Quantum Simulation of Quantum Field Theories

Hossein Mohammadi*
Sharif University of Technology
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CONTENTS

MOTIVATION

It's inspiring to use quantum mechanics to study itself, in some sense we use the formidable power of quantum mechanics to help us attack hard problems (in our case ,ironically, this problem was posed by quantum mechanics itself.) One of these problems (and old ones) is computing scattering amplitude more effectively.[1]

Feynman diagrams provides a clear picture and systematic method to compute these amplitudes, still it works for low-coupling limits and for increasing of accuracy we should sum on diagrams,these diagrams increase with the precision on scattering amplitudes, with a super-polynomial behavior.

Here we present a framework for computing scattering amplitudes assisted by digital quantum simulation. It turns out that this set-up works very well and solves the problem of finding amplitudes in a polynomial time, while classical algorithms can solve this problem in super-polynomial times. Also this algorithm works beyond the region of perturbation theory and could be used for probing different possibilities of strong-coupling.

* hossein.mohammadi.00427@gmail.com

I. THE SET-UP

Here we present the set-up and fix our notation in this paper.

Let $\Omega = a\mathbb{Z}_L^d$ be an $L \times L \times \cdots \times L$ square lattice, with d spatial dimensions and spacing a, which has periodic boundary condition. This lattice has $\mathcal{V} = L^d$ sites and $\{\hat{r}_j\}_{j=1}^d$ are unit vectors along j-th direction, as you can see in fig 1.

We should also define our field's degrees of freedom. We want to simulate the simplest field theory, so we choose our field to be a real scalar field and for each $\mathbf{x} \in \Omega$, let the $\phi(\mathbf{x})$ be the value of the field, which is a real scalar (one degree of freedom.) Similarly, we let $\pi(\mathbf{x})$ denote the value of the conjugate momentum.

In canonical quantization of a lattice, these field are promoted to operators and each degree of freedom (at each $\mathbf{x} \in \Omega$) should be treated quantum mechanically, which means that it should obey the following commutation relation:

$$\begin{aligned} [\phi(\mathbf{x}), \pi(\mathbf{y})] &= i a^{-d} \delta_{\mathbf{x},\mathbf{y}} \mathbb{1} \\ [\phi(\mathbf{x}), \phi(\mathbf{y})] &= 0 \\ [\pi(\mathbf{x}), \pi(\mathbf{y})] &= 0 \end{aligned} \tag{1}$$

And finally we should define Lagrangian or Hamiltonian on this lattice, as we will see later, Hamiltonian is much more useful than Lagrangian since the evolution of this field theory is governed by Hamiltonian easily. In

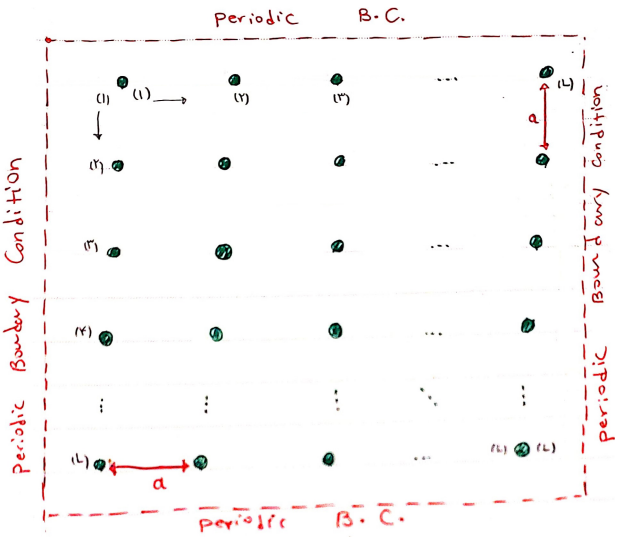

FIG. 1. Sketch of the $\Omega = a\mathbb{Z}_L^d$ lattice (for $d = 2$ dimension.)

