Lattice Simulations of Strong Interactions in Background Fields

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In this talk I will discuss the computational challenges and some recent achievements regarding the investigation of QCD in external background fields

Why is that important?

- The response of a medium to external sources in a well known strategy to extract its properties;
- Our world is not just strong interactions. The response of QCD to external backgrounds can help elucidate the properties of hadronic matter in the context of other interaction (e.g., electromagnetic);
- That can be of particular interest for some contexts.

For Lattice QCD computations, the focus is presently on external backgrounds for which the path integral measure is real and positive, so that standard Monte-Carlo simulations are feasible (no sign problem appears):

- external backgrounds/parameters leading to a complex distribution
  - real chemical potentials
  - electric background fields
  - ...
- external backgrounds/parameters leading to a positive distribution
  - imaginary chemical potentials
  - imaginary electric fields
  - magnetic background fields
  - ...

The focus of my talk will be mostly on the physics of strong interactions in magnetic background fields.

Why is that important?

Quarks represents the connection between electromagnetic (e.m.) and strong interactions, they carry both electric and color charges. However e.m. interactions usually imply just small corrections to strong interaction physics.

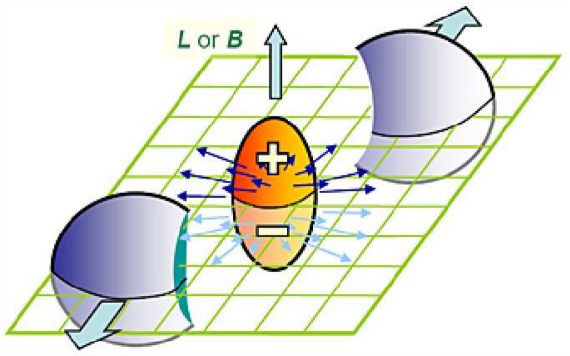
This is not the case in the presence of strong e.m. background fields which are at the scale of strong interactions by themselves. Was does that mean?

$$eB \sim \Lambda_{QCD}^2 \quad \Longrightarrow \quad B \sim 10^{15}\ \mathrm{Tesla}$$

Is there any context where such huge magnetic fields play a role?

- One expects $B \sim 10^{10}$ Tesla on the surface of a class of neutron stars known as magnetars (Duncan-Thompson, 1992). Fields might be larger inside
- Large magnetic fields, exceeding 10^{16} Tesla, might have been produced at the cosmological electroweak phase transition (Vachaspati, 1991)

However, we can reach such fields also in laboratory!

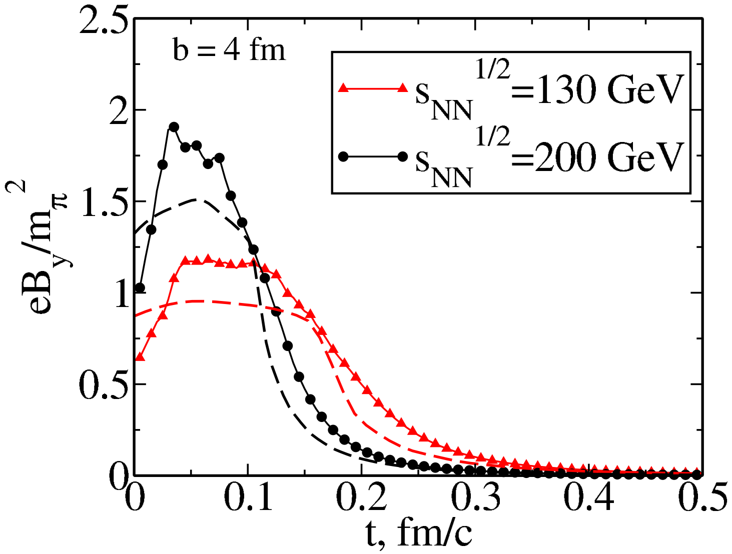


in non-central heavy ion collisions, largest magnetic fields ever created on Earth, with B going up to 10^{15} Tesla at RHIC (Brookhaven) and fairly exceeding that at LHC (CERN).

The largest field are expected in the early stages of the collision, then undergoing a fast decay

Estimate of eB time evolution @ RHIC for $Au - Au$ collisions for two values of $\sqrt{s_{NN}}$.

