado, 2411.09762

Unified, Efficient, Scalable procedure for 3+1 jet evolution

### Quark jet results

Transverse Momenta operator

$$ec{P}_{\perp}^2 = \Bigl(\sum_eta b_eta^\dagger b_eta ec{p}_{\perp} + \sum_eta a_eta^\dagger a_eta ec{p}_{\perp} \Bigr)^2$$

WQ, Li, Kreshchuk, Salgado, 2411.09762



Fock space:  $|q\rangle$ 

### Quark jet results

WQ, Li, Kreshchuk, Salgado, 2411.09762  $ec{P}_{\perp}^2 = \Bigl(\sum_eta b_eta^\dagger b_eta ec{p}_{\perp} + \sum_eta a_eta^\dagger a_eta ec{p}_{\perp} \Bigr)^2$ Transverse Momenta operator 0.014 0.014  $|q\rangle + |qg\rangle + |qgg\rangle$  $|q\rangle + |qg\rangle$ Eikonal,  $|q\rangle$ Eikonal,  $|q\rangle$ 0.012 0.012 Eikonal,  $|qg\rangle$ Eikonal,  $|qg\rangle$ ----------. Medium Eikonal,  $|qgg\rangle$ 0.010 0.010 -\_.\_.. •• A•• Medium  $\langle ec{
m P}_{\perp}^2 
angle / d_p^2 
angle$  $\langle ec{P}_{\perp}^2 
angle / d_p^2 
angle$ 0.004 0.004 0.002 0.002 0.000 0.000 15 20 15 5 10 5 10 20 0  $x^+$  (GeV<sup>-1</sup>)  $x^+$  (GeV<sup>-1</sup>)

#### Quark jet results

Gluon number operator

$$\mathcal{N}_g\equiv\sum_eta a^\dagger_eta a_eta$$

WQ, Li, Kreshchuk, Salgado, 2411.09762



## Future jet work

Meson production for qq pair to hadrons, connecting time evolution with hadron states



Quantum simulation to obtain incoming final state

Variational quantum eigensolver to prepare target meson states

Quantum Antenna (ongoing with Joao, Meijian, Carlos)

 $\langle \psi(x^+)|_{\cdot}$ 

#### Future jet work

Prepare a more realistic QGP background on the circuit directly, surpassing the classical MV model.



## Quantum simulation of jet in HIC - Ultimate path

Full description requires much more but we will get there, together with hardware





Theoretical lab to simulate jet physics!

- Medium property
- Jet as fully quantum object
- Extract useful observable

## 5. Quantum simulation for thermalization

[from 1+1 fermionic/QED/bosonic to speedup in heavy quark thermal]

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Du and WQ, Phys.Rev.D, 2312.16294 WQ and Wu, JHEP, 2404.07912 Ikeda, Kang, Kharzeev, WQ, Zhao, Phys.Rev.D, 2407.21496 Cuntin, WQ, Wu (to appear)

## Quantum field theory at finite temperature

My original goal is understand the medium for QGP...

State preparation itself is super challenging (harder than evolution) involving non-trivial adiabatic process.

So, I started to understand thermal quantum field theory. Essentially:

- Prepare thermal (Gibbs) state
- Measure observables of interests such as energy density, pressure, distribution etc



#### **Classical strategies**

For small system, one can exactly diagonalize the Hamiltonian to compute the thermal average.

$$\langle \hat{O} \rangle_{\beta} = rac{\mathrm{Tr} \left[ e^{-eta \hat{H}} \hat{O} 
ight]}{\mathrm{Tr} \left[ e^{-eta \hat{H}} 
ight]}$$

For large systems with high degrees of freedom, it is more favorable to formulate the problem as a path-integral and use Monte Carlo (MC) methods, such as

$$Z = \operatorname{Tr}[e^{-\beta H}] = \lim_{N \to \infty} \sum_{\{x_{\tau}\}} \langle x_0 | e^{-\frac{\beta}{N}H} | x_1 \rangle \langle x_1 | \dots | x_N \rangle \langle x_N | e^{-\frac{\beta}{N}H} | x_0 \rangle$$

For MC to work, any subpath needs be real and non-negative (Importance sampling) => difficult to deal with non-zero chemical potentials, topological terms, or real-time dynamics... "sign" problem Czajka et al, 2112.03944 & 2210.03062

Here, we use quantum strategies to circumvent it

## Quantum strategies

Because of the non-unitary nature, medium preparation is typically hard on quantum circuit. Still, there are many proposals...