natural units we have:

$$H = \sum_{\mathbf{x}\in\Omega} a^d \Big[\frac{1}{2}\pi(\mathbf{x})^2 + \frac{1}{2}(\boldsymbol{\nabla}_a\phi)^2(\mathbf{x}) + \frac{1}{2}m_0^2\phi(\mathbf{x})^2 + \frac{\lambda_0}{4!}\phi(\mathbf{x})^4\Big] \tag{2}$$

Where $(\boldsymbol{\nabla}_a\phi)^2(\mathbf{x})$ denotes the discretized derivative,

$$(\boldsymbol{\nabla}_a\phi)^2(\mathbf{x}) = \sum_{j=1}^{d}\Big(\frac{\phi(\mathbf{x}+a\hat{\mathbf{r}}_j)-\phi(\mathbf{x})}{a}\Big)^2 \tag{3}$$

To store the data in each site, we should assign qubits to each site, In principle the field $\phi(\mathbf{x})$ is continuous and unbounded variable, but we can cut if off to a maximum value ϕ_{max} and discretize it by increments δ_ϕ. This requires $n_b = O(\log\Big(\frac{\phi_{max}}{\delta_\phi}\Big))$ qubits per site to store value of the field in each site.

II. STEPS OF SIMULATION

The proposed algorithm for simulating ϕ^4-lattice theory consists of the following steps, each of which should be treated carefully, from preparing states to measuring the final states. We try to investigate each state carefully, or at least give some motivation to justify each step.

Collision experiments in colliders are schematically described by figure 2, where a set of in-going momentum states $\{\vec{\mathbf{p}}_i^{\,\text{in}}\}$ are generated at free theory($\lambda_0 = 0$) ,then meet each other in interaction region where the coupling in the Hamiltonian is non-zero, and the final states $\{\vec{\mathbf{p}}_i^{\,\text{out}}\}$ scatter and escape to infinity at very long times where they could be measured to find the result of the collision experiment.

Notice that in this picture it is important to produce in-going states and measure out-going states in a region where $\lambda_0 = 0$, since it's ambiguous to define and measure these states in interacting theories. So we should produce and measure the states in accordance with this fact.

We are now ready to give a brief explanation on each of parts of this algorithm.

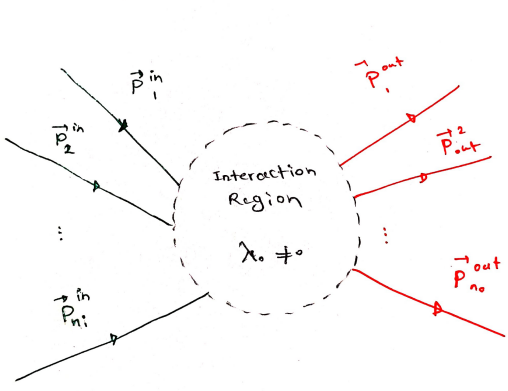

FIG. 2. A typical collision experiment.

A. Preparing $|\text{vac}\rangle$.

After canonical quantization of our free-lattice-theory we found that each of these D.O.Fs behave as if there is a quantum harmonic oscillator on that site. So the vacuum of the free-theory is defined by tensor product of vacuum of all this oscillators, $|\text{vac}\rangle \propto \otimes_{\mathbf{x}\in\Omega}|0\rangle_x$. Remembering that ground state wave-function of quantum harmonic oscillator is $\langle x|\psi\rangle = \mathcal{N}e^{-\frac{m\omega}{2\hbar}x^2}$, we find that ground state of this system should be a Gaussian wave-packet in each site of lattice.

Fortunately, there are algorithms to construct such states, Kitaev and Webb proposed and efficient algorithm and circuit to make such states [2]. The main idea of this algorithm is to prepare a $\mathcal{V}$-dimensional multivariate Gaussian wave-function with a diagonal covariance matrix, and then reversibly change basis to obtain the desired states.

We later review briefly how to code this wave-function of qubits. The next step is to produce in-states.

B. Excite wave-packets.

By simulating a Hamiltonian H_ψ, we obtain the desired wave-packets up to a global phase,(which is irrelevant) and an extra qubit.