The actual decay rate dependes on the electric conductivity of the medium [Skokov, Illarionov and Toneev, '09]



A number of questions that we would like to answer:

- **Does the location and the nature of the QCD transition change as a function of B?**
- **Is strongly interacting matter diamagnetic or paramagnetic?**
- **Does the particle spectrum get modified by B?**
- **Any observable B-induced anisotropies? (Chiral Magnetic Effect? Influence on elliptic flow? Other?)**
- **Any other yet undiscovered effect?**

Most of those questions are linked to the non-perturbative properties of QCD and require a numerical approach

Background fields in Lattice QCD Simulations

As long as background fields are not dynamical, modifications with respect to standard LQCD amounts to a change in the fermion matrix. A $U(1)$ background is the most typical case, leading to a change in the covariant derivative:

$$\mathcal{Z} = \int \mathcal{D}U \, e^{-\mathcal{S}_{YM}} \prod_{f=u,\,d,\,s} \det\left(M^f[U, u^{(f)}]\right)^{1/4}$$

$$D_\mu = \partial_\mu + i\, g A_\mu^a T^a \quad \to \quad \partial_\mu + i\, g A_\mu^a T^a + i\, q a_\mu \quad \text{(continuum)}$$

$$D_\mu \psi \to \frac{1}{2a}\left(U_\mu(n) u_\mu(n) \psi(n+\hat{\mu}) - U_\mu^\dagger(n-\hat{\mu}) u_\mu^*(n-\hat{\mu}) \psi(n-\hat{\mu})\right) \quad \text{(lattice)}$$

$U_\mu \in SU(3)$ **(standard gauge link variable corresponding to gauge fields)**

$\mathbf{u}_\mu \simeq \exp(\mathbf{i\, q\, a}_\mu(\mathbf{n})) \in \mathbf{U(1)}$ **(background field)**

a_μ **may correspond to an e.m. field (real magnetic or imaginary electric, then q is the quark charge)**

$a_i = 0$ **and** $a_0 = \text{constant} \quad \Longrightarrow$ **imaginary chemical potential**

Computationally, the addition of the frozen $U(1)$ phases to the fermion matrix has a negligible overhead

- **Most algorithms used for inverting fermion matrices made up of $SU(3)$ variables, work for $U(3)$ variables as well**
- **the multiplication by a $U(1)$ phase is negligible itself (overhead well below 5%)**

A computational overhead may come from modifications of the physical properties of the medium. An example: at zero T the magnetic field increases the value of the chiral condensate (magnetic catalysis), which is proportional to the density of near-zero eigenvalues of the Dirac operator. The condition number of the fermion matrix worsens, the number of iterations of the inverter grows.

On the whole, the computational needs are at least the same as for standard zero-T or finite-T lattice simulations, easily reaching the order of 100 Tflops $\cdot$ year for projects working with physical quark masses, lattice spacings $a \lesssim 0.1$ fm, physical sizes $La \geq 5$ fm $\sim 3m_\pi^{-1}$. Most of the time is spent for inversion of the fermion matrix.

Which kind of computational resources are needed?

I report the experience from our group:

[C. Bonati (Pisa), M.D. (Pisa), M. Mariti (Pisa), F. Negro (Pisa), F. Sanfilippo (Southampton)]

- exploratory projects, experimenting a new computational strategy or trying to measure a new physical quantity on a simplified discretization of QCD, tipically make use of medium scale local clusters (standard and/or GPU);
- projects aimed at investigating QCD with physical quark masses and with a control over discretization and finite size effects, tipically need large scale supercomputing resources, such as those available within Tier-0 infrastructures (through PRACE or other national calls).

In both cases we make use of homemade codes, usually optimized for the specific architecture.

For example, the code running on the BlueGene/Q makes use of MPI for communications between different nodes and of multi-threading for internal node parallelization. (`https://code.google.com/p/nissa/`)

Various specific strategies are adopted for communication/computation overlap (e.g., SPI layout), which require massive use of the L2 cache and put a lower bound one the number of cores to be used for a specific lattice (around 20k lattice sites per BG/Q node).

# of cores	Time for 1 MD trajectory on a $48^3 \times 12$ lattice (s)	speedup
256	3600	1
512	1870	1.95
1024	840	4.29
2048	240	15
4096	140	26

We reach a peak performance around 35% (in the inverter) on a $48^3 \times 96$ lattice running on 16K cores.

