

Spectral and Transport properties of the Quark Gluon Plasma from Lattice QCD

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[L. Altenkort, OK, R. Larsen, S. Mukherjee, P. Petreczky, H.T. Shu, S. Stendebach, Heavy Quark Diffusion from 2+1 Flavor Lattice QCD, PRL 130 (2023) 231902]

[L. Altenkort, D. de la Cruz, OK, R. Larsen, G.D. Moore, S. Mukherjee, P. Petreczky, H.T. Shu, S. Stendebach Quark Mass Dependence of Heavy Quark Diffusion Coefficient from Lattice QCD, arXiv:2311.01525]

[L. Altenkort, A.M. Eller, OK, L. Mazur, G.D. Moore, Heavy quark momentum diffusion from the lattice using gradient flow, PRD103 (2021) 014511]

[A.Francis, OK, M. Laine, T. Neuhaus, H. Ohno, Nonperturbative estimate of the heavy quark momentum diffusion coefficient, PRD92(2015)116003]

> NHR-Computational Physics Symposium 2023 Online, 03.11.2023



Motivation - Quarkonium in Heavy Ion Collisions



Charmonium+Bottmonium is produced (mainly) in the early stage of the collision

Depending on the Dissociation Temperature

- remain as bound states in the whole evolution
- release their constituents in the plasma



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[Kaczmarek, Zantow, 2005]

Motivation - Quarkonium in Heavy Ion Collisions



Non-relativistic QCD using a complex heavy quark potential (pNRQCD)

- applicable at least for bottomonium
- shift of bound state masses before the states melt
- thermal broadening of the states due to Im[V]



Full relativistic calculations of charmonium and bottomonium difficult, but ongoing...

Motivation – Transport coefficients of Heavy Quarks



Light degrees of freedom can rather well be described by hydrodynamics.

How do heavy quarks propagate in the hot and dense medium?

- What is the kinetic equilibration time for heavy quarks?
- Do heavy quarks thermalize and show collective motion?
- What are the transport coefficients of heavy quarks?

Heavy quark diffusion coefficients are crucial ingredients to study these questions

- Can be calculated from current-current (vector meson) correlation functions
- Or in the heavy quark mass limit using EE or BB correlation functions
- Both methods need spectral recontruction methods to obtain spectral functions

Vector-meson spectral function – hard to separate different scales

$$G(\tau, \vec{p}, T) = \int_{0}^{\infty} \frac{\mathrm{d}\omega}{2\pi} \rho(\omega, \vec{p}, T) K(\tau, \omega, T)$$

$$K(\tau, \omega, T) = \frac{\cosh\left(\omega(\tau - \frac{1}{2T})\right)}{\sinh\left(\frac{\omega}{2T}\right)}$$

Different contributions and scales enter

in the spectral function

- continuum at large frequencies
- possible bound states at intermediate frequencies
- transport contributions at small frequencies
- in addition cut-off effects on the lattice

Spectral functions in the QGP



difficult to extract D_s from vector meson correlation fct.

$$G_{\mu\nu}(\tau, \vec{x}) = \langle J_{\mu}(\tau, \vec{x}) J_{\nu}^{\dagger}(0, \vec{0}) \rangle$$

$$J_{\mu}(\tau, \vec{x}) = 2\kappa Z_{V} \bar{\psi}(\tau, \vec{x}) \Gamma_{\mu} \psi(\tau, \vec{x})$$

→ narrow transport peak hard to resolve
 → large lattices and continuum extrapolation needed
 → use perturbation theory to constrain the UV behavior
 ⇒
 easier to extract heavy quark momentum diffusion

 $\stackrel{\Rightarrow}{\operatorname{coefficient}} \kappa$ in the heavy quark mass limit

 \rightarrow smooth $\omega \rightarrow 0$ limit expected

Heavy Quark Momentum Diffusion Constant κ

Heavy Quark Effective Theory (HQET) in the large quark mass limit

for a single quark in medium

leads to a (pure gluonic) "color-electric correlator"



0.5

1.5

 $q_{\rm s}$

1

2

2.5

- \rightarrow large correction towards strong interactions
- \rightarrow non-perturbative lattice methods required

