

QFT Simulation in the Age of Quantum Computers

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Quantum Field Theory

- Much is known about using quantum computers to simulate quantum systems.

Quantum Field Theory

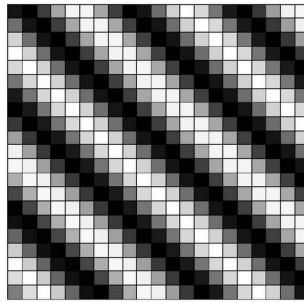
- Much is known about using quantum computers to simulate quantum systems.
- Why might Quantum Field Theory be different?

Quantum Field Theory

- Much is known about using quantum computers to simulate quantum systems.
- Why might Quantum Field Theory be different?
 - Field has infinitely many degrees of freedom
 - Relativistic
 - Particle number not conserved
 - Formalism looks different

Representing Quantum Fields

- A field is a list of values, one for each location in space.



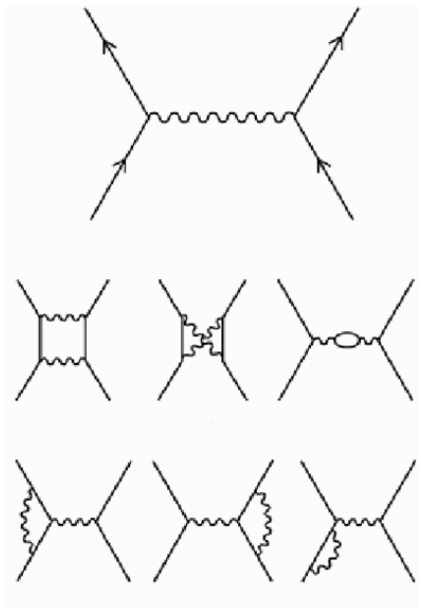
- A quantum field is a superposition over classical fields.

$$\frac{1}{\sqrt{2}} \left| \begin{array}{c} \text{[Horizontal Gradient Field]} \end{array} \right\rangle - \frac{i}{\sqrt{2}} \left| \begin{array}{c} \text{[Diagonal Field]} \end{array} \right\rangle$$

- A superposition over bit strings is a state of a quantum computer.

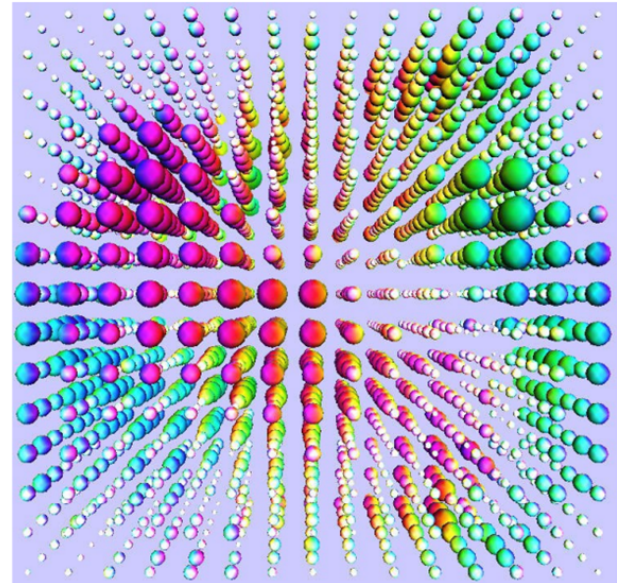
Classical Algorithms

- Feynman Diagrams



- Breaks down at strong coupling or high precision

- Lattice Methods

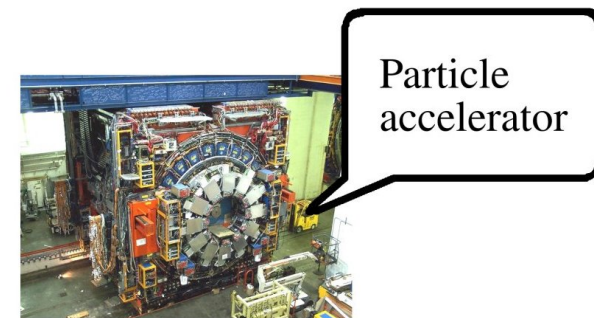
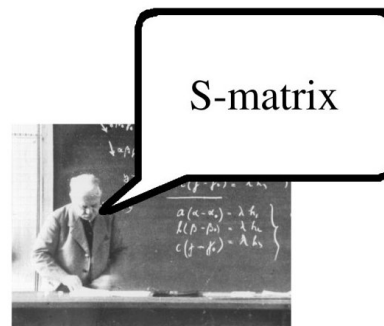
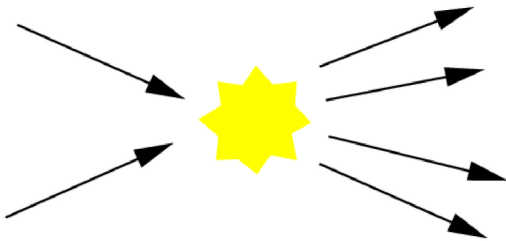


- Good for binding energies.
- Real-time dynamics difficult

There's room for exponential speedup by quantum computing.

Layout of the scattering Problem

- Input:
 - A set of incoming particles with given momenta
 - A Hamiltonian
 - A time of evolution
- The Output of Scattering:
 - A set of particles with their momenta at the end of the evolution time



Bosonic vs Fermionic

- Boson statistics:
 - Map to local operators
 - They can all occupy the same quantum state.
 - The number of qubits per lattice site is proportional to the energy cutoff.
- Fermion statistics
 - Map to non-local operators
 - Jordan-Wigner transformation
 - Workarounds exist
 - Can be represented with a constant number of qubits per site.
 - Fermion doubling

Motivation

- Jordan-Lee-Preskill (2014)
 - Proof of concept for BQP
 - Run-time dominated by state preparation
 - State preparation very slow
 - Limited to the phase directly connected to free theory
- Two paths forward to improve state preparation
 - More efficient state preparation algorithms
 - More general state preparation algorithms

Gross-Neveu Model

- Toy model for QCD
- 1+1d- fermionic
- Asymptotic Freedom
- Has flavors
- Chiral symmetry
 - Broken by mass term m_0



$$\mathcal{L} = \sum_{j=1}^N \bar{\psi}_j (i\partial\!\!\!/ - m_0) \psi^j + \frac{g^2}{2N} \left(\sum_{j=1}^N \bar{\psi}_j \psi^j \right)^2$$