Overview of physics results

In the following I will discuss about some selected topics and results, with a focus on the computational challenges

- **Temperature and nature of the transition as a function of external parameters (chemical potentials and magnetic field)**
- **Magnetic properties of strongly interacting matter: diamagnetic or paramagnetic?**
- **Magnetic-field induced anisotropies**

T_c as a function of external parameters

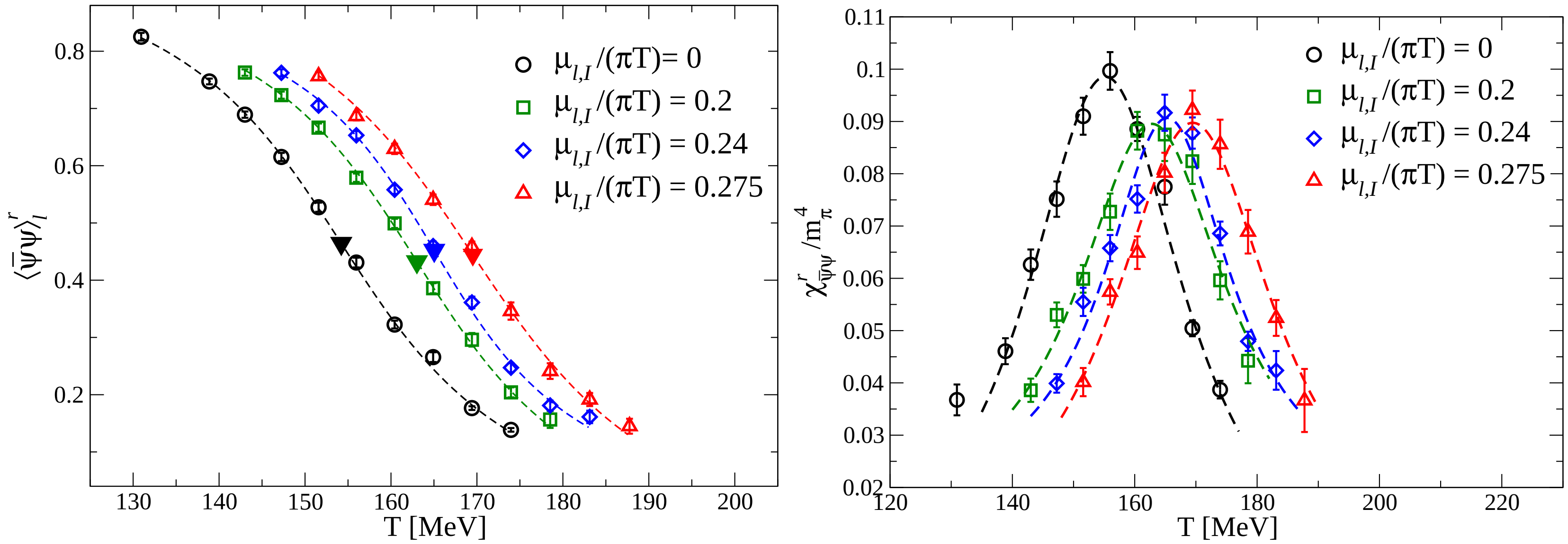
A single finite T simulation may require less computational effort than a zero T simulation: $T = 1/(N_t a)$, hence one lattice dimension is shorter; moreover, as chiral symmetry restores, the number of small eigenvalues diminishes, thus improving the condition number.

However, one needs many different simulations in order to explore a set of different temperatures and locate T_c: in QCD with physical quark masses, chiral symmetry restoration is the leading phenomenon around T_c, so one looks at the chiral condensate and at its susceptibility

That must be repeated for a set of different values of the external parameters in order to determine the dependence of T_c on it. Moreover, different spatial volumes and different lattice spacings should be explored to keep control over finite size and finite cut-off effects.

As for the order of the transition, one needs simulations on different spatial volumes to perform a finite size scaling analysis and determine the critical behaviour. Critical slowing down is an additional problem in this case.

T_c as a function of the baryon chemical potential: curvature of the critical line



