Langevin Dynamics in a Finite Box

Anthony Francis

INT Program on “Gauge Field Dynamics In and Out of Equilibrium”

March 5 - April 13, 2012

JOHANNES GUTENBERG UNIVERSITÄT MAINZ

E-mail: francis@kph.uni-mainz.de

Outline

Diffusion in HIC	• Introduction of the diffusion constant and its connection to the spectral function
Approaches to diffusion	• Methods of computing the diffusion constant via MEM, HQET and Langevin Dynamics
Results from lattice QCD	• Review of a number of recent lattice QCD results
Langevin in a box	• Motivation and set-up of Langevin dynamics in a finite size system
Wightmann correlator	• Computation of the Wightmann correlation function
Spectral functions and Eucl. correlator	• Connection to the relevant spectral functions and Euclidean correlators • The observable effects are highlighted and discussed

Introduction

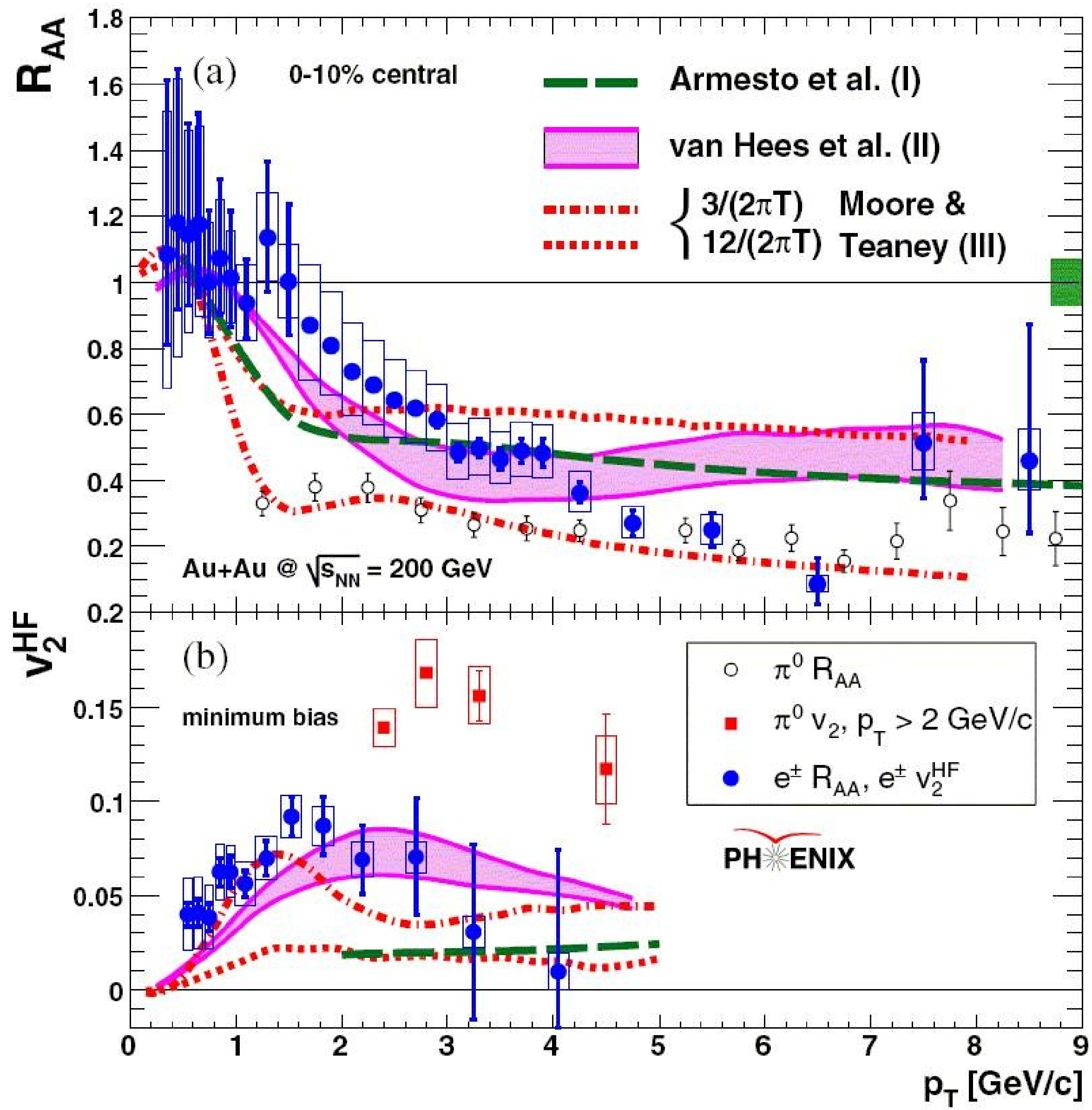
- In heavy ion collision experiments, e.g. @RHIC or @Alice, one can study heavy quark dynamics through ...

  … the elliptic flow

  $$v_2^{HF}$$

  … and the medium modification factor

  $$R_{AA}$$



Adare et al.; Phys.Rev. C84 (2011) 044905

The Diffusion Coefficient

- On the theory side the observed R_{AA} and v_2^{HF} can be related to the diffusion coefficient D:

$$D = \frac{T}{M\eta} = \frac{2T^2}{\kappa}$$

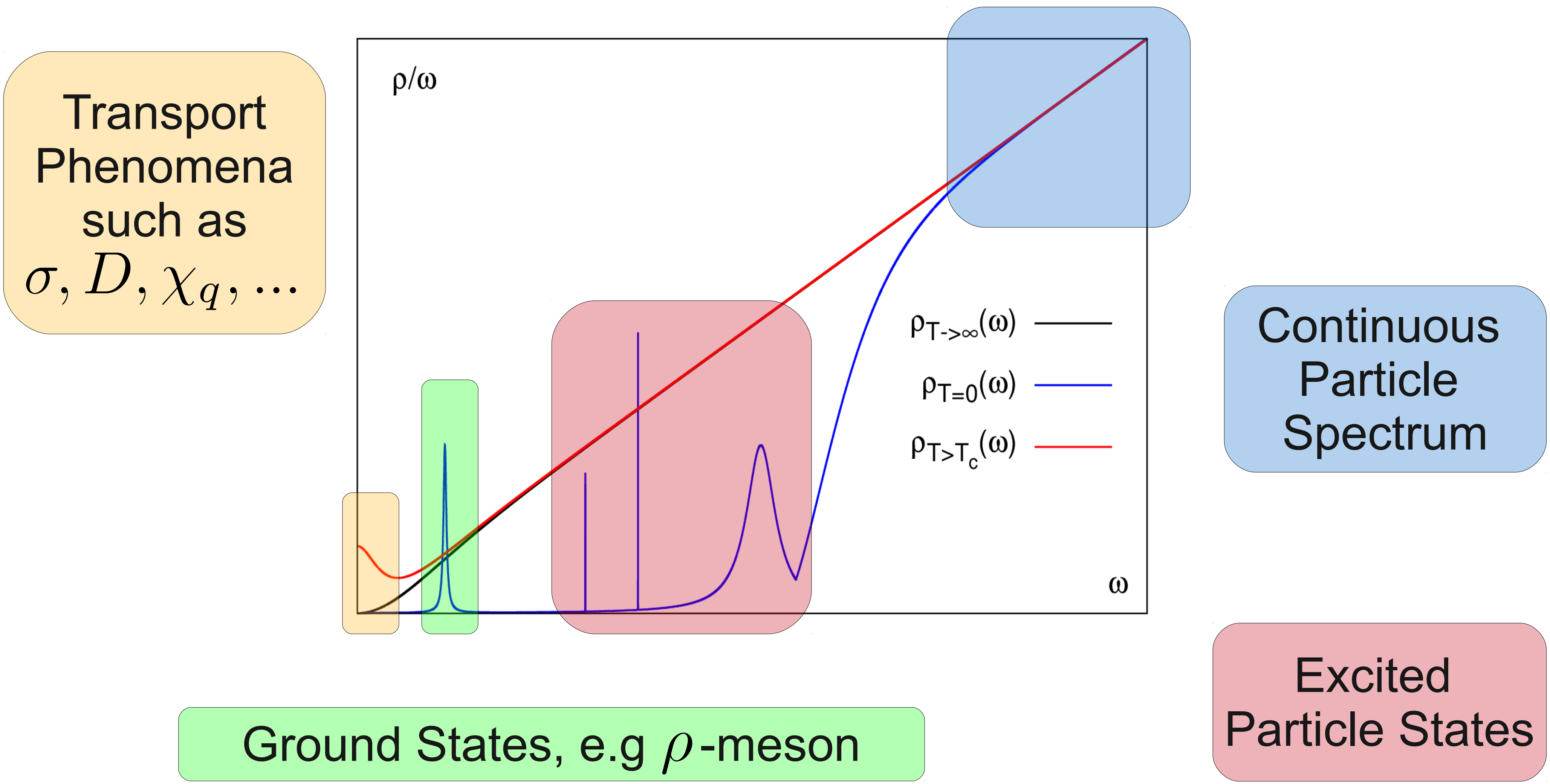
$M =$ Mass of the heavy quark
$\eta =$ Drag coefficient
$\kappa =$ Momentum diffusion