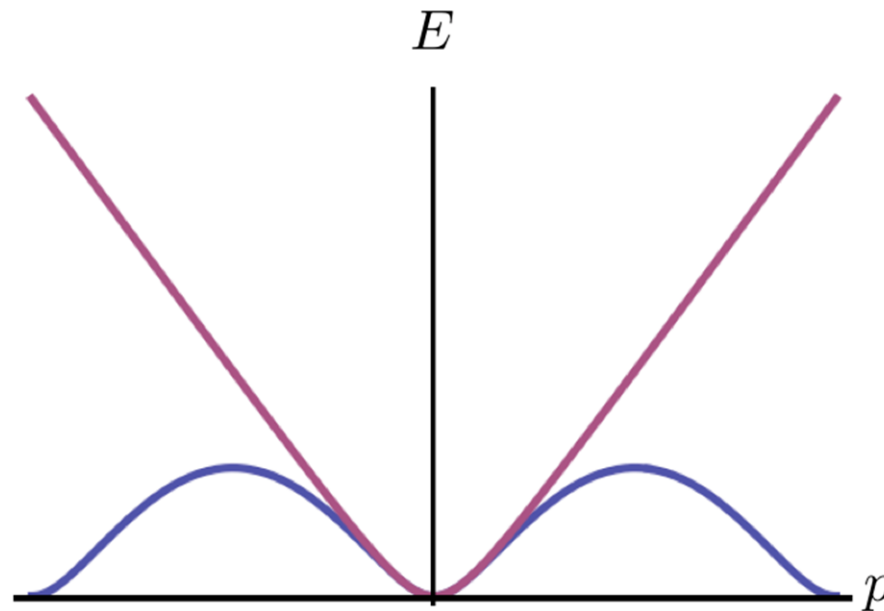
Jordan-Lee-Preskill(2014)

1. Prepare the GS of system, NN-term and g_0 set to zero
2. Adiabatically turn on the NN-term
3. Adiabatically turn on the g_0 term
4. Excite particles by adding a weak sinusoidal source term to the Hamiltonian.
5. Evolve in time
6. Either phase estimate local charges or adiabatically return to free theory then phase estimate number operators of momentum mode.

$$G_{\text{total}} = \begin{cases} O(\epsilon^{-8-o(1)}), & \text{as } \epsilon \rightarrow 0, \\ O(p^{9+o(1)}), & \text{as } p \rightarrow \infty. \end{cases}$$

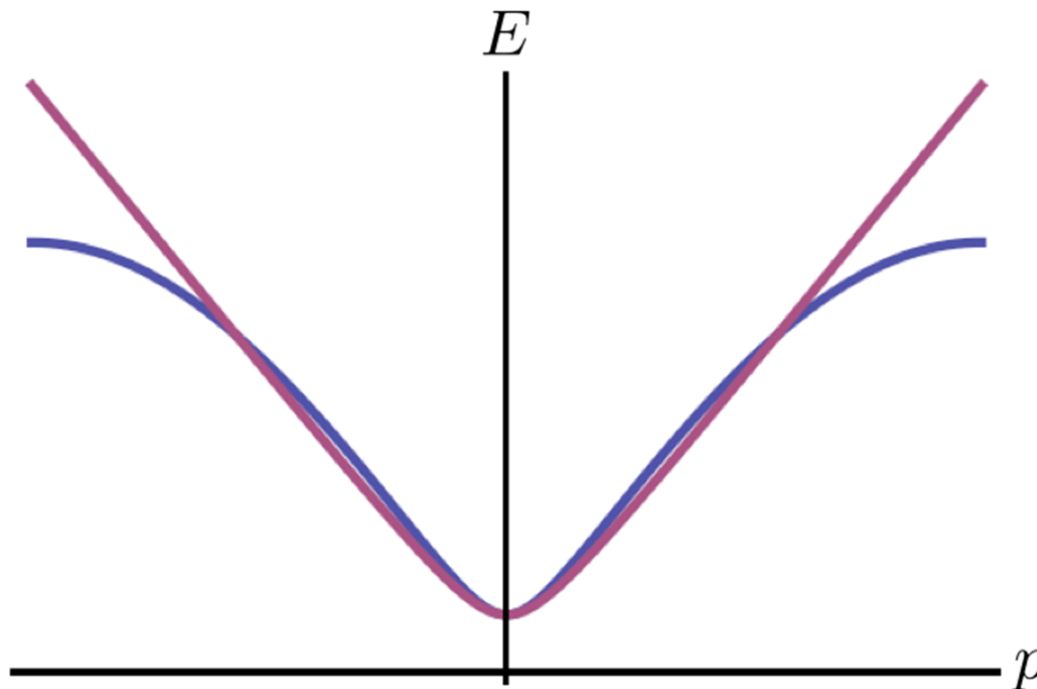
Fermion Doubling Problem

$$\frac{d\psi}{dx} \rightarrow \frac{\psi(x+a) - \psi(x-a)}{2a} \quad \sqrt{p^2 + m^2} \rightarrow \sqrt{\sin^2 p + m^2}$$



Wilson term

$$H \rightarrow H - \frac{r}{2a} \sum_x \bar{\psi} (\psi(x+a) - 2\psi(x) + \psi(x-a))$$



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Faster quantum algorithm to simulate fermionic quantum field theory

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In quantum algorithms discovered so far for simulating scattering processes in quantum field theories, state preparation is the slowest step. We present an algorithm for preparing particle states to use in simulation of fermionic quantum field theory (QFT) on a quantum computer, which is based on the matrix product state ansatz. We apply this to the massive Gross-Neveu model in one spatial dimension to illustrate the algorithm, but we believe the same algorithm with slight modifications can be used to simulate any one-dimensional massive fermionic QFT. In the case where the number of particle species is 1, our algorithm can prepare particle states using $O(\epsilon^{-3.23\dots})$ gates, which is much faster than previous known results, namely, $O(\epsilon^{-8-o(1)})$. Furthermore, unlike previous methods which were based on adiabatic state preparation, the method given here should be able to simulate quantum phases unconnected to the free theory.

DOI: [10.1103/PhysRevA.98.012332](https://doi.org/10.1103/PhysRevA.98.012332)

Faster quantum algorithm to simulate fermionic quantum field theory

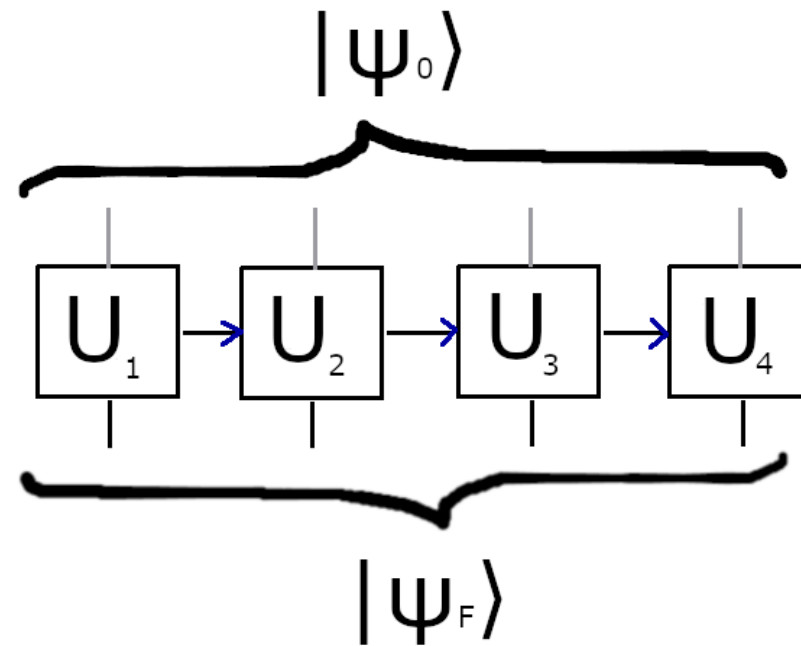
- Discretize and put on a lattice.
- Use DMRG to calculate the GS of interacting theory.
 - Map the MPS to a quantum circuit.
 - Apply the Quantum circuit to get the GS.
- Excite particles using Rabi Oscillations.
 - Floquet's Theorem, guarantees excitation.
- Evolve in time(e.g. Suzuki-Trotter)
- Measure the outcome using phase estimation algorithm.
- Performance, Quantum: $\mathcal{O}\left(\epsilon^{-3-o(1)}\right)$ Classical: $\mathcal{O}\left(\epsilon^{-N/2-1-\sqrt{3N}}\right)$

