Hot Stuff

Sourendu Gupta
Department of Theoretical Physics
Tata Institute of Fundamental Research
Homi Bhabha Road, Mumbai 400005, India October 31, 2012

"The author works on hot matter, a topic which lies at the intersection of particle physics, computer algorithms and quantum field theory. He studied at IIT Kharagpur and TIFR, and has worked in IMSC Chennai, CERN, and Brookhaven National Laboratory. He is also interested in the teaching of physics. His web page address is http://theory.tifr.res.in/~sgupta/"

"Photograph courtesy of Radiya Pacha Gupta. Reproduced with permission."

Abstract : Hot strongly interacting matter once filled the universe, but in the last 14 billion years it has only been briefly produced in relativistic collisions of heavy ions. Its properties can be extracted from a quantum field theory using supercomputers. Now a collaboration of experiments and theory is beginning to test this connection accurately, I describe what has been found, the context, and what we hope to gain in the next few years.

1 Why study hot matter?

To the best of our knowledge, the universe started with a hot big bang. Through its entire history, the universe has been cooling while remaining very nearly in thermal equilibrium (our experience of the universe is atypical, since most of it is now at 3 K). We have very detailed knowledge of the physics that involves the evolution of the universe when it was older than a couple of microseconds. Understanding the earlier history of the universe involves the kind of physics that is the subject of this article: relativistic quantum field theories at very high temperatures.

This era of the universe involves temperatures in excess of 10^9 K (1 trillion K), so the need to study extremely hot matter is clear. But why do we need relativity and quantum field theory?

The reasons are very simple. The kinetic energy of a particle in thermal equilibrium is of the order of the temperature[1] T. When two particles in such a system collide, their center of mass energy is also of order T. Now, if the masses of the particles, M, are much smaller than T, then the Lorentz factor, $\gamma = T/M$, is much larger than unity, and the particles are relativistic. Furthermore, in these circumstances, particles can be produced in every inelastic collision. We know from decades of experiments that quantum mechanics works perfectly well for a system of fixed number of particles. So, for example, quantum mechanics is all that is needed to understand the spectra of atoms and nuclei, transport in nanowires, information processing through the use of entangled states, and many more mundane or exotic fields of research. However, this quantum mechanics is inadequate when particles are produced. Even to adequately understand the simple reaction H H $H^* \rightarrow H + \gamma$ i.e., the decay of an excited hydrogen atom to its ground state with the production of a photon, one has to use quantum field theory. So, to explain the physics of a thermal medium which consists of relativistic particles, one has to use quantum field theory.

2 What kind of matter?

But which quantum field theory should one use for the description of matter at the beginning of the universe? Fortunately, over the last hundred years experiments have narrowed the field until only one theory seems to be adequate for the description of the universe a nanosecond or more after its birth. The story started with the discovery of the atomic nucleus by Rutherford in 1911. Since the nucleus is positively charged (consisting of positively charged protons and neutral neutrons) it was already clear that electromagnetic forces would tear it apart, and a new force

[1]*Throughout this article I will use units such that the Boltzmann constant, k, is unity. Since we will have to use relativity, I will choose units such that the speed of light in vacuum, c, is also unity. Finally, since much of the relevant physics is quantum, I will choose units such that ħ, Planck's constant, is unity.*

was required to bind the nucleus into a stable entity. This was called the strong force.

A detailed understanding of the spectrum of hydrogen showed that the electron and the proton interacted only by the electromagnetic forces. So clearly all matter in the universe was divided into kinds which saw the strong forces (these are called hadrons) and others which did not (these are called leptons). Half a century of discoveries which followed only deepened the mystery. So many more hadrons were observed that it became more and more unlikely that they are all elementary constituents of matter. At the same time all attempts at creating a theoretical model of these particles, considered as elementary, failed. In 1961 the first breakthrough came with the invention of the “quark model” by Gell-Mann [1]. This hypothesized that the elementary constituents of strongly interacting matter were new entities called quarks. In terms of these quarks it was possible to build something like a periodic table of hadrons. The model predicted new hadrons, and was vindicated when they were found.

Within a decade a relativistic quantum field theory of strong interactions had been written and technical difficulties involved in working with it largely solved. In doing this it was discovered that this theory, which was called Quantum Chromo-Dynamics (QCD), had an intrinsic length scale (which is about a femto meter). Strangely, the theory predicted that at distances much shorter than this scale, the strong interactions were rather weak [2]. Experiments soon verified the quantitative theory of the paradoxically weak strong interactions. The physics of long distances, where the strong inter- actions are strong required a reformulation of quantum field theory. Even after this radical invention it turned out that supercomputers were needed to make predictions. Since this forms the core of the method used in the description of the hot stuff at the beginning of time, we will return to this later.