- To compute D one generally exploits a Kubo formula to obtain it from a certain spectral function:

$$D = \lim_{\omega \to 0} c \cdot \frac{\rho(\omega)}{\omega}$$

The Spectral Function

- Spectral functions (SPF) encode the physics of a system:



SPF via lattice QCD

- To compute D from lattice QCD one has to analyze the correlation function of heavy vector currents:

$$J_\mu(\tau,\vec{x}) = \bar{q}(\tau,\vec{x})\gamma_\mu q(\tau,\vec{x})$$

$$G_V(\tau,\vec{p}) = \int d^3x \langle J_\mu(\tau,\vec{x}) J_\mu(0,0)\rangle$$

- The diffusion coefficient can then be read off the corresponding spectral function via

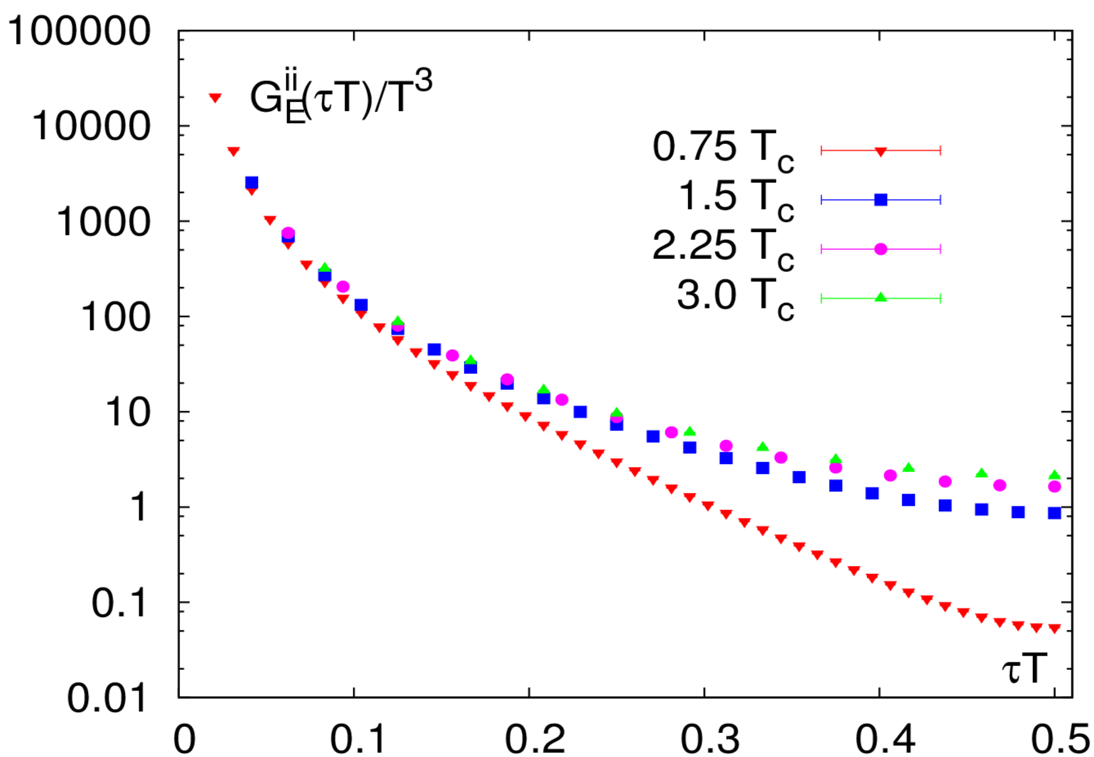
$$D = \lim_{\omega\to 0} \frac{1}{6\chi_{00}} \frac{\rho_V(\omega,\vec{p}=0)}{\omega}$$

SPF via lattice QCD

- The vector-current correlator is connected to the SPF via:

$$G_V(\tau,\vec{p},T) = \int_0^\infty \frac{d\omega}{2\pi} \frac{\cosh(\omega(\tau - 1/2T))}{\sinh(\omega/2T)} \rho_V(\omega,\vec{p},T)$$

Discrete number of points from the lattice



Continuous SPF

Ill-posed problem

SPF via lattice QCD (MEM)

- Possibility: Use Bayesian analysis in the form of the “maximum entropy method” (MEM) to construct...

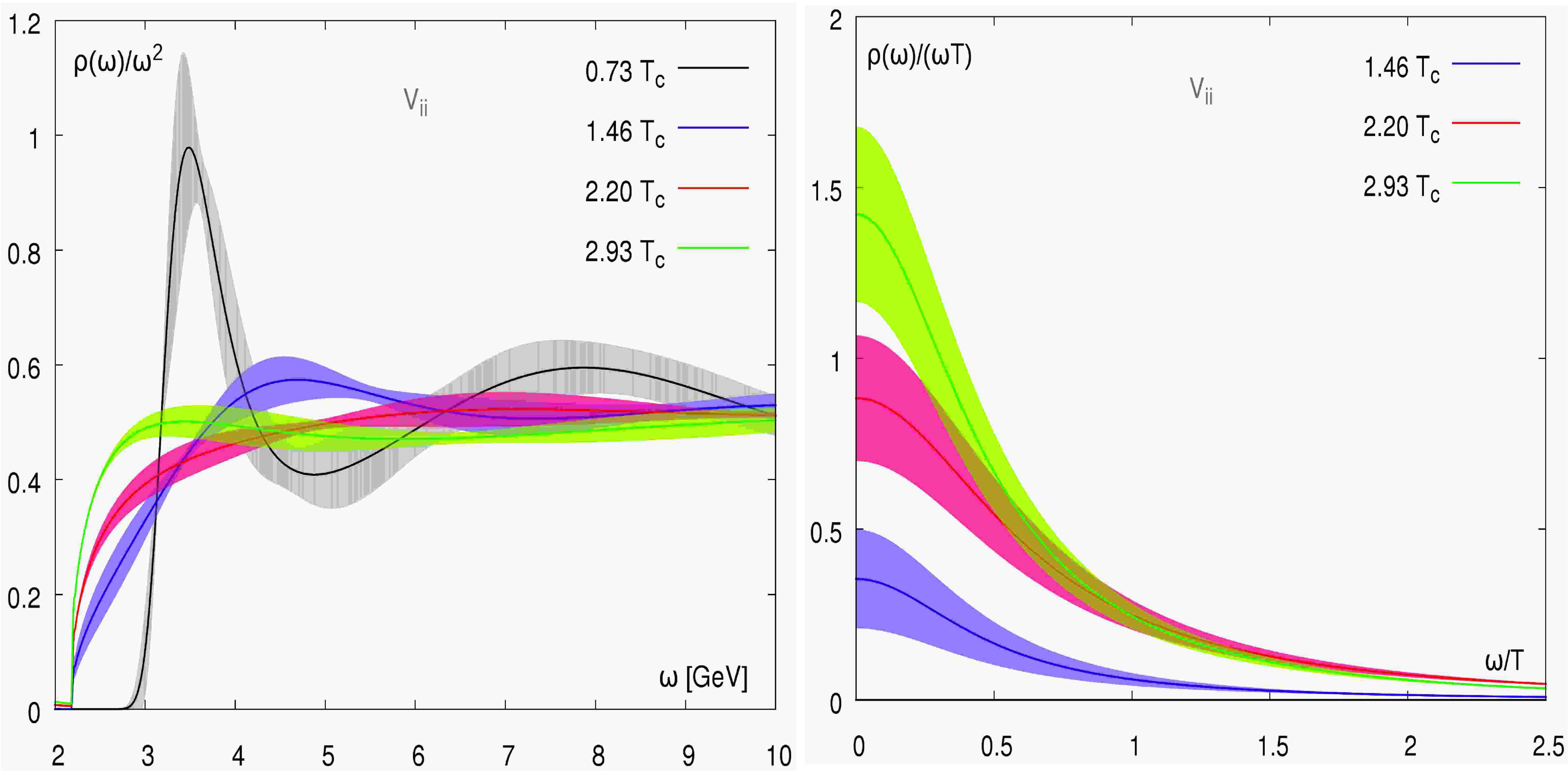
… the most probable SPF given the correlator data with errors AND user specified prior information.