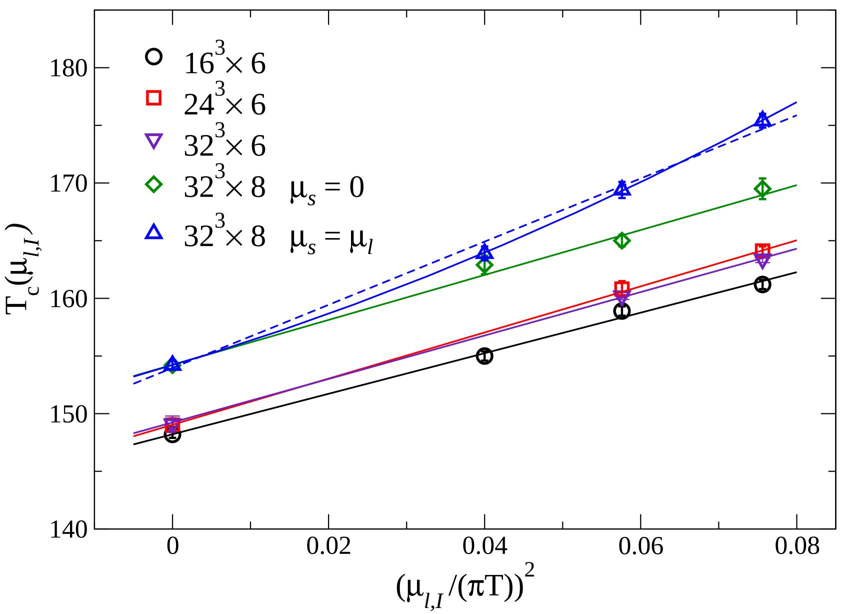
One is interested in T_c as a function of the baryon chemical potential for small values of μ_B

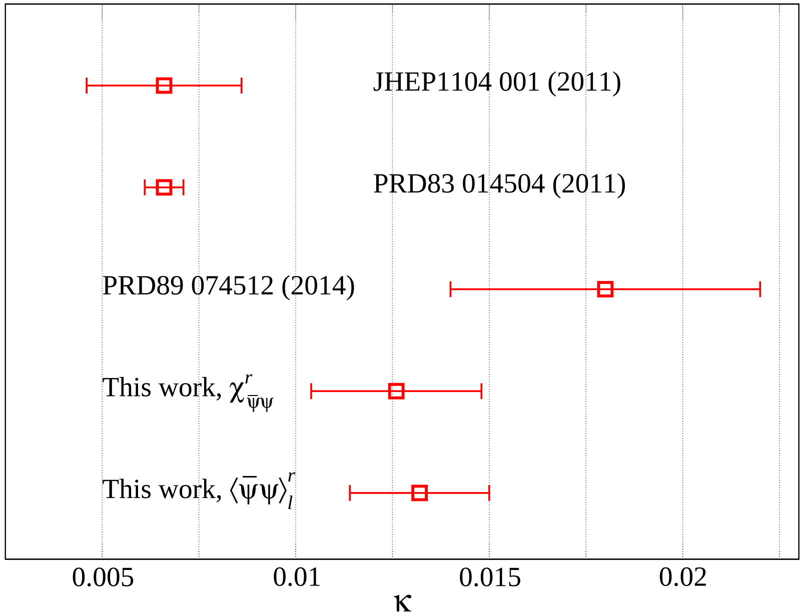
$$\frac{T(\mu_B)}{T_c} = 1 - \kappa \left(\frac{\mu_B}{T}\right)^2 + O(\mu_B^4)\,,$$

κ is the curvature of the pseudo-critical line.

One possibility to avoid the sign problem is to perform simulations at imaginary values of μ_B and then rely on analytic continuation. So, for the light quark chemical potential, one sets $\mu_l = \mu_B/3 = i\mu_{l,I}$

Results for the renormalized chiral condensate (left) and susceptibility (right) on a $32^3 \times 8$ lattice with physical quark masses (C. Bonati, MD, M. Mariti, M. Mesiti, F. Negro, F. Sanfilippo, arXiv:1410.5758)

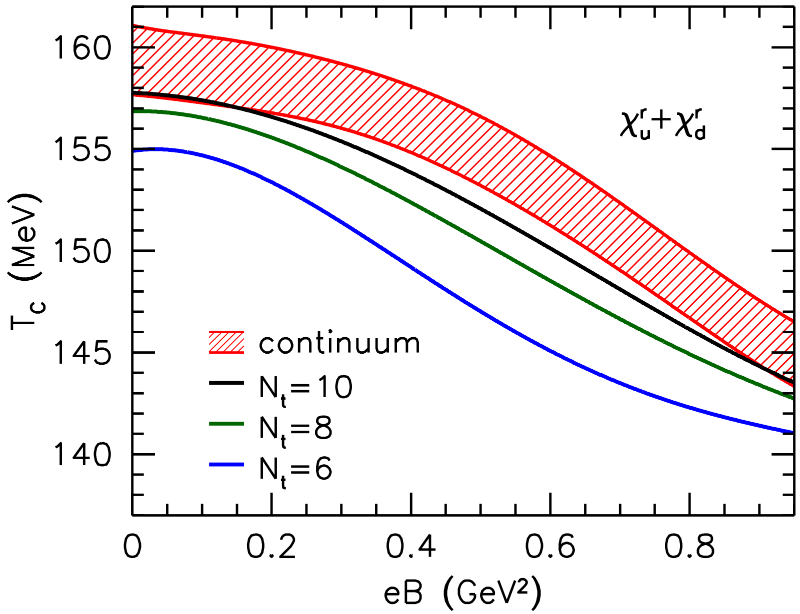




- **LEFT: From determinations of T_c at various $\mu_{l,I}$ one obtains the slope at $\mu_B = 0$, which is associated to κ by analytic continuation**
- **RIGHT: summary of lattice determinations of κ (analytic continuation and Taylor expansion)**

