Lattice calculations of the quark-gluon plasma

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Abstract. The quark-gluon plasma is a novel state of matter in which quarks are no longer confined to bound states such as baryons and mesons. Just after the Big Bang the Universe was filled with a quark-gluon plasma. The cores of neutron stars may well be a quark-gluon plasma. At the Relativistic Heavy Ion Collider (RHIC) at Brookhaven National Laboratory, scientists collide high energy gold beams to produce and study the quark gluon plasma. Lattice gauge theorists use computers to study the properties of the quark-gluon plasma such as the temperature required to produce it and its equation of state. These demanding calculations will require over a Petaflop-year of computing to achieve theoretical goals.

1. Introduction
The Standard Model of Elementary Particle Physics describes three of Nature’s four forces: electromagnetism, the weak force and the strong force. These three forces all have a property called gauge covariance and they are based on the symmetry groups $U(1)$, $SU(2)$ and $SU(3)$, respectively. Gravity, Nature’s fourth force is based on general coordinate covariance, which is so different that the graviton has spin-2, but the other force carriers are all spin-1.

Electromagnetism and the weak force are both relatively weak and can be treated with perturbation theory. The strong force, described by the theory called Quantum Chromodynamics (QCD) is so strong that a nonperturbative treatment is essential to study many of its most interesting consequences. Lattice QCD is the most successful treatment of QCD by a nonperturbative method; however, its application requires large scale numerical computations.

Quarks are spin-1/2 elementary particles that respond to the strong force. The carriers of the force are called gluons because the exchange of gluons makes the quarks stick together forming bound states called hadrons. The fact that we don’t see isolated quarks, just their bound states is called quark confinement, i.e., quarks are not free. In the early days of the quark model every new accelerator was expected to try to produce free quarks, but after several failures the notion of quark confinement was invented.

Among the main goals of lattice QCD are to calculate the masses and decay properties of the hadrons. At very high temperature or density a new state of matter in which quarks are no longer confined has been long predicted and more recently observed. This is called the quark-gluon plasma (QGP). Determining its properties is another major goal of lattice QCD.

An ordinary plasma requires a temperature high enough to liberate electrons from atoms forming a mixture of electrons and ions. This temperature corresponds to an energy of a few electron volts. Since QCD is much stronger than electromagnetism, the temperature to create the QGP is much larger, approximately 200 million electron volts (MeV). It is very challenging...
to study the QGP in the laboratory because the plasma exists only in a very small volume for a very short time and we are only able to observe the ordinary hadronic matter that has left the region of the plasma. We need to find observable consequences of the existence of the plasma that persist after the system cools down and ordinary matter is produced.

2. Quark-gluon plasma in Nature
Just after the Big Bang, the Universe was very hot and quarks were deconfined. As the Universe cooled the quark-gluon plasma disappeared in what may have been a deconfinement-confinement transition, but was more likely a smooth change rather than an abrupt transition. Today, neutron star cores are the most likely place to find a naturally occurring quark-gluon plasma. However, this plasma is cooler than in the early Universe and it is made predominantly of matter, not an equal mixture of matter and antimatter. The Crab Nebula is powered by the Crab Pulsar a neutron star near the center of the nebula. The Hubble Space Telescope provides us with beautiful pictures of this system [1]. An introduction to the physics of neutron stars can be found at the web site of the UNAM Neutron Star Theory Group [2].

3. Quark-gluon plasma in the laboratory
To produce a quark-gluon plasma in the laboratory, we need a high density of very energetic particles. To get the high density, we start with heavy atoms. We ionize the atoms so that we can accelerate them to high energy. Two counterrotating beams are produced and allowed to collide at a few points (intersection regions) where detectors are placed. The Relativistic Heavy Ion Collider (RHIC) [3] at Brookhaven National Laboratory is currently the premier facility for this type of experiment.

By smashing heavy ions such as gold into each other at high energy, a high temperature can be reached in the debris from central collisions. Two large detectors PHENIX and STAR are designed to look at all the charged particles emerging from collisions. Hundreds of charged particles can be tracked from head-on collisions of the gold ions. More glancing collisions result in fewer outgoing particles. Experimentalists determine which particles were produced and their energy and momentum to reconstruct the thermal properties of the system produced by the collision.

4. What theorists study
As the two heavy nuclei collide, the central region of the collision becomes a hot dense state of matter that soon begins to cool as the interacting particles stream away from the collision region. Nuclear theorists model the heating and cooling processes using hydrodynamic-like equations. However, the strongly interacting matter is not an ordinary fluid.

Lattice QCD calculations provide important input to the hydrodynamic models by looking at several important properties of strongly interacting matter:
- Phase Diagram
- Transition Temperature
- Equation of State

The techniques of lattice QCD are better suited to calculating the equilibrium properties of the QGP than to calculating the dynamics of the heating and cooling.

4.1. Phase diagram
Water, of course, is commonly seen in three phases, ice (solid), water (liquid) and steam (gas). The temperature and pressure determine which phase is the equilibrium phase. The phase diagram indicates which phase is favored in the temperature-pressure plane.
For hadronic matter, we use temperature $T$ and baryon chemical potential $\mu$ to plot the phase diagram. When the chemical potential is zero, there are equal amounts of matter and antimatter. With a positive chemical potential, matter is favored over antimatter. Figure 1 shows a rough phase diagram of hadronic matter. We expect that the solid lines are lines of first order phase transitions, and that the dashed line is just a rapid crossover, with no real transition. The solid dots are critical points, and we would like to accurately determine their locations.

