Towards Quantum Simulation of Bound States Scattering - arXiv:2305.07692

Matteo Turco

Instituto Superior Técnico, Universidade de Lisboa
Physics of Information and Quantum Technologies Group, CeFEMA
Portuguese Quantum Institute

QuantHEP Conference
25th-27th September 2023, Bari, Italy

In collaboration with:
Gonçalo Quinta, Prof. João Seixas and Prof. Yasser Omar

TÉCNICO LISBOA

CeFEMA
Center of Physics and Engineering of Advanced Materials

PORTUGUESE QUANTUM INSTITUTE

Introduction

- One of the most promising applications of quantum computation is simulation of real-time evolution in quantum field theory;
- scattering events are basically our only controlled source of information on elementary particle physics;
- scattering is one of the main topics of quantum field theory.

Simulation of scattering is a natural application of quantum computation.

Scattering events

Scattering event:

1. **freely moving incoming particles**
2. **time evolution**
3. **measurements of the outgoing state**

Quantum simulation of scattering:

1. **preparation** of the **incoming state**
   (well separated wavepackets on a lattice)
2. **simulation of time evolution**
3. **measurements**

Elementary and composite particles

A particle can be elementary or composite.
Typically, in quantum field theory:

- an **elementary** particle is directly associated with a field appearing in the Hamiltonian (Lagrangian);
- a **composite** particle is associated with combinations of fields appearing in the Hamiltonian (Lagrangian).

The existing quantum algorithms for scattering simulation are not suitable in presence of incoming composite particles.
The purpose of this work is to present the first strategy to address this problem.

Contents

Structure of this presentation:

1. review of the state of the art;
2. review of the Haag-Ruelle scattering theory;
3. an example with bound states;
4. sketch of the quantum algorithm;
5. conclusions and outlook.

State of the art and goal of the presentation

Paper by Jordan, Lee and Preskill (2011):
Quantum Computation of Scattering in Scalar Quantum Field Theories

Summary of the algorithm:

1. free vacuum preparation
2. free wavepackets excitation from the free vacuum
3. interacting wavepackets preparation through adiabatic transformation
4. time evolution
5. measurements

Steps 1-3 are the initial state preparation. Initial state preparation is typically the hardest part in quantum simulation of scattering.

Lattice quantum field theory

The theory is formulated on a cubic d-dimensional spatial lattice Ω with

- lattice spacing a
- length L
- volume $V = L^d$
- number of sites $\mathcal{V} = \left(\frac{L}{a}\right)^d$

To each site, labelled by $\vec{x}$, we associate

- k qubits
- a pair of operators $\hat{\phi}(\vec{x})$ and $\hat{\pi}(\vec{x})$ such that
  - $\hat{\phi}$ will give us the computational basis;
  - $\hat{\pi}$ is related to $\hat{\phi}$ by Quantum Fourier Transform

The Hamiltonian

The Hamiltonian of the scalar ϕ^4 field theory is

$$H = \sum_{\vec{x}\in\Omega} a^d \left[\frac{1}{2}\hat{\pi}(\vec{x})^2 + \frac{m_0^2}{2}\hat{\phi}(\vec{x})^2 + \frac{1}{2}(\nabla_a\hat{\phi})^2(\vec{x}) + \frac{\lambda_0}{4!}\hat{\phi}(\vec{x})^4 \right]$$

where

$$(\nabla_a\hat{\phi})^2(\vec{x}) = \sum_{j=1}^{d} \left(\frac{\hat{\phi}(\vec{x}+a\hat{r}_j) - \hat{\phi}(\vec{x})}{a} \right)^2$$

The free theory ($\lambda_0 = 0$) is a collection of harmonic oscillators with nearest neighbour interactions given by $(\nabla_a\hat{\phi})^2(\vec{x})$.

