Charmonium and bottomonium spectral functions and the heavy quark diffusion coefficient from lattice QCD

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in collaboration with
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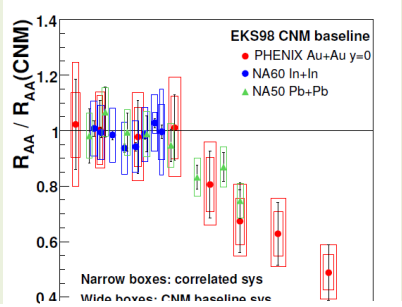
Motivation

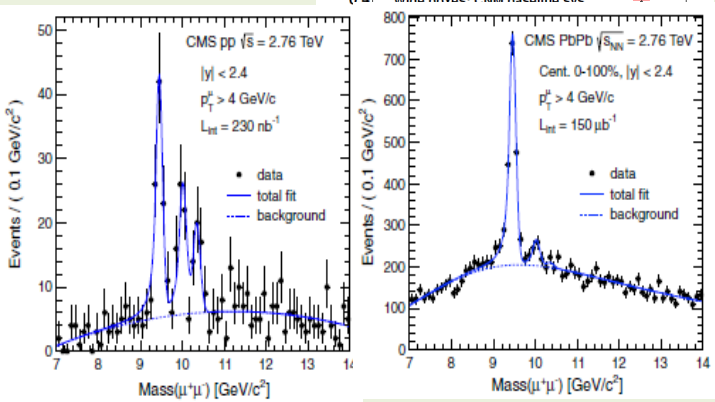
- Quarkonium spectral functions (SPFs)
  - have all information about in-medium properties of quarkonia

Quarkonium dissociation temperature

→ Important to understand quarkonium suppression

N. Brambilla *et al.*, EPJ C71 (2011) 1534





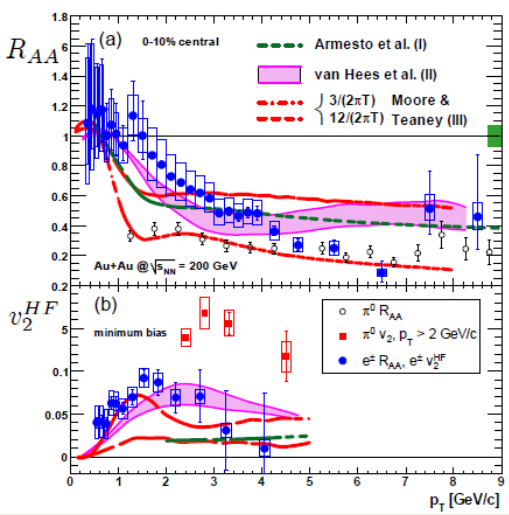
S. Chatrchyan *et al.*, PRL 109 (2012) 222301

Heavy quark diffusion coefficient

$$D = \frac{1}{6\chi_{00}} \lim_{\omega \to 0} \sum_{i=1}^{3} \frac{\rho_{ii}^V(\omega, \mathbf{0})}{\omega}$$

$\rho_{ii}^V(\omega)$: vector SPF

→ Important input for hydro models



Adare *et al.* [PHENIX Collaboration], PRL 98 (2007) 172301

Quarkonium correlation and spectral functions

Euclidian (imaginary time) meson correlation function

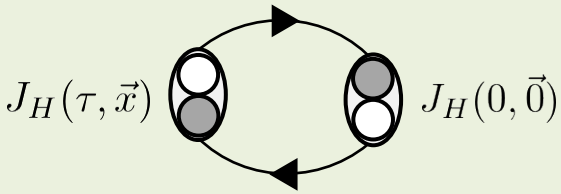
$$G_H(\tau,\vec{p}) \equiv \int d^3x e^{-i\vec{p}\cdot\vec{x}} \langle J_H(\tau,\vec{x}) J_H(0,\vec{0})\rangle$$

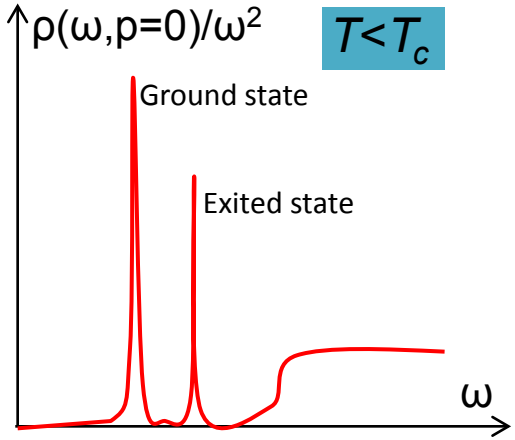
$$= \int_0^\infty \frac{d\omega}{2\pi} \boxed{\rho_H(\omega,\vec{p})} K(\omega,\tau)$$

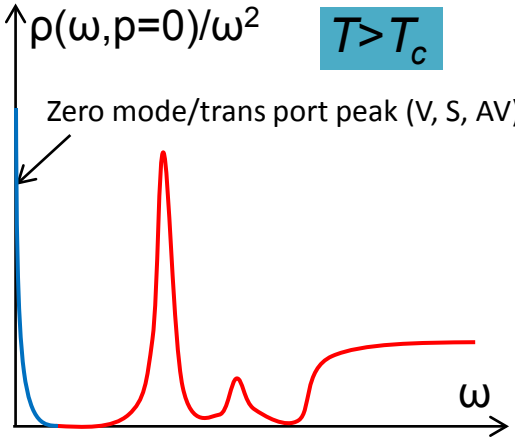
Spectral function

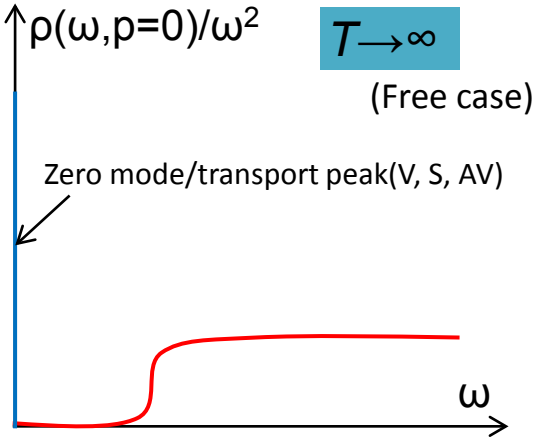
$$J_H(\tau,\vec{x}) \equiv \bar{\psi}(\tau,\vec{x})\Gamma_H\psi(\tau,\vec{x})$$

$$K(\omega,\tau) \equiv \frac{\cosh[\omega(\tau-1/2T)]}{\sinh(\omega/2T)}$$





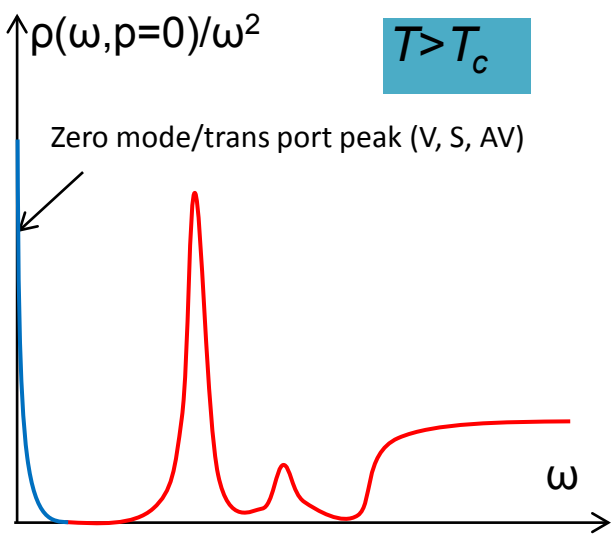




Heavy quark diffusion coefficient

$$D = \frac{1}{6\chi_{00}} \lim_{\omega \to 0} \sum_{i=1}^{3} \frac{\rho_{ii}^{V}(\omega, \mathbf{0})}{\omega}$$

$\rho_{ii}^{V}(\omega)$: spatial component of vector spectral function



χ_{00} : Quark number susceptibility

$\rho_{00}^{V}(\omega) = 2\pi\chi_{00}\omega\delta(\omega)$ ➡ $G_{00}^{V}(\tau) = T\chi_{00}$

D is related to the vector spectral function around zero frequency.

Investigating spectral functions

- Computing SPF → **Ill-posed problem**
  - # of data points of a correlator is $O(10)$ while a SPF needs O(1000) data points.
  - In general, simple χ^2 fitting does not work!
- Indirect ways
  - Spatial correlator → Screening mass
  - Reconstructed correlator
- Several ways to reconstruct SPF
  - Maximum entropy method (MEM) M. Asakawa, T. Hatsuda and Y. Nakahara, Prog.Part.Nucl.Phys. 46 (2001) 459-508
  - A new Bayesian method Y. Burnier and A. Rothkopf, PRL 111 (2013) 18, 182003
  - Stochastic methods A. S. Mishchenko et al., Phys. Rev. B62, 6317 (2000); K.S.D. Beach, arXiv:cond-mat/0403055; S. Fuchs *et al.*, PRE81, 056701 (2010)

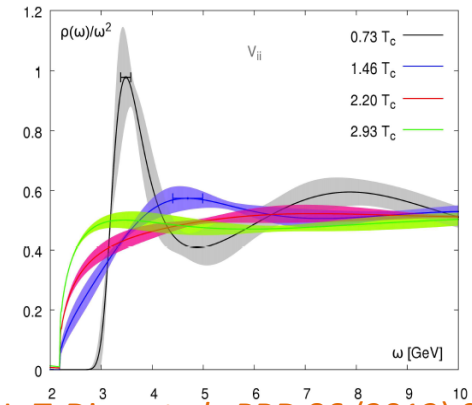
Data quality is also important!