4.2. Transition temperature
We would like to accurately determine the transition (or crossover) temperature $T_c$ as it is important for modeling hadronic matter at RHIC. A lower value of $T_c$ means it is easier to create the QGP. A number of groups have studied the transition temperature using different ways of putting quarks on the lattice. The various calculations are in good agreement at the 10% level. We would like to improve the accuracy of the $T_c$ calculation to the 5% level. This will require a smaller lattice spacing and high statistical accuracy.

4.3. Equation of state
The equation of state expresses the relationship between energy and temperature or pressure and temperature. You probably learned the ideal gas law in chemistry or physics: $pV = nRT$, where $p$ is the pressure, $V$ the volume and $T$ the temperature.

The equation of state for hadronic matter is considerably more complicated. We graph current results from the MILC collaboration in Fig. 2 [6]. We are plotting the pressure divided by $T^4$, which somewhat masks the rapid rise with temperature near 200 MeV. This is where a crossover to a deconfined state of matter is seen.

5. Baryon chemical potential
For quite technical reasons, calculations with a non-zero chemical potential are much harder than those with zero chemical potential. However, in a heavy-ion collider there is more matter than antimatter because the colliding particles are all matter. Thus, it is important to be able to calculate the effect of a small chemical potential. One promising approach is to do a Taylor
expansion in the chemical potential around the zero chemical potential point [7, 8]. Using this approach, initial calculations have been done with a coarse lattice spacing.

6. Who studies the QGP using lattice QCD?
The international community of lattice gauge theorists is strong in Australia, Canada, China, Europe, India, Japan, the U.K. and the U.S. The web site www.lqcd.org has a number of links to the web sites of large collaborations. The International Lattice Data Grid is set up to share data within the community and can be accessed at www.lqcd.org/ildg.

Several collaborations are currently carrying out calculations at non-zero $T$ or chemical potential:

- BNL-Columbia-RIKEN (RBC) and Bielefeld
- MILC
- hotQCD: a new collaboration consisting of LANL, LLNL, MILC, RBC
- Budapest-Wuppertal
- European Twisted Mass Collaboration
- WHOT-QCD: Tokyo-Tsukuba-BNL

Both commercial supercomputers and special purpose computers are used for these calculations. In the US, the BNL QCDOCs and the LLNL BlueGene/L computers are doing most of the current finite $T$ calculations. BlueGene/L is also used in Japan at the KEK Laboratory and in Germany at Julich. The special purpose apeNEXT computer is used in Bielefeld, DESY/Zeuthen and Rome. The Budapest-Wuppertal group uses a large Beowulf cluster and a new computer powered by graphics cards [9].

7. Computational requirements
To perform lattice QCD calculations, the continuum of space-time is approximated as a grid of points in space-time. Also, time is converted to an imaginary quantity so that quantum mechanical oscillatory factors $\exp(-i\omega t)$ become exponential decay factors. The ground state, having the lowest energy, has the slowest exponential decay and is the easiest state to study. Because we have a uniform grid of points in space-time, with periodic or anti-periodic boundary conditions, it is easy to perform domain decomposition to parallelize the codes. Communications take place according to a regular pattern.

One difficulty is that in Nature the up and down quarks are very light. This results in an ill-conditioned sparse matrix that describes the two lightest quarks. To deal with this, we use a heavier value for the quark mass and then extrapolate to the physical value. This extrapolation must be done carefully.

The system must also be placed in a box of finite volume, and one must take care to either do an infinite volume extrapolation or make sure that the effects of the finite volume are very small.

Further, using a grid of space-time points is only an approximation that introduces systematic errors depending on the spacing between the grid points. Thus, one does a series of calculations on ever finer grids and extrapolates to the continuum limit.

If the lattice spacing is denoted by $a$, is it estimated that the cost of the calculation goes like $a^{-11}$. The smallest calculations with non-zero temperature are done on $12^3 \times 4$ or $16^3 \times 4$ grids. Many important calculations have been done with 4 or 6 grid points in the time direction. The next set of calculations will use 8, 10 or 12.

The SciDAC funded USQCD Collaboration recently prepared a series of white papers [5] in which the computational requirements were set out for a wide variety of important QCD calculations. For the next series of calculations with non-zero temperature and baryon chemical
potential it is estimated that almost 1.5 Petaflop-years of computation will be required. This is the actual number of floating point operations required, not the peak machine speed multiplied by the time to complete the calculation.

The calculations described here are done on much smaller grids than those used for zero $T$ calculations. However, there are usually more parameter sets required, and very high statistics can be important. For the most part, these runs require a computer or computers capable of many jobs running at a speed of about 10 TF.

8. SciDAC QCD software

The SciDAC program funds the National Infrastructure for Lattice Gauge Theory software development effort [10]. The effort has produced a series of libraries that can be used to produce efficient programs:

- QLA: for linear algebra on $3 \times 3$ complex matrices and 3-component vectors (or $N \times N$ with less optimization)
- QMP: a simple message passing library for lattice QCD
- QDP: a data parallel library that combines arithmetic and message passing functionality
- QOP: highly optimized versions of particulary important physics functionality
- QIO: a standards based I/O library for storing lattice fields

Several community codes are making use of these libraries:

- Chroma: from Jefferson Lab [11]
- CPS: from Columbia University [12]
- MILC: from MILC Collaboration [13]

The current libraries are being optimized for the Cray XT4 and IBM BlueGene/P leadership class computers. QMC, a multicore library is a current research project. A QCD Physics Toolbox for data analysis and a Workflow project to ease the work of running the many jobs needed for a calculation are also under development. More details of the USQCD software activity can be found in the presentation by Bálint Joó.

References

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