QUACQ:

Quantum utility through advanced computational quantum algorithms

12 September 2024

Objectives

(1) Target problems

(2) Algorithmic primitives

(3) Software

(4) Benchmarking

Thrust 1. Co-design for simulation

Near term: 100s of qubits, ~10^4 gates.

Thrust 2. Quantum algorithms

Both early (~ 10^6 logical ops) and mature fault tolerance (~10^{15} ops).

Thrust 3. Classical benchmarking and verification

E.g. classical resource estimation.

Quantum computing applications

Dirac (1929): “The underlying physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known, and the difficulty is only that the exact application of these laws leads to equations much too complicated to be soluble.”

Feynman (1981): “You can simulate this with a quantum system, with quantum computer elements. It’s not a Turing machine, but a machine of a different kind.”

Artificial intelligence may drive future progress in (strongly correlated) chemistry and materials science. Eventually, quantum computers can accelerate progress by providing abundant training data.

Ground states in chemistry and materials

Dirac: "… equations much too complicated to be soluble."

Yet, heuristic classical algorithms have been very successful.

We are targeting the relatively small "strongly correlated" corner of chemistry and materials science, where such methods falter.

Can quantum computers efficiently solve for ground states in cases where classical methods fail?

Quantum computers cannot find ground states for QMA-hard cases, but that's okay. Nature does not find these states either.

How useful are quantum computers in physically relevant situations that are beyond the reach of classical methods?

Ground states in chemistry and materials

We are seeking problems that are (1) quantumly easy, (2) classically hard, (3) physically relevant.

A patchwork of heuristic classical methods including: HF, DFT, CC, QMC, DMRG, TN, NN, … These lack performance guarantees, but often work. Cost need not scale exponentially with problem size.

Quantum algorithms are heuristic, too. We need an initial state that has sufficient overlap with the ground state.

Strong correlations can result in competing phases, first-order quantum phase transitions, … Adiabatic state preparation may fail.

Garnet Chan et al., Evaluating the evidence for exponential quantum advantage in ground-state quantum chemistry (2023)

Ground states in chemistry and materials

We are seeking problems that are (1) quantumly easy, (2) classically hard, (3) physically relevant.

Perhaps exponential quantum advantage should not be expected.

But a significant polynomial advantage is a reasonable expectation and could be quite impactful.

These applications require deep quantum circuits. Fault-tolerant quantum computation will be needed, at a high cost in physical qubits and gates.

Garnet Chan et al., Evaluating the evidence for exponential quantum advantage in ground-state quantum chemistry (2023)

Simulating quantum dynamics

Classical computers are especially bad at simulating quantum *dynamics.* Quantum computers will have a big advantage.

But …

Many-body localized (MBL) systems, which equilibrate slowly, are only slightly entangled, and *might* therefore be easy to simulate classically.

Systems with strong quantum chaos become highly entangled and are therefore hard to simulate classically. But they might be boring – perhaps they quickly converge to thermal equilibrium and after that “nothing interesting” happens.

If we ask the right questions, scientifically informative surprises should be expected (quantum many-body scars, diabatic evolution in quantum spin liquids, …)

Digital vs. Analog quantum simulation

Near-term quantum simulators can be either *digital* (circuit based) or *analog* (tunable Hamiltonians).

Analog quantum simulation has been an active research area for 20 years or more; digital quantum simulation is just getting started in the past few years.

Digital provides more flexible Hamiltonian and initial state preparation. But gate based simulations of time evolution are expensive.

Analog platforms include: ultracold (neutral) atoms and molecules, trapped ions, superconducting circuits, etc. These same platforms can also be used for circuit-based computation.

Although they are becoming more sophisticated and controllable, analog simulators are limited by imperfect control. They are best suited for studying "robust" properties that can be accessed using noisy quantum systems.

Eventually, digital (circuit-based) quantum simulators will surpass analog quantum simulators for studies of quantum dynamics, but perhaps not until fault tolerance is feasible.

Experience with near-term digital simulators will lay foundations for fault-tolerant simulations in the future (applies to NISQ more broadly).

Prototypical quantum dynamics simulation task

(1) State preparation. E.g., incoming scattering state.

(2) Hamiltonian evolution. E.g. Trotter approximation.

(3) Measure an observable. E.g., a simulated detector.

Goal: sample accurately from probability distribution of outcomes.

Determine how computational resources scale with: error, system size, particle number, total energy of process, energy gap, …

Resources include: number of qubits, number of gates, …

Hope for polynomial scaling! Or even better: polylog scaling.