From MPS to Quantum Circuit

- **DMRG:**

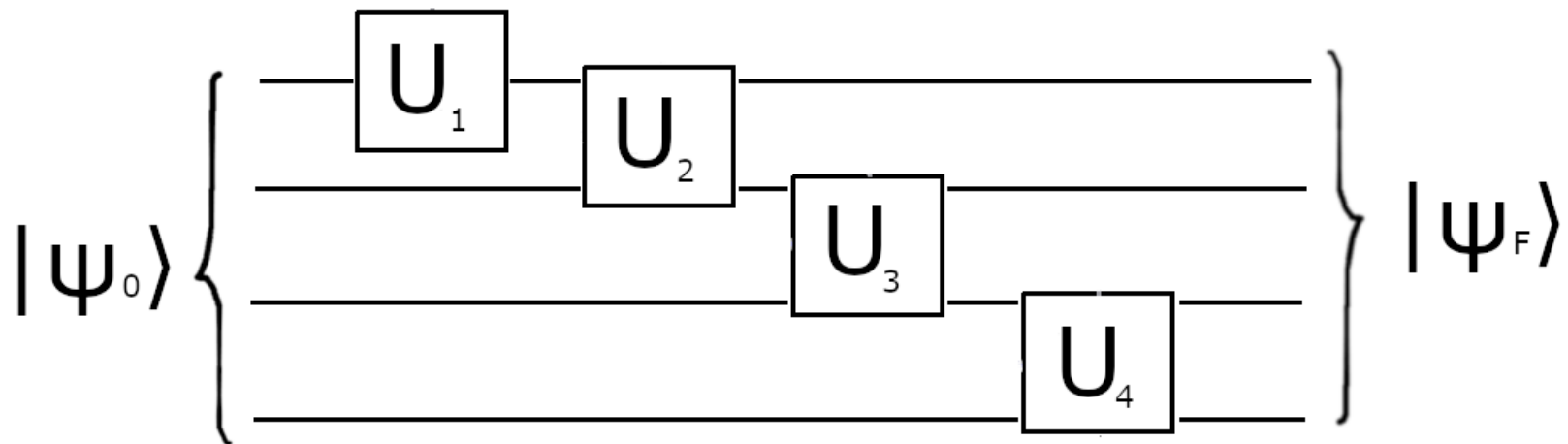
$$|\psi_F\rangle = \begin{array}{cccc} \boxed{M_1} & - & \boxed{M_2} & - & \boxed{M_3} & - & \boxed{M_4} \\ | & & | & & | & & | \end{array}$$

- **SVD:**



From MPS to Quantum Circuit

- Quantum Circuit:



- Each of these classical steps, run in time:

$$\mathcal{O}(n\chi^3)$$

Exciting Initial Particles

- Starting in the ground state of interacting Hamiltonian, simulate dynamics with a sinusoidal source term(Rabi Oscillations):

$$H(t) = H_0 + \lambda \sin(\omega t)W$$

- ω is chosen so it resonates with our desired state:

$$\omega = \sqrt{p^2 + m^2}$$

- Ensure the desired momentum with W :

$$W = \int dx (f(x)\psi(x) + f^*(x)\psi^\dagger(x))$$

$$f(x) \propto e^{ipx - x^2/\sigma^2}$$

Few-Level Approximation

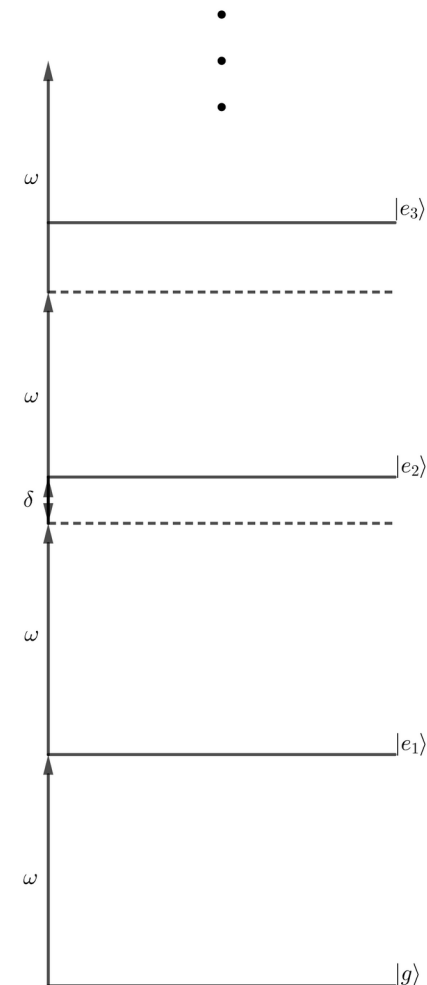
Theorem 1. Assume we have a Hamiltonian $H_0 + \lambda \cos(\omega t)W$ with $\|W\| = 1$. Let $\rho(t)$ be the projector onto the state obtained at time t starting with the ground state of H_0 at $t = 0$. Let $\rho^{(-)}$ be the projector onto the state at time t obtained by projecting $H_0 + \lambda \cos(\omega t)W$ onto the span of the lowest ν eigenstates of H_0 and solving the resulting Schrodinger equation in this ν -dimensional Hilbert space. Then

$$|\text{Tr}[\rho^{(-)}(t)\rho(t)]| \geq 1 - (2\nu\lambda + 3\nu\lambda^2t)\frac{1}{\delta}, \quad (28)$$

where δ is the minimum detuning from one of the other excited states (i.e., minimum energy distance between $\{E_0 + \omega, \dots, E_{\nu-1} + \omega\}$ and the rest of the spectrum of H_0).

Two-Level Approximation

- $\downarrow \nu$ and $\uparrow \delta =$ better approximation
- ν is the degeneracy in the rotating frame = number of states on resonance
- 2-levels for anharmonic asymmetric case.



Applying Floquet's Theorem

Theorem 2. Assume we have a two-level Hamiltonian:

$$H = -\frac{\Delta}{2}\mathbb{Z} + \lambda \cos(\omega t)\mathbb{X}, \quad (29)$$

where \mathbb{X} and \mathbb{Z} are Pauli matrices and $\Delta > 0$ is a real number. We initialize our state at time $t = 0$ to be $|0\rangle$ in the standard basis. For $\lambda \ll \omega$, after time $t = \frac{\pi}{\lambda}$,

$$\left| \left\langle 1 \left| \psi \left(\frac{\pi}{\lambda} \right) \right\rangle \right| \geq 1 - \frac{1}{\sqrt{3}} \left(\frac{\lambda}{\omega} \right)^2 - \mathcal{O} \left[\left(\frac{\lambda}{\omega} \right)^4 \right]. \quad (30)$$

Exciting Initial Particles, Bounds

- Two ingredients go into our analysis of the success rate of exciting particles:

1. 2-level approximation. Error bound:

$$|\langle \psi(t) | \psi_2(t) \rangle| \geq 1 - (2\lambda + 3\lambda^2 t) \frac{1}{\delta}$$

2. Analyze 2-level system with Floquet's theory:

$$|\langle \mathbf{1} | \psi_2(\pi/\lambda) \rangle| \geq 1 - \frac{1}{\sqrt{3}} \left(\frac{\lambda}{\omega} \right)^2$$

Limitations

- Jordan-Lee-Preskill:

- Not practical:

$$\mathcal{O}\left(\epsilon^{-8-o(1)}\right)$$

- Adiabatic state preparation:

- Limited to the phase adiabatically connected to the free phase of the theory.