Gradient flow D_{t} diffusion equation for the gauge fields along extra dimension, flow-time t

$$\mathcal{O}(x,t) \xrightarrow{t \to 0} \overline{\partial t} \sum_{k} q_{k}(t,t) \mathcal{O}_{k}^{R}(x) - \frac{\partial S_{\mathrm{YM}}}{\partial A_{\mu}}$$

$$A_{\mu}(t=0,x) = A_{\mu}(x)$$



- continuous smearing of the gauge fields, effective smearing radius: $r_{\text{smear}} \sim \sqrt{8t}$ - $ga_{uge}^{T_{uge}^{R}}$ fields $\begin{pmatrix} U_{\mu\nu}(t,x) \\ become^{+}s_{ue} \\$
- no UV divergences at finite flow-time $t \rightarrow$ operators of flowed fields are renormalized
- UV fluctuations effectively reduces \rightarrow noise reduction technique
- applicable in quenched and full QCD
- methods developed in quenched studies now applied in full QCD

What is the flow time dependence of correlation functions?

How to perform the continuum and $t \rightarrow 0$ limit correctly?

Gradient flow - *diffusion* equation for the gauge fields along extra dimension, *flow-time t* [M. Lüscher, 2010]



- continuous smearing of the gauge fields, effective smearing radius: $r_{
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What is the flow time dependence of correlation functions? How to perform the continuum and $t \rightarrow 0$ limit correctly? LO perturbative limits

for the flow-time dependence:

 $\tilde{\tau}_f < 0.1136(\tau T)^2$ $G_{\tau_F}^{\rm norm}(\tau)$ $\sqrt{8\tau_F}T =$ 0.00. cont 10^{4} 0.00. latt 0.05, cont0.05, latt 0.10, cont+0.10, latt 10^{3} 10^{2} 10^{1} τI $10^{0}_{0.0}$ 0.50.1 0.2 0.3 0.4[A.M Eller, G.D. Moore, PRD97 (2018) 114507]

2+1-flavor lattice QCD results on the flow dependence of the color-electric correlator:



Effective reduction of UV fluctuations \rightarrow good noise reduction technique Signal gets destroyed at flow times above the perturbative estimate Linear behavior at intermediate flow times

Lattice set up

2+1-flavor lattice QCD on large and fine isotropic lattices at four temperatures above $T_{\rm c}$

- HISQ action with physical strange quark mass and $m_s/m_l=5~(m_\pi \approx 300~MeV)$
- using gradient flow method to improve the signal

$T [{\rm MeV}]$	T/T_c	$a[{\rm fm}]$	β	N_{σ}	N_{τ}	$\# \operatorname{conf}$
195	1.09	0.0505	7.570	64	20	5899
		0.0421	7.777	64	24	3435
		0.0280	8.249	96	36	2256
220	1.22	0.0449	7.704	64	20	7923
		0.0374	7.913	64	24	2715
		0.0280	8.249	96	32	912
251	1.40	0.0393	7.857	64	20	6786
		0.0327	8.068	64	24	5325
		0.0280	8.249	96	28	1680
293	1.63	0.0336	8.036	64	20	6534
		0.0306	8.147	64	22	9101
		0.0280	8.249	96	24	688



[L. Altenkort, OK, R. Larsen, S. Mukherjee, P. Petreczky, H.T. Shu, S. Stendebach, Heavy Quark Diffusion from 2+1 Flavor Lattice QCD, PRL 130 (2023) 231902]

1) perform the continuum limit, $a{\rightarrow}~0~\leftrightarrow~N_t{\rightarrow}\infty$

2) perform the flow time to zero limit of the continuum correlators

3) determine κ in the continuum using an Ansatz for the spectral fct. $\rho(\omega)$

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Gradient Flow method – 1) $a \rightarrow 0$ limit at fixed flow time

- cut-off effects get reduced with increasing flow time
- continuum limit, $a \rightarrow 0$ ($N_t \rightarrow \infty$), at fixed physical flow time:



well defined continuum correlators for different finite flow times
 next step: flow time to zero extrapolation of continuum correlators

Gradient Flow method – 1) $a \rightarrow 0$ limit at fixed flow time

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well defined continuum correlators for different finite flow times
 next step: flow time to zero extrapolation of continuum correlators