Need an efficient preparation of initial state.

Approximating a continuous system incurs discretization cost (smaller lattice spacing improves accuracy).

Is circuit based dynamical simulation too expensive for the NISQ era?

Huang et al., Classically estimating observables of noiseless quantum circuits, 2409.01706

Estimate expectation of (local) observable after evolution.
Heisenberg picture, truncate the Pauli path integral.
Works for noisy circuits because high weight operators are highly damped.
Works for noiseless circuits, too, if “locally scrambling.”
Use classical shadow of the input state.

Begušić and Chan, Real-time operator evolution in two and three dimensions via sparse Pauli dynamics, 2409.03097

Validated by 1D, 2D, and 3D simulations.

D-Wave, Computational supremacy in quantum simulation, 2403.00910.

Spin glass dynamics. Fast quench (7 ns) in TFIM with > 5000 qubits.
Kibble-Zurek exponents consistent with quantum phase transition.
Programmable J_{ij}.

Harvard, Quantum Kibble-Zurek mechanism and critical dynamics on a programmable Rydberg simulator, Nature 2019.

51 qubits, Z2, Z3, Z4 universality classes.

Google, Dynamics of magnetization at infinite temperature in Heisenberg spin chain, Science 2024.

1D Heisenberg with ZZ deformed from 1 (XXZ model).
Total Z magnetization conserved → emergent hydrodynamics.
Spin transport: $\langle M(t) \rangle \sim t^{1/z}$: Ballistic (z=1), diffusive (z=2), or superdiffusive (z=3/2, the KPZ prediction).

46-qubit simulation on Google hardware.
Higher moments of M(t) depart from KPZ expectations.
Further study requires high initial temperature and long times.

Being Cool

Rule of thumb: Exotic phases when temperature is about 100 times smaller than natural energy scale. (Why?)

An impediment if we wish to study e.g. high-temperature superconductivity with an analog simulator.

Chen et al., Local minima in quantum systems, 2309.16596

Quantum thermal gradient descent algorithm from Lindblad dynamics.
Finding local minima of the energy is quantumly easy.
It is also BQP-hard, hence classically hard.

What are the classically hard instances?
After optimizing classically, detect classically that a quantum algorithm could do better.

Quantum simulation of quantum field theory

50 years since Ken Wilson proposed lattice gauge theory!

Real-time evolution (collider physics), nonzero chemical potential (early universe, neutron stars), …

What's classically hard? Processes that produce highly entangled states, e.g., multiparticle production, quench, …

Laying the foundations for more revealing future work.

Stepping stone to quantum gravity.

New concepts and insights?

Entanglement in high-energy scattering

Two incoming high-energy particles, many soft outgoing particles. Crudely model the outgoing particles as a thermal ensemble with temperature T = O(1).

The overall state is pure – the thermodynamic entropy of left-movers and right-movers is really entanglement entropy.

If the particles are emitted from the interaction region in a time t ~ L, they occupy a region of size L. Entropy S, particle number N, energy E, are related by

$$S \sim N \sim TL \sim E / T$$

The bond dimension is *exponential in the entropy*, therefore a classical simulation of the scattering would be very difficult for about 20 particles.

We could measure time-dependence of the outgoing particle flux, particle-particle correlations, etc.