Recent lattice studies on quarkonium melting

- Charmonia
  - Several studies both in quenched QCD and with dynamical quarks
  - Using MEM
  - **Dissociation temperatures are still not conclusive**

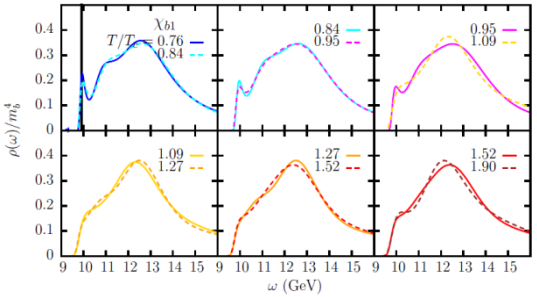
    J/Ψ seems to survive up to 1.5T_c

    P-wave states may melt just above T_c

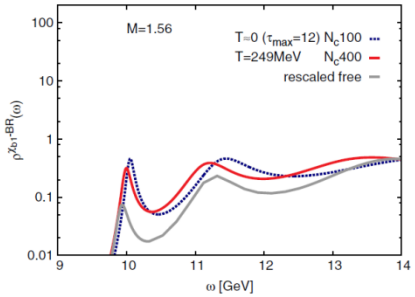


H.-T. Ding *et al.*, PRD 86 (2012) 014509

- Bottomonia
  - NRQCD
  - Using MEM or the new Bayesian method
  - **Υ(1S) seems to survive at least up to 2T_c**
  - **Different conclusions on melting of a P-wave state with different methods.**



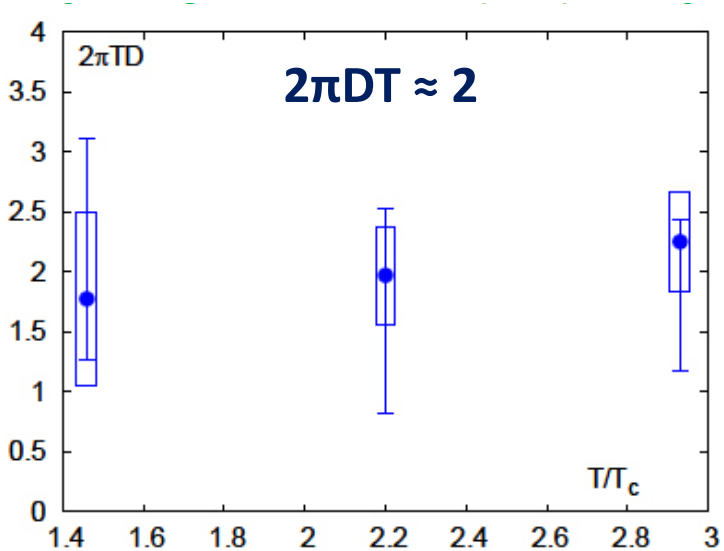
G. Aarts *et al.*, JHEP1407(2014)097



S. Kim *et al.*, PhysRevD.91.054511

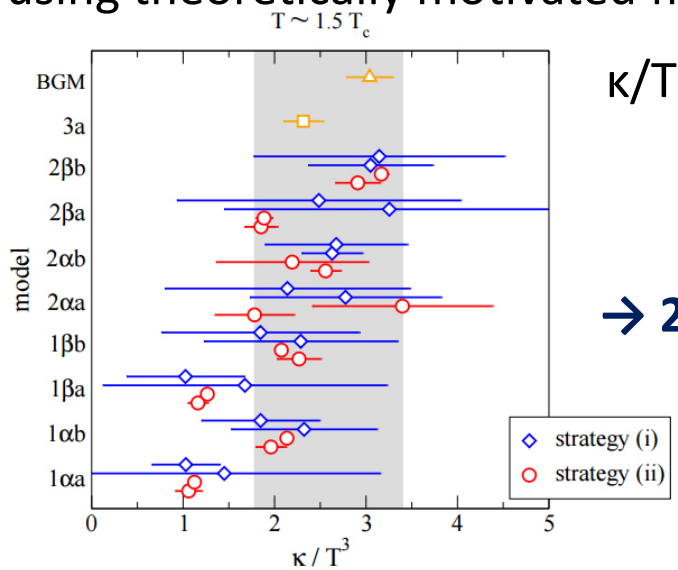
Recent lattice studies on heavy quark diffusion coefficient

- Quenched QCD, using MEM



H.-T. Ding *et al.*, PRD 86 (2012) 014509

- Heavy quark effective theory, continuum limit, using theoretically motivated fits



$\kappa/T^3 = 1.8 - 3.4$

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

→ **2πDT ≈ 3.7—7.0**

A. Francis, O. Kaczmarek, M. Laine, T. Neuhaus and HO, PRD 92 (2015) no.11, 116003

- Perturbative estimate

  2πDT ≈ 71.2 in LO

  Moore and Teaney, PRD 71 (2005) 064904

  2πDT ≈ 8.4 in NLO

  Caron-Hout and Moore, PRL 100 (2008) 052301

- Strong coupling limit

  2πDT ≈ 1

  Kovtun, Son and Starinets, JHEP 0310 (2004) 064

It is important to crosscheck previous results with more precise SPFs given on larger and finer lattice and by different methods.

This study

- Finite temperature lattice QCD simulations
  - large and fine isotropic lattices
  - quenched approximation
    (no dynamical quark)
  - both charm and bottom quarks
  - vector (V) channel

β	N_σ	a [fm]	N_τ	T/T_c
7.192	96	0.0184	48	0.75
			32	1.1
			28	1.25
			24	1.5
			16	2.2
7.793	192	0.00905	96	0.75
			64	1.1
			56	1.25
			48	1.5

- Investigating quarkonium SPFs (and heavy quark diffusion)
  - indirectly with the correlation functions
  - directly by using both MEM and stochastic methods

Screening mass

Spatial meson correlation function

Screening mass

$$G(z) \equiv \int dxdy \int_0^{1/T} d\tau \langle J_H(\tau, \vec{x}) J_H(0, \vec{0}) \rangle \underset{z >> 1/T}{\longrightarrow} e^{-\boxed{M_{\rm scr}} z}$$

If there is a lowest lying bound state

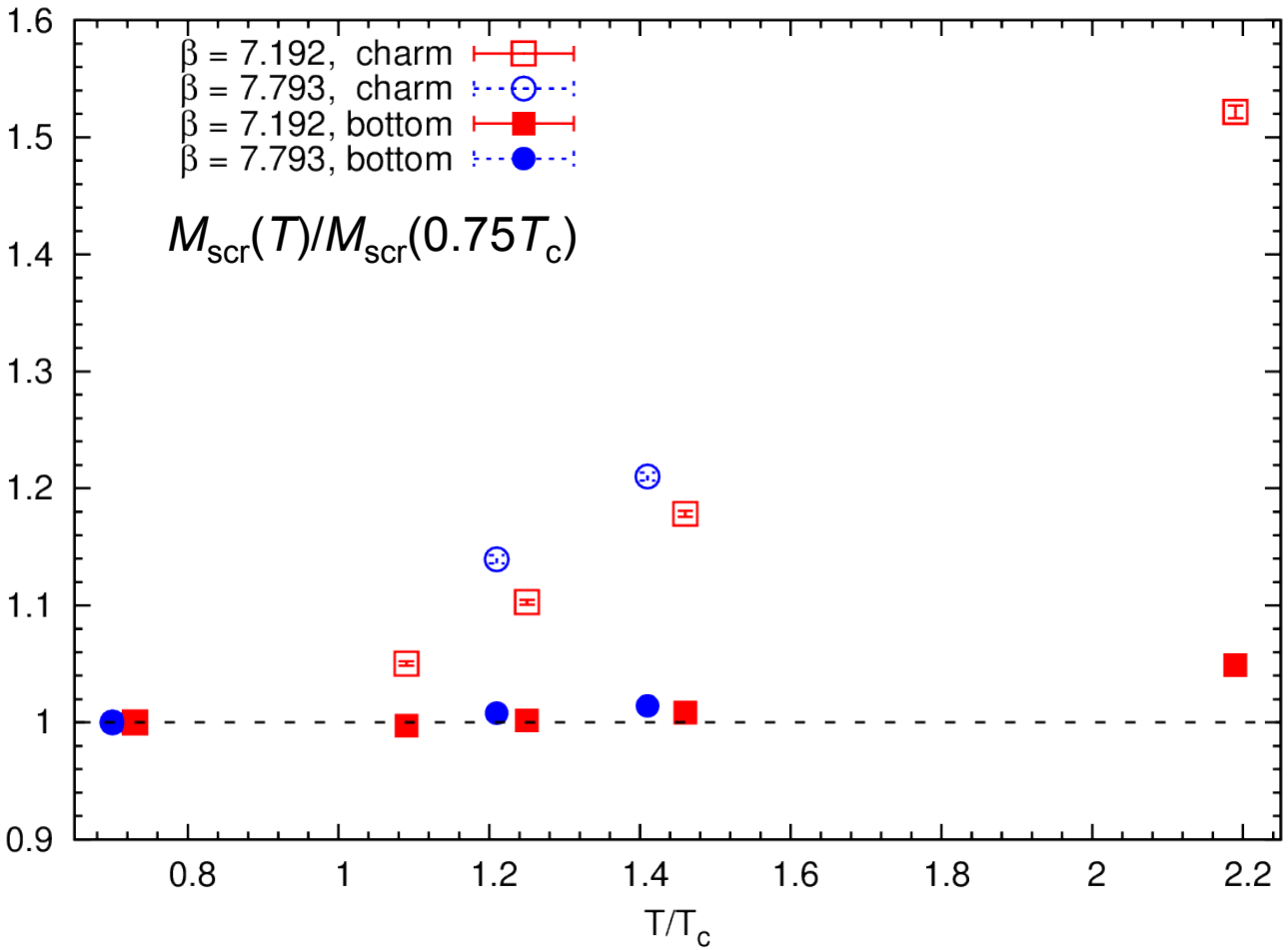
$$\boxed{M_{\rm scr} = M}$$

High *T* limit (free case)

Quark mass

$$\boxed{M_{\rm scr} = 2\sqrt{(\pi T)^2 + m_q^2}}$$

Screening mass for V channel



M_{scr} increases monotonically as increasing temperature.

