今後の将来展望: HΦ

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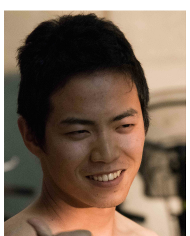
1. Finite-*T* linear response

Computational Science Alliance
The University of Tokyo

New function will be implemented: Finite-T linear response

Combination of TPQ and Kω

Y. Yamaji, T. Suzuki, & M. Kawamura, arXiv:1802.02854.



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Finite-Temperature Spectra

$$\mathcal{G}_\beta^{AB}(\omega) = \sum_{n,m} \frac{e^{-\beta E_n}}{Z(\beta)} \frac{\langle n|\hat{A}^\dagger|m\rangle\langle m|\hat{B}\ |n\rangle}{\omega + i\delta + E_n - E_m}$$

$$Z(\beta) = \sum_n e^{-\beta E_n}$$

$$\mathcal{G}_\beta^{AB}(\omega) = \sum_{n} \frac{e^{-\beta E_n}}{Z(\beta)} \langle n|\hat{A}^\dagger \frac{1}{\omega + i\delta + E_n - \hat{H}} \hat{B}\ |n\rangle$$

Complexity	$\mathcal{O}(N_{\mathrm{H}}^3)$
Memory	$\mathcal{O}(N_{\mathrm{H}}^2)$

Is it necessary? Answer is No

Finite-Temperature Spectra by Real-Time Evolution of Wave Functions

T. Iitaka and T. Ebisuzaki, Phys. Rev. Lett. 90, 047203 (2003).
R. Steinigeweg, J. Gemmer, and W. Brenig, Phys. Rev. Lett. 112, 120601 (2014).
T. Monnai and A. Sugita, J. Phys. Soc. Jpn. 83, 094001 (2014).
C. Karrasch, D. M. Kennes, and J. E. Moore, Phys. Rev. B 90, 155104 (2014).
F. Jin, R. Steinigeweg, F. Heidrich-Meisner, K. Michielsen, and H. De Raedt,
Phys. Rev. B 92, 205103 (2015).

Finite-Temperature Spectra by Micorocanonical Ensemble

M. W. Long, P. Prelovsek, S. El Shawish, J. Karadamoglou, and X. Zotos,
Phys. Rev. B 68, 235106 (2003).
X. Zotos, Phys. Rev. Lett. 92, 067202 (2004).

An Intuitive Description of TPQ States and Green's Function at Finite Temperature

A normalized TPQ state

$$|\psi_\beta\rangle \equiv \frac{|\phi_\beta\rangle}{\sqrt{\langle\phi_\beta|\phi_\beta\rangle}} \sim \sum_n e^{i\varphi_n} \frac{e^{-\frac{\beta}{2}E_n}}{\sqrt{Z(\beta)}} |n\rangle$$

Spectral projector

$$\hat{P}_n = |n\rangle\langle n|$$

Green's function rewritten by using a TPQ state

$$\mathcal{G}_\beta^{AB}(\zeta) \sim \sum_n \langle\psi_\beta|\hat{P}_n \hat{A}^\dagger \frac{1}{\zeta + E_n - \hat{H}} \hat{B} \hat{P}_n |\psi_\beta\rangle$$

An Alternative to Spectral Projection

T. Kato, Progress of Theoretical Physics 4, 514 (1949).

$$\hat{P}_{\gamma,\rho} = \frac{1}{2\pi i} \oint_{C_{\gamma,\rho}} \frac{dz}{z - \hat{H}}$$

$$z = \rho e^{i\theta} + \gamma$$

$$|\phi\rangle = \sum_n d_n |n\rangle$$

$$\hat{P}_{\gamma,\rho}|\phi\rangle = \sum_{E_n \in (\gamma-\rho, \gamma+\rho)} d_n |n\rangle$$

T. Sakurai and H. Sugiura,
J. Comput. Appl. Math. 159, 119 (2003).
T. Ikegami, T. Sakurai, and U. Nagashima,
J. Comput. Appl. Math. 233, 1927 (2010).

