Lattice calculations of the heavy quark diffusion coefficient using gradient flow

INT - Heavy Flavor Production in Heavy-Ion and Elementary Collisions

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Outline

Introduction: Motivation of the Quark Gluon Plasma

- Quark Gluon Plasma (QGP) generated at particle accelerators such as LHC/RHIC
- The QGP can be described in terms of transport coefficients
- We are interested in Heavy quark physics as they probe the medium consisting of light quarks well
- Here: we focus on the heavy quark momentum coefficient κ:
  Spatial diffusion coefficient $D_{\mathrm{S}} = 2T^2/\kappa$
  Drag coefficient $\eta_{\mathrm{D}} = \kappa/(2MT)$
  Heavy quark relaxation time $\tau_{\mathrm{Q}} = \eta_{\mathrm{D}}^{-1}$
- κ related to experimental quantities Nuclear modification factor R_{AA}, and Elliptic flow ν_2
- Multiple theoretical models predicting wide range of values

→ Non-perturbative lattice simulations needed

Introduction: Theoretical constructions for the Lattice

(Casalderrey-Solana and Teaney PRD 74 (2006)), (Caron-Huot et.al. JHEP04 (2004))

- In the $M \to \infty$ limit we can define:

$$\kappa = \frac{1}{3T\chi} \sum_{i=1}^{3} \lim_{\omega \to 0} \left[\lim_{M \to \infty} M_{kin}^2 \int_{-\infty}^{\infty} dt e^{i\omega(t-t')} \int d^3x \left\langle \frac{1}{2} \left\{ \frac{\hat{\mathcal{J}}^i(t,x)}{dt}, \frac{\hat{\mathcal{J}}^i(0,x)}{dt} \right\} \right\rangle \right]$$

- Where $\hat{\mathcal{J}}^i(x) = \bar{\psi}(x)\gamma^\mu\psi(x)$ is the heavy quark current
- The heavy quark force in static limit:

$$M \frac{d\hat{\mathcal{J}}^i}{dt} = \{\phi^\dagger E^i \phi - \theta^\dagger E^i \theta\}$$

- Where ϕ, θ are HQ and $\mathrm{H\bar{Q}}$ operators, E^i chromoelectric field
- Now the euclidean correlator is defined as:

$$\kappa = \sum_{i=3}^{3} \lim_{M \to \infty} \frac{\beta}{3\chi} \int dt d^3x \left\langle \frac{1}{2} \left\{ \left[\phi^\dagger g E^i \phi - \theta^\dagger g E^i \theta\right](t,x), \left[\phi^\dagger g E^i \phi - \theta^\dagger g E^i \theta\right](0,x) \right\} \right\rangle$$

Introduction: Theoretical constructions for the Lattice

(Caron-Huot et.al. JHEP04 (2004))

- Switch to Euclidean electric fields:

$$G_{\mathrm{E}} = -\frac{1}{3T\chi}\sum_{i=3}^{3}\lim_{M\to\infty}\int d^3x \left\langle \frac{1}{2}\left[\phi^\dagger gE^i\phi - \theta^\dagger gE^i\theta\right](\tau,x)\left[\phi^\dagger gE^i\phi - \theta^\dagger gE^i\theta\right](0,x)\right\rangle$$

- After simplifying the propagators of ϕ and θ in $M\to\infty$:

$$G_{\mathrm{E}}(\tau) = -\frac{1}{3}\sum_{i=1}^{3}\frac{\langle \mathrm{ReTr}[U(\beta,\tau)gE_i(\tau,0)U(\tau,0)gE_i(0,0)]\rangle}{\mathrm{ReTr}[U(\beta,0)]}$$

- Related to the Diffusion coefficient by:

$$G_{\mathrm{E}} = \int_0^\infty \frac{d\omega}{\pi}\rho(\omega)\frac{\cosh\left(\frac{\beta}{2}-\tau\right)\omega}{\sinh\frac{\beta\omega}{2}}, \kappa = \lim_{\omega\to 0}\frac{2T}{\omega}\rho(\omega)$$

- In general, inversion problem ill defined
- No $\omega\to 0$ transport peak

Introduction: Theoretical constructions for the Lattice

(A. Bouttefeu and M. Laine JHEP 12 (2020) 150, M. Laine JHEP 06 (2021) 139)

