今後の将来展望: HΦ

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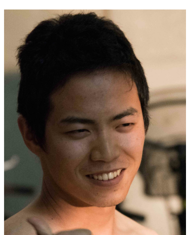
1. Kωの応用: Finite-T linear response
2. 今後の開発目標 Perspective

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).

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

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

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

Discretized by Riemann sum

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).

$$\hat{P}_{\gamma,\rho,M} = \frac{1}{M}\sum_{j=1}^{M} \frac{\rho e^{i\theta_j}}{\rho e^{i\theta_j} + \gamma - \hat{H}} \qquad \theta_j = 2\pi(j-1/2)/M$$

Shifted Krylov Subspace Method

$$\vec{x} = \frac{1}{\rho e^{i\theta_j} + \gamma - \hat{H}} \vec{b}$$

Liner equations

$$(z\mathbf{1} - H)\vec{x} = \vec{b}$$

$$\Rightarrow G_{\hat{O}}(z) = \vec{b}^{\dagger}\vec{x}$$

$$\vec{b} \doteq \hat{O}|\psi\rangle$$

$$\vec{x} \doteq (z\mathbf{1} - \hat{H})^{-1}\hat{O}|\psi\rangle$$

←Solvable by Shifted Krylov subspace method

A. Frommer (1995, 2003)

T. Sogabe, T. Hoshi, S. L. Zhang, and T. Fujiwara, *A numerical method for calculating the Green's function arising from electronic structure theory*, In Frontiers of Computational Science. pp.189-195, 2007.

Shifted CG: Algorithm

Initial $\vec{r}_0 = \vec{b},\ \alpha_{-1} = 1,\ \rho_{-1} = +\infty,$
$\pi_0^\sigma = \pi_{-1}^\sigma = 1,\ \vec{p}_{-1}^\sigma = \vec{x}_{-1}^\sigma = \vec{0}$

For $k = 0, 1, \ldots, m$

-Seed equations

$$
\begin{aligned}
\rho_k &= \vec{r}_k^T \vec{r}_k \\
\beta_{k-1} &= \frac{\rho_k}{\rho_{k-1}} \\
\alpha_k &= \frac{\rho_k}{\vec{r}_k^T A \vec{r}_k - \beta_{k-1} \frac{\rho_k}{\alpha_{k-1}}} \\
\vec{r}_{k+1} &= \left(1 + \frac{\alpha_k \beta_{k-1}}{\alpha_{k-1}}\right) \vec{r}_k - \alpha_k A \vec{r}_k - \frac{\alpha_k \beta_{k-1}}{\alpha_{k-1}} \vec{r}_{k-1}
\end{aligned}
$$

-Shifted equations

$$
\begin{aligned}
\pi_{k+1}^\sigma &= (1 + \alpha_k \sigma) \pi_k^\sigma - \frac{\alpha_k \beta_{k-1}}{\alpha_{k-1}} (\pi_{k-1}^\sigma - \pi_k^\sigma) \\
\vec{p}_k^\sigma &= \frac{1}{\pi_k^\sigma} \vec{r}_k + \beta_{k-1} \left(\frac{\pi_{k-1}^\sigma}{\pi_k^\sigma}\right)^2 \vec{p}_{k-1}^\sigma \\
\vec{x}_k^\sigma &= \vec{x}_{k-1}^\sigma + \frac{\pi_k^\sigma}{\pi_{k+1}^\sigma} \alpha_k \vec{p}_k^\sigma
\end{aligned}
$$

Seed switch

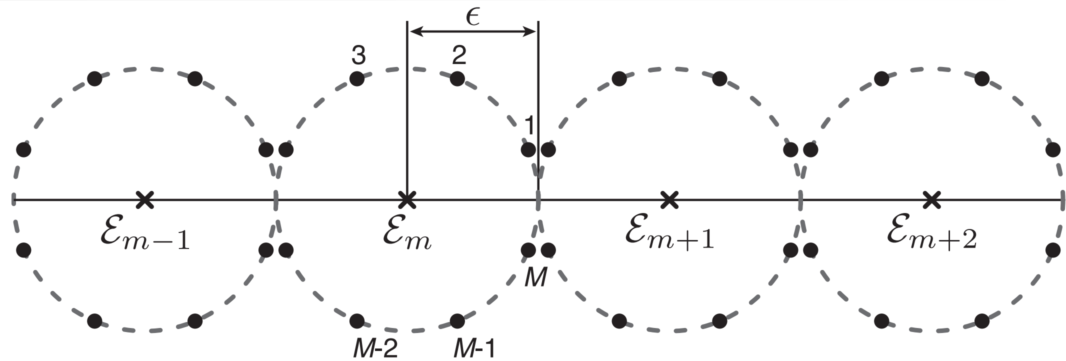
S. Yamamoto, *et al.*,
J. Phys. Soc. Jpn. 77, 114713 (2008).