Discretized by Riemann sum

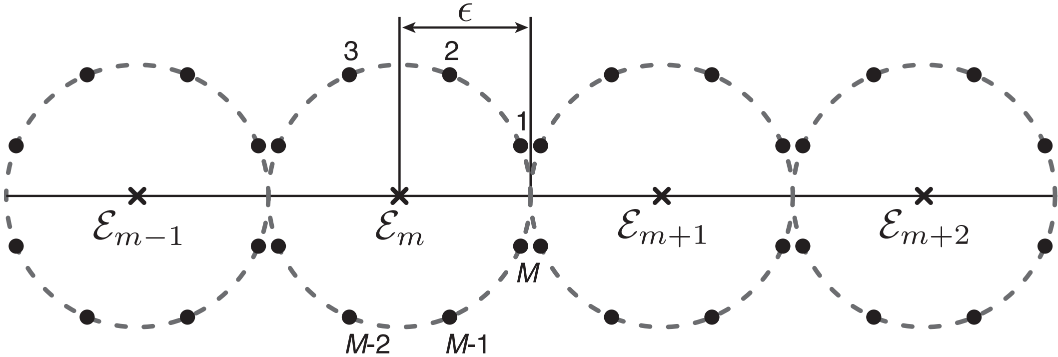
$$\hat{P}_{\gamma,\rho,M} = \frac{1}{M} \sum_{j=1}^{M} \frac{\rho e^{i\theta_j}}{\rho e^{i\theta_j} + \gamma - \hat{H}}$$

$$\theta_j = 2\pi(j - 1/2)/M$$

Finite-Temperature Green's Function by Typical Pure States

$$|\psi^m_{\beta,\boldsymbol{\delta}}\rangle = \hat{P}_{\mathcal{E}_m,\epsilon,M}|\psi_\beta\rangle$$

$$\boldsymbol{\delta} = (E_0, \epsilon, M)$$



$$\mathcal{E}_m = E_0 + (2m-1)\epsilon$$

Green's funtion

$$\widetilde{\mathcal{G}}^{AB}_{\beta,\boldsymbol{\delta}}(\zeta) = \sum_{m\geq 0}\langle\psi^m_{\beta,\boldsymbol{\delta}}|\hat{A}^\dagger\frac{1}{\zeta+\mathcal{E}_m-\hat{H}}\hat{B}|\psi^m_{\beta,\boldsymbol{\delta}}\rangle$$

$$\mathcal{G}^{AB}_{\beta}(\zeta) = \lim_{\epsilon\to+0}\lim_{M\to+\infty}\mathbb{E}\left[\widetilde{\mathcal{G}}^{AB}_{\beta,\boldsymbol{\delta}}(\zeta)\right]$$