- Note: The details of D depend on the shape of a transport peak in the low-ω region.
- But: The correlator encodes basically only the area under the transport peak

⇒ Difficult to extract the transport peak properties

- Additional difficulty: Heavy quarkonium (dissociation) and transport phenomena are both encoded in the same SPF

SPF via lattice QCD (MEM)



H.T.Ding, A.F, O.Kaczmarek, F.Karsch, H.Satz, W.Soeldner; J.Phys.G G38 (2011) 124070

SPF via lattice QCD (HQET)

- In HQET the relevant SPF may be obtained from a force-force correlator:

$$G_E(\tau) = \lim_{M\to\infty} \frac{1}{\chi_{00}} \int d^3x \langle J_F(\tau,\vec{x}) J_F(0,0)\rangle$$

where the leading force is the chromo-electric force gE

$$J_F = \phi^\dagger g E_i \phi - \theta^\dagger g E_i \theta$$

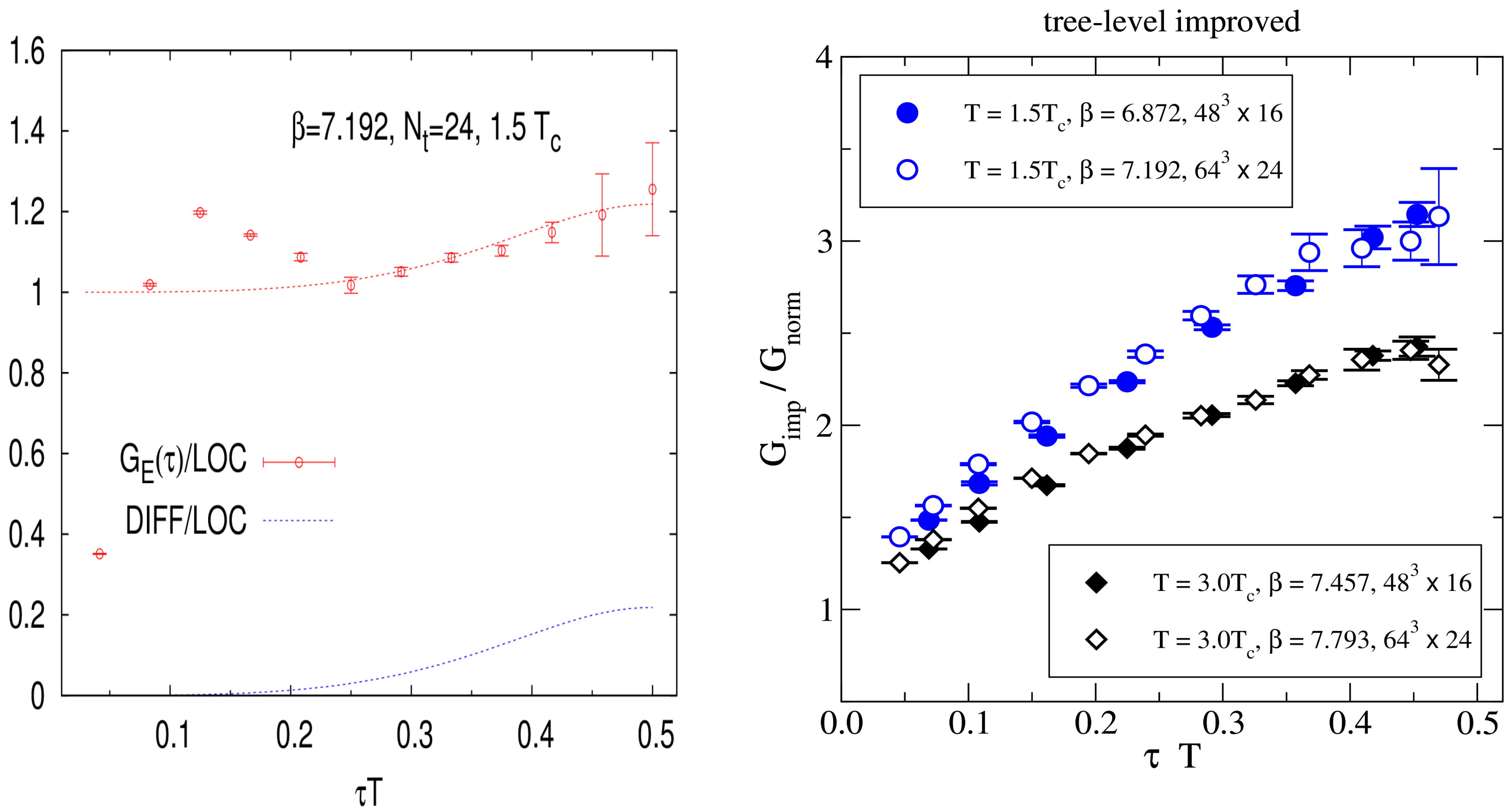
- D is then obtained by: $$D^{-1} = \lim_{\omega\to 0} \frac{\rho(\omega)T}{\omega}$$

- As before, analytical continuation is necessary
- It can be shown that the SPF does not possess a transport peak

→ More direct handle on D from correlator

S.Caron-Huot, M.Laine, G.D.Moore; JHEP 0904 (2009) 053

SPF via lattice QCD (HQET)



D.Banerjee et al.; Phys.Rev. D85 (2012) 014510

A.F., O.Kaczmarek, J.Langelage, M.Laine; PoS LATTICE2011 (2011) 202

SPF via Langevin Dynamics

- For heavy quarks the diffusion is of a time-scale $\sim M/T^2$

Possibility to model the interaction of the heavy quark with the medium as uncorrelated momentum kicks

- Langevin equations:

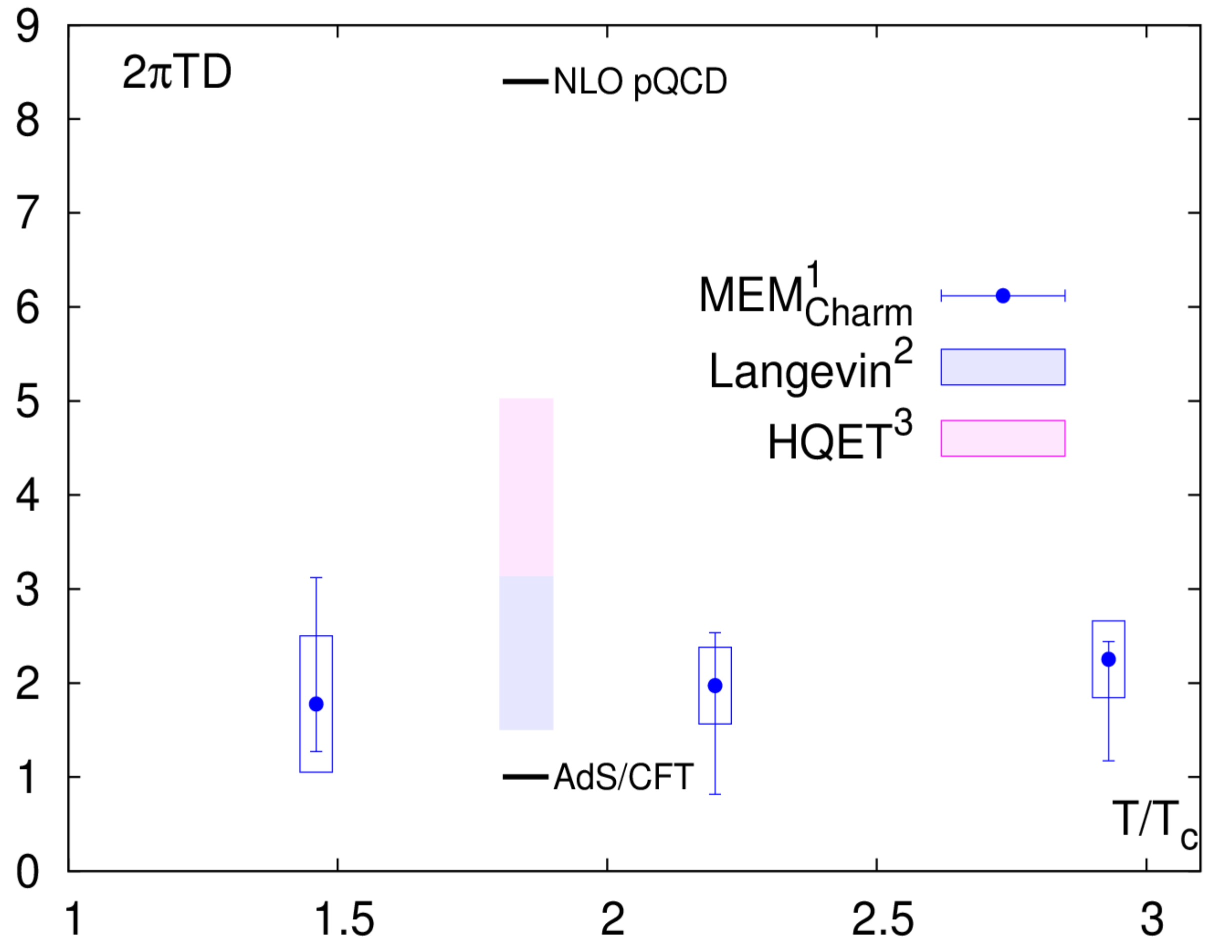
$$\frac{d\vec{x}}{dt} = \frac{\vec{p}}{M} \quad , \qquad \frac{\vec{p}}{dt} = \vec{\xi}(t) - \eta\vec{p}(t)$$

$$\langle \xi^i(t)\xi^j(t')\rangle = \kappa\delta^{ij}\delta(t-t')$$

- This description can be extended into a Langevin-Boltzmann model to yield R_{AA} and v_2^{HF} as functions of D

G.D.Moore, D.Teaney; Phys.Rev. C71 (2005) 064904

Diffusion from MEM, HQET and Langevin



1) H.T.Ding, A.F, O.Kaczmarek, F.Karsch, H.Satz, W.Soeldner; J.Phys.G G38 (2011) 124070

2) G.D.Moore, D.Teaney; Phys.Rev. C71 (2005) 064904

3) A.F., O.Kaczmarek, J.Langelage, M.Laine; PoS LATTICE2011 (2011) 202

- The results from all approaches indicate $2\pi TD \simeq 1-5$
- For lattice QCD the greatest obstacle is the analytic continuation

Langevin Dynamics in a Finite Box

- All lattice results are obtained at finite volumes

➡ Are there de facto finite size effects that must be included?

- Analytic continuation poses the greatest obstacle

➡ Can we determine features of the SPF from finite size effects?

- Model system to address these questions:

➡ Langevin dynamics in a finite size system

Setting up the Box

- To set up the box we assume:

  - The box walls constrain the position of the particle between 0 and l
  - There is an instantaneous reversal of momentum p when the particle hits the wall
  - The dynamics inside the box can be described in terms of a freely diffusing particle

  - Note: This work is done in $(1+1)$-dimensions

Setting up the Box

- In $1D$ the probability $w_0(x,p,t|x_0,p_0,t_0)$ of finding a particle at x and p starting at $t_0 = 0 = x_0 = p_0$ is given by the motion of a Brownian particle in the absence of an external field

$$w_0(x,p,t|0) = \frac{1}{2\pi m\sqrt{FG - H^2}} \cdot \exp\left[-\frac{GR^2 - 2HRS + FS^2}{2(FG - H^2)} \right]$$

$$R = x - x_0 - \eta^{-1}\frac{p_0}{m}(1 - e^{-\eta t})$$

$$S = \frac{p - p_0 e^{-\eta t}}{m}$$

$$F = \frac{T}{m\eta^2}(2\eta t - 3 + 4e^{-\eta t} - e^{-2\eta t})$$

$$G = \frac{T}{m}(1 - e^{-2\eta t})$$

$$H = \frac{T}{m\eta}(1 - e^{-\eta t})^2$$

S. Chandrasekhar; Rev.Mod.Phys 15 (1943) 1

Setting up the Box

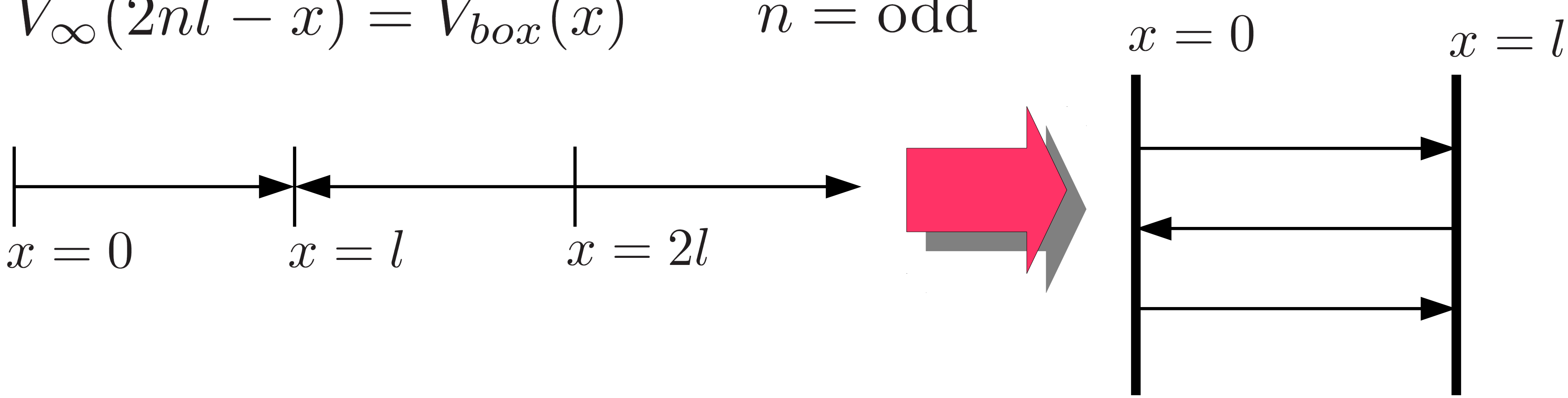
- Implementing the box assumptions then leads to:

$$w(x,p,t|0) = \sum_{n=-\infty}^{\infty} \Big(w_0(x+2nl,p,t|0) + w_0(2nl-x,-p,t|0) \Big)$$