State preparation

We will focus our attention on state preparation, namely

1. free vacuum preparation
2. free wavepackets excitation from the free vacuum
3. adiabatic transformation to the interacting theory

1. in the first step we prepare the vacuum state of the free theory

$$|0 \dots 0\rangle \rightarrow |\text{free vac}\rangle$$

Free wavepackets excitation

2. once we have $|\text{free vac}\rangle$, we want to excite a wavepacket $|\psi\rangle$ with wavefunction $\psi(\vec{x})$.
   To do that in the free theory:
   - we can introduce creation operator in $\vec{x}$, $\hat{a}^\dagger_{\vec{x}}$
   - the wavepacket we want is $|\psi\rangle = \hat{a}^\dagger_\psi |\text{free vac}\rangle$, with

$$\hat{a}^\dagger_\psi = \sum_{\vec{x}\in\Omega} a^d \psi(\vec{x}) \hat{a}^\dagger_{\vec{x}}$$

   - $\hat{a}^\dagger_\psi$ can be written as linear combination of $\hat{\phi}(\vec{x})$ and $\hat{\pi}(\vec{x})$:

$$\hat{a}^\dagger_\psi = \sum_{\vec{x}} \left[f_\psi(\vec{x})\hat{\phi}(\vec{x}) + g_\psi(\vec{x})\hat{\pi}(\vec{x}) \right]$$

   it can be implemented with one ancillary qubit

Adiabatic transformation

2. the procedure can be repeated with well separated wavepackets

$$|\text{free vac}\rangle \to |\psi_1\rangle\,|\psi_2\rangle$$

3. in the last step of state preparation we make an adiabatic transformation from the free theory to the interacting theory

$$|\psi_1\rangle\,|\psi_2\rangle \to |\psi_{1,\text{int}}\rangle\,|\psi_{2,\text{int}}\rangle$$

Important: we need to ensure that $|\psi_{1,\text{int}}\rangle$ and $|\psi_{2,\text{int}}\rangle$ are one-particle states each

Summary

State preparation can be summarized by

$$|0\dots0\rangle \to |\text{free vac}\rangle \to |\psi_1\psi_2\rangle \to |\psi_{1,\text{int}}\psi_{2,\text{int}}\rangle$$

The goal of this presentation is to show how to construct interacting wavepackets starting from the interacting vacuum

$$|\text{int vac}\rangle \to |\psi_{1,\text{int}}\psi_{2,\text{int}}\rangle$$

In order to do this we need some notions of axiomatic quantum field theory

- Axiomatic quantum field theory is a rigorous formulation of quantum field theory based on a bunch of axioms incorporating principles of quantum mechanics and special relativity.
- It is built on canonical quantization of field theory, fixing some technical problems already present in free theories.
- It is formulated without distinguishing between free and interacting theories.
- For many interesting theories it is hard to get a rigorous proof that they fulfil the axioms.

Smeared operators

$\hat{\phi}(x)$, with x a spacetime coordinates, is not a well defined operator, but rather a *operator-valued tempered distribution*. In practice we need to smear it with a Schwartz function:

$$\phi_f = \int d^4x\, f(x)\hat{\phi}(x)$$

Recall that a Schwartz function is perfectly smooth (C^∞) and decays faster than any power of x as x goes to ∞.

Generators of translations

Since the theory is Lorentz invariant, there have to exist the generators of translations $P = (H, \vec{P})$ such that

$$e^{iP\cdot a}\hat{\phi}(x)e^{-iP\cdot a} = \hat{\phi}(x + a)$$

We can connect with the Schrödinger operators by

$$\hat{\phi}(x) = \hat{\phi}(t, \vec{x}) = e^{iHt}\hat{\phi}(\vec{x})e^{-iHt}$$

We can also define coordinate dependent smeared operators

$$\phi_f(x) = e^{iP\cdot x}\phi_f e^{-iP\cdot x} = \int d^4y\, f(x - y)\hat{\phi}(y)$$

Spectrum of P

The mass-squared operator $P^2 = P_\mu P^\mu$ has a disconnected spectrum made of

- 0, isolated eigenvalue of the vacuum
- m^2, isolated eigenvalue of one-particle states
- $[4m^2, \infty[$, continuum of multi-particle states

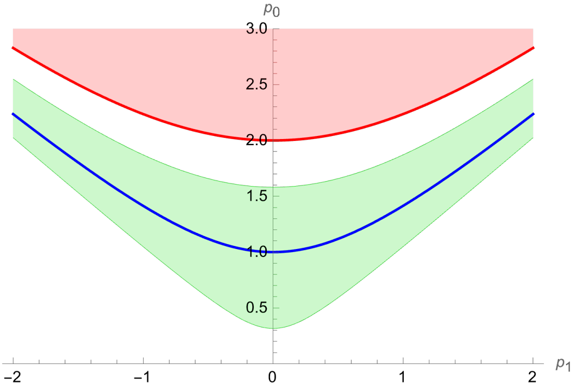
Correspondingly the spectrum of P_μ has three disconnected subsets:

- $p_\mu = 0$, eigenvalue of the vacuum
- $p^2 = m^2$, one-particle mass hyperboloid
- $p^2 \geq 4m^2$, continuum of multi-particle states

For a two-particle state:
$(p_1 + p_2)^2 = 2m^2 + 2p_1 \cdot p_2$ with $p_1 \cdot p_2 \geq m^2$.

Consider the region R (in green):

$$\alpha m^2 < p^2 < \beta m^2 \qquad 0 < \alpha < 1 \qquad 1 < \beta < 4$$



Take a smearing function $f_1(x)$ that is the Fourier transform of a function $\tilde{f}_1(p)$ with support in the region R.

Define

$$\phi_1(x) = \int d^4y\, f_1(x-y)\hat{\phi}(y)$$

The state $\phi_1(x)\,|\textbf{int vac}\rangle$ is guaranteed to be a one-particle state.

Next, take a positive energy solution of the Klein-Gordon equation

$$g(\tau,\vec{x}) = \int \frac{d^3p}{2E(\vec{p})}\tilde{g}(\vec{p})e^{i(\vec{p}\cdot\vec{x}-E(\vec{p})\tau)}$$

Haag-Ruelle Scattering Theory

Define

$$\phi_{1,g}(\tau) = -i \int d^3x \left\{ g(\tau,\vec{x}) \frac{\overleftrightarrow{\partial}}{\partial\tau} \phi_1(\tau,\vec{x}) \right\}$$

with

$$A(\tau)\frac{\overleftrightarrow{\partial}}{\partial\tau}B(\tau) = A(\tau)\dot{B}(\tau) - \dot{A}(\tau)B(\tau)$$

Theorem (Haag Asymptotic)

The state vector

$$|\Psi,\tau\rangle = \phi_{1,g_1}(\tau)\cdots\phi_{1,g_n}(\tau)\,|int\ vac\rangle$$

converges strongly in the limit $\tau \to -\infty$ to the in-state of n one-particle wavepackets

$$|\Psi\rangle = \int d^3p_1 \ldots d^3p_n\, \tilde{\psi}_{1,g_1}(\mathrm{p}_1)\cdots\tilde{\psi}_{1,g_n}(\mathrm{p}_n)\,|\mathrm{p}_1\ldots\mathrm{p}_n\rangle_{in}$$

Bound States in the Haag-Ruelle Formalism

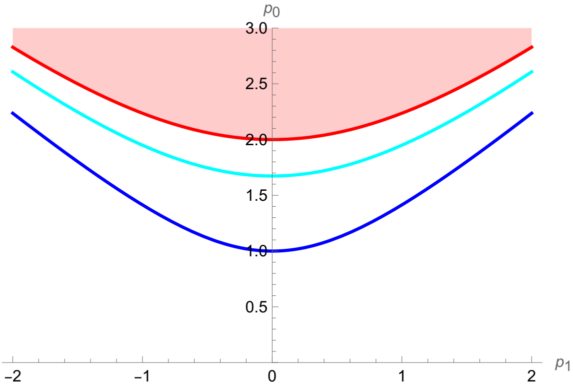
Consider a scalar theory with (weak) interactions $\lambda(\hat{\phi}^6 - \hat{\phi}^4)$ in one space dimension.
It has

- an elementary particle with mass m;
- a composite particle with mass $m_b \in]m, 2m[$.

Moreover:

- $\hat{\phi}(x)$ can be used to create wavepackets of the elementary particle;
- $:\hat{\phi}^2:(x)$ can be used to create wavepackets of the composite particle in, essentially, the same way as described so far.