Small temperature dependence for bottom.

Reconstructed correlator

$$G_{\rm rec}(\tau,T;T') \equiv \int_0^\infty d\omega \rho(\omega,T') K(\omega,\tau,T)$$

$$\frac{G(\tau,T)}{G_{\rm rec}(\tau,T;T')} = \frac{\int_0^\infty d\omega \rho(\omega,T) K(\omega,\tau,T)}{\int_0^\infty d\omega \rho(\omega,T') K(\omega,\tau,T)}$$

different same

equals to unity at all τ

if the spectral function doesn't change at each temperature

S. Datta *et al.*, PRD 69 (2004) 094507

$$\frac{\cosh[\omega(\tau - N_\tau/2)]}{\sinh[\omega N_\tau/2]} = \sum_{\tau'=\tau;\Delta\tau'=N_\tau}^{N'_\tau - N_\tau + \tau} \frac{\cosh[\omega(\tau' - N'_\tau/2)]}{\sinh[\omega N'_\tau/2]}$$

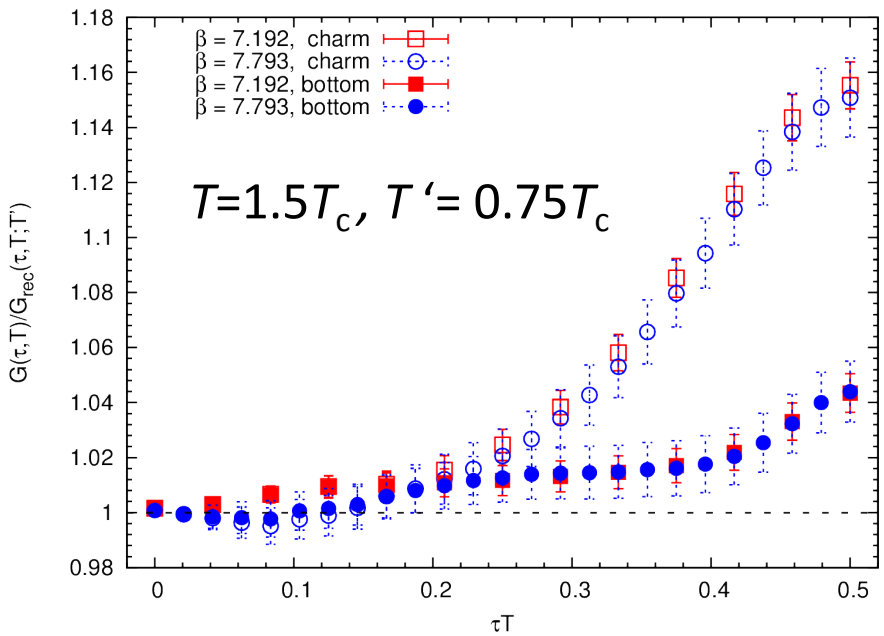
$$T = 1/(N_\tau a) \qquad N'_\tau = mN_\tau \qquad m = 1,2,3,\cdots$$

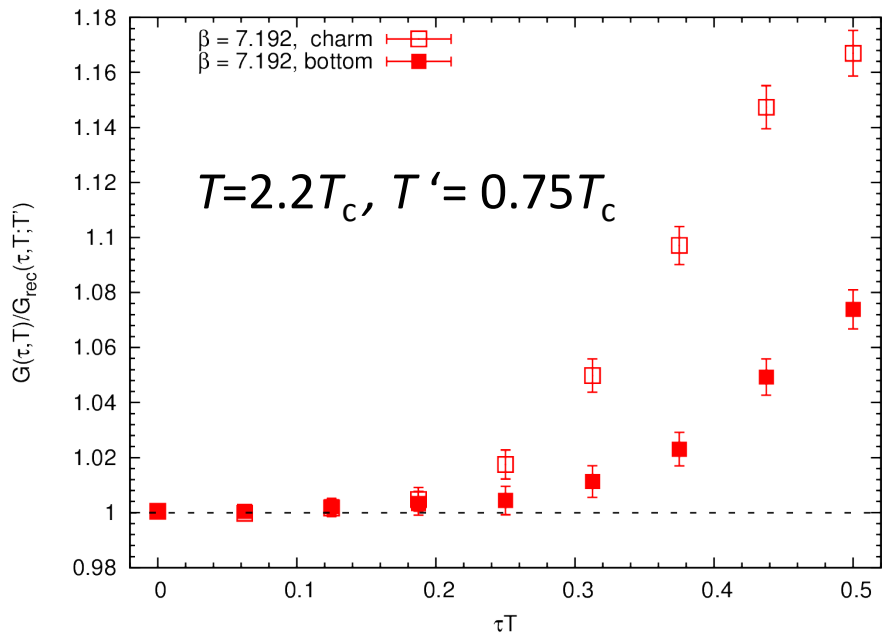
$$G_{\rm rec}(\tau,T;T') = \sum_{\tau'=\tilde{\tau};\Delta\tau'=N_\tau}^{N'_\tau - N_\tau + \tau} G(\tau',T')$$

H.-T. Ding *et al.*, PRD 86 (2012) 014509

Reconstructed correlator for V channel

$G(\tau,T)/G_{rec}(\tau,T;T')$





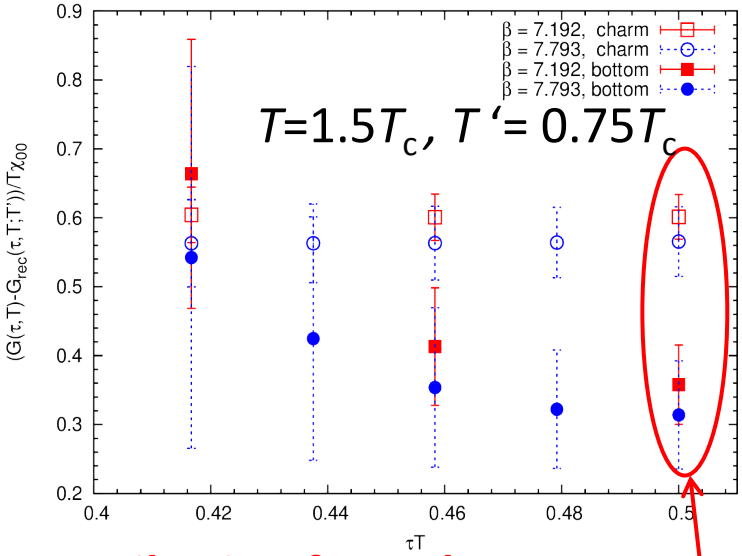
There is strong enhancement at large τ, especially for charm.

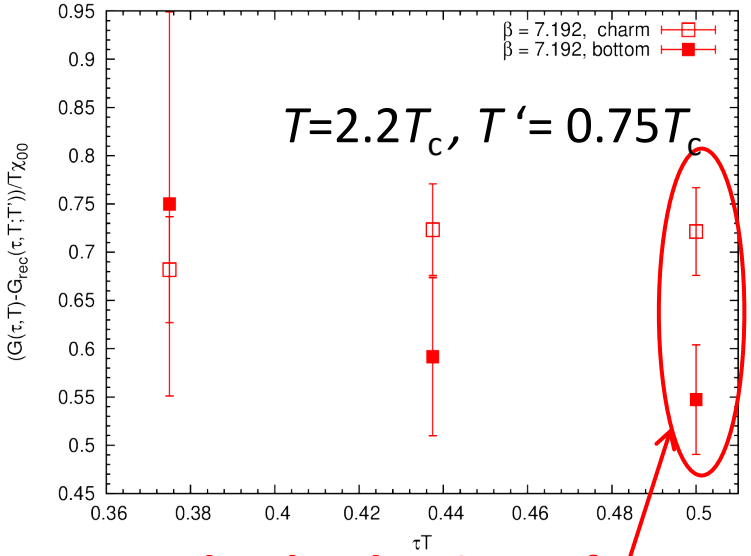
Large τ ↔ Small ω

→ This strong modification might be related to the transport peak.