Notice that we cannot use $\phi(\mathbf{x})$ itself to create a state localized at $\vec{\mathbf{x}}$, simply because this operator is non-unitary and we can't implement it by circuits. Instead given an arbitrary wave-function $\psi(\mathbf{x})$ which is normalized by $a^d\sum_{\mathbf{x}\in\Omega}|\psi(\mathbf{x})|^2 = 1$, consider the following second quantized-operator:

$$a_\psi^\dagger = \eta(\psi)\sum_{\mathbf{x}\in\Omega} a^d\psi(\mathbf{x})a_{\mathbf{x}}^\dagger \tag{4}$$

where $\eta(\psi)$ is added to ensure that $a_\psi a_\psi^\dagger|\text{vac}\rangle = |\text{vac}\rangle$. This operator is interpreted to create state $\psi(\mathbf{x})$ over lattice.

And consider the following Hamiltonian H_ψ with one ancillary qubit:

$$H_\psi = a_\psi^\dagger \otimes |1\rangle\langle 0| + a_\psi \otimes |0\rangle\langle 1| \tag{5}$$

One can easily verify that $|\text{vac}\rangle|0\rangle$ and $|\psi\rangle|1\rangle$ is an invariant subspace that H_ψ acts as:

$$\begin{aligned} H_\psi|\text{vac}\rangle|0\rangle &= |\psi\rangle|1\rangle \\ H_\psi|\psi\rangle|1\rangle &= |\text{vac}\rangle|0\rangle \end{aligned} \tag{6}$$

This immediately leads to

$$e^{-i\frac{\pi}{2}H_\psi}|\text{vac}\rangle|0\rangle = -i|\psi\rangle|1\rangle \tag{7}$$

Hence, by simulating a time evolution according to the Hamiltonian H_ψ, we obtain the desired wave-packet state $|\psi\rangle$, up to an irrelevant global phase and extra qubit,

which can be discarded. After rewriting H_ψ in terms of the operators $\phi(\mathbf{x})$ and $\pi(\mathbf{x})$, one sees that simulating H_ψ is a very similar task to simulating H and can be done with the Suzuki-Trotter formula.

C. Adiabatically turn on the interaction.

To obtain a wave-packet of the interacting theory, we start with the wave-packet of the free theory, constructed in the previous step, and then simulate adiabatic turn-on of the interaction. Consider $H(s)$ to be the following Hamiltonian ($0 \leq s \leq 1$):

$$H(s) = a^d \sum_{\mathbf{x}\in\Omega} \Big[\frac{1}{2}\pi(\mathbf{x})^2 + \frac{1}{2}(\boldsymbol{\nabla}_a\phi)^2(\mathbf{x}) + \frac{1}{2}m_0^2(s)\phi(\mathbf{x})^2 + \frac{\lambda_0(s)}{4!}\phi(\mathbf{x})^4\Big] \tag{8}$$

D. Simulate Hamiltonian time evolution.

E. Adiabatically turn off the interaction.

F. Measure occupation numbers of momentum modes.

APPENDICES

Appendix I - Calculation of ϕ^4 theory on lattice

Here we present proofs of finding energy levels,Green functions and Second quantization of non-interacting ϕ^4-lattice model.

Recall that we discretized the ϕ^4 model to obtain the Hamiltonian (2), with the typical recipe for discretizing a model: Just $\sum_{\mathbf{x}\in\Omega} a^d \to \int d^dx$ as $a \to 0$ in position space, and $\sum_{\mathbf{p}\in\Gamma} \frac{1}{L^d} \to \int \frac{d^dp}{(2\pi)^d}$ as $L \to \infty$.

Also note that equation (3), in descritized lattice means that we have nearest-neighbor coupling, so in each direction j, from d different spatial directions, there are two coupling terms to $\mathbf{x} \pm a\hat{\mathbf{r}}_j$, and equation (3) is actually sum of two terms with $+a$ replaced by $-a$. (For edge sites,periodic boundary condition assures that edge sites still couple to two neighbors.)

First let us solve the E.O.M . For each $\mathbf{x} \in \Omega$ there is one D.O.F in lattice and we can solve for E.O.M of just one of D.O.Fs. We can also ignore the a^d factor in Hamiltonian since it's an overall factor and doesn't contribute to E.O.M.

