

## Quantum Computation towards a determination of the Phase Diagram of Quantum Chromodynamics

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A large fraction of HPC resources in theoretical computational physics involved in the "numerical computation" of non-perturbative Quantum-Field Theories

# WHY?

Quantum Chromodynamics, the theory that describes strong interactions among gluons and quarks, is non-perturbative in the low-energy regime. Many aspects of our world are not understable within standard perturbation theory:

- Quark Confinement
- Hadron masses and the origin of most of the visible mass around us
- Many other properties

## Is confinement a permanent state of matter?

**N. Cabibbo and G. Parisi, 1975:** conjecture for the existence of a deconfined phase at high T and/or high baryon density: **Quark-Gluon Plasma (QGP)?** 

Such state of matter is relevant to the early Universe, interior of compact stars, ...



## **Possible checks?**

- Theoretical: Numerical Computations of QCD
  - $T_c\simeq 155~{\rm MeV}\sim 1.8~10^{12}~^{\circ}{\rm K}~\sim 10^{-6}{\rm s}$  after Big-Bang, not a real phase transition
- Experimental: Heavy Ion Collisions (LHC, RHIC, ....) point to a similar  $T_c$

## How do we compute QCD and QCD thermodynamics, usually?

QCD is a (not-solvable) quantum system.

**Quantum thermodynamics:** 

$$\langle O \rangle_T = \frac{\text{Tr}\left(Oe^{-\beta H}\right)}{\text{Tr}\left(e^{-\beta H}\right)} = \frac{\sum_n \langle n|Oe^{-\beta H}|n\rangle}{\langle n|e^{-\beta H}|n\rangle} = \frac{1}{Z} \sum_n \langle n|O|n\rangle e^{-\beta E_n}$$

however Hamiltonian eigenstates |n
angle and their matrix elements are unknown

### **Generic Quantum Monte-Carlo approach**

- rewrite as a classical sum over an (infinite) number of computable terms
- if all terms are positive, sample them by Monte-Carlo methods

### An example: the path-integral approach

The most widely used approach in Quantum Field Theories

- $\bullet\,\,{\rm Look}$  at  $e^{-\beta H}$  as evolution in Euclidean (imaginary) time  $\hbar\beta$
- $\bullet\,$  Divide "imaginary evolution" in N steps, then send  $\to\infty\,$

$$e^{-\beta H} = \left(e^{-(\beta/N)H}\right)^N$$

• Choose a basis  $|x\rangle$  (the "computational basis") where matrix elements of  $\exp(-\beta H/N)$  are easily computable (at least for large N)

 $|x\rangle$ : position eigenstates in QM, field eigenstates in QFT,  $\hat{z}$ -component eigenstates (standard bits) for quantum spin systems

• rewrite traces over the computational basis:

$$\operatorname{Tr}(e^{-\beta H}) = \sum_{x} \langle x | \left( e^{-\frac{\beta}{N}H} \right)^{N} | x \rangle = \sum_{x} \sum_{x_{1}} \dots \sum_{x_{N-1}} \langle x | e^{-\frac{\beta}{N}H} | x_{N-1} \rangle \langle x_{N-1} | \dots | x_{1} \rangle \langle x_{1} | e^{-\frac{\beta}{N}H} | x \rangle$$

#### Lattice QCD has been and is still a continuous stimulus to the development of HPC

#### An example: the series of APE machines "made in INFN"

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#### THE APE COMPUTER: AN ARRAY PROCESSOR OPTIMIZED FOR LATTICE GAUGE THEORY SIMULATIONS

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#### APE, 1988, 250 Mflops $\rightarrow$ APE100 $\rightarrow$ APEmille $\rightarrow$ apeNEXT, 2006, 10 TeraFlops

Nowadays: Large clusters, GPU-based processors, approaching the exascale ...

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Finite temperature computations well under control, but when we turn on a baryon chemical potential, we get into trouble ...



The product of matrix elements over the computational basis becomes complex

The "infamous sign problem", leaving much of the QCD phase diagram out of our reach.

Many attempts to solve the problem within a classical approach ... unsuccessful so far

This is why the problem is considered as a one of the major motivations for Quantum Computations ...

## But HOW would Quantum Computation solve the problem?

Waiting for real Quantum Computers capable of encoding QCD, we are trying to answer the question on simple models sharing the same problems The problem is in the computational basis, everything is well defined and positive in the physical states basis:

$$Z(T,\mu_B) = \sum_{n} \langle n | e^{-\beta(H-\mu_B N_B)} | n \rangle = \sum_{n} e^{-\beta(E_n-\mu_B N_{B,n})}$$

You don't know the physical states and how to deal with them, but the Quantum Computer does, because the QC encodes (digitally or analogically) the quantum physical system itself!

**TASK:** devise a quantum algorithm capable of sampling the quantum physical states according to the grand-canonical distribution, then taking measures on them Non-triviality:  $\exp(-\beta H)$  is not a unitary operator ...

**Our choice:** Quantum Metropolis algorithm  $\Rightarrow$  talk by Marco Cardinali

## A poor classical man facing the quantum world

#### A "classical" Metropolis Markov chain:

- explore the state space by a stochastic path made up of "try-and-reject" steps

- along the path, take measurements of the quantities you are interested in, to approximate ensemble averages

#### **Dealing with Metropolis on a Quantum Computer:**

- The "reject" step becomes non-trivial: no-cloning theorem

- Taking measurements in QM is not cheap: quantum collapse in general destroys the state