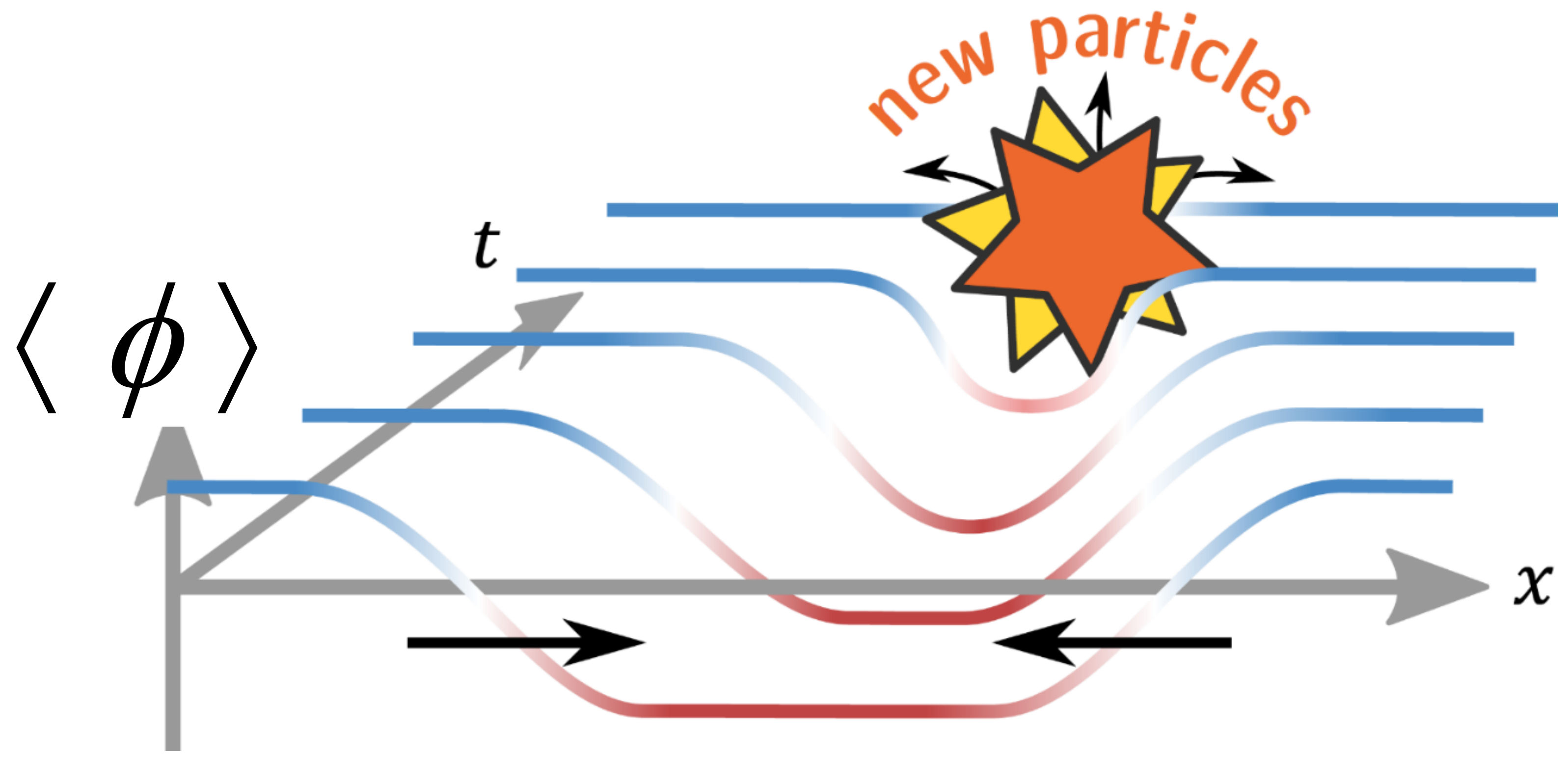
Bañuls et al., Real-time scattering in the lattice Schwinger model, 2402.18429.

Stable particles, vector and scalar (scalar is bound state of two vectors).
Inelastic scattering VV → SS.
Second-order Trotter, 100 sites, bond dimension 50.
Far from the continuum (makes state prep easier).

Farrell et al., Quantum simulations of hadron dynamics in the Schwinger model using 112 qubits, 2401.08044.

112 qubits (56 lattice sites), 13,858 2Q gates on IBM.
Build wavepacket at infinite coupling, then adiabatically turn on the kinetic term.
Truncate interactions over distance > correlation length.
Optimize circuit to reduce depth.
Physics circuit and mitigation circuit, rescale observables in physics circuit.
Measure chiral condensate to detect meson after evolution.

Milsted, Liu, Preskill, Vidal, Collisions of false-vacuum bubble walls in a quantum spin chain, PRX Quantum 2022.