Continuum limit, $a \rightarrow 0 (N_t \rightarrow \infty)$, Flow time limit, $t \rightarrow 0$, followed by at fixed physical flow time: for each distance: 0.250.250.300.30 G_E G_E $\sqrt{8 au_{
m F}}/ au_{
m F}$ 10^{-10} Inorm $\gamma_{\rm norm}$ au T**1**0.500 9 τT **1**0.472 6 **1**0.500 **I** 0.444 8 **I** 0.458 **I** 0.417 **1**0.417 **I** 0.389 **I** 0.375 7**I** 0.361 5**I** 0.333 **I** 0.333 **1**0.292 6**I** 0.306 **I** 0.250 **I** 0.278 **I** 0.250 54 T=293MeV T=195MeV $8\tau_{\rm F}/\tau^2$ $8\tau_{\rm F}/$ 40.05 0.000.05 0.000.100.10

 \rightarrow well defined continuum and flow time extrapolation

 \rightarrow well defined renormalized correlation function

Continuum extrapolated correlation function

Continuum extrapolated color-electric correlation function from

2+1-flavor lattice QCD at four temperatures above T_c



Determine κ in the continuum using various Ansätze for the spectral function $\rho(\omega)$ fitted to the continuum extrapolated correlation functions

$$G(\tau, \vec{p}, T) = \int_{0}^{\infty} \frac{\mathrm{d}\omega}{2\pi} \rho(\omega, \vec{p}, T) K(\tau, \omega, T) \qquad K(\tau, \omega, T) = \frac{\cosh\left(\omega(\tau - \frac{1}{2T})\right)}{\sinh\left(\frac{\omega}{2T}\right)}$$

Models for the spectral function

Spectral function models with correct asymptotic behavior

 $\rho_{\rm uv}(\omega) = \frac{g^2(\bar{\mu}_\omega)C_F\omega^3}{6\pi}$ $\rho_{\rm ir}(\omega) = \frac{\kappa\omega}{2T}$

modeling corrections to ρ_{IR} in various ways

Label	$ ho_{ m model}$	μ	Fit parameters
\max_{LO}	$\max(\Phi_{ID}, \Phi_{ID})$	$\max(\mu_{ ext{eff}},\omega)$	$\kappa/T^3 K$
\max_{NLO}	$\max(\Psi_{\mathrm{IR}},\Psi_{\mathrm{UV}})$	$\max(\mu_{\mathrm{eff}}, \mu_{\mathrm{opt}})$	<i>n/1</i> , n
$\mathrm{smax}_{\mathrm{LO}}$	$\sqrt{\Phi^2 + \Phi^2}$	$\max(\mu_{ ext{eff}},\omega)$	$\kappa/T^3 K$
$\mathrm{smax}_{\mathrm{NLO}}$	$\bigvee \Psi_{\rm IR} + \Psi_{\rm UV}$	$\max(\mu_{ ext{eff}},\mu_{ ext{opt}})$	n/1, n
$plaw_{LO}$	$\theta(\omega_{\rm IR}-\omega)\Phi_{\rm IR}+$	$\max(\mu_{ ext{eff}},\omega)$	$\kappa/T^3 K$
$plaw_{NLO}$	$ heta(\omega - \omega_{ m IR}) heta(\omega_{ m UV} - \omega) p(\omega) +$	$\max(\mu_{ ext{eff}},\mu_{ ext{opt}})$	n/1, m
	$ heta(\omega - \omega_{\mathrm{UV}})\Phi_{\mathrm{UV}}$		

using continuum extrapolated lattice correlators

to fit the models and extract κ

$$G_{\text{model}}(\tau) \equiv \int_0^\infty \frac{\mathrm{d}\omega}{\pi} \rho_{\text{model}}(\omega) \frac{\cosh\left(\frac{1}{2} - \tau T\right)\frac{\omega}{T}}{\sinh\frac{\omega}{2T}}$$

error estimates using fully bootstrapped analysis

$$\kappa/T^3 = \lim_{\omega \to 0} \frac{2T\rho_{\rm E}(\omega)}{\omega}$$

Heavy Quark Momentum Diffusion Constant – spectral reconstruction 18



Heavy Quark Momentum Diffusion Constant – spectral reconstruction 19



Spatial heavy quark diffusion coefficient



close to T_c charm quark kinetic equilibration appears to be almost as fast as that of light partons.