A proper comparison with phenomenological freeze-out curves will need the exploration of finer lattices ($N_t = 10$ and $N_t = 12$) for a controlled extrapolation to the continuum limit.

T_c in a magnetic background field



G. Bali et al., JHEP 1202, 044 (2012), $N_f = 2 + 1$, stout smeared staggered fermions, physical masses

- In this case $T_c(B)$ is obtained directly, by looking at the chiral susceptibility, since simulations at real B are feasibile.
- T_c decreases as a function of B, by about 10-20% at $|e|B \sim$ 1 GeV^2.
- Naive expectation is that B should increase chiral symmetry breaking (magnetic catalysis) and delay the transition. So this is an unexpected result from LQCD simulations (inverse catalysis), which is fostering many further theoretical studies.

The magnetic susceptibility of strongly interacting matter

Which kind of material is "strongly interacting matter"?

- **DIAMAGNETIC? free energy density f increases with B, pressure decreases**
- **PARAMAGNETIC? free energy density decreases with B, pressure increases**

The question is, in principle, simple and well posed:

We need the magnetization $M = -\partial f / \partial B$ and the magnetic susceptibility $\chi = -\partial^2 f / \partial B^2$ which are in principle perfectly computable equilibrium quantities.

$\chi > 0 \implies$ **PARAMAGNETIC** $\chi < 0 \implies$ **DIAMAGNETIC**

NUMERICAL PROBLEM: in the usual lattice setup (compact manifold with periodic b.c.), B is quantized (total flux must vanish, like for magnetic monopoles), and the derivative is not well defined.

That has represented a challenge in early studies.

Thermodynamic integration approach

C. Bonati, M. D., M. Mariti, F. Negro and F. Sanfilippo, Phys. Rev. Lett. 111, 182001 (2013) [arXiv:1307.8063]

- **The idea is to compute free energy differences instead of derivatives, so as to reconstruct its B-dependent part** $\Delta f(B,T) = -\frac{T}{V}\log\left(\frac{Z(B,T,V)}{Z(0,T,V)}\right)$

- **However, a direct determination of the ratio of partition functions is hardly feasible**

$$\frac{Z(B,T,V)}{Z(0,T,V)} = \frac{\int \mathcal{D}U e^{-S_G[U]} \det M[U,B]}{\int \mathcal{D}U e^{-S_G[U]} \det M[U,0]} = \left\langle \frac{\det M[U,B]}{\det M[U,0]} \right\rangle_{B=0}$$

difficulties emerge both in computing the observable and in correctly sampling it

- **A standard trick is to rewrite the ratio as the product of intermediate, easily computable ratios of interpolating partition functions, possibly also a continuous interpolation $\rightarrow$ derivative method**

$$\log\left(\frac{Z'}{Z}\right) = \log\left(\frac{Z'}{Z_N}\frac{Z_N}{Z_{N-1}}\cdots\frac{Z_2}{Z_1}\frac{Z_1}{Z}\right) = \log\frac{Z}{Z_N} + \cdots + \log\frac{Z_1}{Z} \rightarrow \int_Z^{Z'} dx \frac{d\log Z(x)}{dx}$$

This method is usually known as thermodynamic integration

Any interpolation is good! Provided the reconstruction is unambiguous

Various implementations:

- C. Bonati, M. D., M. Mariti, F. Negro and F. Sanfilippo, arXiv:1307.8063, arXiv:1310.8656

  Integration path is over non-quantized values of B (connecting quantized ones)

- G. S. Bali, F. Bruckmann, G. Endrodi S. D. Katz and A. Schaefer, arXiv:1406.0269

  Integration path is over the quark mass (a return ticket to the quenched limit)

In both cases the computational challenge is to perform enough intermediate simulations to allow for a smooth integration. The reward in statistical accuracy is worth that