The strong interactions turn out to be the hardest theoretical and experimental challenge in physics until now. They are understood adequately enough for people to work with, but not enough to be considered solved and done with. At the end of a century about 30 Nobel prizes, to more than 50 people, have been awarded for the strong interactions alone; the most recent was in 2010. This makes it the most awarded field in physics — a good indication of the continuing interest in the subject. Today it stands as the hardest part of the Standard Model of particle physics: a theory now verified through the recent discovery of the Higgs boson in the Large Hadron Collider (LHC) in CERN, and ready for application to the problem of the early evolution of the universe.

In order to have any confidence in our ability to do this, one has to design experiments to test the predictions of quantum field theory at high temperature. This is where the strong interactions come in. It turns out that the easiest way to produce hot matter is to bang heavy nuclei together in a high energy collider. The kinetic energy is converted to the thermal energy of a fireball which expands and cools, roughly in the same way that the universe did. These little bangs are full of strongly interacting matter.

As a result, although QCD is the hardest part of the Standard Model, it turns out to be the most relevant at the present stage of testing our notions about the universe in its infancy.

3 Supercomputing in quantum field theory

When interactions are weak, the usual method of computation in any quantum theory is by developing a perturbation series. This works beautifully in the quantum theory of electrodynamics, making it the most precisely tested physical theory of all times. However, this method is not available to us for strong interactions. Instead we rely on a reformulation which rests on two legs — the path integral method of Feynman and the grand synthesis of Wilson.

The origin of quantum mechanics and wave-particle duality is seen in the two-slit interference experiment. A quantum particle, such as an electron, is described by a probability amplitude. When an electron impinges on a screen with two slits then it goes through both; the amplitudes of it taking either path have to be added. A detector placed on the other side of the screen can detect the electron at some position with a probability proportional to the square of the summed amplitude. This gives rise to the usual interference patterns. If a stream of electrons is sent through the apparatus then the detector sees more electrons in the regions where the interference maxima are, and less where there is destructive interference. This much was known from the 1920s. Feynman’s insight in the 1940s was that the number of slits could be increased indefinitely, and all the different paths that the particle could take would still interfere. In fact, the screen could be removed altogether and the resultant infinity of paths would still interfere. Therefore the amplitude of a quantum particle to travel from the position x_i at time t_i to a position x_f at time t_f would be the sum (integral) of the amplitudes for all possible paths [3].

An interesting duality was noticed in quantum mechanics since its beginning. Time evolution in quantum mechanics involves the unitary operator exp (iHt) where H is the Hamiltonian operator of the system and t is the time. At the same time,

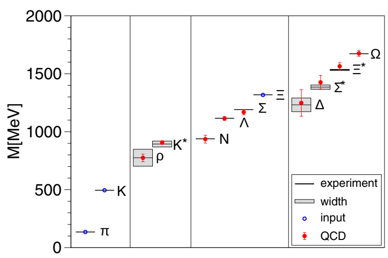

Figure 1: A comparison of experimentally determined masses of hadrons with those predicted by QCD. Three parameters of the theory are adjusted by input of the masses of the π, K and Σ. The remainder are predictions [5].

the statistical mechanics of the same quantum system involves a density matrix exp $(-H/T)$ where T is the temperature. The two are related by the identification $t \rightarrow i/T$, and their path integral representations are also similarly related. Exploiting this, Wilson was able to convert all the technical problems of quantum field theory into the statistical mechanics of particles on a space-time lattice, while being able to control the limit in which the lattice spacing goes to zero [4]. This is the grand synthesis of modern theoretical physics, as a result of which amplitudes in quantum field theory can be computed by a numerical evaluation of the corresponding statistical mechanics. In the 1970s when Wilson created the grand synthesis, numerical methods for statistical mechanics had already been evolving for a decade or so, and could be turned to the lattice formulation of QCD and other quantum field theories immediately.

Such a treatment of quantum field theory turns out to require incredibly large computing power. The biggest supercomputers available today, IBM's Blue Gene series, was first designed by field theorists to solve the problem of QCD, and has now been turned to other uses such as hydrodynamics, drug design, code breaking and weather prediction, and much more. The result is that some predictions of QCD are now marvelously precise. Two years ago there was a superb calculation of the masses of all hadrons up to twice the mass of the proton, in which QCD was seen to work beautifully (see Figure 1).