- Moosavian-Jordan:

- 1+1 space-time dimensions

- Bottlenecked by classical heuristic algorithm:

$$\mathcal{O}\left(\epsilon^{-N/2-1-\sqrt{3N}}\right)$$

Site-by-site quantum state preparation algorithm for preparing vacua of fermionic lattice field theories

Site-by-site quantum state preparation algorithm for preparing vacua of fermionic lattice field theories

Ali Hamed Moosavian, James R. Garrison, Stephen P. Jordan

(Submitted on 8 Nov 2019)

Answering whether quantum computers can efficiently simulate quantum field theories has both theoretical and practical motivation. From the theoretical point of view, it answers the question of whether a hypothetical computer that utilizes quantum field theory would be more powerful than other quantum computers. From the practical point of view, when reliable quantum computers are eventually built, these algorithms can help us better understand the underlying physics that govern our world.

In the best known quantum algorithms for simulating quantum field theories, the time scaling is dominated by initial state preparation. In this paper, we exclusively focus on state preparation and present a heuristic algorithm that can prepare the vacuum of fermionic systems in more general cases and more efficiently than previous methods. With our method, state preparation is no longer the bottleneck, as its runtime has the same asymptotic scaling with the desired precision as the remainder of the simulation algorithm. We numerically demonstrate the effectiveness of our proposed method for the 1+1 dimensional Gross-Neveu model.

Comments: 10 pages, 6 figures

Subjects: **Quantum Physics (quant-ph)**

Cite as: [arXiv:1911.03505](https://arxiv.org/abs/1911.03505) [quant-ph]

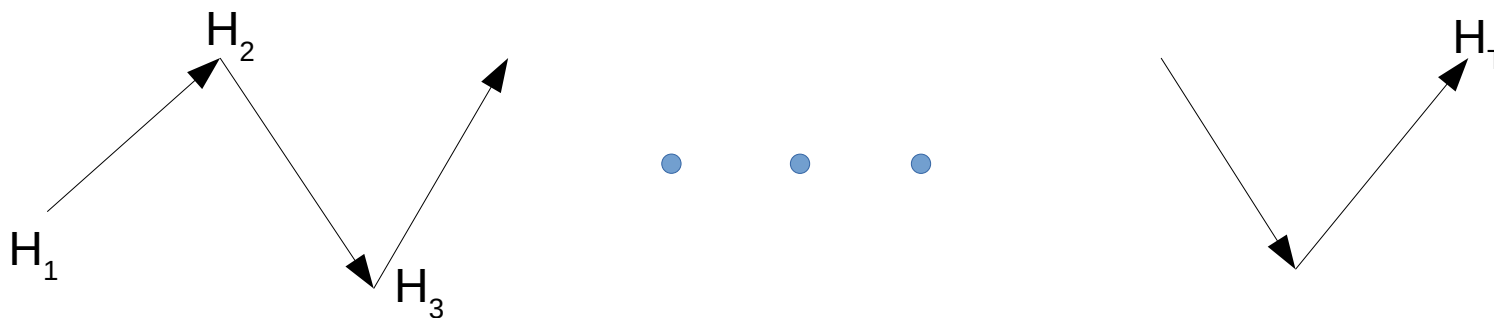
(or [arXiv:1911.03505v1](https://arxiv.org/abs/1911.03505v1) [quant-ph] for this version)

Overview of the Algorithm

- Start with the ground state of a small system:
 - Can be explicitly calculated
- We add sites to the ground state, one site at a time
- Two requirements:
 - The spectral gap doesn't close:
 - Mass gap
 - The inner product between consecutive ground states is not exponentially close to zero:
 - Physical intuition: with finite correlation length, the inner product should approach a constant.

Jagged Adiabatic Path Lemma

LEMMA 1.3 (the jagged adiabatic path lemma). *Let $\{H_j\}_{j=1}^{T=\text{poly}(n)}$ be a sequence of bounded norm, simulatable Hamiltonians on n qubits, with nonnegligible spectral gaps, $\Delta(H_j) \geq n^{-c}$, and with known ground-values, such that the inner product between the unique ground-states $\alpha(H_j), \alpha(H_{j+1})$ is at least n^{-c} for all j . Then there exists an adiabatic state generator with $\alpha(H_0)$ as its initial state and $\alpha(H_T)$ as its final state. In particular there exists an efficient quantum algorithm that takes $\alpha(H_0)$ to within arbitrarily small distance from $\alpha(H_T)$.*



Preparing PEPS on a QC

Theorem 1: Let $G = (V, E)$ be an interaction graph with bounded degree and some total order defined on V . Let $\{A^{(v)}\}_{v \in V_{[t]}}$ be a set of injective PEPS projectors of dimension $d \times D^k$ associated with each v in V up to vertex t (according to the total vertex order) describing a sequence of PEPS $|\psi_t\rangle$, and let $\kappa = \max_{v \in V} \kappa(A^{(v)})$ be the largest condition number of all PEPS projectors. Let $\Delta = \min_t \Delta(H_t)$, where $\Delta(H_t)$ is the spectral gap of the parent Hamiltonian H_t of the PEPS $|\psi_t\rangle$. Then there exists a quantum algorithm generating the final PEPS $|\psi_{|V|}\rangle$ with probability at least $1 - \varepsilon$ in time $\tilde{O}\left(\frac{|V|^2 |E|^2 \kappa^2}{\varepsilon \Delta} + |V| k d^6\right)$.

Modified Jagged Path Lemma

Theorem 1 (Modified Jagged Path Lemma).

- Sequence $\{H_j\}_{j=1}^N$ of geometrically local, bounded norm, gapped Hamiltonians