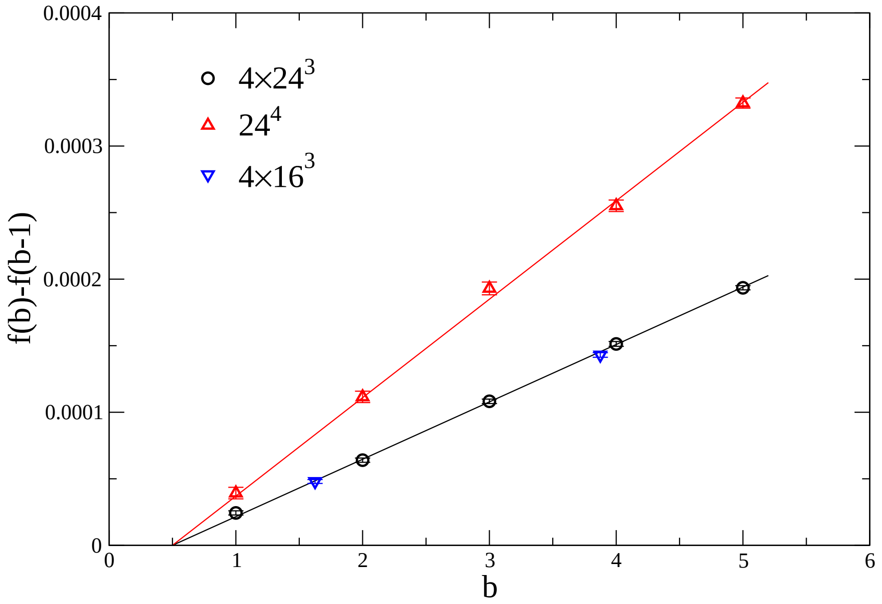
Alternative solutions:

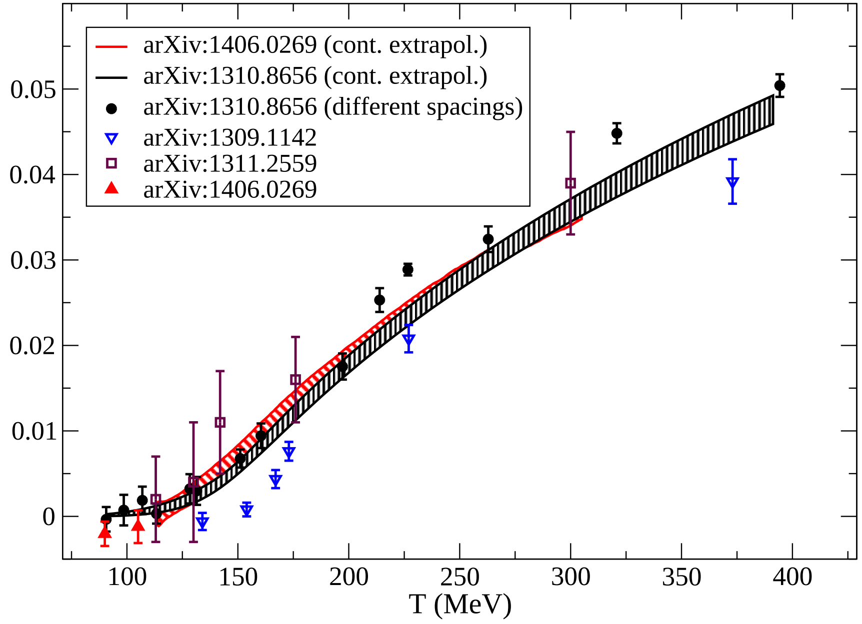
- L. Levkova and C. DeTar, arXiv:1309.1142

  Half-half method: a constant B for half of the lattice, and a constant $-B$ for the other half. Zero magnetic flux for every B: no quantization is required. But interface effects at the boundary must be kept under control.

- G. S. Bali, F. Bruckmann, G. Endrodi and A. Schaefer, arXiv:1311.2559

  computation of the magnetization based on pressure anisotropies $N_f = 2 + 1$ stout staggered fermions





LEFT: free energy differences between quantized values at zero and non-zero T, the difference provides a renormalized quantity

RIGHT: Renormalized magnetic susceptibility, QCD at the physical point, various methods

- The Quark-Gluon Plasma (QGP) is characterized by strong paramagnetism
- QGP shows a linear response for a magnetic fields up to 0.2 GeV^2
- That might have observable consequences in heavy ion collisions (Paramagnetic squeezing, G. S. Bali, F. Bruckmann, G. Endrodi and A. Schaefer, arXiv:1311.2559)
- Below T_c: should be diamagnetic (pion gas), but statistical errors still do not allow a definite statement.

Is confinement affected by a magnetic background?