Bound States in the Haag-Ruelle Formalism



- in blue, the hyperboloid of mass m
- in cyan, the hyperboloid of mass m_b
- in red, the multi-particle continuum

Two particles in the continuum

Consider two single-particle incoming states.

$$\phi_{1,g_1}(\tau)\phi_{1,g_2}(\tau)\,|\text{int vac}\rangle =$$
$$e^{iH\tau}\int d^4x_1\,\psi_1(x_1;\tau)e^{iH(t_1-\tau)}\hat{\phi}(\vec{x}_1)e^{-iH(t_1-\tau)}\times$$
$$\times\int d^4x_2\,\psi_2(x_2;\tau)e^{iH(t_2-\tau)}\hat{\phi}(\vec{x}_2)\,|\text{int vac}\rangle$$

Provided we choose appropriate initial conditions for ψ_1 and ψ_2, we can take $\tau = 0$ (in full generality).

Two particles on the lattice

Assuming this holds as an approximation on the lattice, we have

$$\phi_{1,g_1}(0)\phi_{1,g_2}(0)\,|\text{int vac}\rangle =$$
$$\sum_{\vec{x}_1}\int_{-\infty}^{+\infty} dt_1\,\psi_1(x_1)e^{iHt_1}\hat{\phi}(\vec{x}_1)e^{-iHt_1}\times$$
$$\times\sum_{\vec{x}_2}\int_{-\infty}^{+\infty} dt_2\,\psi_2(x_2)e^{iHt_2}\hat{\phi}(\vec{x}_2)\,|\text{int vac}\rangle$$

Next, we will sketch how to implement the operator

$$\sum_{\vec{x}}\int_{-\infty}^{+\infty} dt\,\psi(x)e^{iHt}\hat{\phi}(\vec{x})e^{-iHt}$$

on a quantum computer.

Implementation on a quantum computer

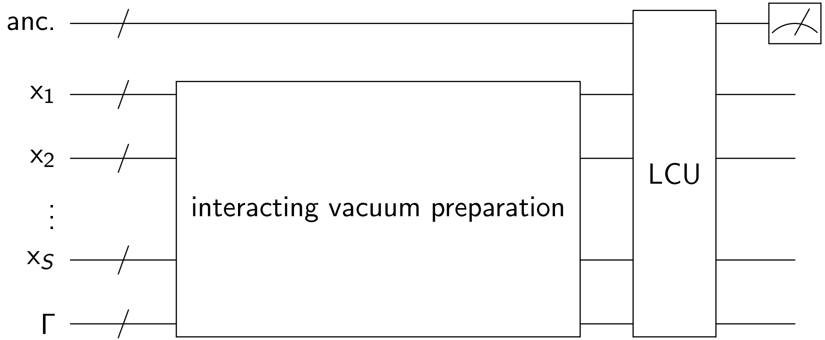
- label by $1 \dots S$ the lattice sites where ψ is significantly different from zero;
- t is constrained around zero by ψ;
- truncate and discretize the integral over t in N points;

$$\sum_{i=1}^{N} \sum_{j=1}^{S} \psi(t_i, \vec{x}_j) e^{iHt_i} \hat{\phi}(\vec{x}_j) e^{-iHt_i}$$

- $\hat{\phi}(\vec{x})$ can be written as a linear combination of k Z Pauli matrices.

We can use **linear combination of unitaries** (LCU), with $\log_2(kNS)$ ancillary qubits.

Preparation of interacting wavepackets



- LCU requires a time evolution simulation for a time $T = t_N - t_1$ (temporal size of ψ);
- successfully completed upon measuring the ancillary register with result $|0 \dots 0\rangle$.

Conclusions

We have a strategy to prepare interacting wavepackets starting from the interacting vacuum

$$|\text{int vac}\rangle \to |\psi_{1,\text{int}}\psi_{2,\text{int}}\rangle$$

rather than

$$|\text{free vac}\rangle \to |\psi_1\psi_2\rangle \to |\psi_{1,\text{int}}\psi_{2,\text{int}}\rangle$$

What is the usefulness of this?

Conclusions

$$|\text{int vac}\rangle \to |\psi_{1,\text{int}}\psi_{2,\text{int}}\rangle \quad (1)$$

$$|\text{free vac}\rangle \to |\psi_1\psi_2\rangle \to |\psi_{1,\text{int}}\psi_{2,\text{int}}\rangle \quad (2)$$

1. (2) does not allow for preparation of incoming bound states in (1) elementary particles and composite particles are treated in the same way.