By using Hamilton equations of motion we get:

$$\dot{\phi}(\mathbf{x}) = \frac{\partial H}{\partial \pi(\mathbf{x})} = \pi(\mathbf{x})$$
$$\dot{\pi}(\mathbf{x}) = -\frac{\partial H}{\partial \phi(\mathbf{x})} \tag{9}$$

The second equation becomes:

$$= -\frac{1}{2}\Big[\frac{1}{a^2}\big[\sum_j \big(2\phi(\mathbf{x}) - \phi(\mathbf{x}+a\hat{\mathbf{r}}_j) - \phi(\mathbf{x}-a\hat{\mathbf{r}}_j)\big)\big] + 2m_0^2\phi(\mathbf{x})\Big] = \frac{1}{a^2}\Big[\sum_j \big[-2\phi(\mathbf{x}) + \phi(\mathbf{x}+a\hat{\mathbf{r}}_j) + \phi(\mathbf{x}-a\hat{\mathbf{r}}_j)\big]\Big] - m_0^2\phi(\mathbf{x})$$

As you see this is like coupled oscillators in d spatial dimensions, and know how to quantize such theories.

In order to proceed more we differentiate first equation of (9) and substitute the second one:

$$\ddot{\phi}(\mathbf{x}) = \frac{1}{a^2}\Big[\sum_j \big[-2\phi(\mathbf{x}) + \phi(\mathbf{x}+a\hat{\mathbf{r}}_j) + \phi(\mathbf{x}-a\hat{\mathbf{r}}_j)\big]\Big] - m_0^2\phi(\mathbf{x}) \tag{10}$$

We introduce the Fourier transform of $\phi(\mathbf{x})$ in reciprocal lattice $\Gamma = \frac{2\pi}{La}\mathbb{Z}_L^d$ by:

$$\phi(\mathbf{x}) = \frac{1}{a^d}\sum_{\mathbf{p}\in\Gamma} e^{i\mathbf{p}.\mathbf{x}}\phi(\mathbf{p}) \tag{11}$$

By placing this transformation in equation (10) you can see that we reach at $\ddot{\phi}(\mathbf{p}) = -\omega^2(\mathbf{p})\phi(\mathbf{p})$ where:

$$\omega^2(\mathbf{p}) = m_0^2 + \frac{1}{a^2}\sum_{j=1}^{d}\big[2 - e^{ia\mathbf{p}.\hat{\mathbf{r}}_j} - e^{-ia\mathbf{p}.\hat{\mathbf{r}}_j}\big]$$

By easy manipulation we reach at

$$\omega(\mathbf{p}) = \sqrt{m_0^2 + \frac{4}{a^2}\sum_{j=1}^{d}\sin^2\big(\frac{a\mathbf{p}.\hat{\mathbf{r}}_j}{2}\big)} \tag{12}$$

At this stage we can proceed to quantize this lattice by recipe of quantum field theory, just rewrite "suitable" linear combination of $\phi(\mathbf{x})$ and $\pi(\mathbf{x})$ as creation and annihilation operators (similar to this process in quantum harmonic oscillator).

$$a_{\mathbf{p}} = \sum_{\mathbf{x}\in\Omega} a^d e^{-i\mathbf{p}.\mathbf{x}}\phi(\mathbf{p})\Big[\sqrt{\frac{\omega(\mathbf{p})}{2}}\phi(\mathbf{x}) + i\sqrt{\frac{1}{2\omega(\mathbf{p})}}\pi(\mathbf{x})\Big] \tag{13}$$

$a_{\mathbf{p}}$ annihilates a completely delocalized state at $\mathbf{p}$ momentum which is a superposition of annihilation operators at different positions, similarly $a_{\mathbf{p}}^\dagger$ creates a completely delocalized state at $\mathbf{p}$ which is a superposition of creation operators at different positions. Note that all

this operators are defined for $H = H_{(0)}$ system or non-interacting system.