- Considering full Lorentz force:

$$F(t) = \dot{p} = q(E + v \times B))(t)$$

- $\langle v^2 \rangle \sim \mathcal{O}(T/M)$ corrections to HQ momentum diffusion

$$\kappa_{\mathrm{tot}} \simeq \kappa_{\mathrm{E}} + \frac{2}{3}\langle v^2 \rangle \kappa_{\mathrm{B}}$$

- κ_{B} related to correlation of chromo magnetic fields:

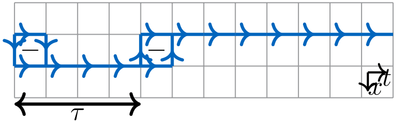
$$G_{\mathrm{B}}(\tau) = \frac{1}{3}\sum_{i=1}^{3} \frac{\langle \mathrm{ReTr}[U(\beta,\tau)B_i(\tau,0)U(\tau,0)B_i(0,0)]\rangle}{\langle \mathrm{ReTr}[U(\beta,0)\rangle}, \kappa_{\mathrm{B}} = \lim_{\omega\to 0}\frac{2T\rho_{\mathrm{B}}(\omega)}{\omega}$$

- Same tree level expansion as G_{E}, but NLO has divergence

$$\rho_{\mathrm{B}} = \frac{g^2 C_f \omega^3}{6\pi}\left[1 - \frac{g^2 C_A}{(4\pi)^2}\frac{2}{\epsilon} + (\text{finite})\right] + \mathcal{O}(g^6)$$

Introduction: Lattice discretization

- G_{E} correlator:



- E-field discretization:

$$a^2 E_i(\tau, x) = U_4(\tau, x) U_i(\tau + 1, x) - U_i(\tau, x) U_4(\tau, x + \hat{i})$$

- Similar for B-field discretization:

$$a^2 B_i(\tau, x) = \epsilon_{ijk} U_j(\tau, x) U_k(\tau, x + \hat{j})$$

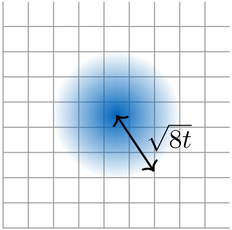
- Both, $G_{\mathrm{E/B}}$ have a finite extension which leads to unphysical self-energy contributions
- κ-physics at large τ, but bad signal-to-noise ratio there

➡ Need to renormalize the correlators for obtaining a proper continuum limit, e.g. $Z_{\mathrm{E,B}}$

Introduction: Gradient flow

- Evolve gauge fields along fictitious time t:

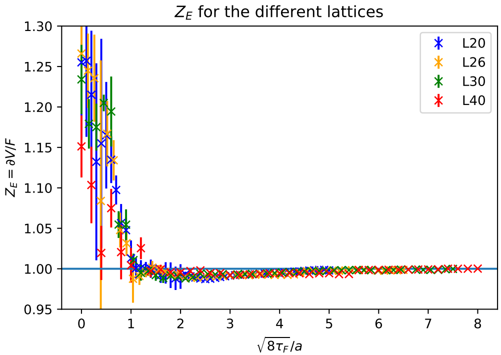
$$\partial_t B_{\tau_F,\mu} = -\frac{\delta S_{YM}}{\delta B} = D_{\tau_F,\mu} G_{\tau_F,\mu\nu}\,,$$
$$G_{\tau_F,\mu\nu} = \partial_\mu B_{\tau_F,\nu} - \partial_\nu B_{\tau_F,\mu} + [B_{\tau_F,\mu}, B_{\tau_F,\nu}]\,.$$
$$B_{0,\mu} = A_\mu \;\leftarrow\; \text{the original gauge field}$$



- Diffuses the inital gauge field with radius $\sqrt{8\tau_F}$, "diffuses" discretization effects
- Automatically renormalizes gauge invariant observables
- Zero flowtime limit $\mathcal{O}(x,\tau_F) \xrightarrow{\tau_F \to 0} \sum_j d_j(\tau_F)\mathcal{O}_j^R(x)$
- Could allow un-quenched simulations
- Issue with $G_\mathcal{B}$: divergence at zero flowtime

Introduction: Gradient flow

- From force measurement: non-perturbative Z_E determination
- For $\sqrt{8\tau_F} > a$: $Z_\mathrm{E} \to 1$
- Gradient flow renormalizes field insertions if enough flowtime is applied