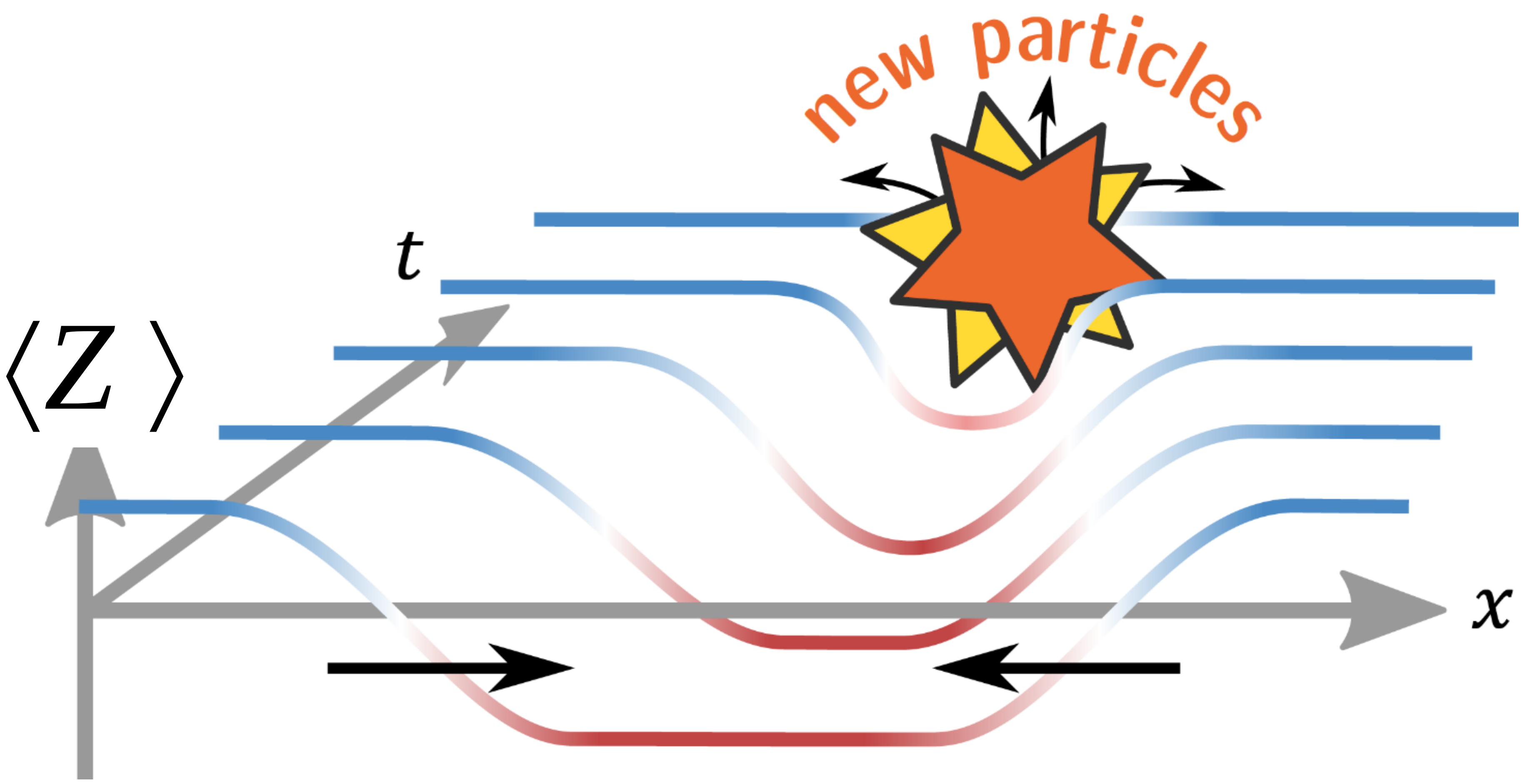


Kink-antikink scattering: Lots of entropy generated, so hard to simulate classically.

Excitations are nonperturbative (cf. proton in large-*N* QCD). A baby version of what we'll need in QCD.

And it's not obvious what happens at strong coupling.

Emergent field theory in a spin system. Heuristic, but more likely to be feasible using near-term platforms. And interesting in its own right. (Cf. colliding bubble walls in the early universe.)