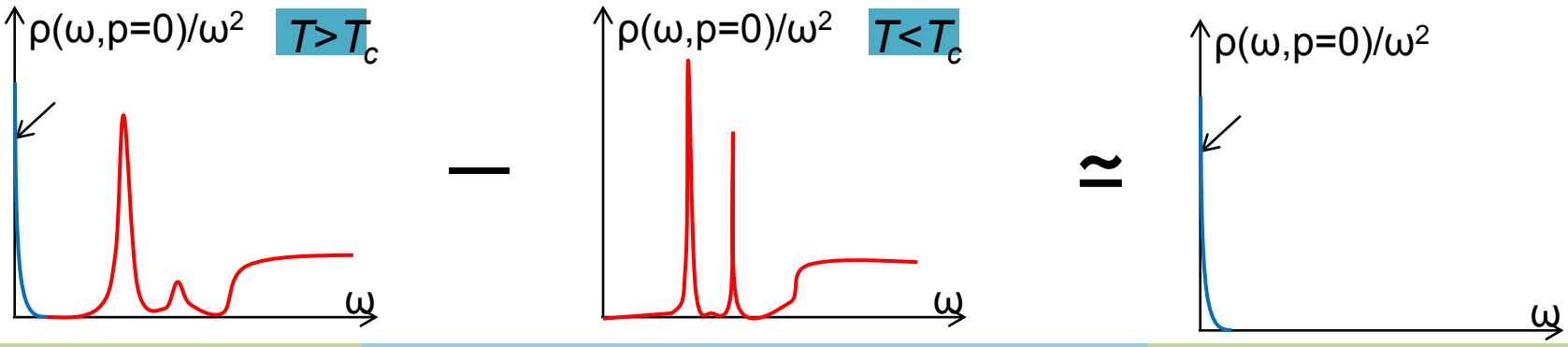
Estimating the heavy quark diffusion coefficient

$G(\tau,T) - G_{rec}(\tau,T;T')$





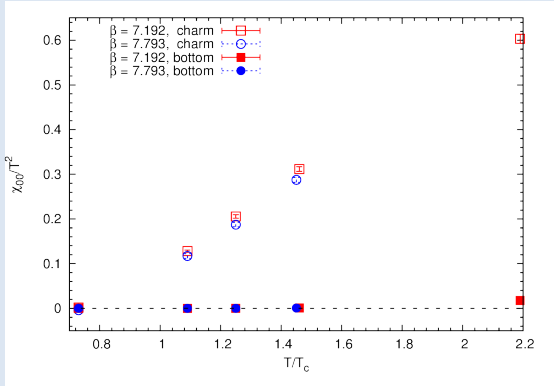
Contribution from the transport peak is assumed to be dominant for $G - G_{rec}$ at $\tau T = ½$.



Estimating the heavy quark diffusion coefficient (cont'd)

χ_{00} : Quark number susceptibility

$\rho^V_{00}(\omega) = 2\pi\chi_{00}\omega\delta(\omega)$ ➡ $G^V_{00}(\tau) = T\chi_{00}$



Heavy quark diffusion coefficient

$$D = \frac{1}{6\chi_{00}} \lim_{\omega\to 0} \sum_{i=1}^{3} \frac{\rho^V_{ii}(\omega, \mathbf{0})}{\omega}$$

H.-T. Ding *et al.*, PRD 86 (2012) 014509

Ansatz: $$\rho^V_{ii}(\omega << T) = 2\chi_{00}\frac{T}{M}\frac{\omega\eta}{\omega^2+\eta^2} \qquad \eta \equiv \frac{T}{MD}$$

M = 1—1.5 GeV

Charm: $2\pi TD \approx 0.6$—1 ($\beta = 7.192$), $2\pi TD \approx 0.5$—0.8 ($\beta = 7.793$) at $1.5T_c$

$2\pi TD \approx 0.6$—0.8 ($\beta = 7.192$) at $2.2T_c$

Bottom: no solution for M > 4 GeV

Reconstruction of SPFs : methods

MEM

- Most likely solution

$$\max P[A|\bar{G}] \leftrightarrow \min F \leftrightarrow \frac{\delta F}{\delta A} = 0$$

where

$$P[A|\bar{G}] \propto e^{-F} \quad F \equiv \chi^2/2 - \alpha S$$

- Prior information

$$S \equiv -\int d\omega\, A(\omega) \ln\left(\frac{A(\omega)}{D(\omega)}\right)$$

- Eliminating α

$$P[\alpha|\bar{G}] \propto P[\alpha] \int \mathcal{D}A\, e^{-F[A]}$$

where

$$P[\alpha] = 1,\ 1/\alpha$$

➡

$$\langle A(\omega)\rangle = \int d\alpha A_\alpha(\omega) P[\alpha|\bar{G}]$$

Stochastic methods

- Most likely solution

$$\mathcal{D}'n \equiv \mathcal{D}n\, \Theta[n]\delta\left(\int dx\, n(x) - \bar{G}(\tau_0)\right)$$

Stochastically evaluate

$$\langle n(x)\rangle_\alpha = \int \mathcal{D}'n\, n(x) e^{-\chi^2/2\alpha} \quad \text{for } n(x) \equiv \frac{A(\phi^{-1}(x))}{D(\phi^{-1}(x))}$$

SAI (Stochastic Analytical Inference)

S. Fuchs *et al.*, PRE81, 056701 (2010)
HO, PoS LATTICE 2015, 175 (2016)

- Prior information

$$x \equiv \phi(\omega) = \frac{1}{\mathcal{N}} \int_{-\infty}^{\omega} d\omega' D(\omega')$$

- Basis

δ functions

- Eliminating α

$$P[n|\bar{G}] \propto P[\alpha] \int \mathcal{D}'n\, e^{-\chi^2[n]/2\alpha}$$

➡ $$\langle\langle n(x)\rangle\rangle = \int d\alpha \langle n(x)\rangle_\alpha P[n|\bar{G}]$$

SOM (Stochastic Optimization Method)

A. S. Mishchenko *et al.*, PRB62, 6317 (2000)
H.-T. Shu *et al*, PoS LATTICE 2015, 180 (2016)

- Prior information

None ($x = \omega$)

dose not rely on DM!

- Basis

Boxes

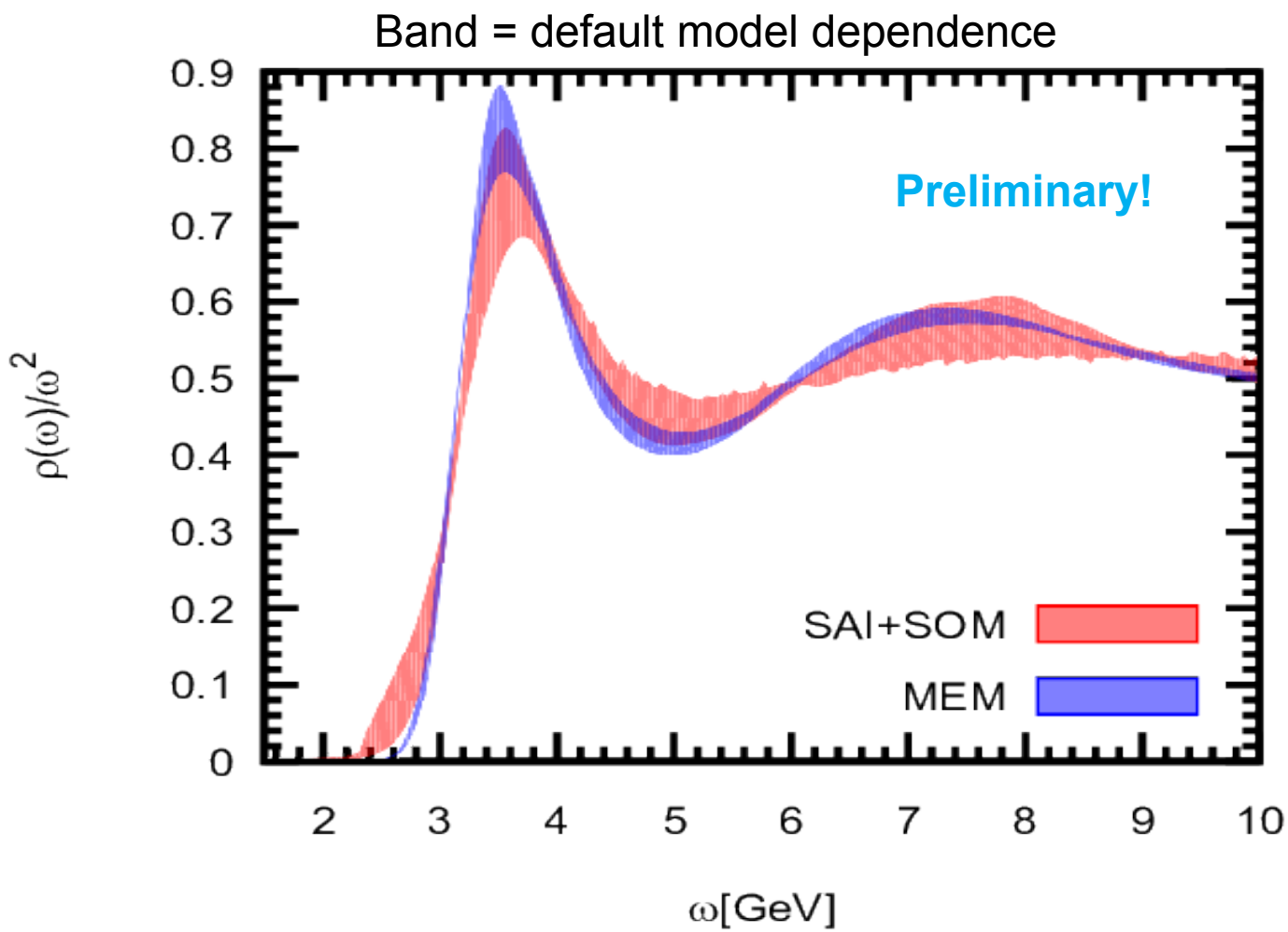
- Eliminating α

Choosing α
at a critical point of $\langle\chi^2\rangle_\alpha$

Reconstruction of SPFs : setup

- Using the finer lattice (β=7.793)
- Only charmonium SPFs at $0.75T_c$ and $1.5T_c$ have been analyzed so far
- With both MEM and the stochastic methods
- Various default models have been tested
  - ω^2
  - Free SPF
  - A resonance peak at several locations
  - Transport peak