- For illustration: In terms of a potential with and without the box

$$V_\infty(x+2nl) = V_{box}(x) \qquad n = \text{even}$$

$$V_\infty(2nl-x) = V_{box}(x) \qquad n = \text{odd}$$



I.Oppenheim, P.Mazur; Physica 30 (1964) 1833

The Wightmann Correlator

- We can now compute the Wightmann correlation function

$$W_p(t) = \langle p_0 \bar{p}(t) \rangle$$

$$\int_{-\infty}^{\infty} dp_0 \int_0^l dx_0 \, f_0(x_0, p_0) \, p_0 \int_{-\infty}^{\infty} dp \int_0^l dx \, w_0(x, p, t|0) \, p$$

where $f_0(x_0, p_0)$ is the initial probability distribution

$$f_0(x_0, p_0) = \frac{1}{l\sqrt{2\pi m T}} \cdot \exp\left[- \frac{p_0^2}{2mT} \right]$$

The Wightmann Correlator

- The Wightman correlator is made up of three parts

$$W_p(t) = W_p^{(0)}(t) + W_p^{(1)}(t) + W_p^{(2)}(t)$$

- The first is the well known result of the infinite volume case:

$$W_p^{(0)}(t) = MTe^{-\tau}$$

where $\tau = \eta t$

- In $W_p^{(1)}(t)$ and $W_p^{(2)}(t)$ a new dimensionless parameter dependent on the box extent l appears

$$\lambda = \frac{l^2 \eta^2 M}{2T} = \frac{l^2 \eta}{2D}$$

⇒ $W_p^{(1)}(t)$ and $W_p^{(2)}(t)$ do not survive the infinite volume limit

The Wightmann-Correlator

- The second term then is

$$W_p^{(1)}(\tau) = MT \cdot \, (-1) \, (\frac{2}{\pi}) \sqrt{\lambda} \phi(\tau) e^{-\tau} \sum_{n=-\infty}^{\infty} \cdot$$

$$\int_0^1 d\chi \int_{-\infty}^{\infty} d\bar{p} \bar{p}^2 e^{-\bar{p}^2} \int_{P_{2n-1}}^{P_{2n}} dP e^{-\lambda P^2 / \phi(\tau)}$$

- This can be approximated to

$$W_p^{(1)}(\tau) \simeq MT \frac{\tau^{11/2}}{\sqrt{\lambda}} \qquad \text{for} \quad \tau \ll 1$$

$$W_p^{(1)}(\tau) \simeq -MT \frac{\tau^2}{\sqrt{\lambda}} e^{-\tau} \qquad \text{for} \quad \tau \gg 1$$

The Wightmann-Correlator

- The third is given by

$$W_p^{(2)}(\tau) = MT \cdot (-1)\sqrt{\frac{2}{\pi}} \frac{2D\eta^{-1}(1-e^{-\tau})^3}{\ell \cdot \sqrt{2D\eta^{-1}(\tau - 1 + e^{-\tau})}} \cdot \sum_{n=-\infty}^{\infty} (-)^n e^{-n^2\ell^2/(4D\eta^{-1}(\tau-1+e^{-\tau}))}$$

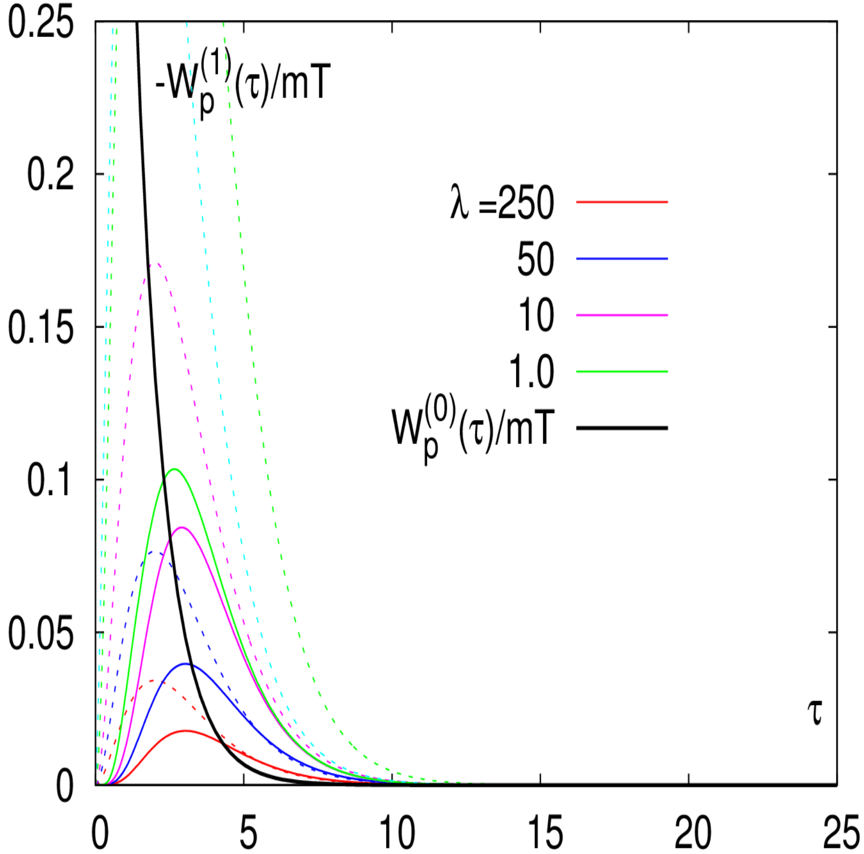
- This can be approximated to

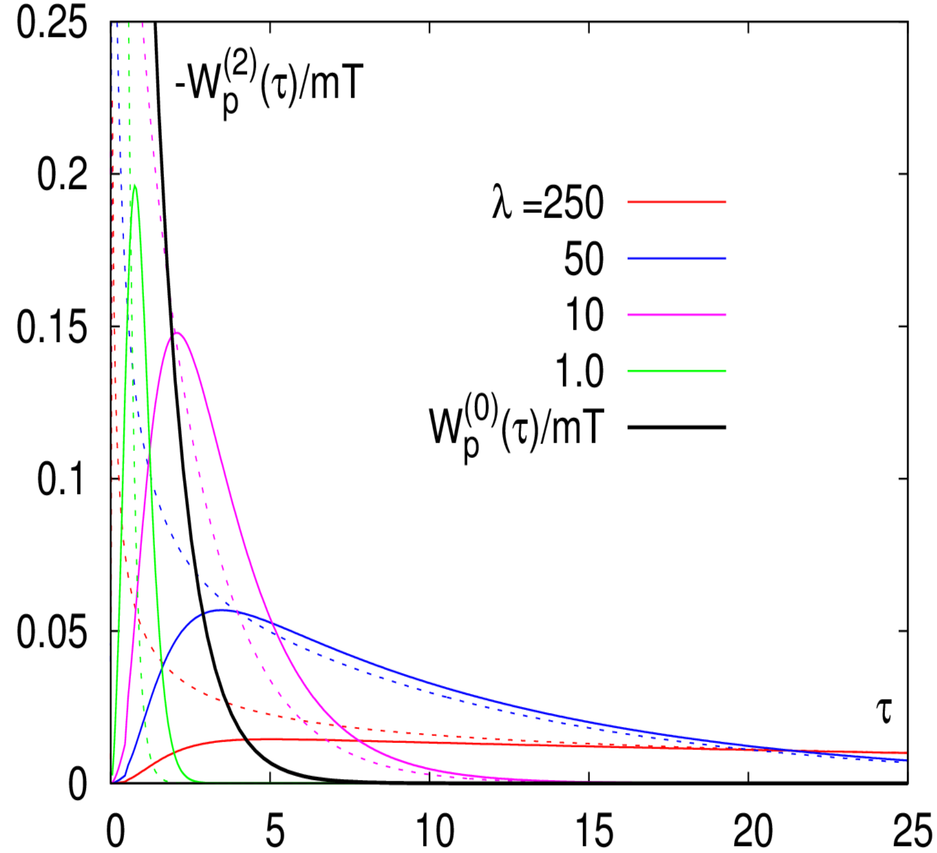
$$W_p^{(2)}(\tau) \simeq -\frac{2}{\sqrt{\pi}} MT \frac{\tau^2}{\sqrt{\lambda}} \qquad \text{for} \quad \tau \ll 1$$

$$W_p^{(2)}(\tau) \simeq -\frac{2}{\lambda} MT \sum_{k=-\infty}^{\infty} e^{-(2k+1)^2\pi^2\tau/2\lambda} \qquad \text{for} \quad \tau \gg 1$$