Introduction: Our aim

- Perform simulations at $T = 1.5T_C$ and $T = 10^4T_C$
- So far for κ_{E}:
  1. Measure flowed G_{E} and perform continuum limits
  2. Obtain renormalized G_{E} with the zero flowtime limit
  3. Model ρ_{E} and obtain κ_{E}
- To target κ_{B} try new procedure for κ_{E}:
  1. Measure flowed G_{E} and perform continuum limits
  2. Model ρ_{E} at finite flowtime and obtain flowed $\kappa_{\mathrm{E}}(\tau_F)$
  3. Perform zero flowtime limit for κ_{E}
  4. Compare with the traditional approach
- Perform the same for $\kappa_{\mathrm{B}}/G_{\mathrm{B}}$

Outline

Analysis: Lattice setup

- Set scale for $1.5T_C$ and 10^4T_C through
  (A. Francis et.al. PRD 91 (2015))
- Simulation parameters:

T/T_C	N_t	N_S	β	N_{conf}
1.5	20	48	7.044	4290
	24	48	7.192	4346
	28	56	7.321	5348
	34	68	7.483	3540
10000	20	48	14.635	1890
	24	48	14.792	2280
	28	56	14.925	2190
	34	68	15.093	1830

- Configurations produced with Wilson action, Gradient flow with Symanzik action
- For the largest lattice, adaptive gradient flow solver is used, fixed stepsize for the others

Analysis: Lattice perturbative

- Continuum perturbative correlator is known:
  (Caron-Huot et.al. JHEP04 (2009))

$$\frac{G_{\mathrm{E}}^{\mathrm{pert,LO}}}{g^2 C_f} = \pi^2 T^4 \left[\frac{\cos^2(\pi\tau T)}{\sin^4(\pi\tau T)} + \frac{1}{3\sin^2(\pi\tau T)} \right]$$

- Lattice perturbative correlator is known (flowed correlator more complicated):
  (A. Francis et.al. PoSLattice (2011))

$$\frac{G_{\mathrm{E}}^{\mathrm{LOlatt}}(\tau)}{g^2 C_{\mathrm{F}}} = \int_{-\pi}^{\pi} \frac{d^3 q}{(2\pi)^3} \frac{\tilde{q}^2 e^{\bar{q} N_t (1-\tau T)} + \bar{q}^2 e^{\bar{q} N_t \tau T}}{3a^4 (e^{\bar{q} N_t} - 1) \sinh(\bar{q})}, \bar{q} = 2\mathrm{arsinh}\left(\frac{\sqrt{\bar{q}^2}}{2}\right), \quad \tilde{q}^n = \sum_{i=1}^{3} 2^n \sin^n\left(\frac{q_i}{2}\right)$$

- By perturbative behavior and experience, the valid flowtime range is

$$a \leq \sqrt{8\tau_F} \leq \frac{\tau}{3}, \qquad \frac{a}{\tau} \leq \frac{\sqrt{8\tau_F}}{\tau} \leq \frac{1}{3}$$

- We use the ratio $\sqrt{8t}/\tau$ as the relevant scale

Analysis: Measurement preparation

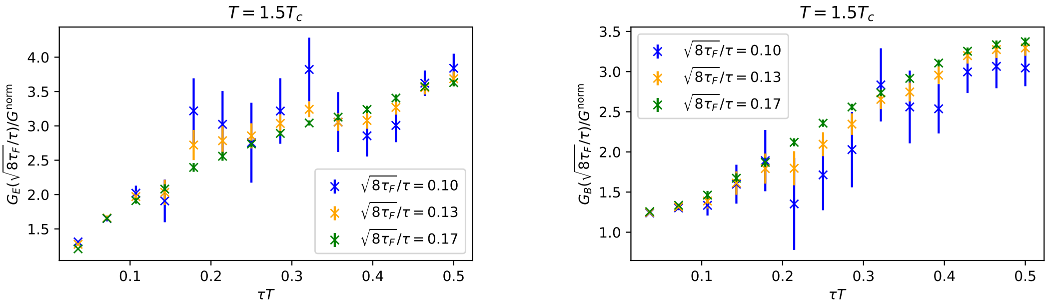
- We use the ratio $\sqrt{8t}/\tau$ as the relevant scale
- Normalizing the correlator with $G^{\mathrm{norm}} = G_{\mathrm{E}}^{\mathrm{pert,LO}}/g^2 C_f$
- Tree level improvement through multiplicative factor

$$\frac{G_{\mathrm{E}}^{\mathrm{pert,LO}}}{G_{\mathrm{E}}^{\mathrm{LOlatt}}} \times \frac{G_{\mathrm{E}}^{\mathrm{meas}}}{G^{\mathrm{norm}}} = \frac{G_{\mathrm{E}}^{\mathrm{meas}}}{G_{\mathrm{E}}^{\mathrm{LOlatt}}/g^2 C_f}$$

