Comparison to relativistic free spectrum (see. hep-lat/0507004)

$$\rho(\omega) = \Theta(\omega^2 - 4M^2)\, \frac{N_c}{8\pi\omega} \sqrt{\omega^2 - 4M^2}\, \big(1 - 2n_F(\omega/2)\big)\big(\omega^2 k + 4M^2 k\big) + 2\pi\,\omega\,\delta(\omega)\, N_c\, \gamma$$

$\underset{\omega\to\infty}{\approx} \omega^2$

Now the lattice NRQCD version: We get the dispersion relation from our time evolution operator $K_{x,\tau+1} = \left(1 - a\frac{p^2}{2M}\right) K_{x,\tau} \Rightarrow aE_p = -\log\left(1 - \frac{p^2}{2Ma}\right)$

C++ exercise: Compute the NRQCD free spectral function for $Ma = 5$

Let us have a look at some actual real-world NRQCD data:

HotQCD $N_f = 2+1$ HISQ ensembles $48^3 \times 12$ $(T>0)$ $48^3 \times 32, 48, 64$ $(T\approx 0)$

$M_b a \in [2.8 \ldots 0.9]$ $n=4$ $\boxed{\text{Fig 8}}$ $\boxed{\text{Fig 9}}$ (see also: 1409.3630; 1402.6210; 1109.4496)

⇒ Notice mass difference between different lattice spacings → NRQCD energy shift

⇒ First hint at in-medium modification from correlator ratios. $\boxed{\text{Fig 10}}$ $\boxed{\text{Fig 11}}$

Correlators only give us information about global in-medium changes but we are interested in changes of individual states. Need spectral information (mass & width @ $T>0$). Once peaks acquire thermal width effective mass analysis fails (no plateau!)

Spectral function reconstruction using Bayesian inference

In general we have the relation $D(\tau) = \int d\omega\, K(\tau,\omega)\,\rho(\omega)$ which needs to be inverted. Since ρ can contain many features needs to be well resolved along ω: $D_i = \sum_{l=1}^{N_\omega} \delta\omega_l\, K_{il}\, \rho_l$

Relativistic $Q\bar{Q}$: $K = \frac{\cosh(\omega(\tau - \beta/2))}{\sinh(\omega\beta/2)}$

NRQCD $Q\bar{Q}$: $K = e^{-\omega\tau}$

Inversion is $\underbrace{\text{ill-posed}}_{N_\tau \ll N_\omega}$ and $\underbrace{\text{ill-conditioned}}_{D_i = D_i^{\text{ideal}} + \eta}$:

∞ solutions to χ^2 fit

Naive inversion in the case $N_\tau = N_\omega$ leads to exponential increase of noise.

Question: How to systematically regularize the problem?

Personal answer: Bayesian inference that allows to incorporate additional prior information on the spectrum. Subjective view of probability, assign $P[X]$ even if X is not random variable.

Multiplication law for prob.

$$P(\rho, D, I) = P[\rho|D,I]\cdot P[D|I] = P[D|\rho,I]\, P[\rho|I]$$

$$\underbrace{P[\rho|D,I]}_{\text{Posterior}} = \frac{\overbrace{P[D|\rho,I]}^{\text{Likelihood}}\ \overbrace{P[\rho|I]}^{\text{Prior}}}{\underbrace{P[D|I]}_{\text{Evidence}}}$$

↑ test function

see also: Phys. Rep. 269 (1996) 133

Likelihood: How compatible is the data with current spectrum?
Prior: How compatible is ρ with prior information.

- For sampled data sets, due to the law of large numbers we can assume Gaussian distributed data: $P(D|\rho,I] = e^{-L}$ $L = \sum_{ij} (D_i - D_i^\rho) C_{ij}^{-1} (D_j - D_j^\rho)$

$$C_{ij} = \frac{1}{N_m(N_m-1)} \sum_{e=1}^{N_m} (D_i^e - D_i)(D_j^e - D_j)$$

- The second ingredient is the prior probability
$P[\rho|I] = e^{-\alpha S[\rho,m]}$

α is a so called hyperparameter that weighs influence of data vs. prior information.

Prior information enters in two ways: By the functional form of S and by the choice of a function m, which fullfills $\frac{\delta S}{\delta \rho}\Big|_{\rho=m} = 0$ the so called default model. By definition it corresponds to the correct spectrum in the absence of data.

$\Rightarrow$ Eventually $\frac{\delta}{\delta\rho} P[\rho|D,I]\Big|_{\rho=\rho^{Bayes}} = 0$ defines the most probable spectrum in the Bayesian sense. Competition btw L & S.

On the market different implementations that differ in $P[\rho|I]$ and handling of α.

- Tikhonov: $S = \int d\omega\, (\rho - m)^2$

tune α such that $L = N_\tau$
(correct spectrum sampled with Gaussian noise gives $L = N_\tau$)

issue: pulls the result very strongly towards m

- Maximum Entropy Method (MEM): $S_{SJ} = \int d\omega \left(\rho - m - \rho \log\frac{\rho}{m}\right)$

tune α such that $P[D|I]$ extremal
(positive definite spectra, Shannon-Jaynes entropy derived from arguments in 2d image reconstruction)

issue: flat directions make numerical search difficult.