Quantum imaginary time evolution (QITE)

Motta et al, 1901.07653 Davoudi et al, 2208.13112



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Variational Quantum Thermalizer

Verdon et al, 1910.02071

"Maxwell demon", quantum fridge

Thermofield Double States

Open quantum system approaches

Ball and Cohen, 2212.06730

Cottrell et al, 1811.11528

de Jong et al, 2010.03571 & 2106.08394 Cleve and Wang, 1612.09512 Kamakari et al, 2104.07823

## Quantum imaginary time evolution

Key idea: trotterize the non-unitary evolution by replacing imaginary time with real time evolution

$$|\psi(\beta/2)\rangle = e^{-\beta\hat{H}/2} |\psi_0\rangle \approx \prod_{i=1}^{N_s} e^{-\Delta\beta\hat{H}/2} |\psi_0\rangle \qquad \qquad |\psi_{i+1}\rangle = e^{-\Delta\beta\hat{H}/2} |\psi_i\rangle = e^{-i\Delta\beta\hat{A}_i/2} |\psi_i\rangle \sqrt{c_i(\Delta\beta)} + \mathcal{O}(\Delta\beta^2)$$

$$|k
angle \not -e^{-i\Deltaeta A_0/2} - e^{-i\Deltaeta A_{1/2}} - \cdots - e^{-i\Deltaeta A_{N_s-1/2}} - |\phi_k
angle$$
  
 $N_s = eta/\Deltaeta$  trotter steps using quantum gates

Practical advantage:







No ancilla qubits



#### Recent QITE applied to field theories

Davoudi et al, 2208.13112 (Lattice gauge theory) Czajka et al, 2112.03944 (Chemical potentials) Pedersen et al, 2311.11616 (Schwinger topological) WQ and Wu, 2404.07912 (Fermion systems)

## QITE + Thermal sampling

QITE + QMETTS (quantum minimally entangled typical thermal state) algorithm to compute thermal observable.

$$\langle \hat{O} \rangle_{\beta} = \sum_{k \in \mathcal{S}} \frac{P_k}{Z} \left\langle \phi_k | \hat{O} | \phi_k \right\rangle \qquad \qquad |\phi_k\rangle = P_k^{-1/2} e^{-\beta \hat{H}/2} \left| k \right\rangle \qquad P_k = \left\langle k | e^{-\beta \hat{H}} | k \right\rangle \qquad Z = \sum_{k \in \mathcal{S}} P_{k+1} \left| e^{-\beta \hat{H}/2} | k \right\rangle \qquad Z = \sum_{k \in \mathcal{S}} P_{k+1} \left| e^{-\beta \hat{H}/2} | k \right\rangle \qquad Z = \sum_{k \in \mathcal{S}} P_{k+1} \left| e^{-\beta \hat{H}/2} | k \right\rangle \qquad Z = \sum_{k \in \mathcal{S}} P_{k+1} \left| e^{-\beta \hat{H}/2} | k \right\rangle \qquad Z = \sum_{k \in \mathcal{S}} P_{k+1} \left| e^{-\beta \hat{H}/2} | k \right\rangle$$

Super efficient for large systems because state collapsing picks out dominant contribution  $N_S \ll |S|$ 

$$\langle \hat{O} \rangle_{\beta} \approx \frac{1}{N_S} \sum_{k=1}^{N_S} \langle \hat{O}_k \rangle_{\beta} \qquad |\langle k' | \phi_k \rangle|^2 \sim P_{k'}/Z$$



WQ and Wu, 2404.07912

We study the Majorana Fermions in 1+1 dimensions and use Majorana representation:

$$\mathcal{L} = rac{1}{2} ar{\psi} (i \partial \!\!\!/ - m) \psi - \mathcal{H}_I(\psi) \, ,$$