$$\Delta(H_j) \geq m_j > 0$$

- Non-vanishing overlap of ground states

$$|\langle g_j | g_{j+1} \rangle| \geq \eta > 0$$

- Predictions of GS energies

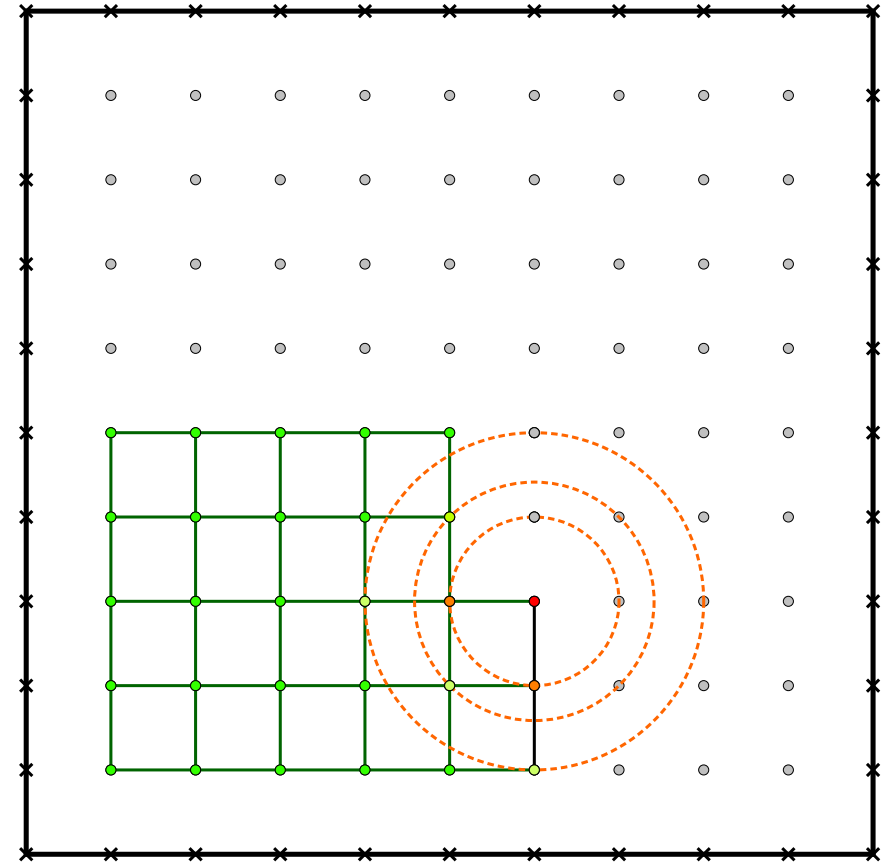
→ QA $|g_1\rangle \rightarrow |g_N\rangle$ in run-time $O\left(\frac{Nn}{m\eta} \text{polylog}(1/\epsilon)\right)$

The Algorithm

- Set Lattice Spacing $a \propto \epsilon/p$
- Discretize the Hamiltonian
- Prepare the GS of a small system $|g_{N_0}\rangle$
- Apply a unitary, e.g. Hadamard on the rest of the system
- Repeat:
 - Transform $|g_j\rangle \otimes |Q_{j+1}\rangle$ to $|g_{j+1}\rangle$ using Theorem 1
- Runtime: $O\left(\frac{V^2}{a^{2D}\eta} \text{polylog}\left(\frac{1}{\epsilon}\right)\right)$

Adding sites

- Keep the shape as close to a D-dimensional hypercube as possible.
- This ensures the overlaps do not vary too much during the preparation algorithm.
- If correlation length is finite, only a finite amount of sites will be affected.



The Conjecture

Conjecture 1 (Overlap of ground states). *Assume a properly discretized massive fermionic QFT that obeys the Wightman axioms, in particular, the energy-momentum spectral condition [42]. Let $|g_j\rangle$ be the ground state of the system with j sites and η be defined as $\lim_{j \rightarrow \infty} |(\langle g_j| \otimes \langle Q|) |g_{j+1}\rangle|$, where $|Q\rangle$ is an unentangled state that is present to make the Hilbert spaces compatible. Then there exists $|Q\rangle$ for which $\eta > 0$.*

The Conjecture

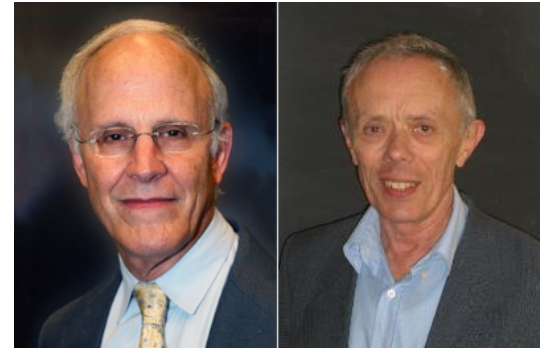
- Proven cases:
 - GS is injective PEPS
Phys. Rev. Lett. 108,
110502 (2012).
 - GS is topological
PEPS
Phys. Rev. A - At. Mol.
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The Conjecture

- Proven cases:
 - GS is injective PEPS
Phys. Rev. Lett. 108, 110502 (2012).
 - GS is topological PEPS
Phys. Rev. A - At. Mol. Opt. Phys. 88, 1–5 (2013).
- Counter example:
 - AKLT
- Does not have a single site coarse continuum limit!
- Solution:
 - Add two sites at a time

Testing on Classical Computers

- Gross-Neveu model
- Pick some reasonable variables:
 - m_0, g_0
- Calculate GS using DMRG for different system sizes:
 - up to 50 sites
- Calculate inner product between GS of consecutive systems.



Mass Renormalization & Correlation Length

- How to calculate the gap? How about CL?
- Continuous Free Theory:

$$\langle 0 | \psi_0(x) \bar{\psi}_0(y) | 0 \rangle = \frac{m_0}{2\pi} K_0(m_0 |x - y|)$$

- Discretized and Interacting Theory:

$$\langle 0 | \psi_0(x) \bar{\psi}_0(y) | 0 \rangle \propto K_0(m|x - y|) + O(a)$$

- Where m is the renormalized mass and is inversely proportional to the correlation length χ .

$$K_0(\zeta) \sim \sqrt{\frac{\pi}{2\zeta}} e^{-\zeta} \left(1 - \frac{1}{8\zeta} + \frac{9}{128\zeta^2} + O\left(\frac{1}{\zeta^3}\right) \right)$$

Choosing an appropriate parameters

- A reasonable correlation length should be much larger than lattice spacing and much smaller than system size at the same time.

$$a \ll \chi \ll L \Rightarrow \chi \approx \frac{L}{\sqrt{51}} \approx \frac{L}{7.14}$$

