FASTSUM: simulations of hot and dense QCD

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Outline

FASTSUM members

Gert Aarts (Swansea)
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Maria-Paola Lombardo (Firenze)
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Current students

Sergio Chaves, Alan Kirby,
Sam Offler, Thomas Spriggs,
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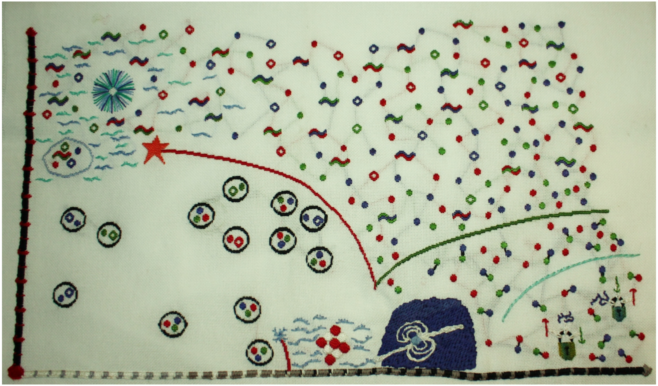
Luke Gayer (TCD)

Former members

Ale Amato (Swansea→Helsinki→)
Davide de Boni (Swansea→)
Wynne Evans (Swansea→)
Pietro Giudice (Swansea→Münster→)
Jonas Glesaaen (Swansea→)
Tim Harris (TCD→Mainz→Milano)
Aoife Kelly (Maynooth→)
Buğra Oktay (TCD→Utah→)
Kristi Praki (Swansea→)
Ryan Quinn (Maynooth→)
Don Sinclair (Argonne)

Background

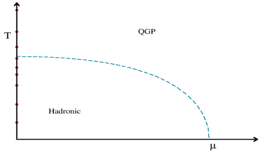


Challenges

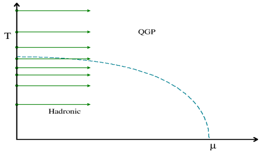
- Nature of transition as $m_{ud} \to 0$
- Equation of state, higher order cumulants (skewness, kurtosis)
- Existence of critical point at $(T, \mu) > 0$
- **Transport properties** (conductivity, viscosity, jet quenching)
- **Hadron properties**:
  in-medium modifications, heavy quarkonium
- Effect of magnetic field, chiral magnetic effect
- **Cold dense QCD** (sign problem)

Projects

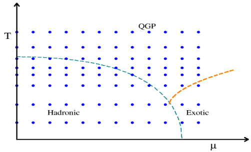
Spectroscopy at high T



Taylor expansion



Complex Langevin



Dynamical anisotropic lattices

Temperature $T = \frac{1}{L_\tau} = (N_\tau a_\tau)^{-1}$
Main thermodynamics interest: spectral properties

$$\rho(\omega) = \mathrm{Im}\, G_R(\omega) = \mathrm{Im} \int_0^\infty G_R(t) e^{-i\omega t}$$

$$G_E(\tau; T) = \int_0^\infty d\omega K(\omega, \tau; T) \rho(\omega; T)$$

- A large number of points in time direction required
- Fixed-scale approach
  - $\rightarrow$ vary T by varying N_τ (not a)
  - $\rightarrow$ need only 1 $T = 0$ calculation for renormalisation
  - $\rightarrow$ independent handle on temperature

- Introduces 2 additional parameters
- Non-trivial tuning problem

  [PRD **74** 014505 (2006); HadSpec Collab, PRD **79** 034502 (2009)]

Other approaches

Fixed-N_τ approach

- Isotropic lattices, $a_s = a_\tau = a$
- Fix N_τ, vary T by varying a
- T can be changed continuously near T_{pc}
- Current state-of-the-art: $N_\tau = 12$–16, N_{cfg} =10k-1M per temperature
- Most studies use staggered fermions

Isotropic Wilson fermion simulations

- WHOT-QCD: Clover, fixed-scale ($N_\tau = 16$-4), Wilson flow
- tmfT: twisted-mass, using ETMC parameters, $N_\tau = 24$–4.
- Mainz: Fixed T, using CLS parameters + smaller a for continuum extrapolation

Simulation parameters

[PRD **76** 194513 (2007), HadSpec Collab, PRD **79** 034502 (2009)]