20

Spatial heavy quark diffusion coefficient



Next steps:

- determine the quark mass correction:
- correction may be important for charm
- extend to physical 2+1 flavor QCD
- $\kappa \simeq \kappa_E + rac{2}{3} \langle v^2
 angle \kappa_B$, $\langle v^2
 angle pprox rac{3T}{M_{kin}} \left(1 rac{5T}{2M_{kin}}
 ight)$

[L. Altenkort, OK, R. Larsen, S. Mukherjee, P. Petreczky, H.T. Shu, S. Stendebach,

[A. Bouttefeux, M. Laine, HEP 12 (2020) 150] [M. Laine, JHEP 06 (2021) 139]

- determine charm and bottom quark diffusion coefficient from vector meson correlators

21

previous project: 81 TB gauge field configurations

$96^3 x N_{\tau}$ lattice

64 ³ xN $_{ au}$ lati	ices
----------------------------------	------

$N_{ au}$	36	32	28	24	20
T [MeV]	195	220	251	293	352
# conf.	2256	912	1680	688	2488

~55.000 gauge field configurations with m_{π} = 320 *MeV*

[MeV]	β	am_s	am_l	N_{τ}	# conf.
195	7.570	0.01973	0.003946	20	5899
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251	7.857	0.01479	0.002958	20	6786
	8.068	0.01204	0.002408	24	5325
293	8.036	0.01241	0.002482	20	6534
	8.147	0.01115	0.002230	22	9101

Generated on supercomputing resources Perlmutter, JUWELS, Marconi



current project: ~200 TB gauge field configurations

 128^3 xN_{τ} and 96^3 xN_{τ} lattices with physical pion masses compute projects on Frontier and LUMI-G ~ 8 Mio GPU-hours for one year





All gauge field configurations will be stored in the International Lattice Data Grid (ILDG)

Measurement of observables on GPU HPC systems

Operators and correlation functions need to be calculated on each gauge field configuration

Needs optimized multi-GPU code measurement routines in SIMULATeQCD

Measurement of correlation functions on Bielefeld GPU Cluster



Measurement of fluctuations and correlations of charm and conserved charges on Noctua 2



https://github.com/LatticeQCD/SIMULATeQCD https://doi.org/10.5281/zenodo.7994982 https://arxiv.org/abs/2306.01098

SIMULATEOCD: A simple multi-GPU lattice code for OCD calculations

Lukas Mazur^{a,*}, Dennis Bollweg^{b,*}, David A. Clarke^{e,*}, Luis Altenkort^d, Olaf Kaczmarek^{d,*}, Rasmus Larsen^e, Hai-Tao Shuf, Jishnu Goswami^g, Philipp Scior^b, Hauke Sandmeyer^d, Marius Neumann^d, Henrik Diek^d, Sajid Ali^{d,h}, Jangho Kimⁱ, Christian Schmidt^d, Peter Petreczky^b, Swagato Mukherjee^{b,*},

(HotQCD collaboration)

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un Abstract

2023

-The rise of exascale supercomputers has fueled competition among GPU vendors, driving lattice QCD developers to write code that supports multiple APIs. Moreover, new developments in algorithms and physics research require frequent 0 updates to existing software. These challenges have to be balanced against constantly changing personnel. At the same , time, there is a wide range of applications for HISQ fermions in QCD studies. This situation encourages the development of software featuring a HISQ action that is flexible, high-performing, open source, easy to use, and easy to adapt. In this technical paper, we explain the design strategy, provide implementation details, list available algorithms and modules, _ and show key performance indicators for SIMULATEQCD, a simple multi-GPU lattice code for large-scale QCD calculations, The mainly developed and used by the HotQCD collaboration. The code is publicly available on GitHub.