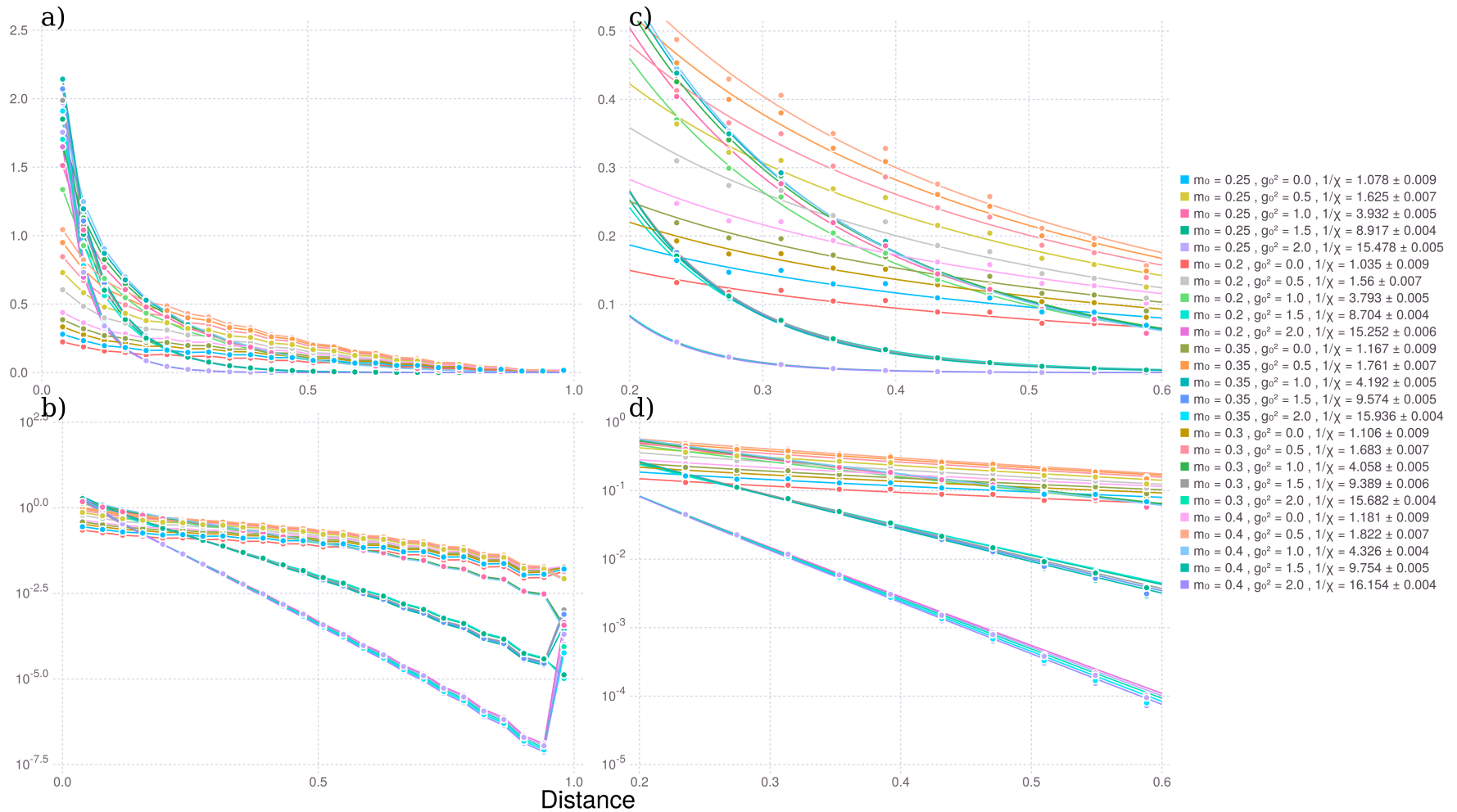
- Preliminary numerical investigation:

$$g_0^2 \in [0, 2.0] \quad m_0 \in [0.2, 0.4]$$

Two point correlation functions

Two-point correlation functions

$$\langle \psi_0 \left(\frac{1}{2} - \frac{\Delta x}{2} \right) \bar{\psi}_0 \left(\frac{1}{2} + \frac{\Delta x}{2} \right) \rangle$$

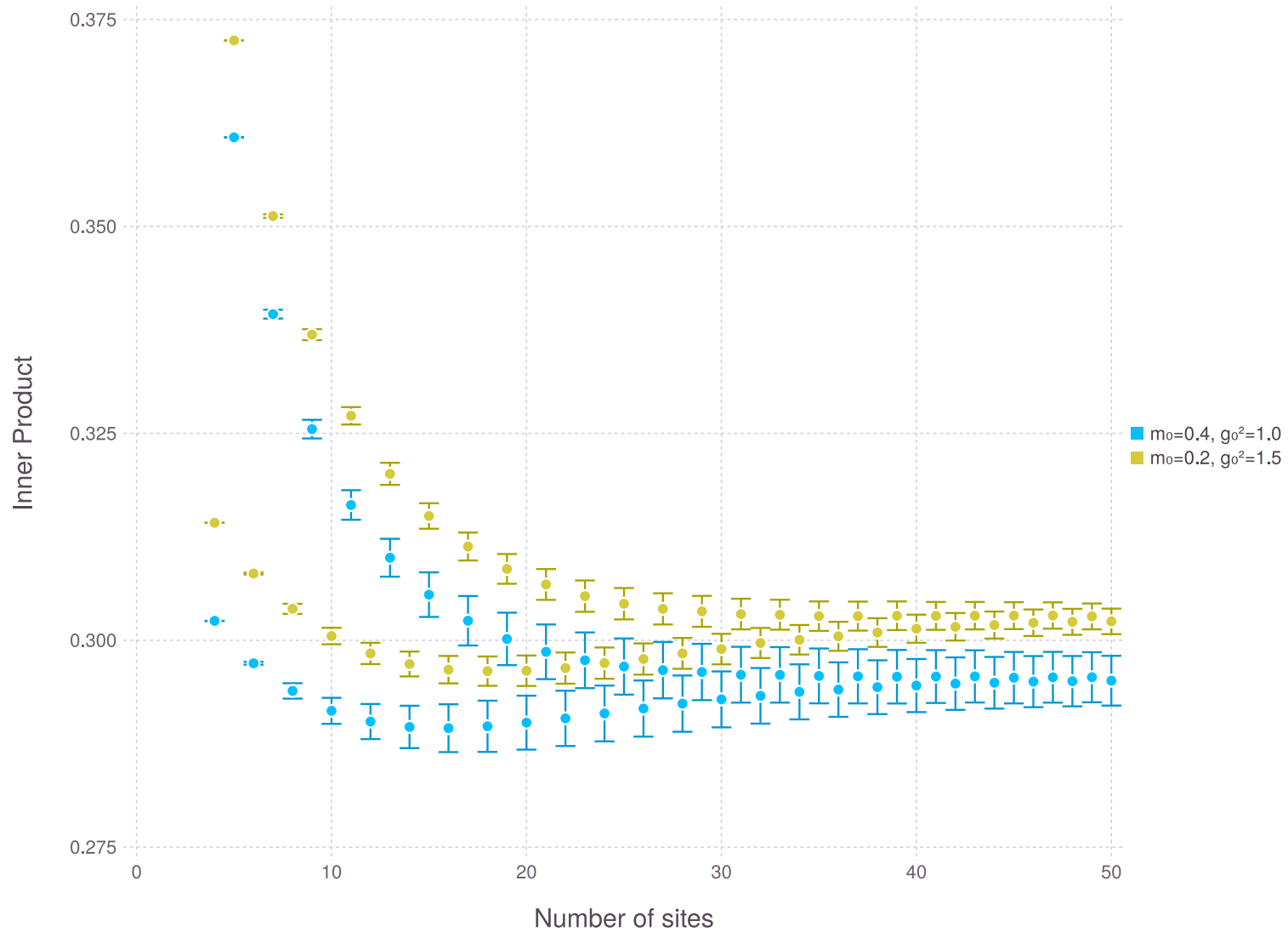


Correlation lengths

■ $m_0 = 0.25$, $g_0^2 = 0.0$, $1/\chi = 1.078 \pm 0.009$
■ $m_0 = 0.25$, $g_0^2 = 0.5$, $1/\chi = 1.625 \pm 0.007$
■ $m_0 = 0.25$, $g_0^2 = 1.0$, $1/\chi = 3.932 \pm 0.005$
■ $m_0 = 0.25$, $g_0^2 = 1.5$, $1/\chi = 8.917 \pm 0.004$
■ $m_0 = 0.25$, $g_0^2 = 2.0$, $1/\chi = 15.478 \pm 0.005$
■ $m_0 = 0.2$, $g_0^2 = 0.0$, $1/\chi = 1.035 \pm 0.009$
■ $m_0 = 0.2$, $g_0^2 = 0.5$, $1/\chi = 1.56 \pm 0.007$
■ $m_0 = 0.2$, $g_0^2 = 1.0$, $1/\chi = 3.793 \pm 0.005$
■ $m_0 = 0.2$, $g_0^2 = 1.5$, $1/\chi = 8.704 \pm 0.004$
■ $m_0 = 0.2$, $g_0^2 = 2.0$, $1/\chi = 15.252 \pm 0.006$
■ $m_0 = 0.35$, $g_0^2 = 0.0$, $1/\chi = 1.167 \pm 0.009$
■ $m_0 = 0.35$, $g_0^2 = 0.5$, $1/\chi = 1.761 \pm 0.007$