Confinement is a property of gauge fields, which are not coupled to e.m. fields directly. However significant effects on them may come through quark loop effects, which are epected to be important in the non-perturbative regime.

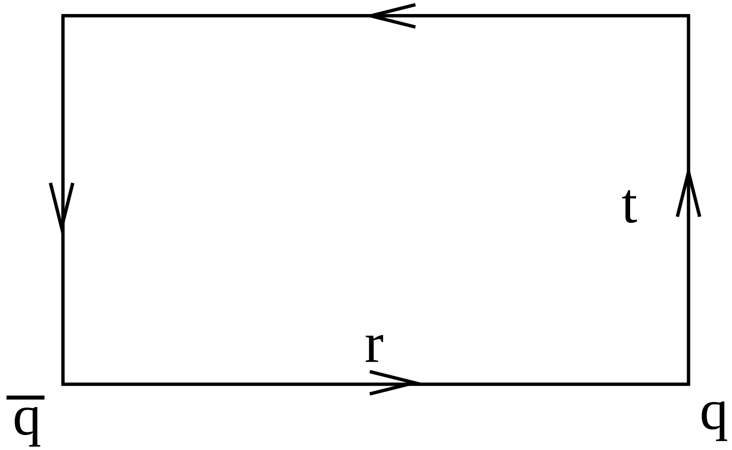
May we expect an effect on the static quark-antiquark potential? This is the starting point for many computations of the heavy quarkonia spectrum. Usual Cornell parametrization:

$$V_{Q\overline{Q}}(\vec{r}) = C + \sigma|\vec{r}| + \frac{\alpha}{|\vec{r}|}$$

$\sigma \equiv$ is the ***string tension***

$\alpha \equiv$ is the Coulomb coupling parameter

The magnetic field breaks rotational invariance, does the breaking propagates to pure gauge quantities? Does the potential becomes anisotropic?



$V_{\bar{Q}Q}$ **can be extracted by computing the Wilson Loop**

$$\mathbf{W}(\vec{\mathbf{R}},\mathbf{T})$$

A rectangular $R \times T$ loop built up of link variables $U_\mu(n)$.

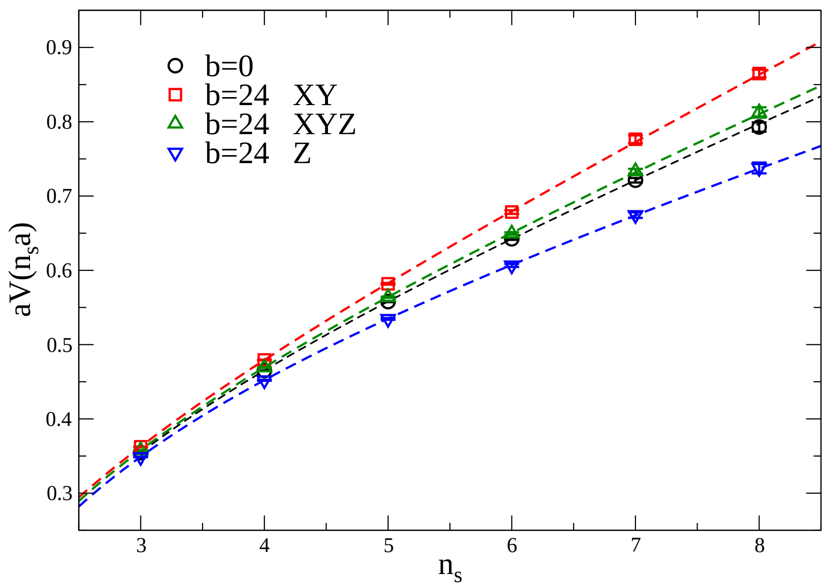
$$\boxed{aV_{Q\overline{Q}}(a\vec{n}) = \lim_{n_t \to \infty} \log \left(\frac{\mathbf{W}(a\vec{n}, an_t)}{\mathbf{W}(a\vec{n}, a(n_t+1))} \right)}$$