Keywords: lattice QCD, CUDA, HIP, GPU

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- Developed by HotQCD collaboration (Bielefeld, Brookhaven,...)
- Highly optimized lattice QCD code for multi-GPU (Nvidia and AMD GPUs)
- Optimized for supercomputing resources
- Currently used on Frontier, LUMI-G, Leonardo, Summit, Perlmutter, JUWELS. Noctua2....
- SIMULATeQCD selected for EuroHPC JU extraordinary support program (ESP) (with AMD and HPE for LUMI-G)

All analysis performed on Bielefeld compute server

All data and lattice and analysis software as well as a workflow (bash/python)

of the project published as open access



https://doi.org/10.4119/unibi/2979080

All raw and derived data is already openly available gauge field configurations will be published soon on ILDG

All data and analysis software of this project is openly available

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Analysis Software developments

Analysis Toolbox Software development

https://github.com/LatticeQCD/AnalysisToolbox

Heavy quark diffusion analysis based on this

https://github.com/luhuhis/correlators flow

In leading order in 1/M the quark mass dependence of κ depends on another transport coefficient, $\kappa_{\rm B}$,

$$\kappa \simeq \kappa_E + \frac{2}{3} \langle v^2 \rangle \kappa_B$$

$$\langle v^2 \rangle \approx \frac{3T}{M_{kin}} \left(1 - \frac{5T}{2M_{kin}} \right)$$

 $\kappa_{\rm B}$ can be determined from the color-magnetic correlator

$$G_B(\tau, T) = \sum_{i=1}^{3} \frac{\langle \operatorname{ReTr} \left[U(\beta, \tau) B_i(\mathbf{x}, \tau) U(\tau, 0) B_i(\mathbf{x}, 0) \right] \rangle}{3 \langle \operatorname{ReTr} U(\beta, 0) \rangle}$$

and the corresponding spectral function

$$G_B(\tau, T) = \int_0^\infty \frac{\mathrm{d}\omega}{\pi} \ \rho_B(\omega, T) \frac{\cosh[\omega \tau - \omega/(2T))]}{\sinh[\omega/(2T)]}$$

Problem: In contrast to G_E , G_B has a non-trivial anomalous dimension and the renormalization and continuum extrapolation is more involved.

[A. Bouttefeux, M. Laine, HEP 12 (2020) 150] [M. Laine, JHEP 06 (2021) 139]

- Gradient flow serves as a non-perturbative renormalization scheme and the continuum extrapolated correlators are renormalized at the scale $\mu_F = 1/\sqrt{8\tau_F}$
- The renormalization group invariant physical correlators can be obtained via oneloop pQCD matching

$$G_B^{\text{phys.}}(\tau, T) = \lim_{\tau_{\text{F}} \to 0} Z_{\text{match}}(\bar{\mu}_T, \bar{\mu}_{\tau_{\text{F}}}, \mu_{\text{F}}) G_B(\tau, T, \tau_{\text{F}}).$$

- This involves three components:
 - matching from gradient flow to \overline{MS} scheme at a scale $\bar{\mu}_{\tau_F}$
 - matching from \overline{MS} to the heavy quark effective theory at a scale $\overline{\mu}_T$
 - running of the anomalous dimension of the operator from $\bar{\mu}_T$ to $\bar{\mu}_{\tau_F}$
- Estimate uncertainties from unknow higher-order effects by varying the scales

$$\bar{\mu}_T = 2\pi T \dots 19.18T$$
 and $\bar{\mu}_{\tau_F} = \mu_F \dots 1.4986\mu_F$

[L. Altenkort, D. de la Cruz, OK, et al., arXiv:2311:01525]

$$G_B^{\text{phys.}}(\tau, T) = \lim_{\tau_{\rm F} \to 0} Z_{\text{match}}(\bar{\mu}_T, \bar{\mu}_{\tau_{\rm F}}, \mu_{\rm F}) G_B(\tau, T, \tau_{\rm F}).$$

$$\ln Z_{\text{match}} = \int_{\bar{\mu}_T^2}^{\bar{\mu}_{\tau_F}^2} \gamma_0 g_{\overline{\text{MS}}}^2(\bar{\mu}) \frac{d\bar{\mu}^2}{\bar{\mu}^2} + \gamma_0 g_{\overline{\text{MS}}}^2(\bar{\mu}_T) \left[\ln \frac{\bar{\mu}_T^2}{(4\pi T)^2} - 2 + 2\gamma_{\text{E}} \right] - \gamma_0 g_{\overline{\text{MS}}}^2(\bar{\mu}_{\tau_F}) \left[\ln \frac{\bar{\mu}_{\tau_F}^2}{4\mu_{\text{F}}^2} + \gamma_{\text{E}} \right]$$