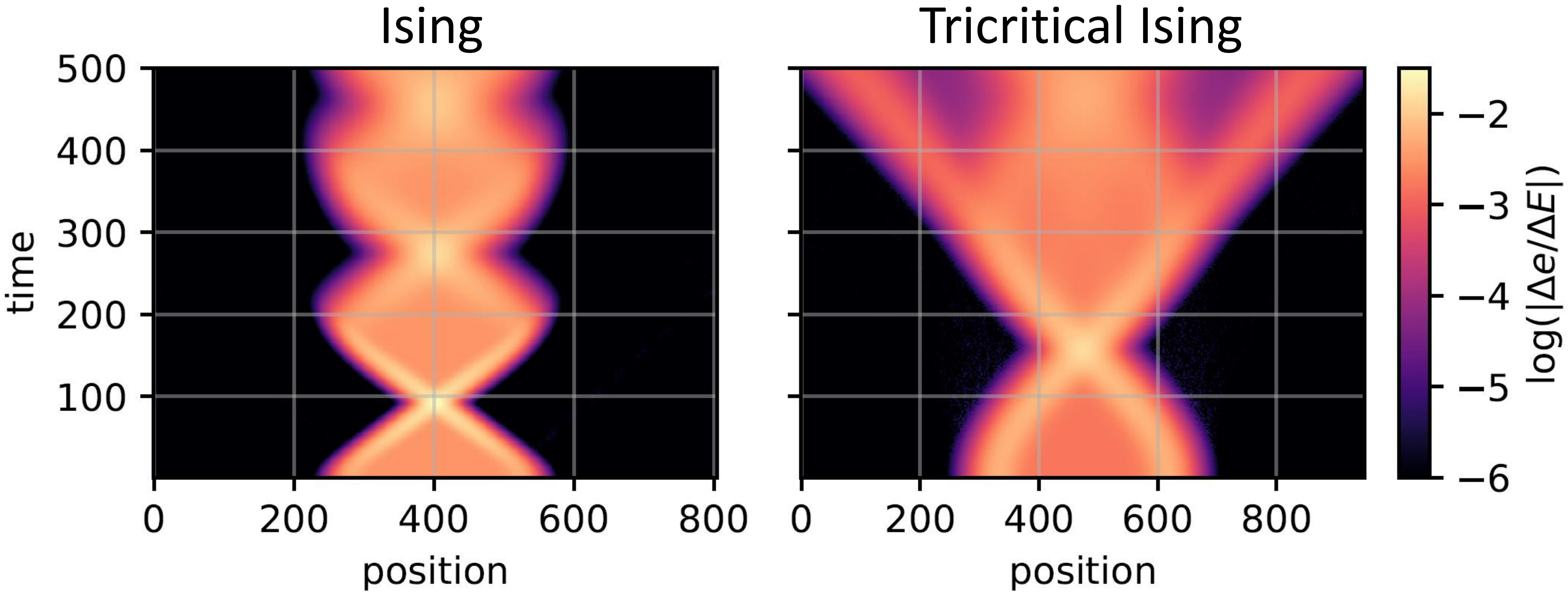


Explicit symmetry breaking (false vacuum)

$$H = \sum_{j=1}^{N} \left[-Z_j Z_{j+1} - gX_j - hZ_j + \lambda \left(X_j Z_{j+1} Z_{j+2} + Z_j Z_{j+1} X_{j+2} \right) \right]$$

We want a spin chain with these features:

-- Emergent Lorentz-invariant field theory
-- Spontaneously broken discrete symmetry
-- Not integrable (or too close to integrable)

