# Final Technical Report for Grant Award DE-SC0016431: Quantum Complexity Theory and High Energy Physics

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## 1 Improved State Preparation for Simulating Quantum Field Theories on Quantum Computers

In quantum algorithms discovered so far for simulating scattering processes in quantum field theories, state preparation is the slowest step. We have developed a new 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 applied 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 one, our algorithm can prepare particle states using $O(\epsilon^{-3.23})$ gates, which is much faster than previous known results, namely $O(\epsilon^{-8})$. 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.

Our algorithm simulates scattering of fermionic particles in the Gross-Neveu quantum field theory with a mass term. The mass term ensures that the theory is gapped, *i.e.* that there is a nonzero energy difference between the ground state and first excited state in the infinite volume limit. This allows us to construct the vacuum (ground state) efficiently by classically computing a Matrix Product State (MPS) description of the vacuum state and then compiling that description directly into a quantum circuit for preparing that state. We then use Rabi oscillations to efficiently excite single-particle wavepackets. This completes the state preparation phase of the simulation, after which the scattering of the particles off each other can be simulated using high order Suzuki-Trotter formulae exactly as in [1] or using newer results for lattice hamiltonian simulation as in [2]. Relative to previous state of the art [1] our new state preparation method has better asymptotic complexity in the limit of high precision and is able to simulate the symmetry-broken phase of the Gross-Neveu model, which was inaccessible to prior state preparation methods, which simulated an adiabatic process starting from the free theory.

We have published this work in Physical Review A [3].

## 2 Applying Tensor Networks to High Energy Physics

In the proposal for this grant, one of the ideas was to adapt tensor networks, which had been a successful variational ansatz for quantum systems with finite-dimensional Hilbert spaces, to apply to quantum systems with continuous degrees of freedom, such as Bosonic lattice quantum field theories. Over the course of this project we discovered that, in our formulation, the constraints on the tensors which would be needed to ensure that the network represents a valid quantum state were highly nontrivial and interesting. Eventually, it became clear that with a sufficiently complete understanding of the constraints we could abandon the tensor network ansatz entirely and obtain *lower bounds* on the vacuum energy of the quantum field theories, in contrast to conventional variational methods, which yield *upper bounds*.

To understand this idea, it is helpful to consider the harmonic oscillator as a simple example. The Hamiltonian is given by $H = ap^2 + bx^2$ where $x$ and $p$ are the canonically conjugate position and momentum operators, and $a, b$ are arbitrary real positive coefficients. One can formulate the problem of finding the ground energy $\langle H \rangle$ as an optimization problem expressed in terms of the expectation values of $x^2$ and $p^2$. Namely, one wishes to minimize $\langle H \rangle = a\langle p^2 \rangle + b\langle x^2 \rangle$ subject to the constraint that the quantities $\langle p^2 \rangle$ and $\langle x^2 \rangle$ are achievable as expectation values of a physially allowed quantum state. One well known constraint imposed by this condition is Heisenberg's uncertainty principle, which in natural units is $\langle x^2 \rangle \langle p^2 \rangle \geq \frac{1}{4}$. One finds that minimizing $\langle H \rangle = a\langle p^2 \rangle + b\langle x^2 \rangle$ subject to Heisenberg's uncertainty principle yields the exact value of the ground state energy of the Harmonic oscillator.

For more general Hamiltonians, such as anharmonic oscillators (or lattices of coupled anharmonic oscillators arising from discretizatino of the $\phi^4$ quantum field theory), this procedure will always yield a lower bound on the ground energy, because there is an infinite tower of constraints on the expectation values of monomials constructed from canonically conjugate observables. In a practical computer calculation one will only incorporate a finite subset of these constraints. For the harmonic oscillator it turns out that this neglection of higher order constraints causes no error, but in general neglecting constraints in a minimization problem will yield an underestimate of the value of the minimum. Our approach is to incorporate higher order constraints until we converge to a tight estimate of the ground energy. A procedure for generating the complete tower of higher order constraints has been derived by the quantum optics community [4]. In the end, the resulting optimization problem ends up as a semidefinite program, which can, at least in principle, be solved by polynomial time classical algorithms. In practice, there can be many subtleties in obtaining good convergence. Consequently, the application of this method to concrete physical problems is work in progress. However, the effort that we have invested over the course of this grant has not gone to waste. Rather, the technical knowledge that we obtained in this area helped to inform a project that we are now pursuing in a DOE-funded Quantum Algorithms Team project entitled QOALAS (Quantum Optimization And Learning And Simulation).

## 3 Simulating Relativistic Wave Equations on Quantum Computers

We developed a quantum algorithm for simulating wave equations, subject to nontrivial boundary conditions. In particular, the algorithm can simulate the scattering of a wavepacket off of scatterers of arbitrary shape, with either Dirichlet or Neumann boundary conditions. We considered

specifically the application of this algorithm to relativistic wave equations such as Maxwell's equations and the Klein-Gordon equation. The output of the simulation is in the form of a quantum state proportional to the solution to the wave equation. By measuring this state one obtains a sample from a distribution proportional to the square of the amplitude, which in this case can be interpreted as the intensity of the wave.

Compared to classical algorithms, our method uses a number of qubits that scales only logarithmically with the number of lattice sites, whereas classical methods require a number of bits scaling linearly with the number of lattice sites. Additionally, for simulating the wave equation in a region of diameter $\ell$ in $D$-dimensions, discretized onto a lattice of spacing $a$, our quantum algorithm has a state-preparation step with time complexity $\widetilde{O}(D^2\ell/a)$ and a Hamiltonian simulation step with time complexity $\widetilde{O}(TD^2/a)$, where $T$ is the evolution time for the wave equation. In contrast, all classical algorithms, whether based on finite difference methods or finite element methods, must have time complexity scaling at least linearly with the number of lattice sites, *i.e.* as $\Omega((\ell/a)^D)$. Relative to prior quantum algorithms [5, 6], we achieve quadratically better scaling with lattice spacing.

The improved scaling of our algorithm relies on higher order approximations of the Laplacian operator and their factorizations using hypergraph incidence matrices. We describe how to find their operators and their hypergraph incidence matrices, and we provide numerical values for up to fifth order. These higher order Laplacians also allow us to improve how errors scale with respect to lattice spacing at the cost of simulating more complex (less sparse) Hamiltonians. In particular, a $s$ sparse Hamiltonian used to simulate the wave equation in $D$ dimensions produces error on the order of $(\ell/a)^{2(s/D)-2}$, so $\ell/a$ scales as $\epsilon^{D/2(s-D)}$. Expressing the time complexity of our algorithm in terms of $\epsilon$ and $s$, we find that the state preparation has time complexity $\widetilde{O}(sD^2\epsilon^{D/2(s-D)})$ and the Hamiltonian simulation has time complexity $\widetilde{O}(sTD^2\epsilon^{D/2(s-D)})$.

We have posted a preprint of our results to arXiv.org [7] and have submitted our paper for consideration at Physical Review A.

## References


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