- We use the same normalization for G_{B}
- Normalized quantities are dimensionless
  $\rightarrow$ suitable for continuum limits

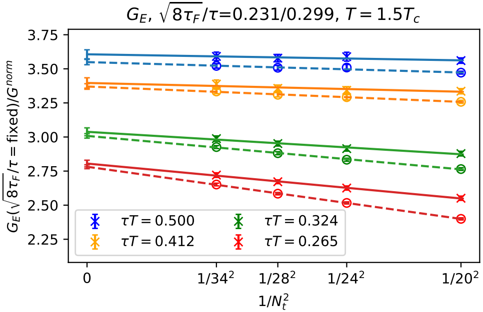
Analysis: Correlator measurement

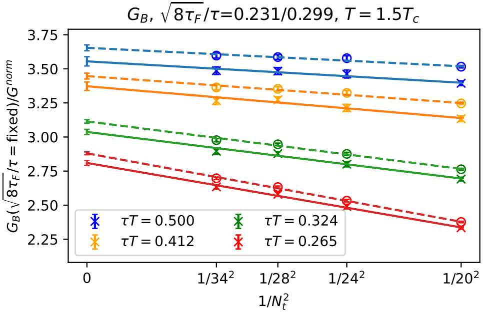
Measured correlator for the $N_t = 28$ lattice



- Increasing flowtime decreases statistical error
- With increasing flowtime converge towards a common shape

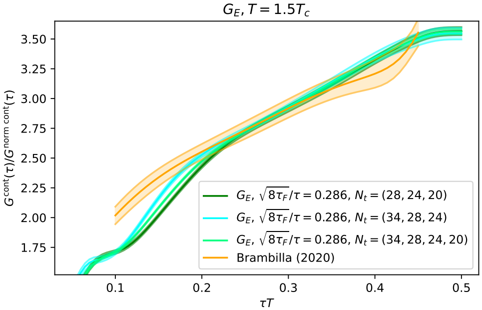
Analysis: Continuum extrapolation

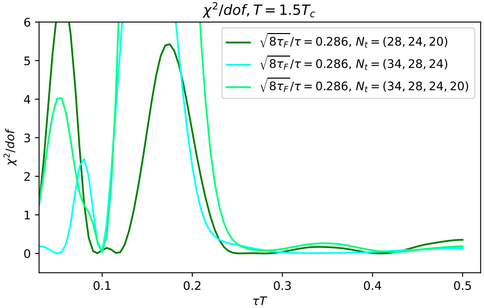




- linear in a^2 fit $\hat{=}$ linear in $1/N_t^2$ fit
- works well within the flowtime range of interest

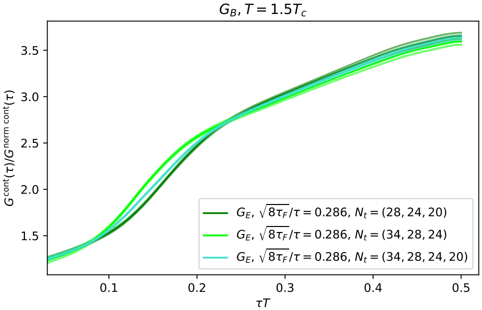
Analysis: Continuum extrapolation for G_{E}

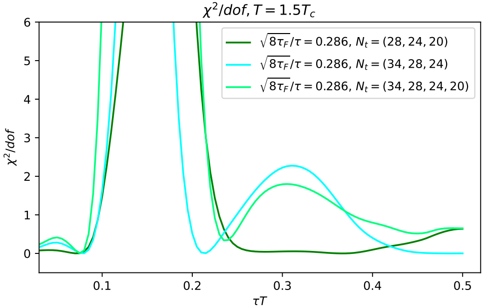




- Largest systematic error source is the interpolation
- For large τT all lattice data can be used
- For small τT continuum limit is restricted to the largest lattices