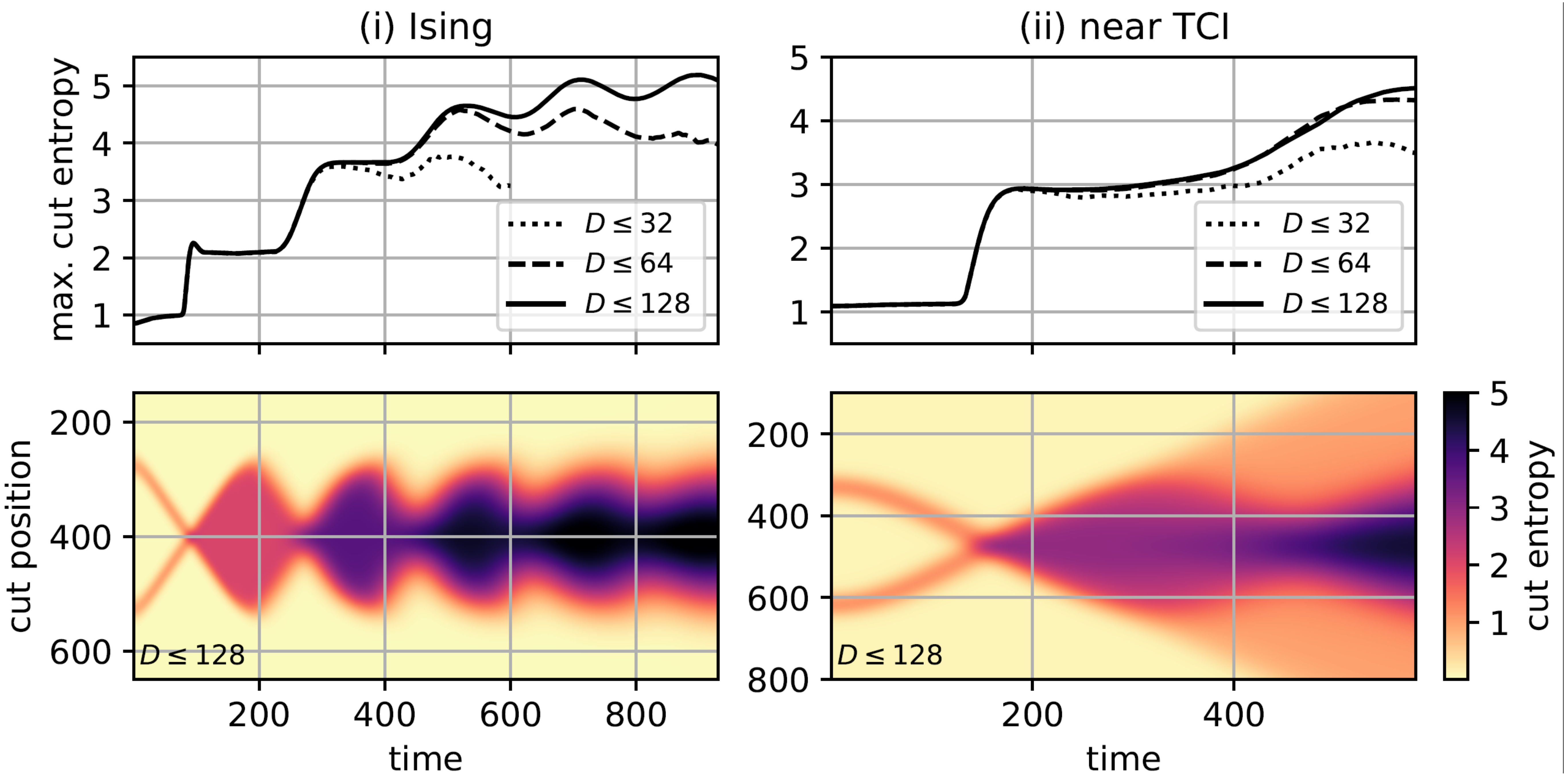


Here excess energy density (relative to the true vacuum) is plotted as a function of position and time.

A kink-antikink pair with false vacuum in between is confined. They collide repeatedly.

The IR limit of the Ising model with $Z2$ symmetry broken ($\lambda = 0$) is an integrable theory. Kinks “bounce” --- no new particles are produced.

The tricritical Ising model ($\lambda \neq 0$) is a nonintegrable field theory. Unconfined “mesons” are produced which propagate ballistically.

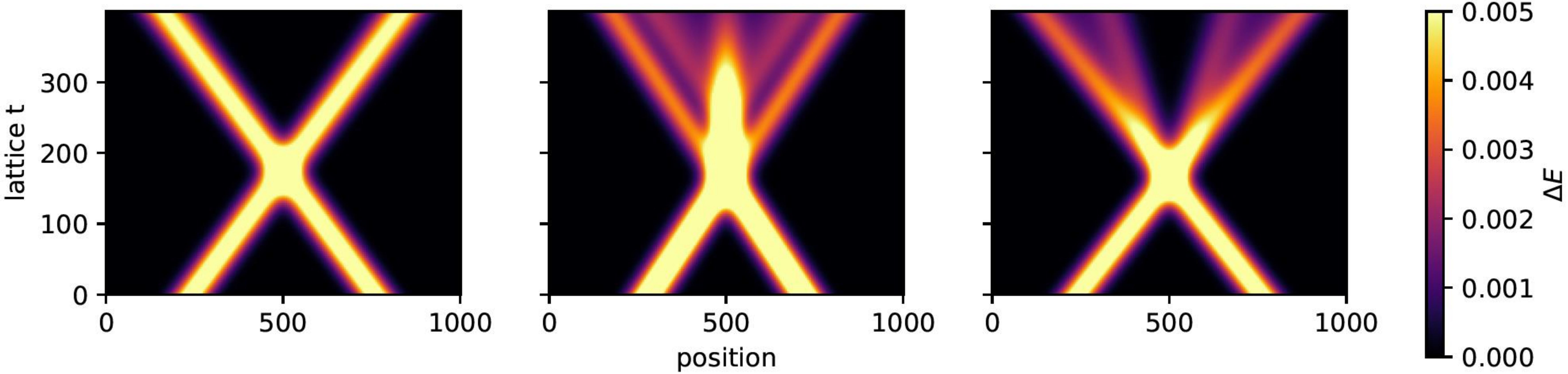


Here entanglement entropy across a cut is plotted as a function of time.