The quantum-field-theoretic inputs we need are

- **spectrum** of the theory (which particles are there?);
- **interpolating fields**

$$\langle\alpha_\text{e}|\,\hat{\phi}(x)\,|\text{int vac}\rangle \neq 0 \qquad \langle\alpha_\text{b}|\,:\hat{\phi}^2:(x)\,|\text{int vac}\rangle \neq 0$$

where $|\alpha_\text{e}\rangle$ and $|\alpha_\text{b}\rangle$ are one-particle state of the elementary and composite kind.

Outlook

What is left to do:

- what are the consequences of putting the Haag-Ruelle formalism on the lattice?
- what happens with gauge theories?
- how to find interpolating fields theory by theory?
- which strategy performs better when both are suitable?

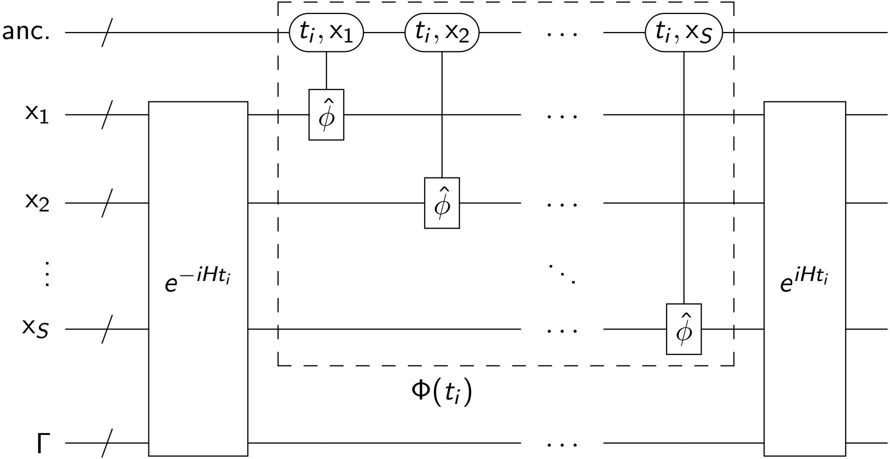
Thanks for listening!

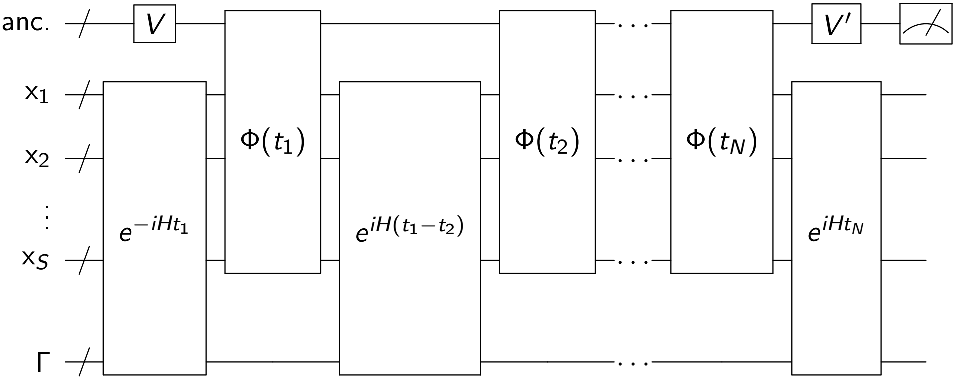
To implement

$$\sum_{i=1}^{N}\sum_{j=1}^{S}\psi(t_i,\vec{x}_j)e^{iHt_i}\hat{\phi}(\vec{x}_j)e^{-iHt_i}$$

- label the computational basis of the ancillary register as $|t_i, \mathrm{x}_j\rangle$
- we need to prepare the ancillary register in the state

$$\sum_{i=1}^{N}\sum_{j=1}^{S}\sqrt{\psi(t_i,\mathrm{x}_j)}\,|t_i,\mathrm{x}_j\rangle$$


anc.
x_1
x_2
x_S
Γ
e^{-iHt_i}
t_i, x_1
t_i, x_2
t_i, x_S
$\hat{\phi}$
$\hat{\phi}$
$\hat{\phi}$
$\Phi(t_i)$
e^{iHt_i}


anc.
V
Φ(t1)
Φ(t2)
Φ(tN)
V′
x1
x2
xS
Γ
e−iHt1
eiH(t1−t2)
eiHtN