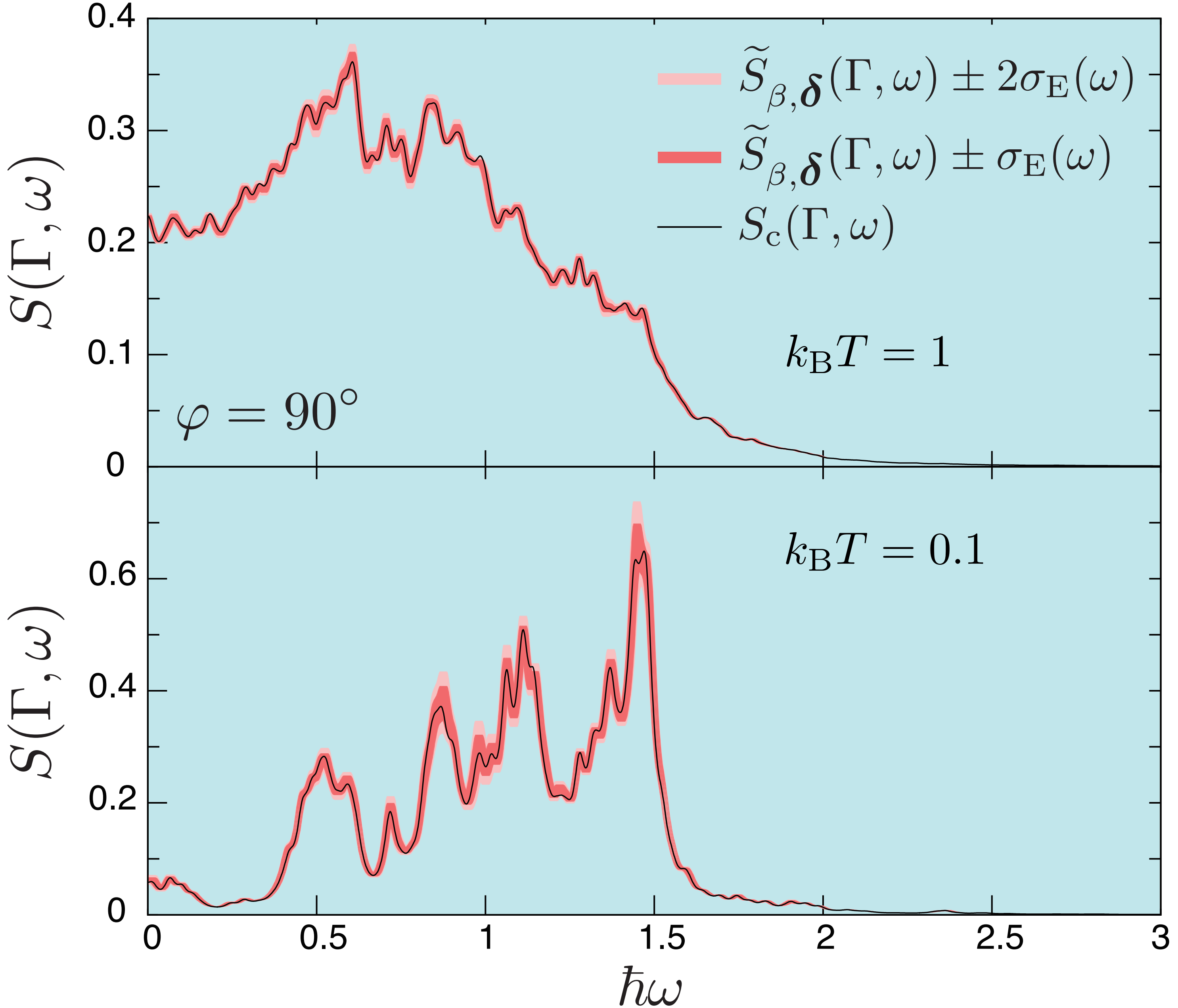
Probability distribution

$$\widetilde{P}_{\boldsymbol{\delta}}(\mathcal{E}_m) = \langle\psi^m_{\beta,\boldsymbol{\delta}}|\psi^m_{\beta,\boldsymbol{\delta}}\rangle$$