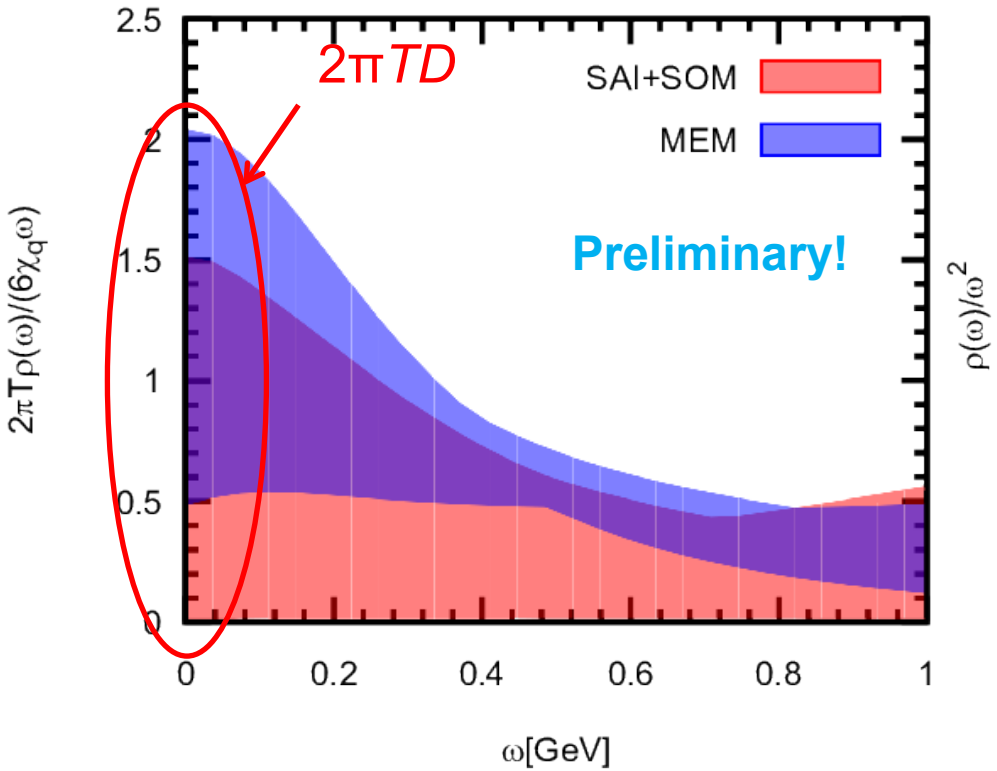
Charmonium SPF for V channel at $0.75T_c$

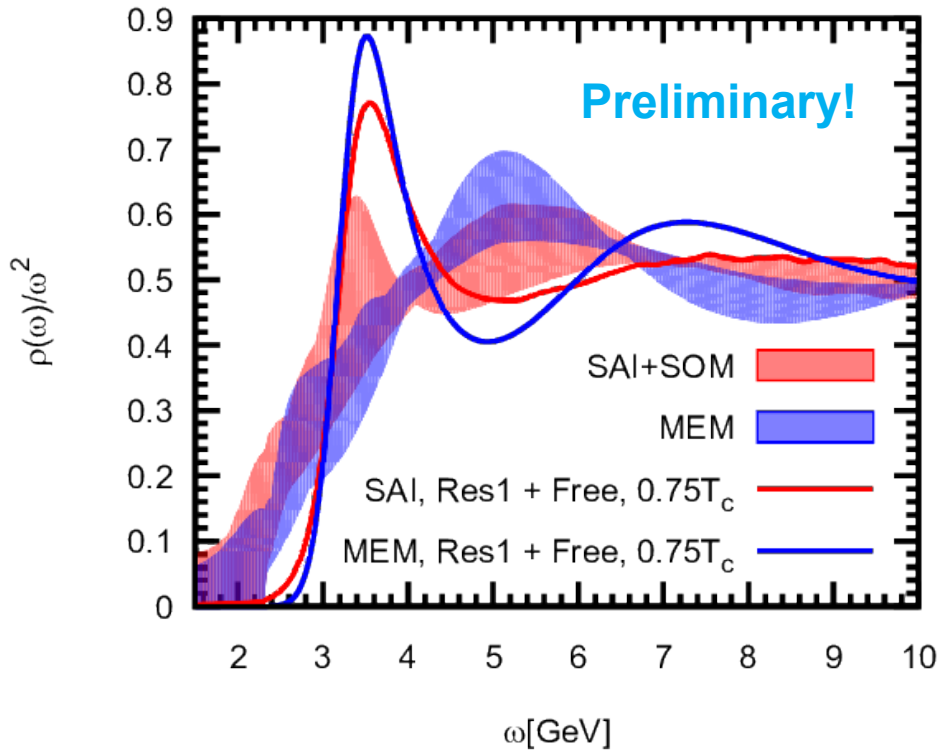


Default model and method dependence is weak.
There is a stable J/Ψ peak.

Charmonium SPF for V channel at 1.5T_c

Band = default model dependence





Melting of J/Ψ is not conclusive so far, although most of the cases in our analysis suggest no clear J/Ψ peak.

There seems to be an upper bound of 2π*TD*, which is 1.5—2 in this study, while a lower bound is not clear.

Summary & outlook

- We investigated vector charmonium and bottomonium SPFs on very large and fine quenched lattices in both indirect and direct ways.
- Screening mass results suggest that charmonium states start having thermal effects just above T_c while temperature dependence of bottomonia is relatively small.
- The heavy quark diffusion coefficient was roughly estimated from difference between ordinary and reconstructed correlators, where $2\pi TD$ is around 1 for charm at $1.5T_c$ and $2.2T_c$.
- Charmonium SPFs for the vector channel at $0.75T_c$ and $1.5T_c$ were reconstructed with both MEM and stochastic methods.
  - Both MEM and the stochastic methods gave almost DM-independent stable SPFs having a clear J/Ψ peak at $0.75T_c$.
  - Most of the results suggest that J/Ψ may be melted around $1.5T_c$ but more detailed study is needed to conclude.
  - So far we observed an upper bound of $2\pi TD$, which is 1.5—2 at $1.5T_c$ in this preliminary study.
- More studies on SPF reconstruction are needed.
  - further checks of the DM-dependence and other systematic uncertainties
  - analysis of the temperature and quark mass dependence as well as other channels
  - continuum extrapolation

End

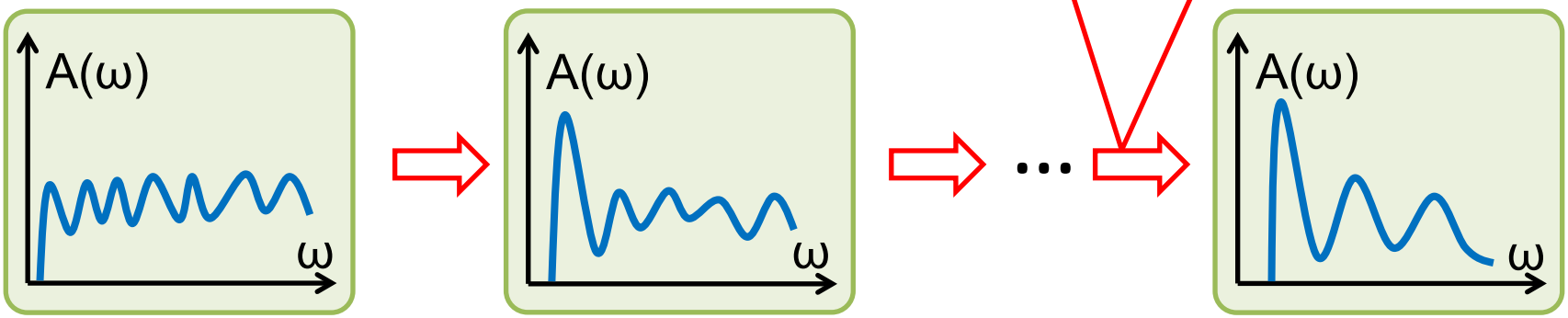
Backup slides

Stochastic method: basic idea

For given α (fictitious temperature, regularization parameter),

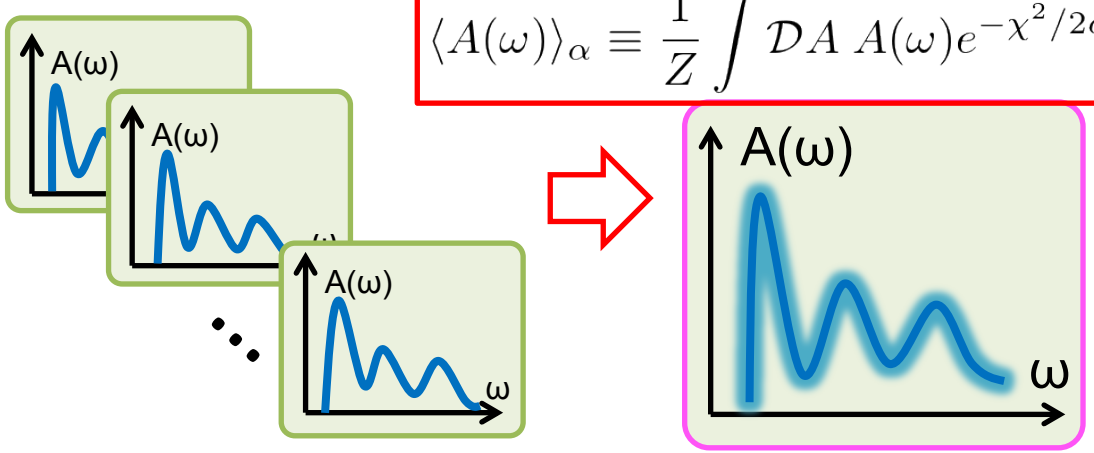
1. generate SPFs stochastically

$$P = \min\{1, e^{-\chi^2/2\alpha}\}$$



2. average over all possible spectra

$$\langle A(\omega)\rangle_\alpha \equiv \frac{1}{Z}\int \mathcal{D}A\; A(\omega) e^{-\chi^2/2\alpha} \qquad Z \equiv \int \mathcal{D}A\; e^{-\chi^2/2\alpha}$$



$$\chi^2 \equiv \sum_{\tau,\tau'} \Delta G(\tau) C^{-1}_{\tau,\tau'} \Delta G(\tau')$$