4 A technical problem and its solution

A decade ago several Indian physicists with interest in lattice QCD got together to form the Indian Lattice Gauge Theory Initiative (ILGTI). The aim of this initiative was to set up the kind of supercomputing facilities which are required for lattice gauge theory. It was first supported by the Department of Atomic Energy, which continues to lend strong support to this program. In the Xth five year plan facilities were set up in TIFR Mumbai, IMSc Chennai and SINP Kolkata. In the XIth five year plan the TIFR facility expanded to become the fifth largest supercomputing center in the country. New centers are coming up in IACS Kolkata and NISER Bhubaneshwar[2] There are enormous opportunities here for anyone who wishes to be part of the initiative, as explained in the web page http://www.ilgti.tifr.res.in.

With these facilities available, Indian collaborations began to look at hard unsolved problems. One problem that was examined by my colleagues and I in the group in TIFR Mumbai was a long-standing puzzle called the "sign problem" which arose in many areas of computational science. In the context of quantum field theory one can state the problem as the following. When the path integral of quantum field theory is converted into statistical mechanics, then it becomes an integral of a function which is defined in an infinite dimensional space but is positive. The lattice reduces this infinity into a very large but finite number of dimensions (typically larger than 10^6).

A method of numerical integration called the Monte Carlo method is then applied. This works only when the integrand is positive. However, in field theory problems when the number of particles and anti-particles is not exactly equal, the integrand is not positive definite but complex, and the method fails. This failure had stopped lattice QCD investigations of the little bang, where the number of baryons exceeds the number of antibaryons. The TIFR group found a generic solution to the sign problem. When particles and antiparticles are not equal in number, one can reformulate this problem in the grand canonical ensemble of statistical mechanics with a chemical potential μ. At $\mu = 0$ the number of particles equals the number of antiparticles, the path integrand is positive, and the Monte Carlo method works. We proposed to set up a Madhava-Maclaurin expansion[3] of the free energy at $\mu = 0$. The series coefficients need to be computed only for $\mu = 0$, and hence the Monte Carlo methods suffices. The series is a good tool as long as it converges, and when it fails to converge the singularity could well be related to the interesting phenomenon of a phase transition in the system [6].

This method was first written down by us in 2002 and applied to a simple model system. The first application to QCD was published in 2005, and we have updated the results subsequently in 2008 and are again in the process of doing so now. Many years of continuous computation on very large supercomputers are needed in order to use this technique. The results allow us to make quantitative and testable predictions for hot quark matter seen in experiments for the first time.

5 Thermodynamic fluctuations

The number of gas molecules in the room you are sitting in right now is perhaps around 10^{28}. When there are so many degrees of freedom, thermodynamics is easily applied. As a result, you can easily measure the pressure, entropy, and enthalpy of the gas. The state of your knowledge

[2]In order to remain globally competitive we need to install petaflops level computing power in the country dedicated to quantum field theory. A flops is an unit of computing power, corresponding to being able to add two floating point numbers in one second. Most desktops currently operate in the range of gigaflops. Computing at higher speeds is needed in many branches of science. This requires parallelization of programs. This is a special skill which need to be taught at the graduate level.

of these quantities is limited only by the accuracy of your instruments. However, if the sample size was smaller, say about 10^6 molecules, then there would be intrinsic physical limits on the accuracy. Repeating accurate measurements would not give the same value, but would reveal thermodynamic fluctuations. The study of these fluctuations about a hundred years ago revealed that new physical information hides here. For example, the fluctuations of energy of such a sample are Gaussian and the width is related to the specific heat of the material.

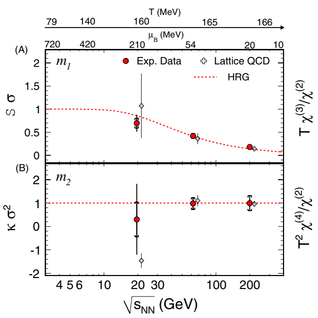

Figure 2: A comparison of the predictions of QCD with experimental determination of the shape of the spectrum of thermodynamic fluctuations in the excess of baryons over antibaryons in heavy-ion collisions [7]. The experimental data comes from an international collaboration called STAR working with a collider in the Brookhaven Laboratory near New York. The lattice predictions come from the Mumbai chapter of the ILGTI.

This looks like a cumbersome way of finding the specific heat, but what if it were so hard to make the material that there was no way to produce enough to do a macroscopic measurement of the specific heat? Then thermodynamic fluctuations may be the only way to relate mesoscopic physics (here of around 10^6 molecules) to microscopic physics (the interactions of the molecules which can be used to compute the specific heat). Quark matter turns out to be like this. Quark matter is produced in the lab in little bangs, creating fireballs which expand and cool. We see only the end result of these collisions. By looking at the relative number of hadrons which are produced in these bangs, one can find the temperature and chemical potential just before the hadrons leave the fireball. This method is analogous to the application of the Saha equations to the Fraunhofer spectra of stars to find their surface temperatures. Knowing T and μ one should be able to predict thermodynamic fluctuations in the fireball.