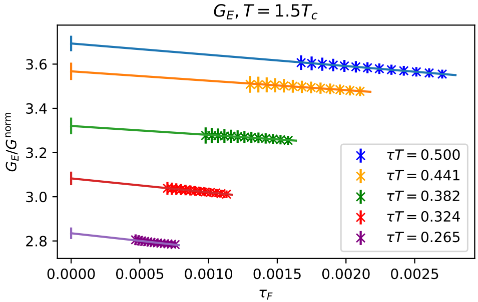
Analysis: Continuum extrapolation for G_{B}

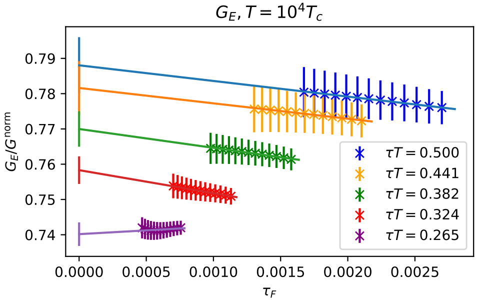




- Largest systematic error source is the interpolation
- For large τT all lattice data can be used
- For small τT continuum limit is restricted to the largest lattices

Analysis: zero flowtime extrapolation





- linear in τ_F fit
- works well for G_{E}

Analysis: Spectral inversion for G_E

- At UV: model ρ at NLO
  - Scale is optimized: $\ln(\mu_\omega) = \ln(2\omega) + \frac{(24\pi^2-149)}{66}$
  - only LO part remains:

$$\rho_\mathrm{E}^\mathrm{LO}(\omega, T) = \frac{g^2(\mu_\omega) C_F \omega^3}{6\pi}$$

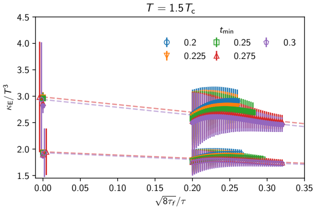
- for $\omega \sim T$ and smaller: $\ln(\mu_\omega) = \ln(4\pi T) - \gamma_\mathrm{E} - \frac{1}{22}$
- At IR: $\rho = \frac{\omega\kappa}{2T}$
- Connect both regimes by
  - line ansatz: scales ω^IR, ω^UV
  - step ansatz: scale Λ

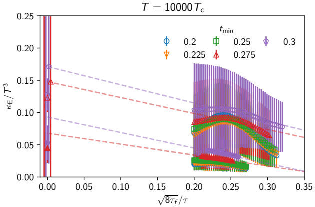
$\rightarrow \rho^\mathrm{Model} \rightarrow$ construct $G_\mathrm{E}^\mathrm{Model}$

Analysis: κ_E extraction

- For κ_E extraction we optimize:
  1. lattice data are normalized such that $G_\mathrm{E}^{\mathrm{lat}}(T\tau_{\mathrm{min}})/G_\mathrm{E}^{\mathrm{Model}}(T\tau_{\mathrm{min}}) = 1$
  2. $G_\mathrm{E}^{\mathrm{lat}}(\tau T > T\tau_{\mathrm{min}})/G_\mathrm{E}^{\mathrm{Model}}(\tau T > T\tau_{\mathrm{min}}) = 1$ within 1.5σ
  3. Estimate systematic errors by model variation
- Result for κ_E:
  - $T = 1.5T_C$: $1.70 \leq \frac{\kappa_\mathrm{E}}{T^3} \leq 3.12$
  - $T = 10^4 T_C$: $0.02 \leq \frac{\kappa_\mathrm{E}}{T^3} \leq 0.16$
- repeat procedure at finite flowtime and perform zero flowtime limit

Finite flowtime effectects negligible compared to model uncertainties





Analysis: Spectral inversion for G_B

- UV part must be modified due to renormalization of G_B:

$$G_\mathrm{B}^{\mathrm{flow,UV}}(\omega,\tau_F) = (1+\gamma_0 g^2 \ln(\mu\sqrt{8\tau_F}))^2 Z_\mathrm{flow} G_\mathrm{B}^{\bar{\mathrm{MS}},\mathrm{UV}}(\tau,\mu)$$