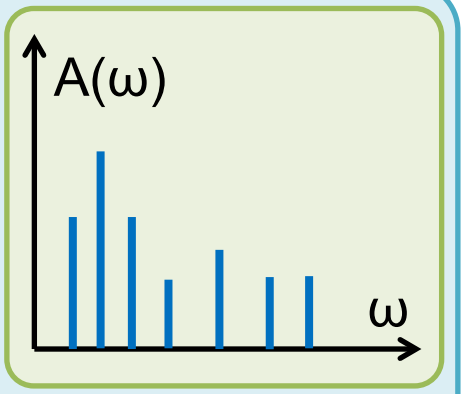
$C^{-1}_{\tau,\tau'}$: covariance matrix

$$\Delta G(\tau) \equiv \bar{G}(\tau) - \int d\omega\; A(\omega)\tilde{K}(\omega,\tau)$$

Stochastic method: basis

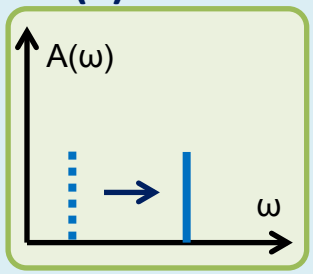
δ functions

$$A(\omega) = \sum_i r_i \delta(\omega - a_i)$$

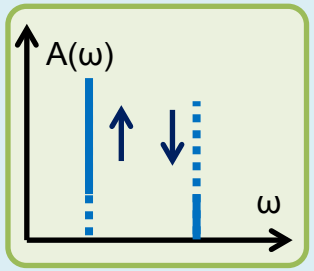


- Update schemes

(a) Shift



(b) Change residues



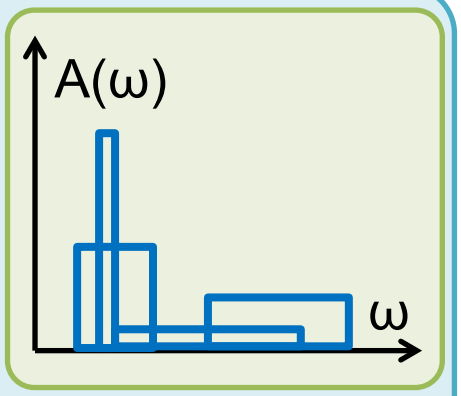
- Constraint

$$\sum_i r_i = \bar{G}(\tau_0)$$

Boxes

$$A(\omega) = \sum_i h_i R(\omega, a_i, w_i)$$

$$R(\omega, a_i, w_i) \equiv \begin{cases} 1 & (a_i - \frac{w_i}{2} \leq \omega \leq a_i + \frac{w_i}{2}) \\ 0 & (\text{otherwise}) \end{cases}$$



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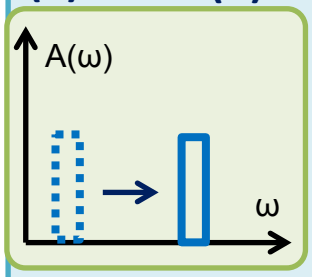
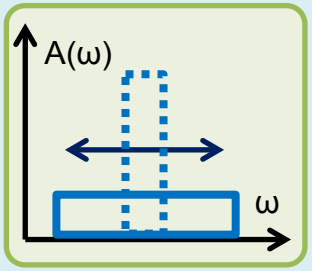
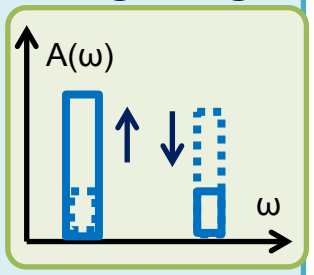


(b) Change width



(c) Change heights



- Constraint

$$\sum_i h_i w_i = \bar{G}(\tau_0)$$

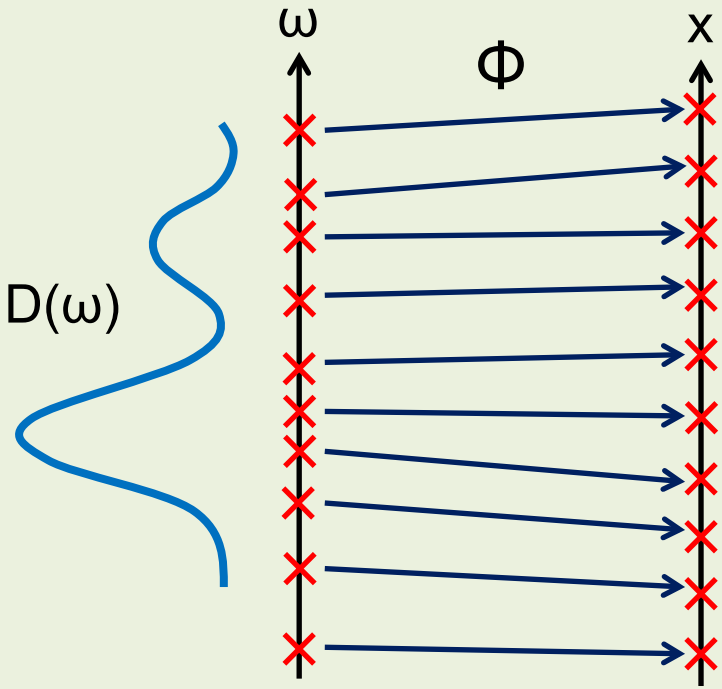
Update schemes which change the number of the basis are also possible.

Stochastic method: default model

K.S.D. Beach, arXiv:cond-mat/0403055

$$x \equiv \phi(\omega) = \frac{1}{\mathcal{N}} \int_{-\infty}^{\omega} d\omega' D(\omega')$$

$D(\omega)$: Default model (prior information)



$$G(\tau) = \int d\omega\ A(\omega)\tilde{K}(\omega,\tau)$$

$$= \int dx\ n(x)\tilde{K}(\phi^{-1}(x),\tau)$$

$$n(x) \equiv \frac{A(\phi^{-1}(x))}{D(\phi^{-1}(x))}$$

$$\bar{G}(\tau_0) - \int dx\ n(x) = 0$$

$$\langle A(\omega)\rangle_\alpha = \langle n(\phi(\omega))\rangle_\alpha D(\omega)$$

Stochastic method: comparison with MEM(1)

Maximum entropy method (MEM)

$$F \equiv \chi^2/2 - \alpha S \qquad S \equiv -\int d\omega\, A(\omega) \ln\left(\frac{A(\omega)}{D(\omega)}\right)$$: entropy

Minimizing F

$$\left.\frac{\delta F}{\delta A}\right|_{A=\bar{A}} = 0 \Rightarrow \bar{A}(\omega)$$: the most likely solution

Stochastic method

K.S.D. Beach, arXiv:cond-mat/0403055

Equivalent!

$$H[n] \equiv \chi^2 = \int dx\, \epsilon(x) n(x) + \frac{1}{2}\int dx dy V(x-y) n(x) n(y)$$: Hamiltonian

Mean filed treatment

$$(n(x) - \bar{n}(x))(n(y) - \bar{n}(y)) \approx 0 \Rightarrow \bar{A}(\omega) = \bar{n}(\phi(\omega)) D(\omega)$$

Stochastic method: comparison with MEM(2)

S. Fuchs *et al.*, PRE81, 056701 (2010)

MEM

$$P[A|\bar{G}] = \frac{P[\bar{G}|A]P[A]}{P[\bar{G}]}$$

- Prior probability

$$P[A] \propto \exp(\alpha S)$$

- Likelihood function

$$P[\bar{G}|A] \propto \exp\left(-\chi^2/2\right)$$

- Posterior probability

$$P[A|\bar{G}] \propto e^{-F}$$

$$\Rightarrow \max P[A|\bar{G}] \leftrightarrow \min F \leftrightarrow \frac{\delta F}{\delta A} = 0$$

Stochastic method

$$P[n|\bar{G}] = \frac{P[\bar{G}|n]P[n]}{P[\bar{G}]}$$

- Prior probability

$$P[n] \propto \Theta[n]\delta\left(\int dx\, n(x) - \bar{G}(\tau_0)\right)$$

- Likelihood function

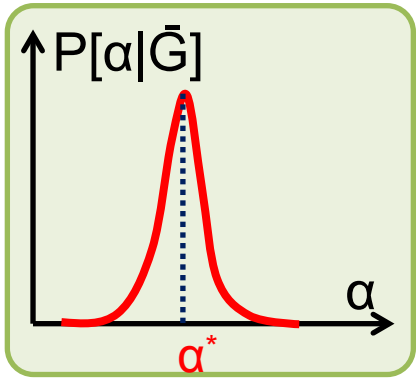
$$P[\bar{G}|n] \propto \exp\left(-\chi^2/2\alpha\right)$$

- Posterior probability

$$P[n|\bar{G}] = \Theta[n]\delta\left(\int dx\, n(x) - \bar{G}(\tau_0)\right) e^{-\chi^2/2\alpha}$$

$$\Rightarrow \langle n(x)\rangle_\alpha = \int \mathcal{D}n\, n(x) P[n|\bar{G}]$$

Stochastic method: eliminating α

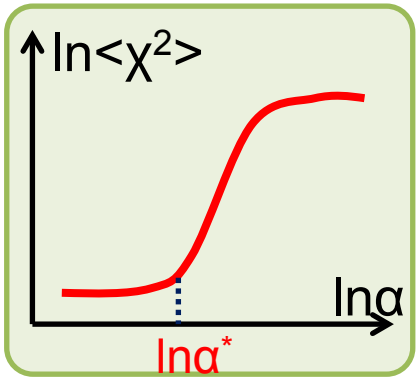


(a) By using the posterior probability P[α|Ḡ]

$$P[\alpha|\overline{G}] \propto P[\alpha] \int \mathcal{D}A\, e^{-\chi^2/2\alpha} \quad P[\alpha] = 1,\ 1/\alpha$$