If this were to be possible then it must also be true that when one selects a sample of fireballs with a fixed T and μ the distribution of a conserved quantity should be Gaussian. One such quantity is the excess of baryons over antibaryons. When this is measured in one little bang after another, it turns out to be approximately Gaussian distributed. The deviations from a Gaussian are as interesting as the width of the Gaussian. It turns out that the Madhava-Maclaurin series coefficients which we compute are precisely the quantities needed to predict the shape of these distributions. Our computations were checked against experimental data and found to agree very well (see Figure 2). This was a major milestone since this was the first time that lattice QCD predictions could be compared to experimental data on hot matter.

6 Implications

Lattice QCD has a very small number of free parameters: the QCD distance scale at which the strong interactions become weak, and the quark masses. Once all the free parameters are fixed everything else is a prediction. Typically the free parameters are fixed by matching them to experimentally determined hadron masses, as shown in Figure 1.

In fact, exactly this was done in the comparison shown in Figure 2. The values of T and μ are required to make a connection between the experiment and prediction. For the experimental data these are determined as explained earlier. For the lattice QCD prediction the lattice computation directly gives the dimensionless ratio T/T_c, where T_c is a conventional scale of temperature called the QCD crossover temperature. At temperatures below T_c strongly interacting matter has a simple hadronic description; above T_c it has a simple description in terms of quarks and gluons. Lattice computations also have predictions for T_c/m where m is a hadron mass. As a result, using computations such as those shown in Figure 1 one can fix T and μ for the lattice computation and make the comparison shown in Figure 2.

However, one need not perform this very round-about comparison. Given the data on fluctuations, one may as well vary the single parameter T_c and check whether the data is well described by the lattice QCD predictions. This was done in a unique collaboration of theorists and experimentalists with the result that an excellent fit to the data is obtained with $T_c = 175^{+1}_{-7}$ MeV.

In more familiar units, T_c is about 2 trillion K. This result is a breakthrough because it is the first time that such a basic parameter of hot primordial matter has been obtained from experiments. Interestingly, this is also the highest measured temperature ever to come out of a terrestrial experiment. It is high enough to melt atomic nuclei into its constituents, the quarks.

Apart from this, it is also an intellectual breakthrough since it closes a circle of reasoning which

[3] *Madhava of Sangamgrama was a member of the 13th century school of mathematics in Kerala and is supposed to have developed the method which was discovered independently several centuries later by Maclaurin. Madhava discovered the method and applied it to the computation of the tangent of any angle.*

was open till now. Single hadron properties could be connected to the properties of strongly interacting hot matter through the analogue of the Saha equations as described earlier. Single hadron properties were explained through lattice QCD, as Figure 1 showed. Lattice QCD connected single hadron properties directly to computations of hot strongly interacting matter. Now the results of the work just described connected lattice QCD with experiments on hot matter.

This is the first time that quantum field theory of hot matter has really been tested in the lab. Clearly new goals and challenges will now emerge, including the quantitative description of the processes occurring in the early universe between the nanosecond and microsecond time scales. One of the questions which I expect to be answered in a few years concerns an interesting phase transition in hot matter [8]. One can well say that the field is heating up.

Acknowledgements

I would like to thank my collaborators in the ILGTI, namely Saumen Datta, Rajiv Gavai, Pushan Majumdar, and Nilmani Mathur. I would also like to thank my experimental colleagues and collaborators, Xiaofeng Luo, Bedangadas Mohanty, Hans-Georg Ritter, and Nu Xu. I would also like to acknowledge the important role played in the ILGTI by our young researchers, Debasish Banerjee, Nikhil Karthik, M. Padmanath, and Sayantan Sarma.

References

[1] M. Gell-Mann, Caltech report CSTL-20 TID-12608 (1961).

[2] D. J. Gross and F. Wilczek, Phys. Rev. Lett. 30 (1973) 1343; H. D. Politzer, Phys. Rev. Lett. 30 (1973) 1346.

[3] R. P. Feynman, Rev. Mod. Phys. 20 (1948) 367.

[4] K. G. Wilson, Phys. Rev. D 10 (1974) 2445.

[5] S. Durr et al., Science 322 (2008) 1224.

[6] R. V. Gavai and S. Gupta, Phys. Rev. D 68 (2003) 034506.

[7] S. Gupta et al., Science 332 (2011) 1525.

[8] M. Stephanov, K. Rajagopal and E. Shuryak, Phys. Rev. Lett. 81 (1998) 4816; R. V. Gavai and S. Gupta, Phys. Rev. D 71 (2005) 114014.