In the discretized theory:

$$\hat{H} = \frac{1}{2} \sum_{n} \bar{\psi}_{n} \left[ -\frac{i}{2a} \gamma^{1} (\psi_{n+1} - \psi_{n-1}) + m\psi_{n} \right] - \frac{r}{4a} \sum_{n} \bar{\psi}_{n} (\psi_{n+1} - 2\psi_{n} + \psi_{n-1}) + \hat{H}_{I}$$
kinetic mass Wilson terms interaction

Map to qubits using Jordan-Wigner encoding: 1 qubit per 1 spatial

$$\psi_n = \begin{pmatrix} \frac{a_n + a_n^{\dagger}}{\sqrt{2}} \\ \frac{a_n^{\dagger} - a_n}{i\sqrt{2}} \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ i & -i \end{pmatrix} \begin{pmatrix} a_n \\ a_n^{\dagger} \end{pmatrix} \equiv R \begin{pmatrix} a_n \\ a_n^{\dagger} \end{pmatrix} \qquad \qquad a_n^{\dagger} = \frac{\sigma_n^X - i\sigma_n^Y}{2} \prod_{i=0}^{n-1} \sigma_i^Z$$

Wilson (1974); Jordan et al, 1404.7115

WQ and Wu, 2404.07912

We study the *N*-fermion systems in thermal equilibrium to approximate the thermal field at  $\beta=1/T$ 

$$\langle \hat{O} \rangle_{\beta} \equiv Z_{\beta}^{-1} \operatorname{Tr}[e^{-\beta \hat{H}} \hat{O}] \qquad \qquad Z_{\beta} \equiv \operatorname{Tr}[e^{-\beta \hat{H}}]$$

From the spectral function, the free-theory thermal distribution is:

$$f_p = \frac{1}{2E_p} \sum_n \left[ \gamma^0 u_p \right]_{\alpha'} \left[ \bar{u}_p \gamma^0 \right]_{\alpha} e^{ipan} \langle \bar{\psi}_n^{\alpha'} \psi_0^{\alpha} \rangle_{\beta} \qquad \qquad f_p = \sqrt{\frac{N}{2E_p}} \langle \hat{a}_p^{\dagger} [\bar{u}_p \gamma^0 \psi_0] \rangle_{\beta} = \langle \hat{a}_p^{\dagger} \hat{a}_p \rangle_{\beta} \qquad \qquad f_p = \frac{1}{e^{\beta E_p} + 1}$$

Energy density  $\hat{\epsilon} \equiv T^{00}$  and pressure  $\hat{P} \equiv T^{11}$  are

#### Free field thermal distribution

WQ and Wu, 2404.07912

We evolve the 4-qubit fermionic fields using QITE algorithm for the free fields. Results agree with analytical distribution of Fermi-Dirac.  $E_p = \sqrt{\left(m + \frac{2r}{a}\sin^2\frac{ap}{2}\right)^2 + p_a^2}, \quad p_a = \frac{1}{a}\sin(pa), \quad \Delta\beta = 0.001.$ 





(b)  $m \gg T$  case

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WQ and Wu, 2404.07912

For simplicity, we consider another external Majorana field  $\psi_M$  that is massive and *homogeneous in space*:

$$L = \int dx \left[ \frac{1}{2} \bar{\psi} (i\partial \!\!\!/ - m_0) \psi - \frac{g}{4} (\bar{\psi}\psi) (\bar{\psi}_B \psi_B) \right] + \frac{1}{2} \bar{\psi}_B (i\gamma^0 \partial_t - M) \psi_B$$

Mass renormalization is solved analytically and two quasiparticles emerge



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#### Extending to bosons in scalar field theory

Similarly, we study Bose Einstein distribution (1 site = (0+1) scalar FT)

Cuntin, WQ, Wu, 2411.19601 (ICHEP 2023) Cuntin, WQ, Wu (work in progress)

The ultimate goal is studying non-equilibrium effects toward thermalization with initial conditions in 1+1



$$\mathcal{L} = \frac{1}{2} \left[ \partial_{\mu} \phi \partial^{\mu} \phi - m \phi^2 \right] - \frac{\lambda}{4!} \phi^4$$

$$\varphi_{\alpha} = \Delta_{\varphi} \left( lpha - rac{N_{\varphi} - 1}{2} 
ight)$$
 ,  $\Delta_{\varphi} = \sqrt{rac{2\pi}{N_{\varphi} \overline{m}}}$ 

