Lattice QCD with anisotropic highly improved staggered quarks

Johannes Heinrich Weber (Michigan State University)

Motivation: quarkonium suppression in a thermal bath of quark-gluon plasma

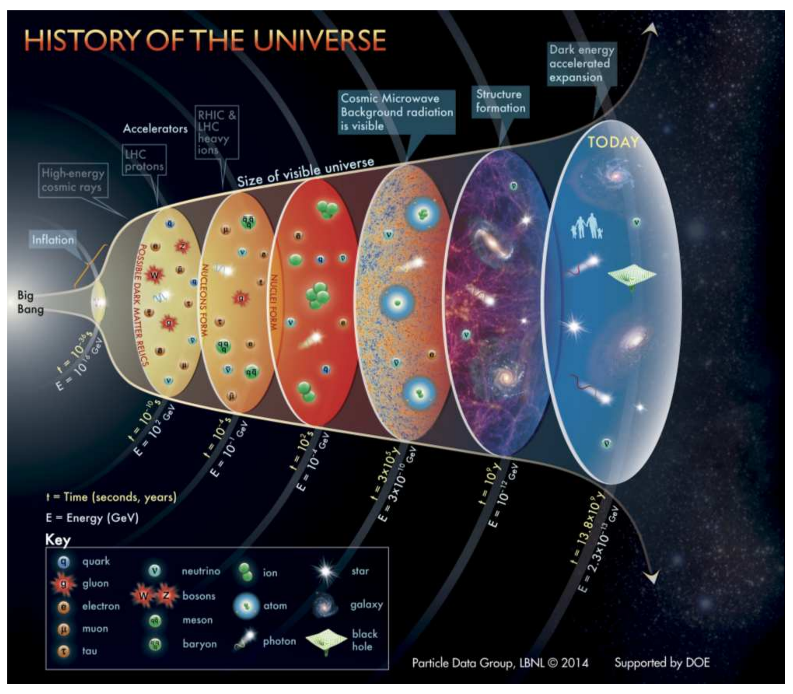

Figure 1: History of the universe: protons and neutrons (the constituents of atomic nuclei), which are made up from mainly light quarks (u and d) and gluons, have frozen out at $t \approx 0.3\,\mu s$. Before the freezeout light quarks and gluons had formed a *quark-gluon plasma* (an almost perfect fluid). Heavy quarks (c and b), travel as bound states or individually through the surrounding *quark-gluon plasma*.

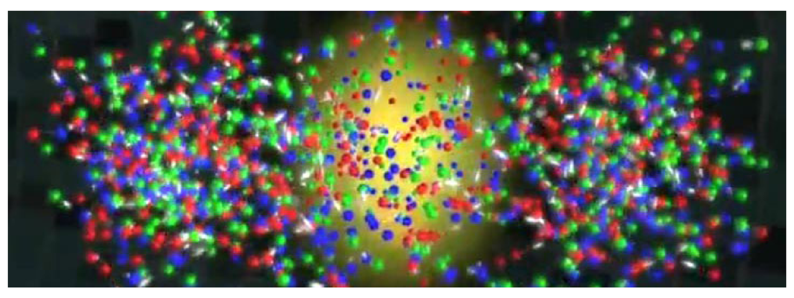

Figure 2: In ultra-relativistic heavy-ion collisions (at RHIC@BNL, LHC@CERN, etc.) an expanding fireball of *quark-gluon plasma* is created.

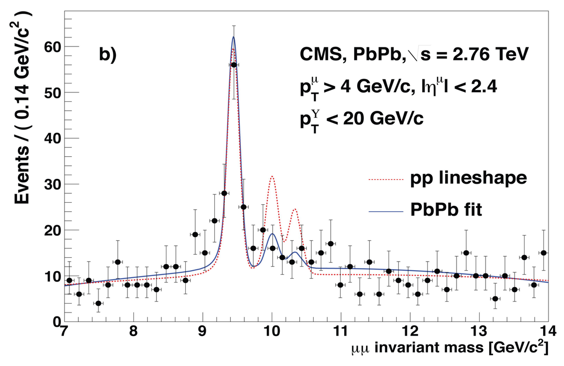

Figure 3: The relative abundances of the bound states of a $b\bar{b}$ pair are different in heavy-ion and proton-proton collisions. This effect is called *quarkonium suppression in quark-gluon plasma.*