■ $m_0 = 0.35$, $g_0^2 = 1.0$, $1/\chi = 4.192 \pm 0.005$
■ $m_0 = 0.35$, $g_0^2 = 1.5$, $1/\chi = 9.574 \pm 0.005$
■ $m_0 = 0.35$, $g_0^2 = 2.0$, $1/\chi = 15.936 \pm 0.004$
■ $m_0 = 0.3$, $g_0^2 = 0.0$, $1/\chi = 1.106 \pm 0.009$
■ $m_0 = 0.3$, $g_0^2 = 0.5$, $1/\chi = 1.683 \pm 0.007$
■ $m_0 = 0.3$, $g_0^2 = 1.0$, $1/\chi = 4.058 \pm 0.005$
■ $m_0 = 0.3$, $g_0^2 = 1.5$, $1/\chi = 9.389 \pm 0.006$
■ $m_0 = 0.3$, $g_0^2 = 2.0$, $1/\chi = 15.682 \pm 0.004$
■ $m_0 = 0.4$, $g_0^2 = 0.0$, $1/\chi = 1.181 \pm 0.009$
■ $m_0 = 0.4$, $g_0^2 = 0.5$, $1/\chi = 1.822 \pm 0.007$
■ $m_0 = 0.4$, $g_0^2 = 1.0$, $1/\chi = 4.326 \pm 0.004$
■ $m_0 = 0.4$, $g_0^2 = 1.5$, $1/\chi = 9.754 \pm 0.005$
■ $m_0 = 0.4$, $g_0^2 = 2.0$, $1/\chi = 16.154 \pm 0.004$

Inner Product



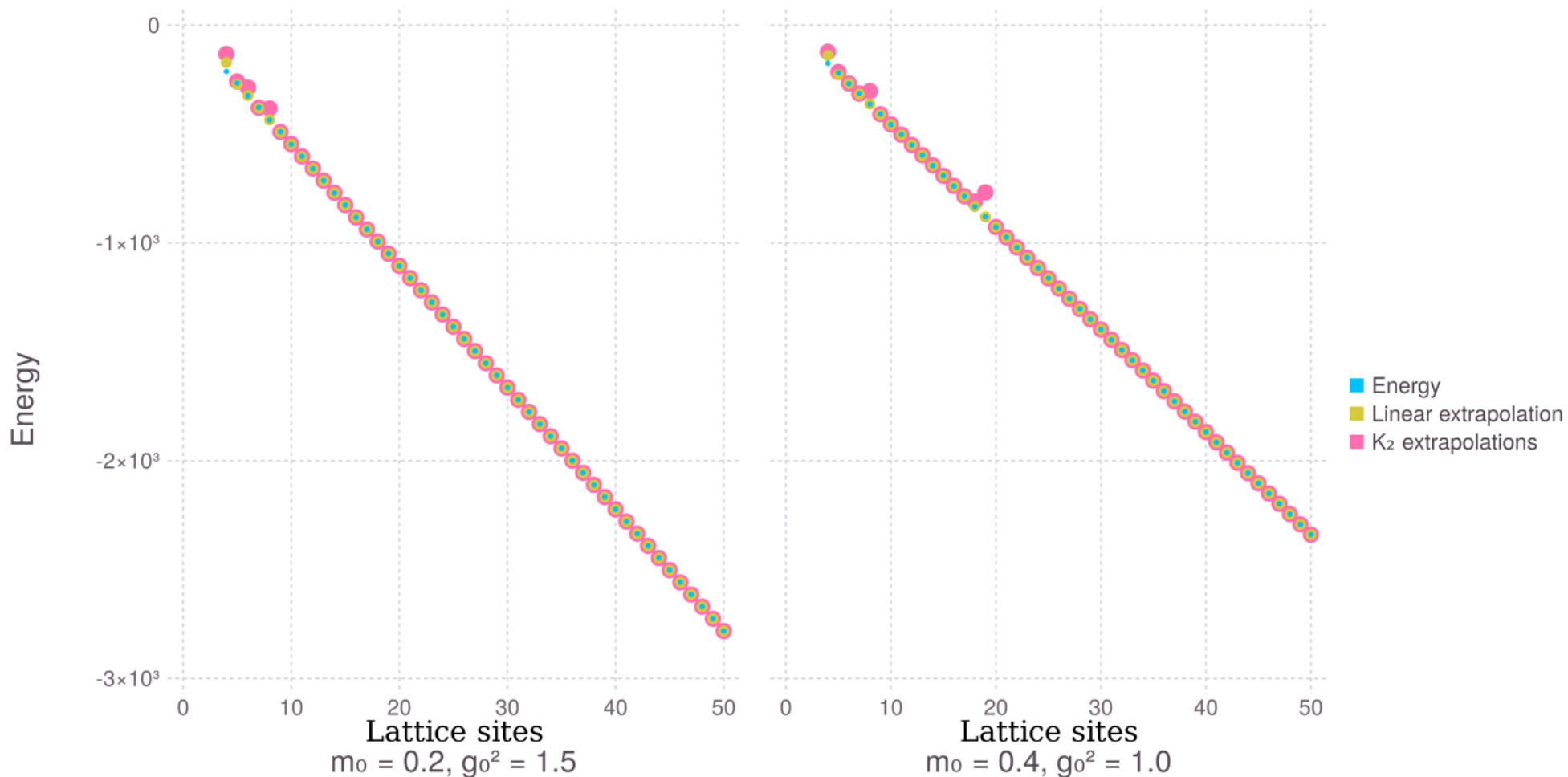
Predicting Ground Energies

- Idea: Use previous energy data to predict the next one.
- Two models were tried:
 - Constant energy density
 - Energy density with Casimir effect corrections