# Extending to QED2

Schwinger model (1+1 QED) with quenched evolution (imbalance of chirality) at finite temperature to study dynamics of charge operators => explain Chiral Magnetic Effect (CME) CME in 1+1, Kharzeev, Yee, 1012

-0.005

-0.010

-0.015

-0.020

CME in 1+1, Kharzeev, Yee, 1012.6026 Ikeda, et al, 2407.21496

CME in 1+1 = generation of electric current



Real & Imag evolution simultaneously!

$$\langle O(t) \rangle_{\beta} = rac{\operatorname{Tr} \left( e^{-\beta H} O(t) \right)}{\operatorname{Tr} (e^{-\beta H})}$$

Vector current

 $J(x) \equiv \bar{\psi}(x) \gamma^1 \psi(x)$ 

Thermal damping controlled by the mass

## Heavy quark thermalization (macroscopic, application of quantum search)

#### Distinguished separation of scales

Two dominant factors:

- Sudden change of momentum from radiation
- Slow change of momentum from environment

Brownian motion can be described by SDE:

- Drag term: Energy loss
- Diffusion term: Momentum broadening

Full SDE (Langevin) equation

$$dx_i = rac{p_i}{E(ec{p})}dt, \quad i = x, y, z,$$
  
 $dp_i = -A(ec{x}, ec{p}, t)p_i dt + \sigma_{ij}(ec{x}, ec{p}, t)dW_j,$   
Drag coefficient Stochastic Wiener process



Rebentrost et al, 1805.00109 Stamatopoulos et al, 905.02666v5 Du and WQ, arXiv:2312.16294

The idea: use Grover-like operator to accelerate the extraction of **expectation** at final step ("maturity") by a square root over classical Monte Carlo methods

$$\mathbb{E}\left[F(\vec{p},T)\right] = \frac{1}{N} \sum_{i=1}^{N} F(\vec{p},T)$$



$$dq_i = -q_i d\tilde{t} + d\tilde{W}_i$$

- Distribution loading gate  $q_i = p_i/M$   $d\tilde{t} = Adt$
- Stochastic Wiener gate  $d\tilde{W}_i \sim \mathcal{N}(0, 2T d\tilde{t}/(M\chi_i^2))$
- Quantum evolution gate  $A = \sigma_{ii}^2 \chi_i^2 / (2MT)$
- Quantum Amplitude Estimation (QAE)  $\epsilon = \mathcal{O}(1/N_q)$  quadratically faster than MC

#### Simulation results (1D)

Du and WQ, arXiv:2312.16294



### Simulation results (1D)

Du and WQ, arXiv:2312.16294

Early time thermalization, aQCMC with QAE



#### Simulation results (2D)

Du and WQ, arXiv:2312.16294



Non-equilibrium initial conditions towards thermalization with medium profiles

Elliptic flow "v2" build up

$$v_2 = \frac{\int f(q, \cos(\phi), t) \cos(2\phi) \mathrm{d}\phi}{\int f(q, \cos(\phi), t) \mathrm{d}\phi} \stackrel{\text{thermal}}{=} \frac{I_1(\frac{1}{2q^2} |\frac{1}{\tilde{\sigma}_x^2} - \frac{1}{\tilde{\sigma}_y^2}|)}{I_0(\frac{1}{2q^2} |\frac{1}{\tilde{\sigma}_x^2} - \frac{1}{\tilde{\sigma}_y^2}|)}$$

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## 6. The future of quantum computing

### Quantum technology is growing at fast pace



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## Quantum technology is growing at fast pace

Our focus is to unlock the full potential of quantum computing by developing a large-scale computer capable of complex, error-corrected computations. We're guided by a roadmap featuring six milestones that will lead us toward top-quality quantum computing hardware and software for meaningful applications.



### Quantum technology is growing at fast pace







Noisy physical qubits

Reliable logical qubits

Quantum supercomputers




Credit: IGFAE



- Quantum computing technology is available today and developing fast.
- Lots of quantum computing applications in experiment and theory for physics.
- Quantum simulation is promising to solve hadron structures, QCD jet evolution, and thermalization. (a conceptually clean, algorithmic proven path)
- We may be in reach of fault-tolerant quantum computing sooner than we expect.





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