The Wightmann Correlator

- The full result has to be computed numerically:





- Both $W_p^{(1)}(\tau)$ and $W_p^{(2)}(\tau)$ decay slowly compared to $W_p^{(0)}(\tau)$

The Wightmann correlator and the SPF

- Connection to the SPF via the fluctuation-dissipation theorem:

$$\rho_p(\omega) = \tanh\left(\frac{\beta\hbar\omega}{2}\right)\int_{-\infty}^{\infty}\frac{dt}{2\pi}\,e^{i\omega t}\Big\langle\{p(t),p(0)\}_+\Big\rangle$$

- In a classical description of heavy quark dynamics this becomes

$$\frac{\pi\rho_p(\omega)}{\omega} = \beta\int_0^{\infty} dt\, W_p(t)\cos(\omega t)$$

- As before $W_p^{(0)}(t)$ leads to the known infinite volume result:

$$\frac{\pi\rho_p^{(0)}(\omega)}{\omega} = M\,\frac{\eta}{\omega^2+\eta^2}$$

see e.g. H.B.Meyer; Eur.Phys.J. A47 (2011) 86

The Wightmann correlator and the SPF

- For $\tau \gg 1$ the expressions simplify considerably and yield

$$\frac{\pi \rho_p^{(1)}(\omega)}{\omega} = -M \frac{2\eta}{\sqrt{\lambda}} \frac{\eta^2 - 3\omega^2}{(\eta^2 + \omega^2)^3}$$

$$\omega \to 0 \simeq -M \frac{2}{\sqrt{\lambda}}$$

$$\frac{\pi \rho_p^{(2)}(\omega)}{\omega} = -\frac{4m}{\lambda} \sum_{k \geq 0} \frac{\gamma_k}{\gamma_k^2 + \omega^2}$$

$$\omega \to 0 \simeq -M \frac{1}{\eta}$$

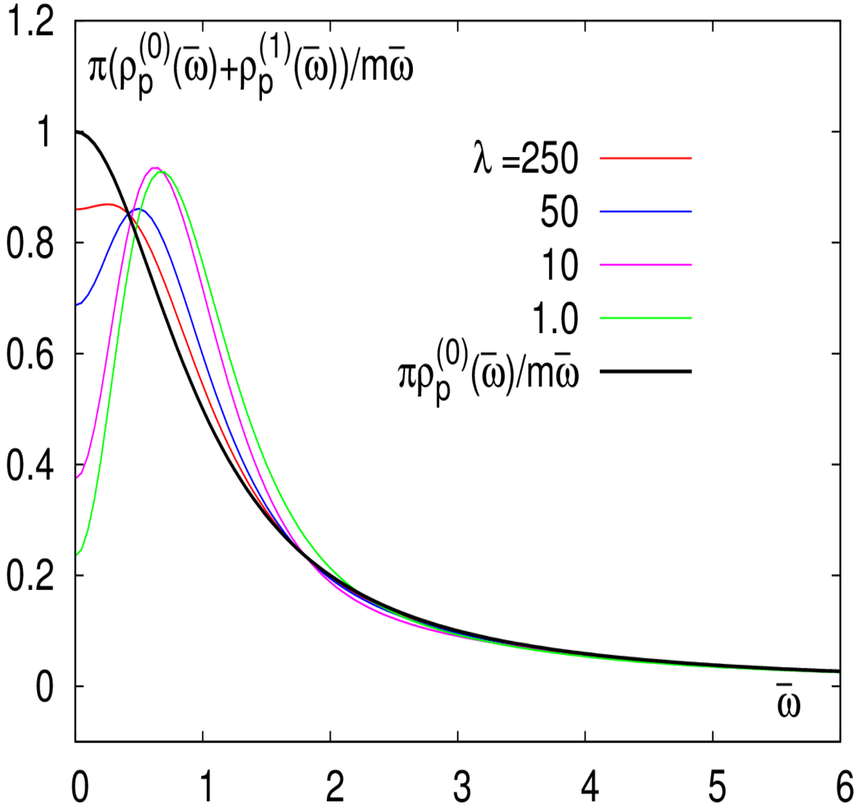
with $\gamma_k = \dfrac{(2k+1)^2 \pi^2 \eta}{2\lambda} = (2k+1)^2 \pi^2 \dfrac{D}{\ell^2}$

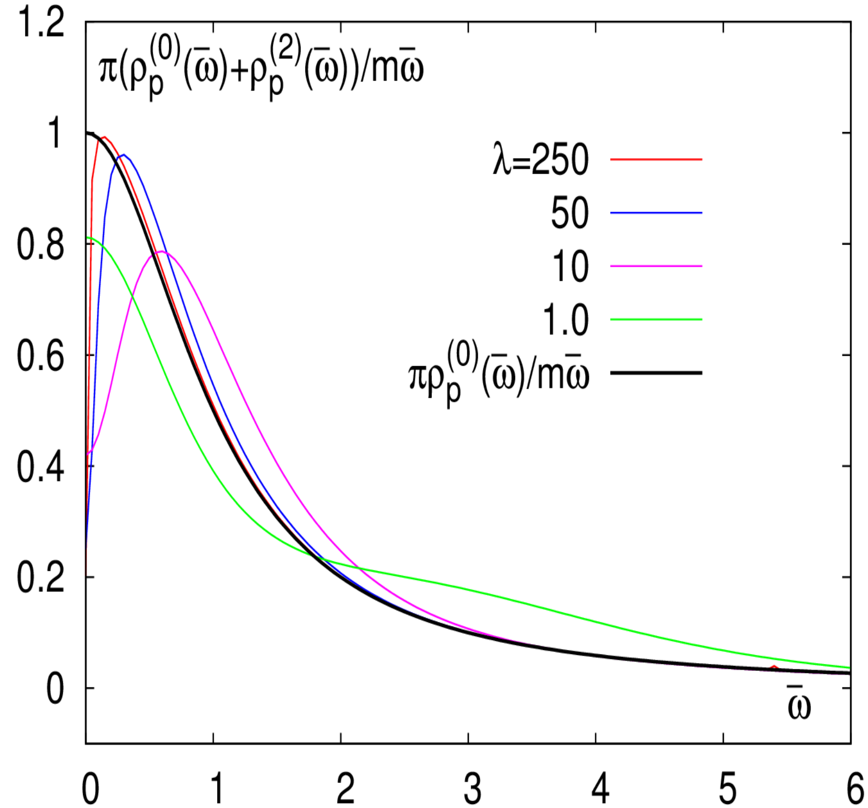
- Note $\rho_p^{(0)}(\omega)$ and $\rho_p^{(2)}(\omega)$ exactly cancel at $\omega = 0$ as

$$\lim_{\omega \to 0} \frac{\pi \rho_p^{(0)}(\omega)}{\omega} \simeq M \frac{1}{\eta}$$

The Wightmann correlator and the SPF

- Still $\rho_p^{(1)}(\omega)$ and $\rho_p^{(2)}(\omega)$ generally have to be calculated numerically





- In the low-ω region there are clearly visible modifications
- Note: $\bar{\omega} = \omega/\eta$