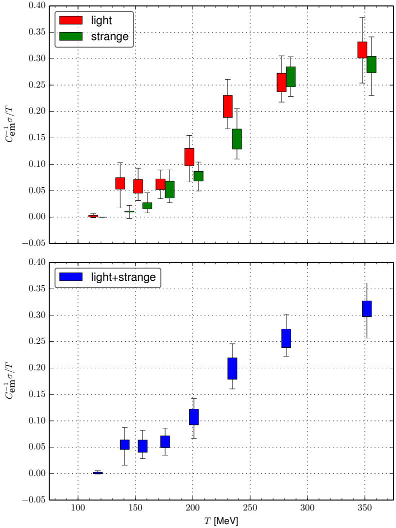
Gen	N_f	ξ	a_s (fm)	a_τ^{-1} (GeV)	m_π (MeV)	N_s	L_s (fm)
1	2	6.0	0.162	7.35	490	12	1.94
2	2+1	3.5	0.123	5.63	390	24	2.95
						32	3.94
2L	2+1	3.5	0.123	5.63	240	32	3.94
3	2+1	7.0	*0.123	*11.66	*390	32	3.94

Simulation parameters: temperatures

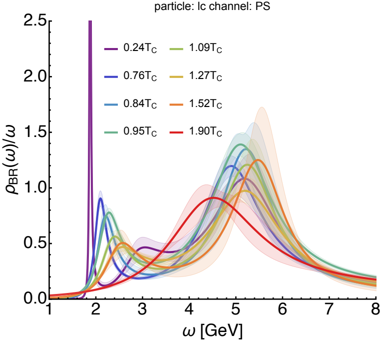
Gen 2			Gen 2L		
N_τ	T (MeV)	T/T_c	N_τ	T (MeV)	T/T_c
128	44	0.24	128	47	0.29
			64	94	0.59
			56	107	0.67
48	117	0.63	48	125	0.78
40	141	0.76	40	150	0.94
36	156	0.84	36	167	1.04
32	176	0.95	32	187	1.17
28	201	1.09	28	214	1.34
24	235	1.27	24	250	1.56
20	281	1.52	20	300	1.87
16	352	1.90	16	375	2.34
			12	500	3.12
			8	750	4.69

Physics highlights

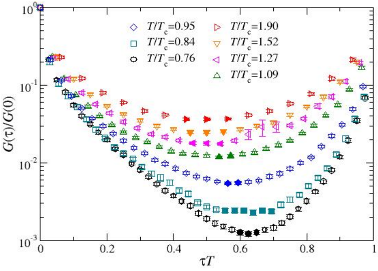
Electrical conductivity

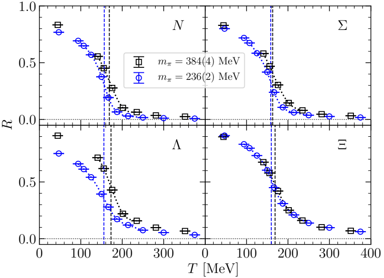


Open charm



Physics highlights — Baryons at high T





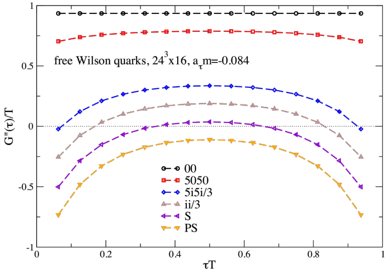
Forward propagating: + parity;
Backward propagating: − parity

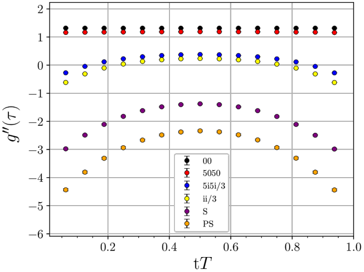
Measure of parity doubling:

$$R(\tau) = \frac{G(\tau) - G\beta - \tau)}{G(\tau) + G(\beta + \tau)}$$

$$R = \sum_{n=0}^{\beta/2-1} \frac{R(\tau_n)/\sigma^2(\tau_n)}{1/\sigma^2(\tau_n)}$$