- Modified UV spectral function

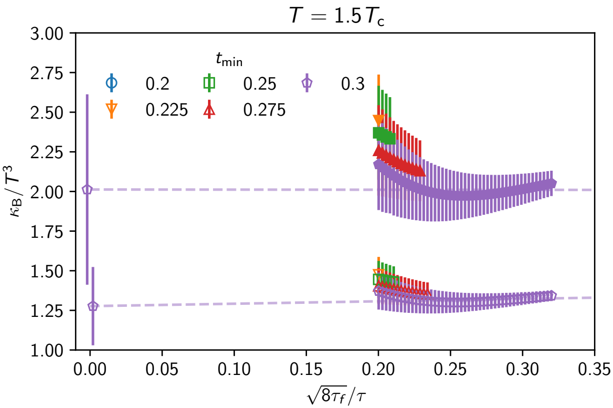
$$\rho_\mathrm{B}^{\mathrm{UV}}(\omega,\tau_F) = Z_\mathrm{flow}\frac{g^2}{6\pi}(1+g(\mu)(\beta_0-\gamma_0)\ln(\mu^2/(A\omega^2)) + g^2(\mu)\gamma_0\ln(8\tau_F\mu^2)$$

$$\gamma_0 = 3/(8\pi^2), \beta_0 = 11/(16\pi^2), A = \exp\left[\frac{134}{35} - \frac{8\pi^2}{5} - \ln 4\right]$$

- Renormalization factor Z_flow fixed by the normalization
- Optimized scale:

$$\mu_\omega = (\sqrt{A}\omega)^{1-\gamma_0/\beta_0}(8\tau_F)^{-\gamma_0/(2\beta_0)}$$

Analysis: κ_B extraction



- Low flowtime dependence
- $1.03 \leq \frac{\kappa_B}{T^3} \leq 2.61$

Analysis: Clover discretization

- Clover discretization of B-field with a^2-improvement:

$$a^2 F_{\mu\nu} = -\frac{i}{8}(Q_{\mu\nu} - Q_{\nu\mu}), Q_{\mu\nu} = U_{\mu\nu} + U_{\nu,-\mu} + U_{-\mu,-\nu} + U_{-\nu,\mu} = Q^{\dagger}_{\nu\mu}$$

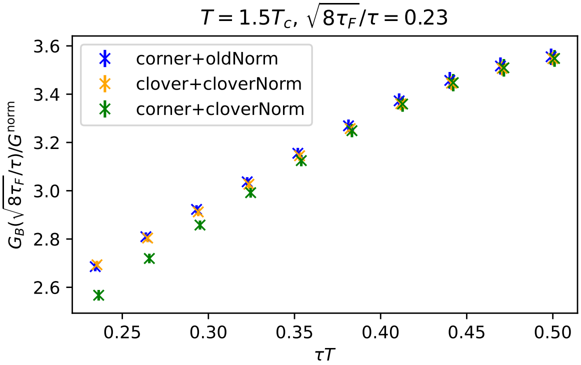
$$a^2 B_i = -\frac{1}{2}\epsilon_{ijk} F_{jk}$$

- new G^{norm}

  (D. Banerjee et.al. JHEP08 (2022) 128)

- Compare three possibilities:
  1. corner discretization + old Norm (our approach)
  2. clover discretization + clover Norm (D. Banerjee et.al.)
  3. corner discretization + clover Norm (for comparison)

Analysis: Clover discretization comparison



- proper choices give the same continuum limit

Outline

Conclusion

- Gradient flow improves qualitatively the signal to noise ratio
- Gradient flow renormalizes the E and B fields
  $\rightarrow$ proper continuum limits of flowed G_{E} and G_{B} possible
- Gradient flow can be used as renormalization scheme
  $\rightarrow$ extract scheme-independent, physical quantities
- Results of the electrical heavy quark diffusion coefficient:
  - $T = 1.5T_C$: $1.70 \leq \frac{\kappa_{\mathrm{E}}}{T^3} \leq 3.12$
  - $T = 10^4 T_C$: $0.02 \leq \frac{\kappa_{\mathrm{E}}}{T^3} \leq 0.16$
- Results of the magnetic heavy quark diffusion coefficient:
  - $T = 1.5T_C$: $1.03 \leq \frac{\kappa_{\mathrm{E}}}{T^3} \leq 2.61$
  - $T = 10^4 T_C$: not enough statistics
- Mass suppressed effects:
  - charm: $\langle v^2 \rangle \approx 0.51 \rightarrow$ 34 $\%$
  - bottom: $\langle v^2 \rangle \approx 0.3 \rightarrow$ 20 $\%$