Choosing α at the peak location of P[α|Ḡ] or
Taking average

$$\langle\langle A(\omega)\rangle\rangle \equiv \int d\alpha\, \langle A(\omega)\rangle_\alpha P[\alpha|\bar{G}]$$



(b) By using the log-log plot of α vs $\langle\chi^2\rangle$

Flat region at large α: default model dominant
Crossover region: both χ^2-fitting and the default model are important
Flat region at small α: χ^2-fitting dominant, overfitting

Choosing α at the kink of $\ln\langle\chi^2\rangle$

K.S.D. Beach, arXiv:cond-mat/0403055

Default models

- Resonance (Res)

$$\rho(\omega) = \frac{\Gamma M}{(\omega^2 - M^2)^2 + M^2\Gamma^2}\frac{\omega^2}{\pi} \qquad \Gamma = \Theta(\omega - \omega_0)\gamma_0 \left(1 - \frac{\omega_0^2}{\omega^2}\right)^5$$

- Transport peak (Trans)

$$\rho(\omega) = \frac{\omega\eta}{\omega^2 + \eta^2}$$

- Free Wilson (Free)

$$\rho(\omega) = \frac{N_c}{L^3}\sum_{\boldsymbol{k}} \sinh\left(\frac{\omega}{2T}\right)\left[b^{(1)} - b^{(2)}\frac{\sum_{i=1}^3 \sin^2 k_i}{\sinh^2 E_{\boldsymbol{k}}(m)}\right] \times \frac{\delta(\omega - 2E_{\boldsymbol{k}}(m))}{(1+\mathcal{M}_{\boldsymbol{k}}(m))^2 \cosh^2 E_{\boldsymbol{k}}(m)}$$

$$\cosh E_{\boldsymbol{k}}(m) = 1 + \frac{\mathcal{K}_{\boldsymbol{k}}^2 + \mathcal{M}_{\boldsymbol{k}}^2(m)}{2(1+\mathcal{M}_{\boldsymbol{k}}(m))}$$

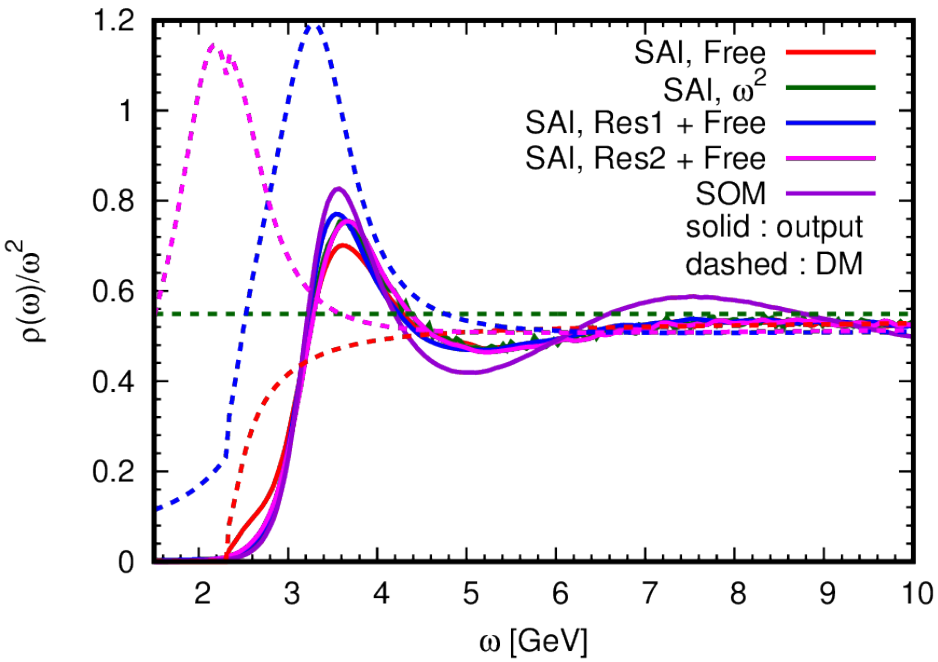
$$\mathcal{K}_{\boldsymbol{k}} = \sum_{i=1}^3 \gamma_i \sin k_i$$

$$\mathcal{M}_{\boldsymbol{k}}(m) = \sum_{i=1}^3 (1 - \cos k_i) + m$$

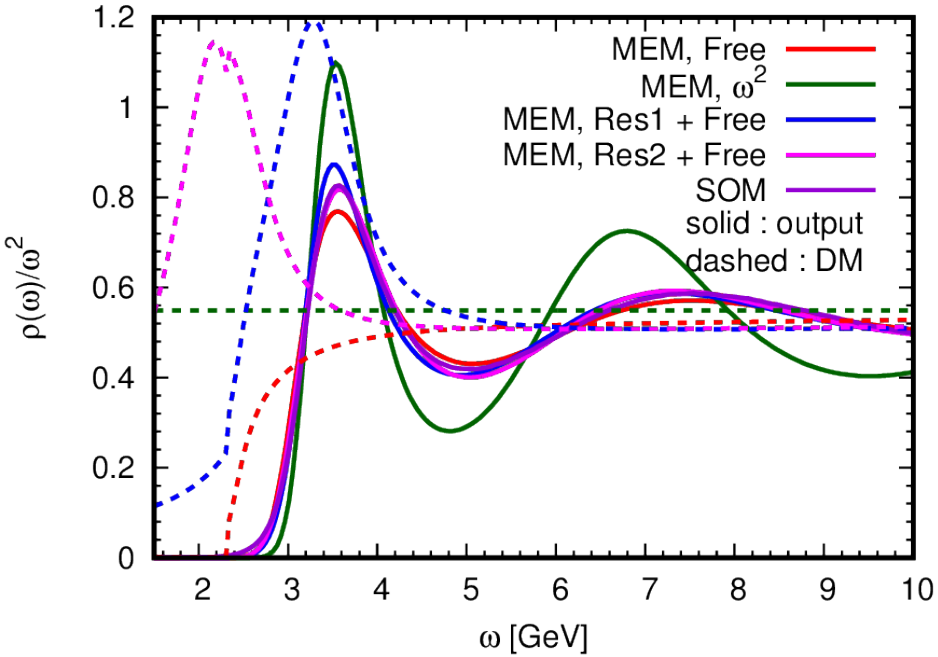
$b^{(1)} = 3$, $b^{(2)} = 1$ for the V channel

Default model dependence at $0.75T_c$ (1)

SAI



MEM



DM = Free, ω^2, Res1 + Free, Res2 + Free

Res1 : peak location ~ J/Ψ mass

Res2 : peak location < J/Ψ mass

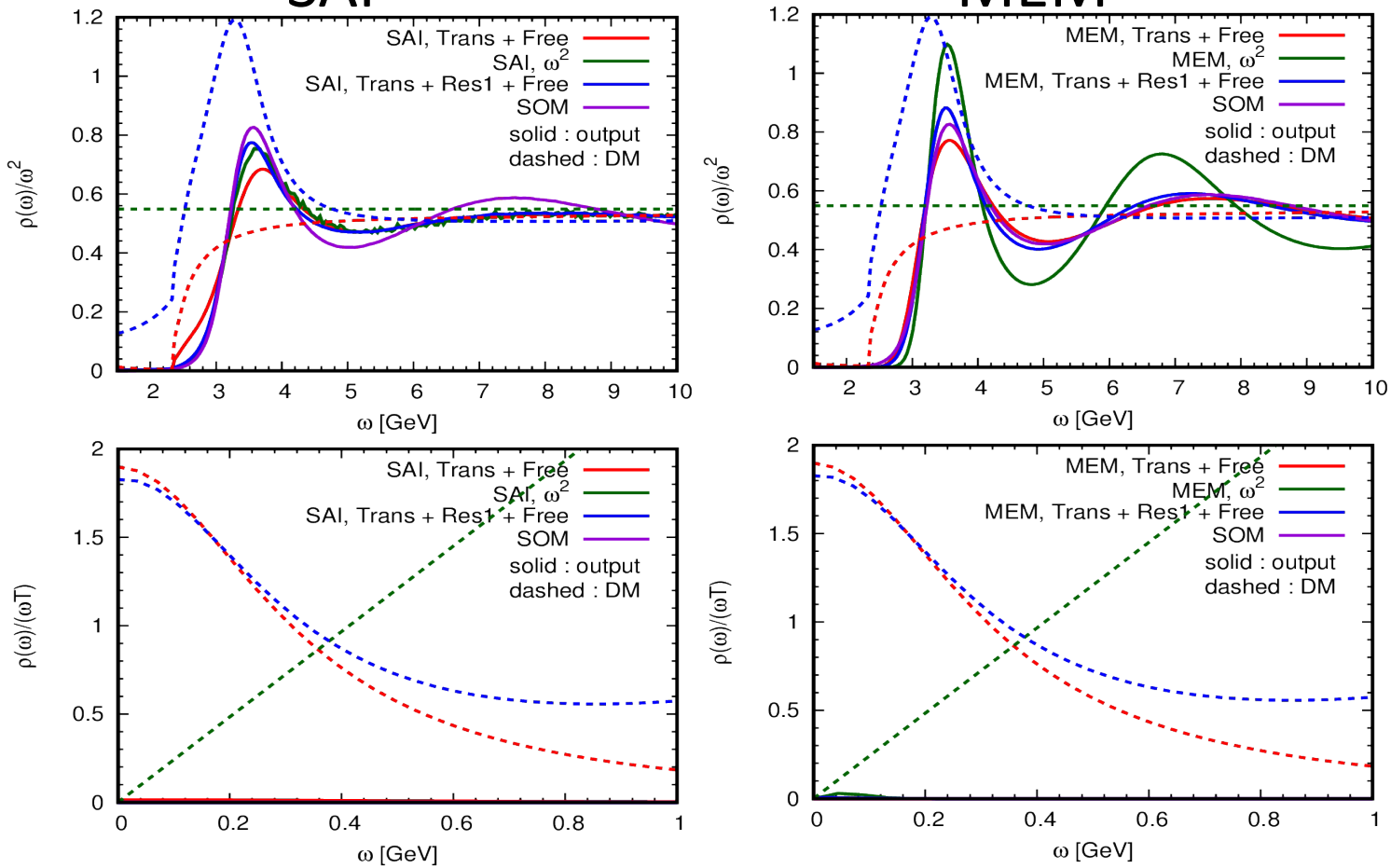
SAI and MEM have weak DM dependence except for $D(\omega) \sim \omega^2$ for MEM.