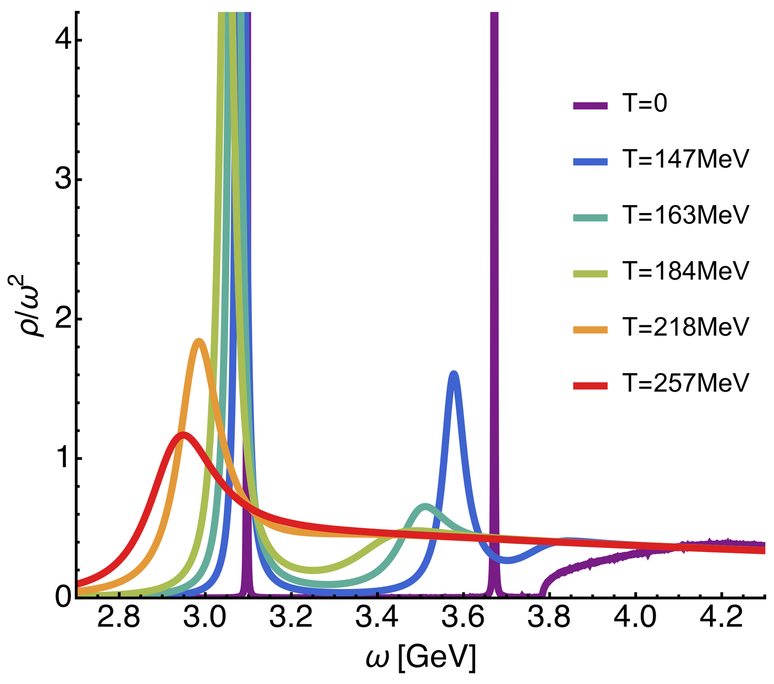

Figure 4: *Spectral function* of S-wave charmonium ($c\bar{c}$) at different temperatures [1] from a theory calculation (a lattice QCD potential used in a nonrelativistic quark model). Peaks broaden and move to lower energy with increasing temperature. Narrow peaks correspond to bound states; the shift of the maximum accounts for changes to the binding energy. The peak width indicates thermal dissociation (and recombination), which are real-time processes.

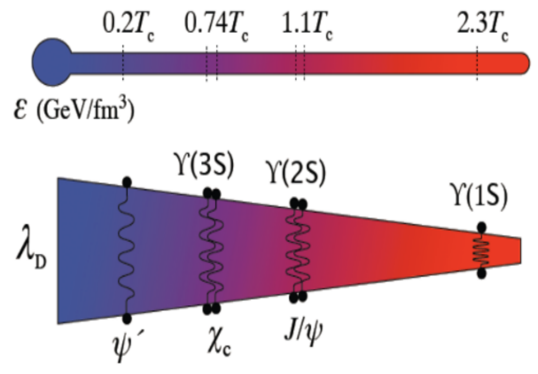

Figure 5: Melting patterns of different $c\bar{c}$ and $b\bar{b}$ states indicate the temperature of the *quark-gluon plasma.* In-medium heavy-quark bound states can be observed through their electromagnetic decays from within the *quark-gluon plasma* formed in heavy-ion collisions. The electromagnetic decay probability of each state is related to the area of the corresponding peak of the *spectral function.*

First-principle lattice QCD instead of model calculations is required to reduce the systematic errors. The intermediate step of retrieving a continuous *spectral function* from the discrete data set of a lattice correlation function along the time direction is an ill-posed problem. This problem is alleviated for *anisotropic lattices* with a much finer temporal lattice spacing.

Lattice QCD

Quantum ChromoDynamics is the non-Abelian $\mathrm{SU}(N_c = 3)$ gauge theory coupled to N_f matter fields (*quarks*) with different masses (this project: $N_f = 2 + 1$, two light quarks and a strange quark). The $N_c^2 - 1 = 8$ gauge bosons are the massless *gluons.* Due to its non-Abelian nature, QCD has an *emergent scale* Λ_{QCD}. A systematic expansion in a small parameter is not feasible for the physical processes involving scales close to Λ_{QCD}. Therefore, nonperturbative methods such as lattice QCD are required.

Imaginary time formalism

Lattice QCD simulations use Markov Chain Monte Carlo algorithms (i.e., Rational Hybrid Monte Carlo) to generate snapshots (*configurations*) of thermally equilibrated nuclear matter on a 4D space-time grid of $N_\sigma^3 \times N_\tau$ sites. Quark fields are defined on the sites and gluon fields on the links between each pair of sites. In order to use importance sampling, simulations have to be performed in a *imaginary time formalism*, i.e., with Euclidean metric (instead of Minkowski metric). In this setup, *real-time dynamics* cannot be studied directly, but is accessible via a detour to *spectral functions.*

Lattice scale and artifacts

The lattice step a or lattice scale is not an input parameter. Instead, the gauge coupling of the non-Abelian gauge theory is the main input parameter, which is related to Λ_{QCD} in a nonlinear way. In a simulation all dimensionful quantities are determined relative to the lattice scale a. Fixing one of these to its experimentally known value fixes the lattice scale a a posteriori.

Discretization artifacts

Unphysical discretization artifacts are removed by taking the *continuum limit*, which is determined from simulations with increasingly finer lattice step a. Variants of the *staggered quark discretization* are the most numerically efficient lattice formulation for quarks, but have the drawback of producing a *distorted spectrum* unless the continuum limit is taken.