Entropy can increase due to either elastic scattering of wave packets (momentum dependence of scattering phase shift), or due to inelastic particle production.

As entropy increases, a larger bond dimension *D* is needed to approximate the state accurately.

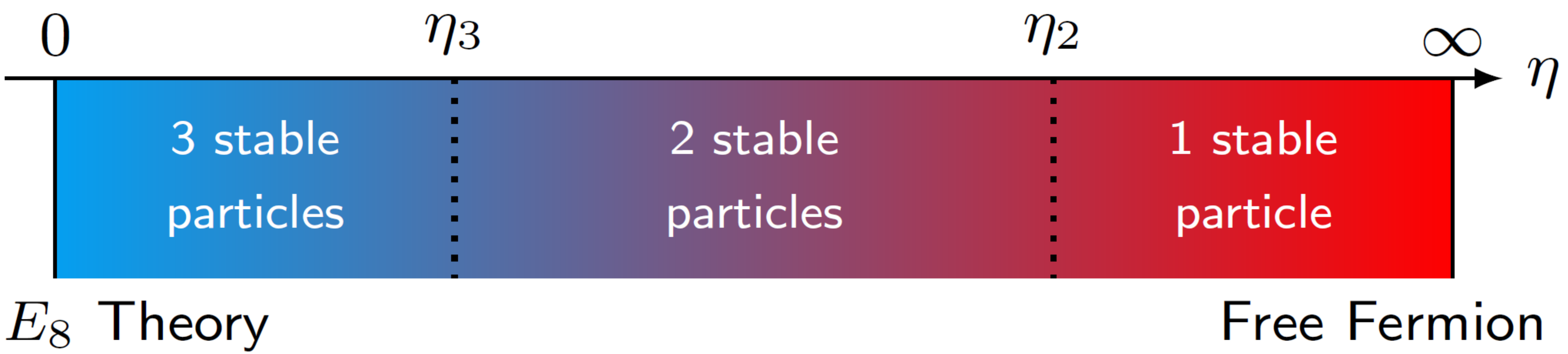
Jha, Milsted, Neuenfeld, Preskill, Vieira, Real-time scattering in Ising field theory using matrix product states, in preparation



elastic resonance inelastic

Ising field theory: A line of nonintegrable theories connecting free fermions and E_8

$$I_{\mathrm{IFT}} = I_{\mathrm{ICFT}} - \tau \int d^2 x \epsilon(x) - h \int d^2 x \sigma(x), \quad \eta \equiv \frac{\tau}{|h|^{8/15}}$$



$$H = -\sum_{j=0}^{N} \left(\sigma_j^z \sigma_{j+1}^z + g_x \sigma_j^x + g_z \sigma_j^z \right), \qquad \eta_{\mathrm{latt}} = \frac{g_x - 1}{|g_z|^{8/15}}$$