The *B*-field correlators in the gradient flow scheme for different temperatures calculated on the finest (open symbols) and coarsest lattices (filled symbols)



Lattice spacing dependence and continuum extrapolation

[L. Altenkort, D. de la Cruz, OK, et al., arXiv:2311:01525]



Flow time extrapolation







T dependence of $G_R^{phys.}$

Spectral function models with correct asymptotic perturbative behavior

$$\rho_B^{\rm uv,LO}(\omega,\mu) = \frac{g_{\rm \overline{MS}}^2(\mu)C_{\rm F}\omega^3}{6\pi},$$

$$\rho_B^{\rm uv,NLO}(\omega,\mu) = \frac{g_{\rm \overline{MS}}^2(\mu)C_{\rm F}\omega^3}{6\pi} \left\{ 1 + \frac{g_{\rm \overline{MS}}^2(\mu)}{(4\pi)^2} \left(N_c \left[\frac{5}{3} \ln \frac{\mu^2}{4\omega^2} + \frac{134}{9} - \frac{2\pi^2}{3} \right] - N_f \left[\frac{2}{3} \ln \frac{\mu^2}{4\omega^2} + \frac{26}{9} \right] \right) \right\},$$

multiplied with $c_B^2(\mu, \bar{\mu}_T) = \exp\left(\int_{\bar{\mu}_T^2}^{\mu^2} \gamma_0 g_{\overline{MS}}^2(\bar{\mu}) \frac{d\bar{\mu}^2}{\bar{\mu}^2}\right)$ to go from \overline{MS} to physical scheme

modeling corrections to $\rho_{\rm \tiny IR}(\omega) = \frac{\kappa\omega}{2T}$ in various ways

Label	$ ho_{ m model}$	μ	Fit parameters
\max_{LO}	$\max(\Phi_{ID}, \Phi_{IUI})$	$\max(\mu_{ ext{eff}},\omega)$	$\kappa/T^3 K$
\max_{NLO}	$\max(\Psi_{\mathrm{IR}},\Psi_{\mathrm{UV}})$	$\max(\mu_{\mathrm{eff}}, \mu_{\mathrm{opt}})$	n/1, R
$\mathrm{smax}_{\mathrm{LO}}$	$\sqrt{\Phi^2 + \Phi^2}$	$\max(\mu_{ ext{eff}},\omega)$	$\kappa/T^3 K$
$\mathrm{smax}_{\mathrm{NLO}}$	$\int \Psi_{\rm IR} + \Psi_{\rm UV}$	$\max(\mu_{ ext{eff}},\mu_{ ext{opt}})$	n/1, R
$plaw_{LO}$	$\theta_{(\omega_{\rm IR}-\omega)}\Phi_{\rm IR}+$	$\max(\mu_{ ext{eff}},\omega)$	$\kappa/T^3 K$
$plaw_{NLO}$	$ heta(\omega - \omega_{\mathrm{IR}}) heta(\omega_{\mathrm{UV}} - \omega) p(\omega) +$	$\max(\mu_{ ext{eff}},\mu_{ ext{opt}})$	n/1, n
	$ heta(\omega-\omega_{ m UV})\Phi_{ m UV}$		

Fitting
$$G_{\text{model}}(\tau) \equiv \int_0^\infty \frac{\mathrm{d}\omega}{\pi} \rho_{\text{model}}(\omega) \frac{\cosh\left(\frac{1}{2} - \tau T\right)\frac{\omega}{T}}{\sinh\frac{\omega}{2T}}$$
 to obtain $\kappa_B/T^3 = \lim_{\omega \to 0} \frac{2T\rho_B(\omega)}{\omega}$





Fit results for κ_B using various models and various scales to estimate systematic uncertainties

T=195 MeV



T=293 MeV



Spatial Diffusion coefficient for charm and bottom quarks