The following equations is verified easily from solving fields in terms of creation and annihilation operators and substituting in Hamiltonian or commutation relation of fields:

$$\begin{aligned}
\phi(\mathbf{x}) &= \frac{1}{L^d}\sum_{\mathbf{p}\in\Gamma} e^{i\mathbf{p}.\mathbf{x}}\sqrt{\frac{1}{2\omega(\mathbf{p})}}\Big(a_{\mathbf{p}} + a^\dagger_{-\mathbf{p}}\Big)\\
\pi(\mathbf{x}) &= \frac{-i}{L^d}\sum_{\mathbf{p}\in\Gamma} e^{i\mathbf{p}.\mathbf{x}}\sqrt{\frac{\omega(\mathbf{p})}{2}}\Big(a_{\mathbf{p}} - a^\dagger_{-\mathbf{p}}\Big)\\
H_{(0)} &= \frac{1}{L^d}\sum_{\mathbf{p}\in\Gamma}\omega(\mathbf{x})a^\dagger_{\mathbf{p}}a_{\mathbf{p}} + E_{(0)}\mathbb{1}\\
[a_{\mathbf{p}}, a^\dagger_{\mathbf{q}}] &= L^d\delta_{\mathbf{p},\mathbf{q}}\mathbb{1}\\
[a_{\mathbf{p}}, a_{\mathbf{q}}] &= [a^\dagger_{\mathbf{p}}, a^\dagger_{\mathbf{q}}] = 0
\end{aligned} \tag{14}$$

Where $E_{(0)} = \frac{1}{2}\sum_{\mathbf{p}\in\Gamma}\omega(\mathbf{p})$ is zero-energy which is irrelevant for our purpose in simulating the ϕ^4-lattice. We also denote $|\text{vac}\rangle$ to be ground state of $H_{(0)}$.

A few comments about spectrum of Hamiltonian, by appropriately using of (14) equations we see that $|\mathbf{p}\rangle = L^{-\frac{d}{2}}a^\dagger_{\mathbf{p}}|\text{vac}\rangle$ is normalized eigenstates of $H_{(0)}$ with $\omega(\mathbf{p})$ energy, and applying more creation operators yields eigenstates with more energy. In this way one can construct the whole spectrum of non-interacting this model.

The operator $\phi(\mathbf{x})$ creates a single-particle localized at position $\mathbf{x}$, we can verify this by using Fourier transformation of creation and annihilation operators:

$$a^\dagger_{\mathbf{x}} = \frac{1}{L^d}\sum_{\mathbf{p}\in\Gamma} e^{-i\mathbf{p}.\mathbf{x}}\sqrt{\frac{1}{2\omega(\mathbf{p})}}a^\dagger_{\mathbf{p}} \tag{15}$$

Green's function is defined by $G(\mathbf{x}-\mathbf{y}) = \langle\text{vac}|\,\phi(\mathbf{x})\phi(\mathbf{y})\,|\text{vac}\rangle$ and by above relation it's easy to see that:

$$G_{(0)}(\mathbf{x}-\mathbf{y}) = \frac{1}{L^d}\sum_{\mathbf{p}\in\Gamma}\frac{1}{2\omega(\mathbf{p})}e^{i\mathbf{p}.(\mathbf{x}-\mathbf{y})} \tag{16}$$

We are able to solve for the spectrum of $H_{(0)}$ in terms of non-interacting particles with sharply defined momentum. In an interacting quantum field theory, the momentum of individual particles is no longer conserved. Nevertheless, total momentum is conserved, and thus the single-particle subspace can be analyzed similarly to the non-interacting case. Specifically, by starting with the single-particle momentum-$\mathbf{p}$ eigenstate of the non-interacting theory, and then adiabatically turning on λ_0, one obtains an eigenstate of H, which can be interpreted as a single particle of momentum $\mathbf{p}$ of the interacting theory.

[1] Stephen P. Jordan, Keith S. M. Lee, and John Preskill. Quantum algorithms for quantum field theories. *Science*, 336(6085):1130–1133, jun 2012.

[2] Alexei Kitaev and William A. Webb. Wavefunction preparation and resampling using a quantum computer. *arXiv: Quantum Physics*, 2008.