Default model dependence at $0.75T_c$ (2)

SAI MEM

High ω

Low ω



DM = Trans + Free, ω^2, Trans + Res1 + Free

The high ω part is insensitive to the transport peak of DM.

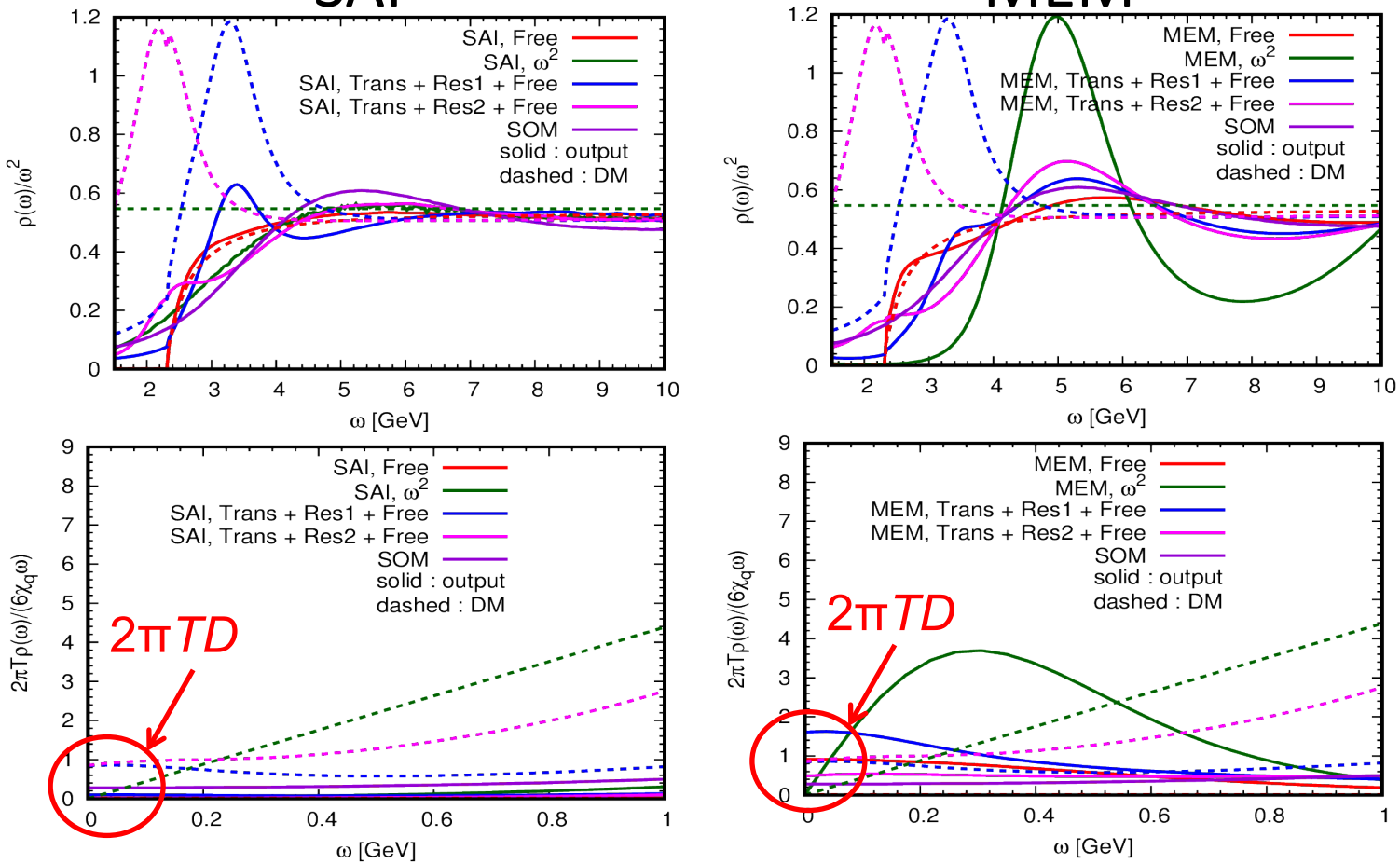
The intercept is quite small.

Default model dependence at 1.5T_c (1)

SAI | MEM

High ω

Low ω



DM = Free, ω^2, Trans1 + Res1 + Free, Trans1 + Res2 + Free Trans1 → 2πTD=1

There is no clear peak around J/Ψ, except for Trans+Res1+Free DM result for SAI.

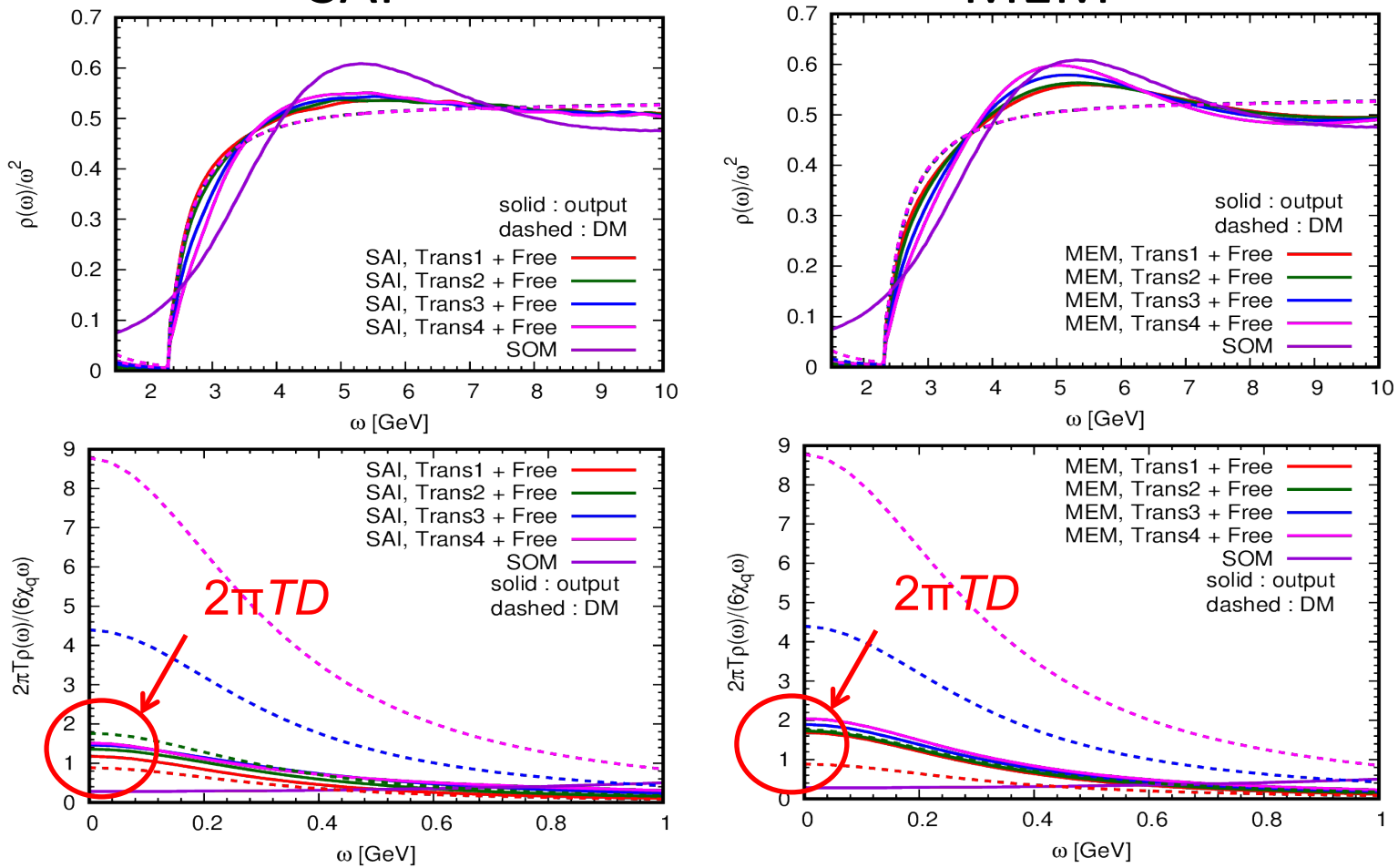
The intercept is quite small for SAI. ω^2 DM result for MEM has strange behavior.

Default model dependence at 1.5T_c (2)

SAI MEM

High ω

Low ω



DM = Trans(1-4) + Free Trans(1-4) → 2π*TD*~1, 2, 4, 9 (fixed width)

There is no clear peak around J/Ψ. The intercept seems to have an upper bound.

The intercept for SAI → 2π*TD* ~ 1.5, for MEM → 2π*TD* ~ 2