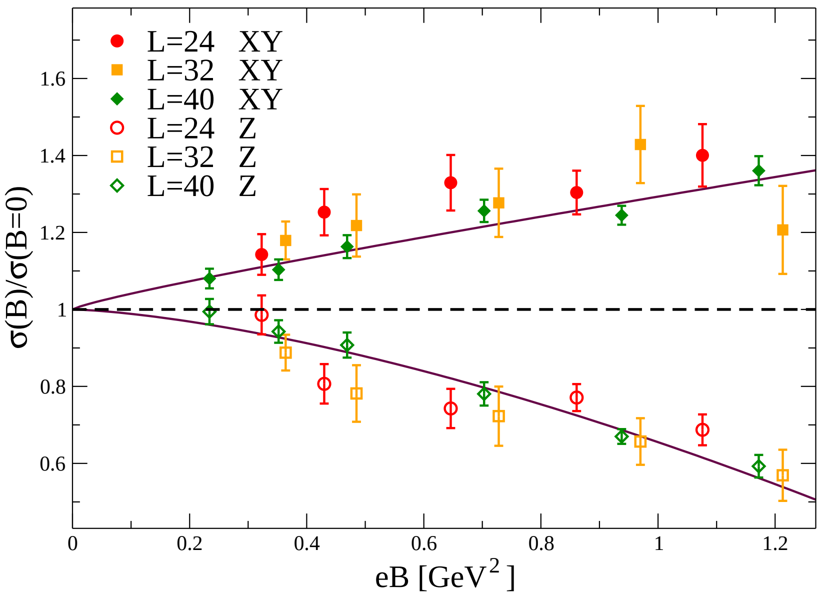
- **creation of a quark-antiquark pair at distance $\vec{\mathbf{R}}$**
- **imaginary time propagation for an interval of time $\mathbf{T}$**
- **annihilation of the pair.**

$$\langle \mathbf{W}(\vec{\mathbf{R}},\mathbf{T}) \rangle \simeq C \exp\left(-\mathbf{T} V_{Q\overline{Q}}(\vec{\mathbf{R}}) \right)$$

An anisotropy clearly emerges

C. Bonati, MD, M. Mariti, M. Mesiti, F. Negro and F. Sanfilippo, arXiv:1403.6094





LEFT: potential parallel (Z) and orthogonal (XY) to B, for $eB \simeq 0.8$ GeV^2, compared to $eB = 0$ and to averaged over directions.

RIGHT: string tension along orthogonal and longitudinal directions as a function of B

The string tension (left) increases in the orthogonal directions and decreases in the longitudinal directions. The Coulomb coupling shows an opposite behaviour.

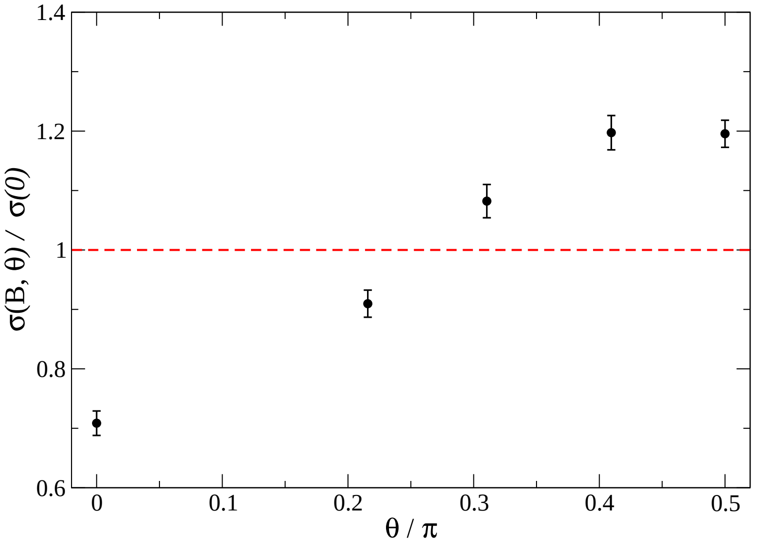
Many perspectives and new questions opened

PRACE (9th call, SISMAF project) is helping us find answers

Continuum extrapolation and detailed angular dependence? Needed to predict effects on quarkonia.

LEFT: Preliminary results for $a \simeq 0.099$ fm and $eB \sim 1$ GeV^2

Simulations performed on BG/Q Fermi machine at CINECA



- **Effects on the heavy meson spectrum? Direct lattice measurement?**
- **Anisotropies in the flux tube formation?**
- **Extension to finite T?**

Final Considerations

- The exploration of QCD under extreme conditions offers a unique opportunity to our theoretical understanding of fundamental interactions and to the search for new physics phenomena

- The non-perturbative properties of strong interactions make numerical Lattice QCD simulations the best investigation tool, based on first principles

- From the very beginning, Lattice QCD has represented a major challenge in the world of scientific computing, fostering the development of new HPC architectures during the last few decades

- Within this context, PRACE represents a unique opportunity for many projects in our field. We hope this opportunity will last for long.