$$E_g(L) = C_0 + C_1 L + C_2 \sum_{h=1}^{\infty} \frac{1}{h^2} K_2(C_3 h L)$$

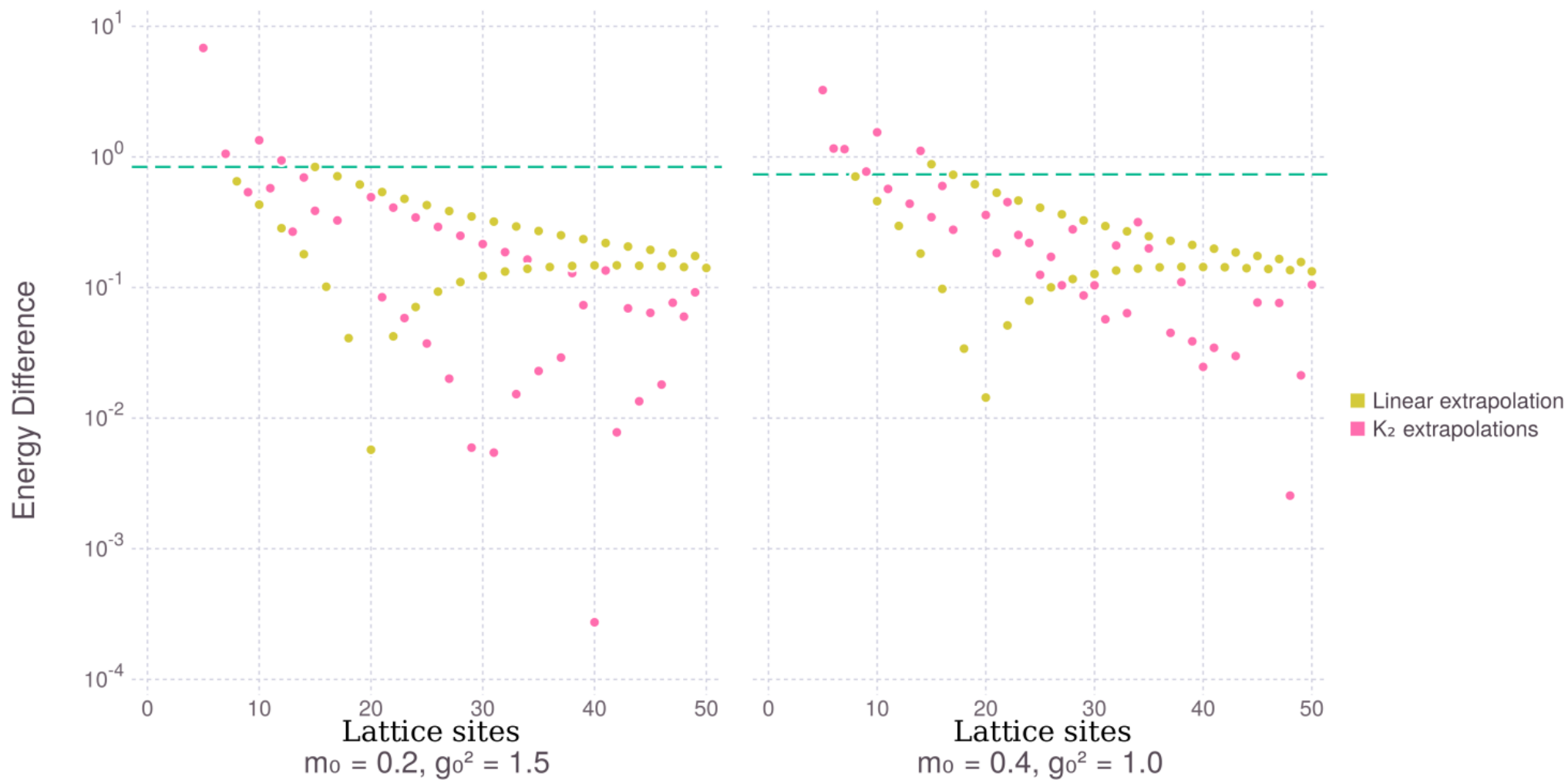
Predicting Ground Energies

The calculated ground energies vs the predictions



Predicting Ground Energies

The difference between fit and the energy value



Summary & Conclusion

- We've looked at two state preparation algorithms
 - MPS
 - Site-by-site
- Direct applications in simulation of fermionic QFTs.
- Other possible applications:
 - Optimization problems
 - Quantum chemistry algorithms

Open Problems

- Future ideas:
 - Prove the conjecture
 - Check with other QFT
 - Check if they can run on NISQ era quantum computers
 - Improve upon bosonic algorithms
 - Quantum Algorithm for hybrid systems
 - The Standard Model

Thank you

Bond Dimension

- It suffices to take $\chi = ke^{S_{1/2}}$ where errors shrink superpolynomially with k , resulting in $k \sim \epsilon^{-\sqrt{N/3}}$
- For lattice spacing small compared to the correlation length, $S_{1/2}$ can be estimated from a CFT argument.

$$S_{1/2} = \frac{N}{6} \log \left(\frac{1}{ma} \right) \quad ma \ll 1$$

- $a \sim \epsilon$ therefore, the complexity for preparing the interacting vacuum is:

$$\mathcal{O} \left(\epsilon^{-N/2 - 1 - \sqrt{3N}} \right) \xrightarrow{N=1} \mathcal{O} \left(\epsilon^{-3.23} \right)$$

Efficient Phase Estimation

Lemma 1 (Phase estimation with $O((n/m) \log(1/\epsilon))$ gates). *Given a simulatable Hamiltonian, H , that acts on n qubits, and a state, $|\psi\rangle$, and a promised lower bound on the spectral gap, $\Delta(H) > m$, and an estimate for the ground energy, \tilde{E} , with a promise that $|\tilde{E} - E| < \frac{m}{2}$, where E is the actual ground energy; we can check whether $|\psi\rangle$ is the ground state of H or not in runtime proportional to $O((n/m) \log(1/\epsilon))$, where ϵ is the probability of making a faulty decision.*

Mapping Overlapping GS

Lemma 2 (Mapping overlapping ground states [39]). *Given two simulatable Hamiltonians, H_1 and H_2 , with known ground energies, E_1 and E_2 , and a minimum overlap between their ground states, $|\langle g_1 | g_2 \rangle| \geq \eta$, one can get from one ground state to the other with $O\left(\frac{\log(2/\epsilon)}{\eta}\right)$ oracle calls to the phase estimation algorithm on these Hamiltonians, where ϵ is the precision goal of the algorithm.*

Proof. This lemma is a direct result of Yoder *et. al.*'s Grover-esque fixed point quantum search [39], when one replaces the oracle in their paper with our phase estimation from Lemma 1.

□

DMRG package in Julia

```
810 function DMRG(H::MPO,ψ0::MPS;ε=10000*eps(Float64),maxiteration=30,DMax=50)
811     #initial random state
812     local eps0 = ε+1.0
813     D = ψ0.BD
814     local MBs
815     l = H.length
816     σ = ψ0.σ
817     Ht = H.tensors
818     ψ1 = ψ0
819     while eps0 > ε && D<DMax
820         println("#####")
821         println("Now using bond dimension D=$(D)")
822         println("#####")
823         if ψ1.BD < D
824             ψ1 = IncreaseBondDimension(ψ1,D)
825         end
826         Ms = RC(ψ1#,D) #Turn into a Right Canonical MPS
827         norm_of_MPS = sqrt(abs(inner(Ms,Ms)))
828         println(norm_of_MPS)
829         Ms.tensors[l] = Ms.tensors[l]/norm_of_MPS
830         norm_of_MPS = sqrt(abs(inner(Ms,Ms)))
831         println(norm_of_MPS)
832         Bs = Ms.tensors #We save the tensors in Bs without
833         Rs = Dict{Int,AbstractArray}() # A list of saved contractions of
834         Ls = Dict{Int,AbstractArray}() # A list of saved contractions of
835         #initializing Rs
836         Bsi = deepcopy(Bs[l])
837         Hi = deepcopy(Ht[l])
838         DummyBsi = Bsi[:, :, 1]
839         DummyHi = Hi[:, :, :, 1]
```

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Related identifiers:

Supplement to

<https://github.com/CNOT/DMRG/tree/v1.0.0>

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