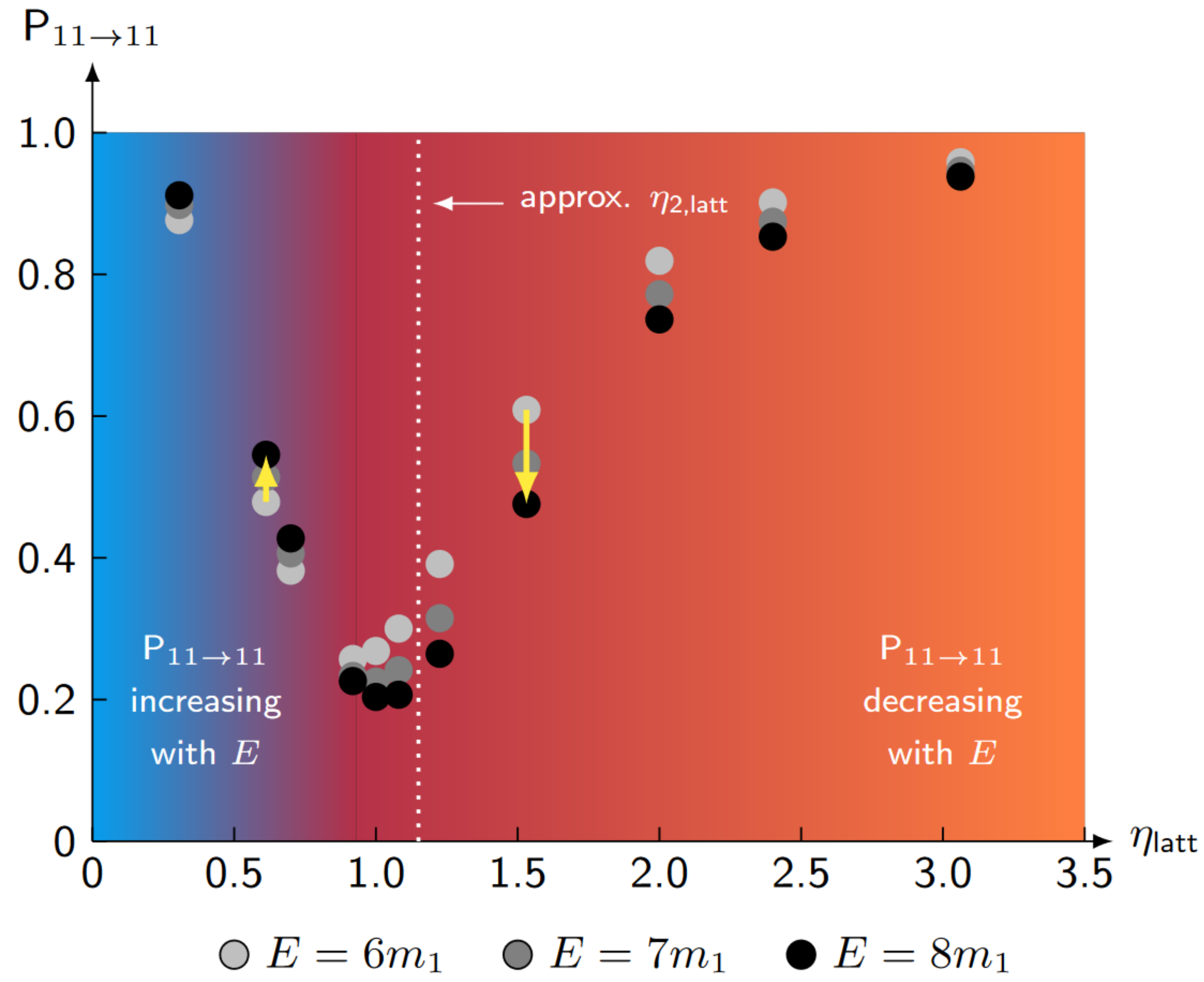
Ising field theory: A line of nonintegrable theories connected free fermions and E_8

Evolve by time-dependent variational principle:
1000 sites, bond dimension 64, correlation length 4-10 sites, wavepacket width 70-100 sites.

Elastic scattering phase shifts from time delay.
Probabilities for inelastic channels 11 → 12, 11→ 13, 11→111.
Perturbation theory near free fermions and E_8.
Strong coupling where previous methods fail.

Track masses and widths of resonances.

“High energy” (up to E = 8m).
As energy increases, probability of elastic scattering increases near E_8, and decreases near free fermions.



Girvin et al., Hybrid oscillator-qubit quantum processors: Simulating fermions, bosons, and gauge fields, 2409.03747.

Circuit QED: Encode bosonic modes and gauge fields in (3D) cavities.
Digital: universal gate constructions. Coupling cavities, e.g. with SNAIL.
Advantage for nonequilibrium dynamics with large occupation number?
QEC: logical bosons encoded in physical bosons.

Tong et al., Provably accurate simulation of gauge theories and bosonic systems, Quantum 2022.

Bounds on growth of local quantum numbers.
E.g. electric field in U(1) and SU(2) gauge theories.

Demler et al., Quantum approximate Bayesian computation for NMR model inference, Nature Machine Intelligence 2020.

Large biomolecule liquid state or high field solid state.
Quantum simulator extracts NMR spectrum of hypothetical model.
Coherent exchange, hard to simulate.
Where does practical utility lie?

Monroe et al, Digital quantum simulation of NMR experiments, Science Advances 2023.

Simulation of zero field NMR with trapped ions, 4 active spins.

Simulating quantum dynamics

Will quantum computers will have a big advantage?
NISQ, early fault tolerance, mature fault tolerance.
Digital vs. analog.

Expect surprises ("discoverinos"). What could be scientifically instructive?

Limitations of classical methods like truncated Pauli path integral, tensor networks, …

Optimizing quantum circuits, e.g. initial state preparation, error mitigation, …