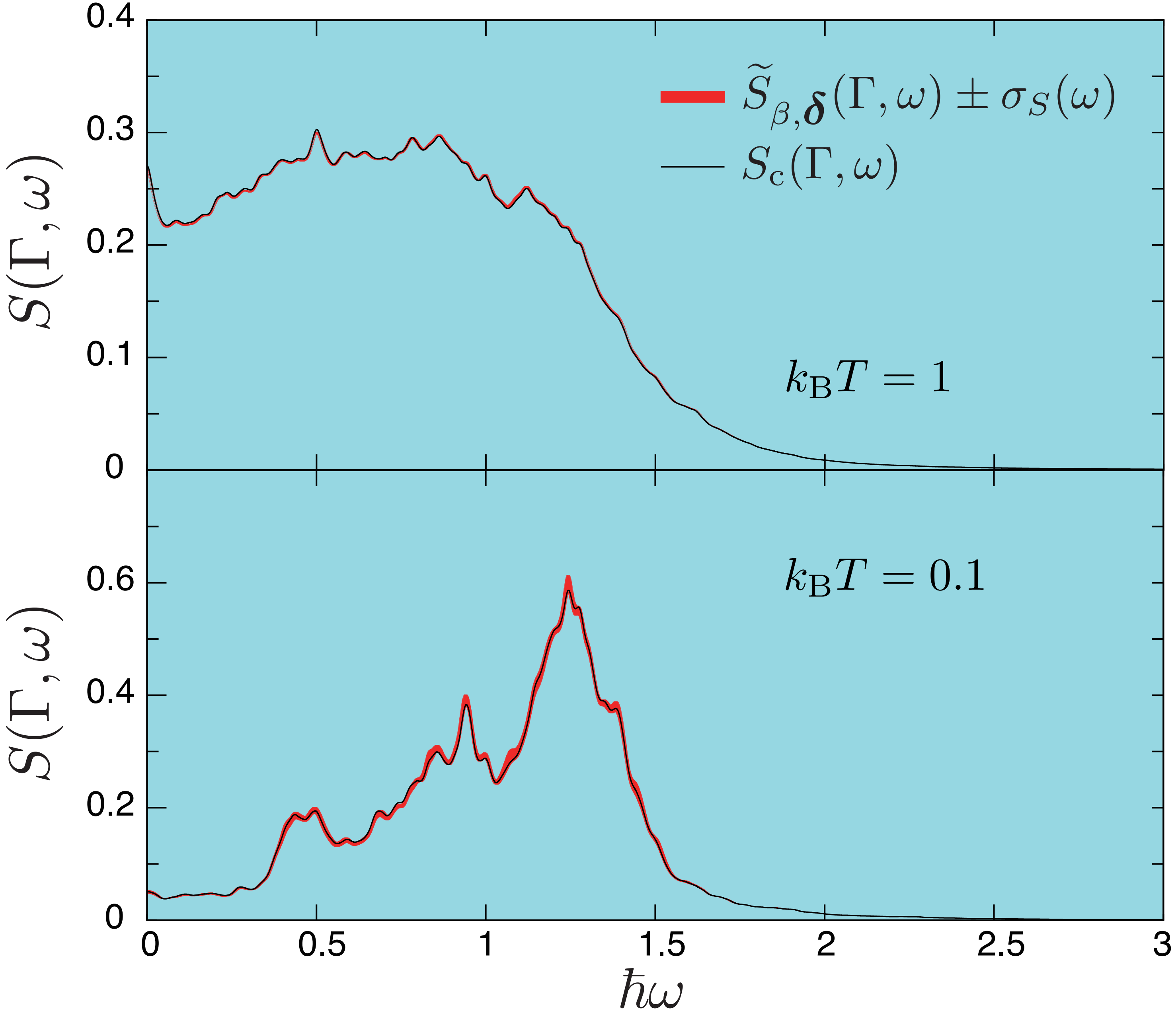
cf.) N. Shimizu, Y. Utsuno, Y. Futamura, T. Sakurai,T. Mizusaki, and T. Otsuka, Physics Letters B 753, 13 (2016).