- Bayesian reconstruction method (BR): $S_{BR} = \int d\omega \left(1 - \frac{\rho}{m} + \log\left(\frac{\rho}{m}\right)\right)$

assume no knowledge of α and integrate out using $P[\alpha]$
enforce $L = N_\tau$ in addition.

issue: for small # of datapoints susceptible to ringing artefacts

<u>How to derive the BR regulator:</u> 4 Axioms (see: 1307.6106)

① <u>Subset independence</u>

Consistently combine prior information in different frequency regimes. (Probabilities multiply)

$S \propto \int d\omega\, s[\rho(\omega), m(\omega)]$

X

② Scale invariance:

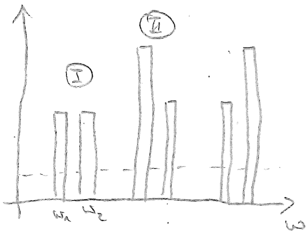
Contrary to statements in the literature, ρ itself does NOT need to behave like a probability distribution. Scaling depends on the corresponding correlator

$\rho^{NRQCD}_{QQ} \sim \sqrt{\omega}$ $\quad \rho^{vel.}_{QQ} \sim \omega^2$ $\quad \rho_{WL} \sim \frac{1}{\omega}$ $\quad \rho_{EMT} \sim \omega^4$

To make the results independent of the units used we only allow ratio of quantities to enter with some scaling. $\Rightarrow$ $S \propto \tilde{\alpha} \int d\omega \; s[\frac{\rho}{m}]$

Introduce a positive hyperparameter with units $[\tilde{\alpha}] = \frac{1}{[d\omega]}$.

③ Smoothness: When the data does not encode peaked structures the spectrum shall remain smooth. Use here maximally un-informative default model. $m(\omega) = m$.



Penalize deviations between neighbouring ρ values: $v_1 = \frac{\rho_1}{\omega_1}$ $\quad v_2 = \frac{\rho_2}{\omega_2}$.

I vs. II $\quad 2s(v) - s(v(1+\epsilon)) - s(v(1-\epsilon)) = \epsilon^2 C_2$

since $v>0$ us multiplicative factor

same penalty for I and II

$\Rightarrow \; -v^2 s''(v) = C_2$

Solution: $S = \tilde{\alpha} \int d\omega \left(C_0 - C_1 \frac{\rho}{m} + C_2 \log\left(\frac{\rho}{m}\right)\right)$

④ Bayesian meaning of S: $\quad S'(v=1) = 0, \quad S''(v=1) < 0$ $\quad$ (convention $S(v=1)=0$)

after absorbing overall positive factor into $\tilde{\alpha}$

$S_{BR} = \alpha \int d\omega \left(1 - \frac{\rho}{m} + \log\frac{\rho}{m}\right)$ $\quad$ is strictly concave $S<0$ $\frac{\delta^2 S}{\delta \rho^2} < 0$, i.e. $-L + \alpha S$ has unique extremum.

How to handle α: Make its role explicit and marginalize

$$P(\rho, D, \alpha, m) = P[D|\rho,\alpha,m]\, P[\rho|\alpha,m]\, P[\alpha|m]\, P[m]$$
$$= P[\alpha|\rho,D,m]\, P[\rho|D,m]\, P[D|m]\, P[m]$$

$P(D|\rho,\alpha,m] = P[D|\rho,m]$

$P[\alpha|m] = P[\alpha] \doteq 1$

$$\Rightarrow \; P[\rho|D,m] = \frac{P[D|\rho,I]}{P[D|I]} \int d\alpha\, P[\rho|\alpha,m]$$

In addition we also enforce $L = N_\tau$ as further constraint.

Show example of spectral reconstruction mock test [Fig 12] [Fig 13]

Different Non-Bayesian methods available

① Backus-Gilbert: Basic idea: if the kernel is a δ-function the correlator equals the spectrum

⇒ Find linear combination of data-points that maximizes "peaked ness" of the kernel.

issue: Implicit prior information in the optimization criterion.

② Padé-approximation: Basic idea: Project the data onto a set of rational basis functions on which the inversion is computed analytically.

issue: Data needs to be extremely precise, otherwise large oscillations when inverting analytically do not cancel.

Show results from actual NRQCD studies $\boxed{\text{Fig 14}}$ $\boxed{\text{Fig 15}}$

<u>Caveats:</u> Temperature changes from: different # of data points, need to disentangle method systematics from in-medium physics.

in NRQCD: Since kernel T independent, truncate T=0 data set to $N_\tau^{T>0}$ and redo reconstruction (As if same spectrum is encoded at higher T)

relativistic: T-dependent kernel, need to compute "reconstructed correlator"

$$G^{rec}(\tau, \underset{\substack{\uparrow \\ \text{meas}}}{T}, \underset{\substack{\uparrow \\ \text{orig}}}{T'}) = \sum_{\tau'=\tau,\, \Delta\tau'=N_\tau}^{N_\tau'-N_\tau+\tau} G(\tau', T')$$

(see also: 1204.4945)

<u>Error analysis:</u>

statistical: Jackknife resampling; repeat the reconstruction with a subset of simulated correlators.

systematic: Change the default model and observe which parts of the reconstructed spectrum remain robust.

BOTH NEED TO BE CARRIED OUT!