Connecting to the Euclidean Correlator

- The Euclidean correlator is the analytic continuation of the Wightmann correlator to imaginary times

$$G_E(t,\vec{k}) = W(-it,\vec{k})$$

- However, in the short distance expansion the connection is

$$\frac{d^2}{dt^2}G_E(t=\hbar\beta/2,0) = -\frac{d^2}{dt^2}W(t,0)\Big|_{t=0}(1+O(\hbar))$$

⇒ they are directly related via the second thermal moment

$$G_E'' = \frac{d^2}{dt^2}G_E(t=\hbar\beta/2) = \int_0^\infty d\omega\,\rho(\omega)\,\frac{\omega^2}{\sinh(\omega/2)}$$

Connecting to the Euclidean Correlator

- Recall for small τ we had

$$W_p^{(1)}(\tau) \simeq MT\frac{\tau^{11/2}}{\sqrt{\lambda}}$$

$$W_p^{(2)}(\tau) \simeq -\frac{2}{\sqrt{\pi}}MT\frac{\tau^2}{\sqrt{\lambda}}$$

➡ there is a $1/\sqrt{\lambda}$ dependent contribution in G''_E

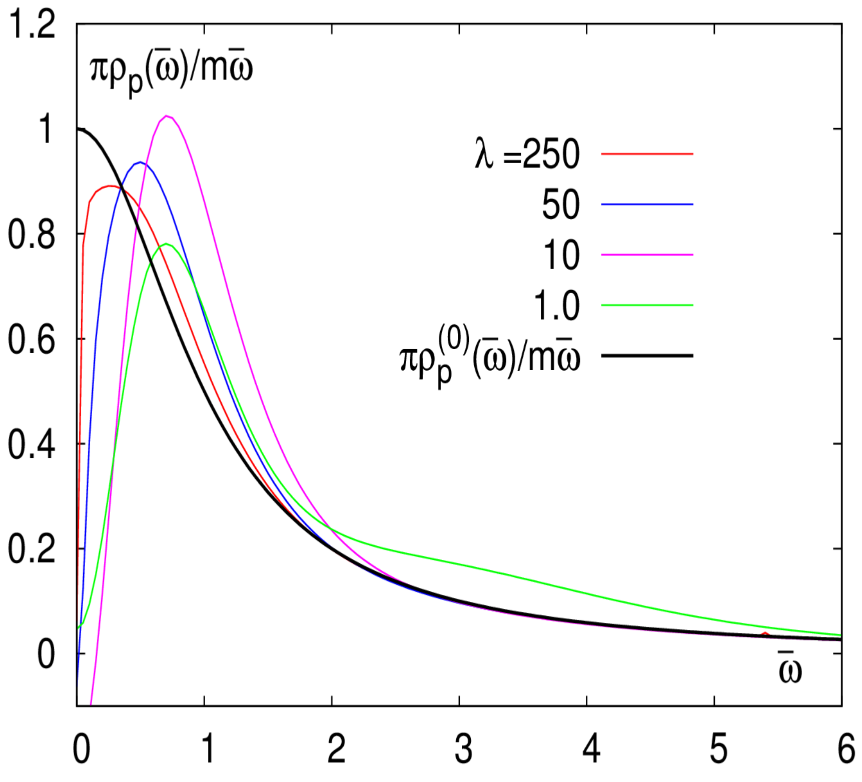
$$G''_E = \frac{d^2}{dt^2}G_E(t=\hbar\beta/2) = \frac{4}{\sqrt{\pi}}MT\frac{\eta^2}{\sqrt{\lambda}} = 8\sqrt{\frac{T^3M}{2\pi}}\frac{\eta}{l}$$

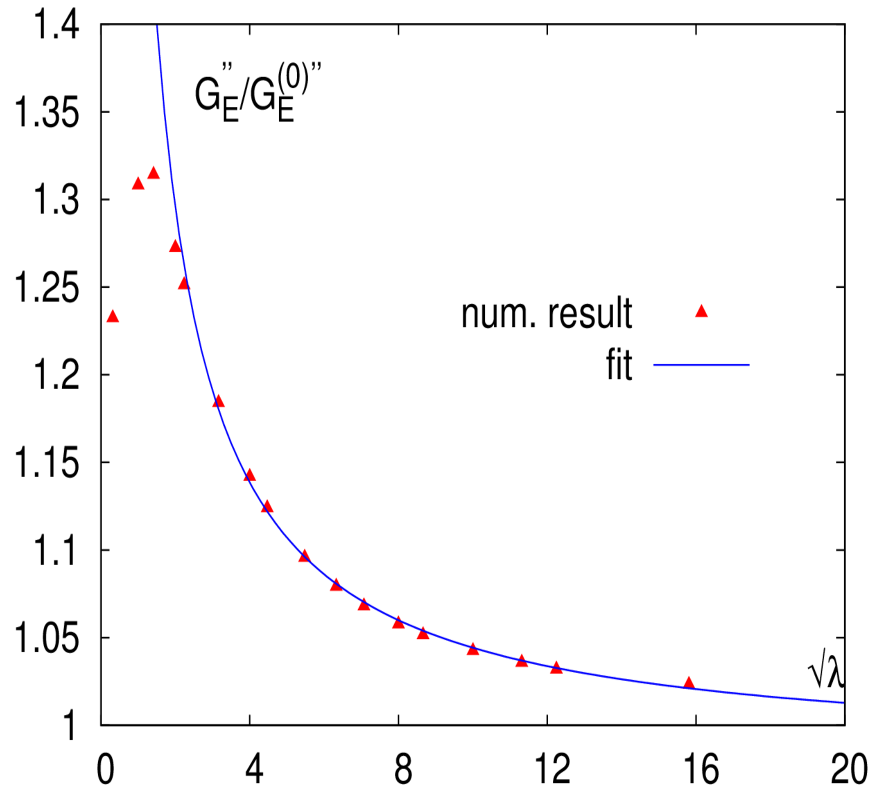
➡ we can extract η directly from the finite size effects in G''_E

Note: A similar idea using a small chemical potential was explored in: P.Petreczky, D.Teaney; Phys.Rev. D73 (2006) 014508

Connecting to the Euclidean Correlator

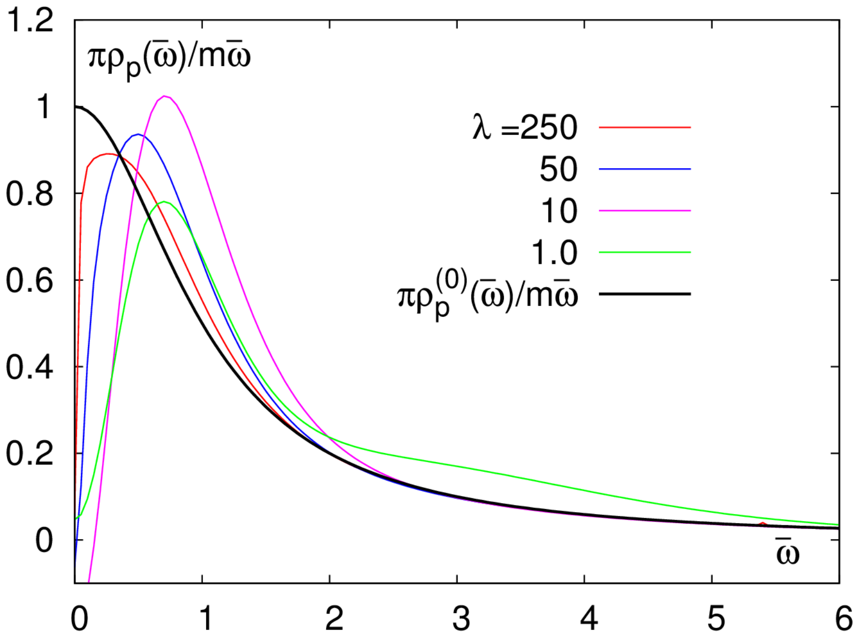
- Numerically we compute the thermal moment via the SPF