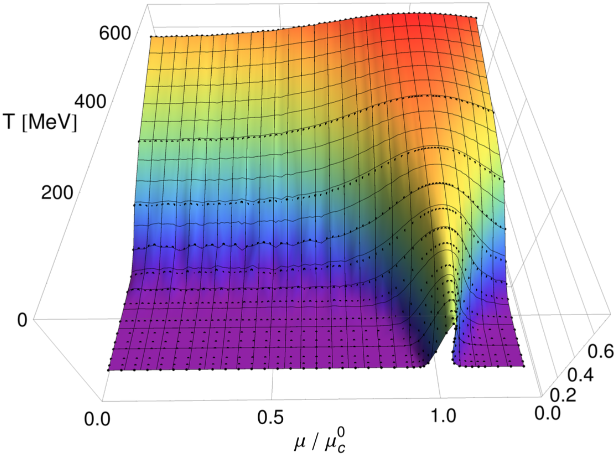
Physics highlights — Taylor expansion





- Part of μ^2 coefficient on Gen2 ensemble
- High temperature
- Free vs interacting: some visible differences

Physics highlights: Complex Langevin



Polyakov loop as function of μ and T, heavy–dense QCD

Recent and current grants

PRACE

- Call 3: 22M (BG/Q JuQueen)
- Call 5: 32M (BG/Q Fermi@CINECA)
- Call 12: 40M (BG/Q Fermi, KNL Marconi@CINECA)
- Call 18: 30M (Broadwell Galileo@CINECA, Rome AMD Irene@CEA)

DiRAC

- Call 1: 200M (BG/Q)
- Call 7: 400M (BG/Q)
- Call 10: 30M (Tesseract)
- Call 11: 375M (Tesseract, DiRAC@Leicester)

Code

OpenQCD

- FASTSUM extension to openQCD 1.6
- Anisotropic
- Stout smearing
- Intel AVX-512 vectorisation
- Fermion matrix inverter
- Meson and baryon correlators
- Taylor expansion coeffs, including condensates, susceptibilities
- Excellent scaling on standard CPUs: Intel, AMD, BlueGene, Xeon Phi, ARM ThunderX2
- Porting to GPU in progress

Computational needs

Strategies

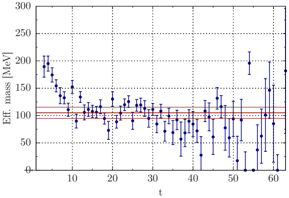
1. Continuum time limit $a_\tau \to 0, a_s$ fixed, $\xi \to \infty$
2. Continuum limit $a_s, a_\tau \to 0, \xi$ fixed
3. Physical quarks $m_q \to m_{ud}, m_s$

Short-term plans

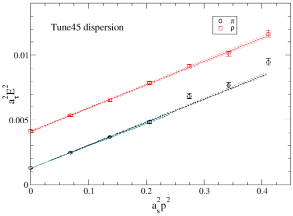
- More chiral: Gen2 $\to$ Gen2L $\to$ Gen2P
- Increase statistics to per-mille on correlators
- Increase spatial volume $32^3 \to 48^3$ or 64^3
- Reduce a_τ: $\xi = 3.5 \to 7$

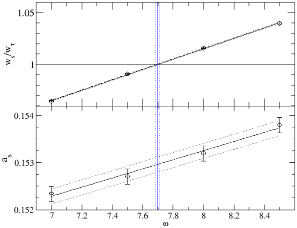
Short–medium term plans

Gen2P: physical quark masses



Gen3: higher anisotropy





Computational needs

Special requirements

- Small steps in $T \to$ “unusual” values for N_τ
- Large spatial volumes for critical scaling, thermodynamics
- Typically larger statistics than $T = 0$ studies
  - $\to$ sub-permille errors for transport, thermal width
  - $\to$ 100k–1M trajectories for higher order Taylor expansion
- Operator traces: $\mathcal{O}(1000)$ sources for susceptibilities, Taylor expansion coefficients

Computational needs

Estimated future needs

- Physical quarks
  - → 1–2 orders of magnitude increase
  - → $\sim$ 2G Tesseract core-hrs, 200TB for full Gen2P ensemble
- Continuum limit
  - → order of magnitude increase per ensemble
  - → significant tuning effort
- Algorithm developments
  - → multilevel for light fermions → viscosity?
  - → Efficient management of high order traces?
  - → Machine learning ideas for spectral functions?

Outlook

- Quantitative understanding of T_{pc}, EoS at $\mu = 0$ obtained
- Replicate staggered results with Wilson (+DW, overlap?)
- Role of topology, $U(1)_A$ restoration?
- Quantitative results for transport and spectral properties?
- Quantitative EoS, transition line for $\mu > 0$?
- Existence of critical point?

Approaches to sign problem

- Complex Langevin is promising
- Lefschetz thimble / flow deformation?
- Density of states
- Dual formulations?
- Ultimate sign problem: real-time simulations