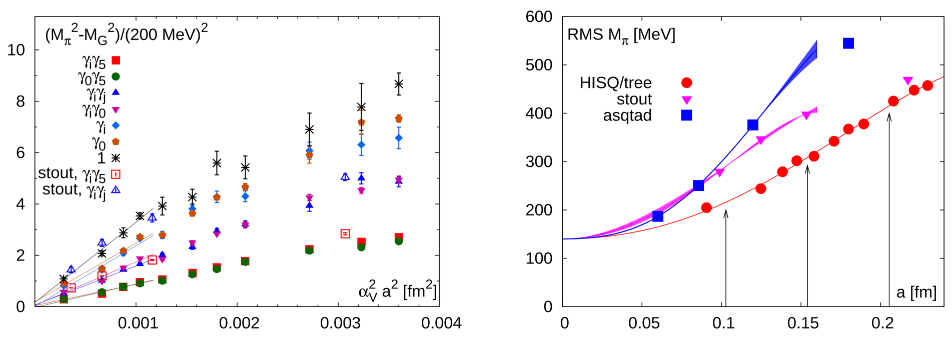

Figure 6: Among the various staggered quark discretizations the highly improved staggered quarks (HISQ) has the smallest distortions of the spectrum [2].

Finite temperature and volume

Euclidean time and inverse temperature

The inverse physical length of the Euclidean time direction plays the role of the equilibrium temperature, $T = 1/(a_\tau N_\tau)$, where N_τ is the number of time steps and a_τ is the lattice step in the time direction. In order to take the *continuum limit at the fixed temperature* T, which removes the artifacts of the lattice approach, one has to *simultaneously decrease* a_τ *and increase* N_τ *keeping* $T = 1/(a_\tau N_\tau)$ *constant.*

The spatial volume is analogous, i.e., $V_3 = (a_\sigma N_\sigma)^3$, where N_σ is the number of steps and a_σ is the lattice step in any of the spatial directions. Effects of the finite volume are negligible if the inverse physical length of each spatial direction is much smaller than the mass gap, i.e., the mass of the would-be Goldstone bosons. At high temperature it is sufficient that $a_\sigma N_\sigma \gg 1/T$.

Continuum limit

To take the *continuum limit* one has to keep temperature, volume, and known physical quantities constant up to discretization artifacts, and one has to know the *scaling relations* of the discretization artifacts with the lattice step a, see Fig. 6, for the case of the *distorted staggered spectrum.*

Anisotropic lattices

Temporal correlators on anisotropic lattices

Lattice correlation functions are usually calculated along the Euclidean time direction. Consequently, reconstructing the *spectral function* from a lattice correlation function is an ill-posed problem. The larger the number of steps in the time direction the less ill-posed the problem is. *Anisotropic lattices* are the only approach that permits *increasing the number of time steps*, while keeping the temperature, the volume and the number of spatial steps fixed.

In anisotropic lattice QCD there are two gauge couplings or a gauge coupling and a *bare anisotropy*, which are related to the two lattice spacings a_τ and a_σ or a lattice spacing $a \equiv a_\sigma$ and a *renormalized anisotropy* $\xi = a_\tau/a_\sigma$ in a nonlinear way. Quarks have a different, nontrivial relation between a bare anisotropy and a renormalized anisotropy ξ. As discretization artifacts are functions of both a_σ and a_τ, the *scaling relations are affected by the anisotropy* ξ. In particular, the *distortions of the HISQ spectrum* (see Fig. 6) are altered, i.e., all degeneracies are lifted, and the dependence of the RMS pion mass on a is distorted.

Project plan

In an initial step, we study the HISQ spectrum in anisotropic pure gauge theory (without dynamical quarks) to *quantify the distortions of the anisotropic HISQ spectrum and its scaling relations.* Our implementation of the *anisotropic HISQ Dslash operator* [3] and the ***vectorized anisotropic pure gauge theory algorithm*** (heatbath with overrelaxation) in the HotQCD code, which is optimized for the KNL architecture, is nearly complete. After establishing control of the *scaling relations* we will adapt the corresponding HMC algorithm for full anisotropic QCD.

Anisotropic QCD with HISQ

- We verify our vectorized anisotropic implementation against the anisotropic branch of the public MILC code [4].
- The *anisotropic HISQ Dslash operator* has identical performance characteristics as its isotropic counterpart [3].
- The bare quark anisotropy may require a reorganization of the HISQ link smearing algorithm, see [3].
- The quark and gauge anisotropies require some reorganization of the HISQ and gauge force algorithms, see [3].

References

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2. A. Bazavov *et al.*, Phys. Rev. D **85**, 054503 (2012).
3. Performance of Staggered Fermion Kernels using Grid.
4. MILC Collaboration, http://www.physics.utah.edu/~detar/milc/milc_qcd.html.

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SciDAC Scientific Discovery through Advanced Computing

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