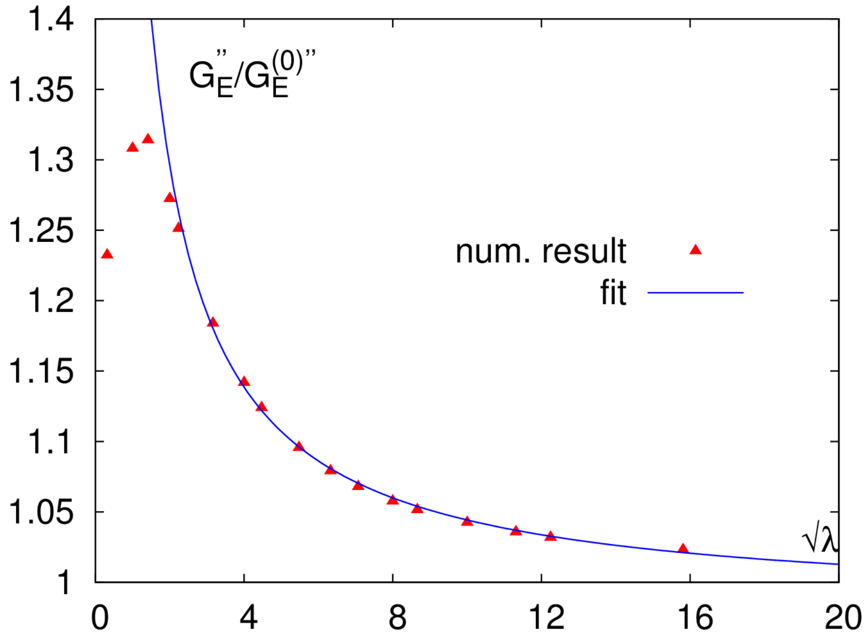




- Dependence in $1/\sqrt{\lambda} \sim 1/l$ in $G_E''/G_E^{(0)''}$

Conclusion





- We implemented hard wall boundary conditions in Langevin dynamics
- We evaluated their impact on the spectral function and the Euclidean correlator
- We found a $1/l$-dependence in the second thermal moment of the Euclidean correlator that is directly proportional to the diffusion constant
- In a next step we hope to observe this type of dependence also in $(1+1)D$ model(s)

Backup Slides

Connecting to the Current-Current Correlator

- The Wightmann correlator describes the correlation of the one-particle momentum
- For normalization check the particle densities:

$$\int d^3x \left\langle \rho_p(t,\vec{x})\rho_p(0,0) \right\rangle = 1$$

$$\int d^3x \left\langle \rho(t,\vec{x})\rho(0,0) \right\rangle = T\chi_s$$

The connection to the heavy quark current is

$$W_{HQ}(t,\vec{k}=0) = \frac{T\chi_s}{M^2} W_p(t)$$

The Wightmann-Correlator

- The second term is

$$W_p^{(1)}(\tau) = MT \cdot \, (-1)\, (\frac{2}{\pi})\sqrt{\lambda}\phi(\tau)e^{-\tau} \sum_{n=-\infty}^{\infty} \cdot$$

$$\int_0^1 d\chi \int_{-\infty}^{\infty} d\bar{p}\bar{p}^2 e^{-\bar{p}^2} \int_{P_{2n-1}}^{P_{2n}} dPe^{-\lambda P^2/\phi(\tau)}$$

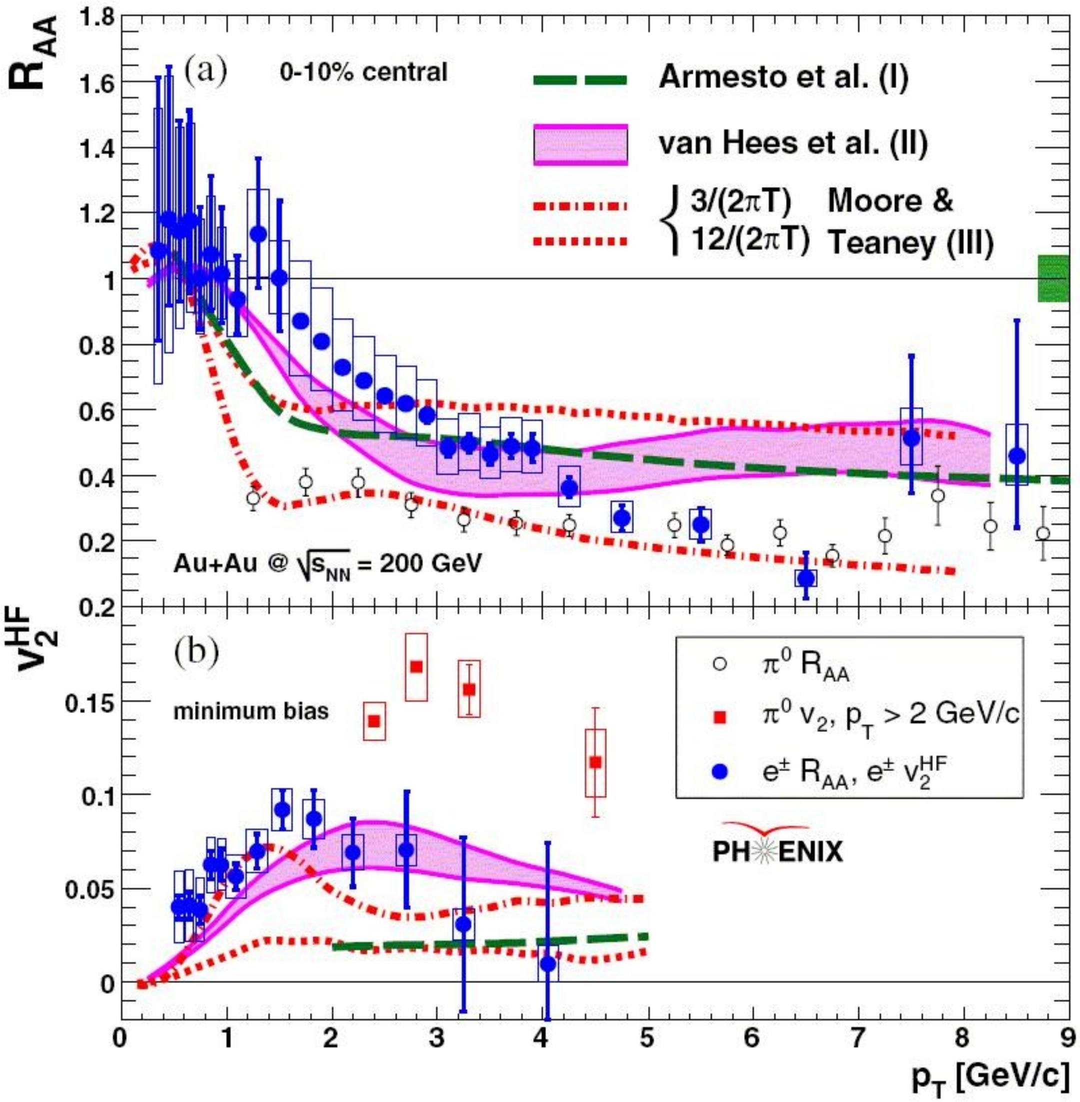
- where

$$\chi = x/l \qquad \phi(\tau) = 2\tau - 3 + 4e^{-\tau} - e^{-2\tau}$$

$$\bar{p} = p/\sqrt{2MT} \qquad P_{2n} = 2n - \chi - \bar{p}(1 - e^{-\tau})/\sqrt{\lambda}$$

$$P = R/l$$

Introduction



Adare et al.; Phys.Rev. C84 (2011) 044905

- Heavy quark dynamics can be studied in experiments, e.g. @RHIC or @Alice

- PHENIX results suggest
  - Radiative energy loss does not explain R_{AA} by itself.
  - Collisional energy loss must also be included
  - v_2^{HF} is larger than initially expected from kinetic theory