12 site AF Kitaev

Standard deviation of averaged values

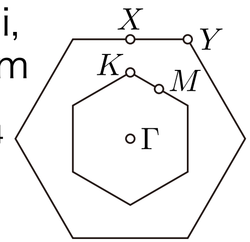


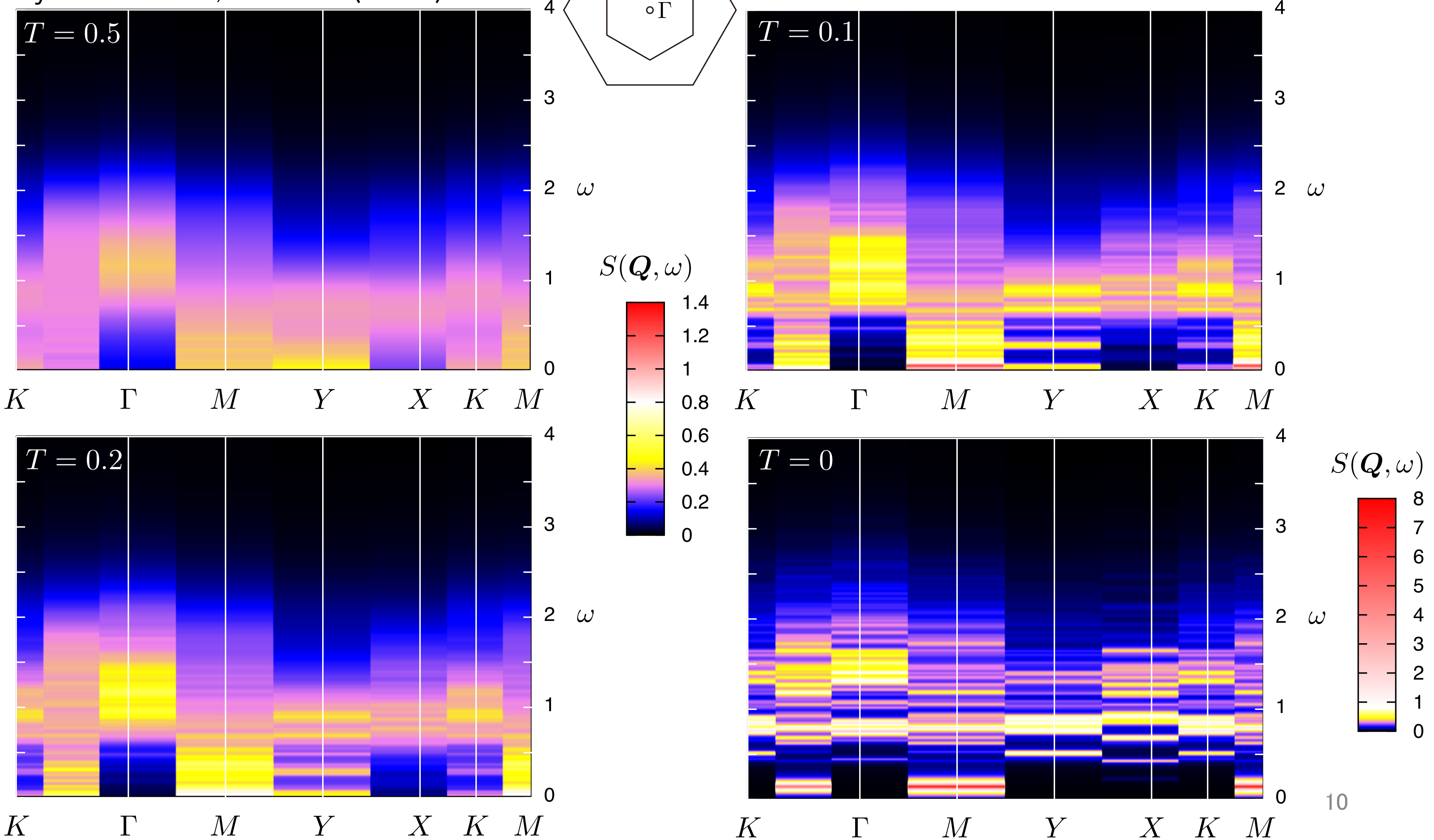
18 site AF Kitaev Standard deviation



Example of Finite-T $S(Q,\omega)$ of Γ model

A. M. Samarakoon, G. Wachtel, Y. Yamaji, D. A. Tennant, C. D. Batista, and Y. B. Kim
Phys. Rev. B 98, 045121 (2018)





Future Plan

New functions will be implemented

1. Finite-T linear response:
   Combination of TPQ and Kω
2. Tool for optimizing model parameters to fit experimental measurements
   -Example: Find an effective spin Hamiltonian that reproduces an observed magnetizaion process
3. Symmetry
   -Reduction of dimension of Hilbert space
   -Analysis of wave fucntions