Library Kω
by Dr. Kawamura (ISSP)

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

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

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

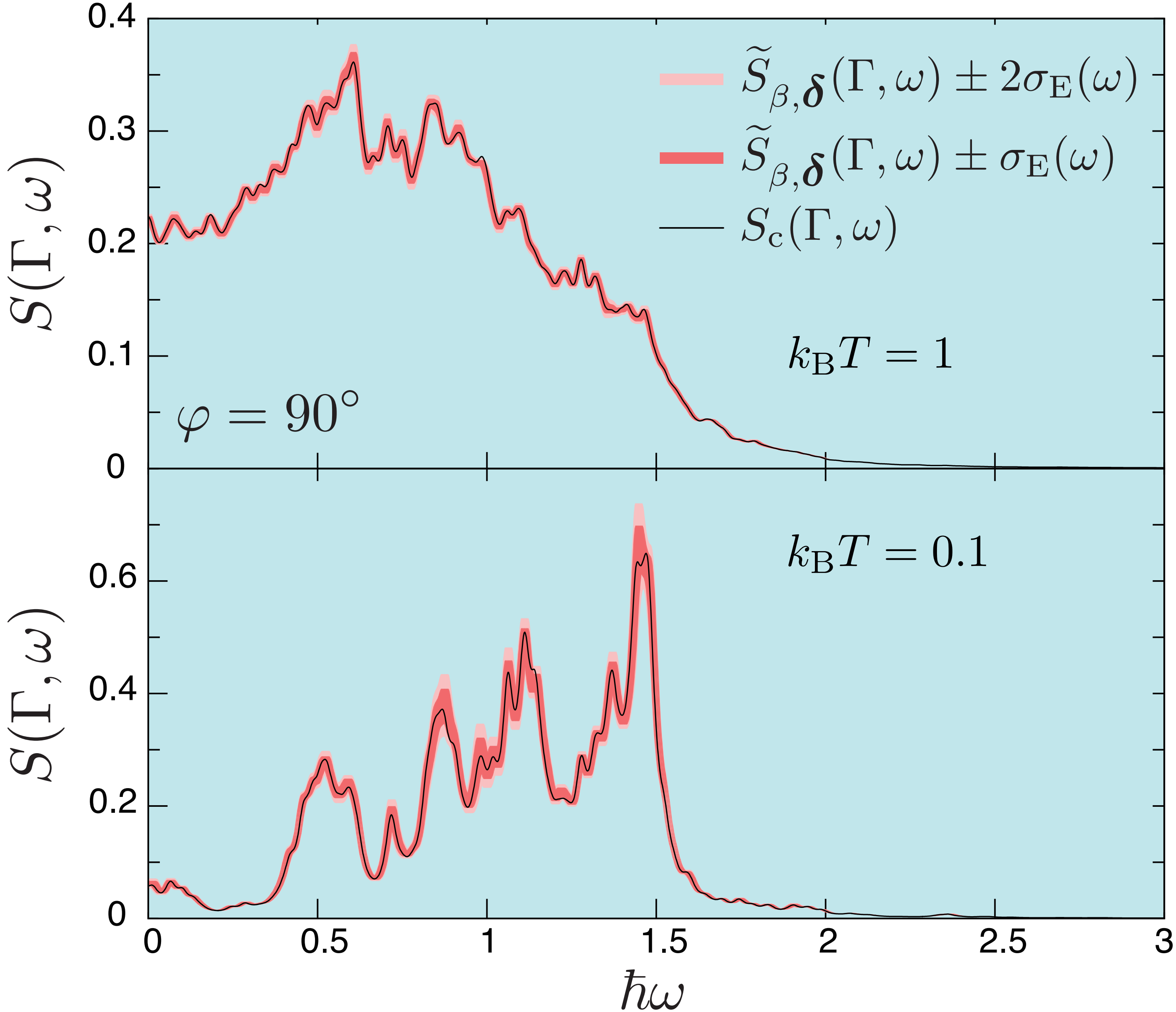
Probability distribution

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

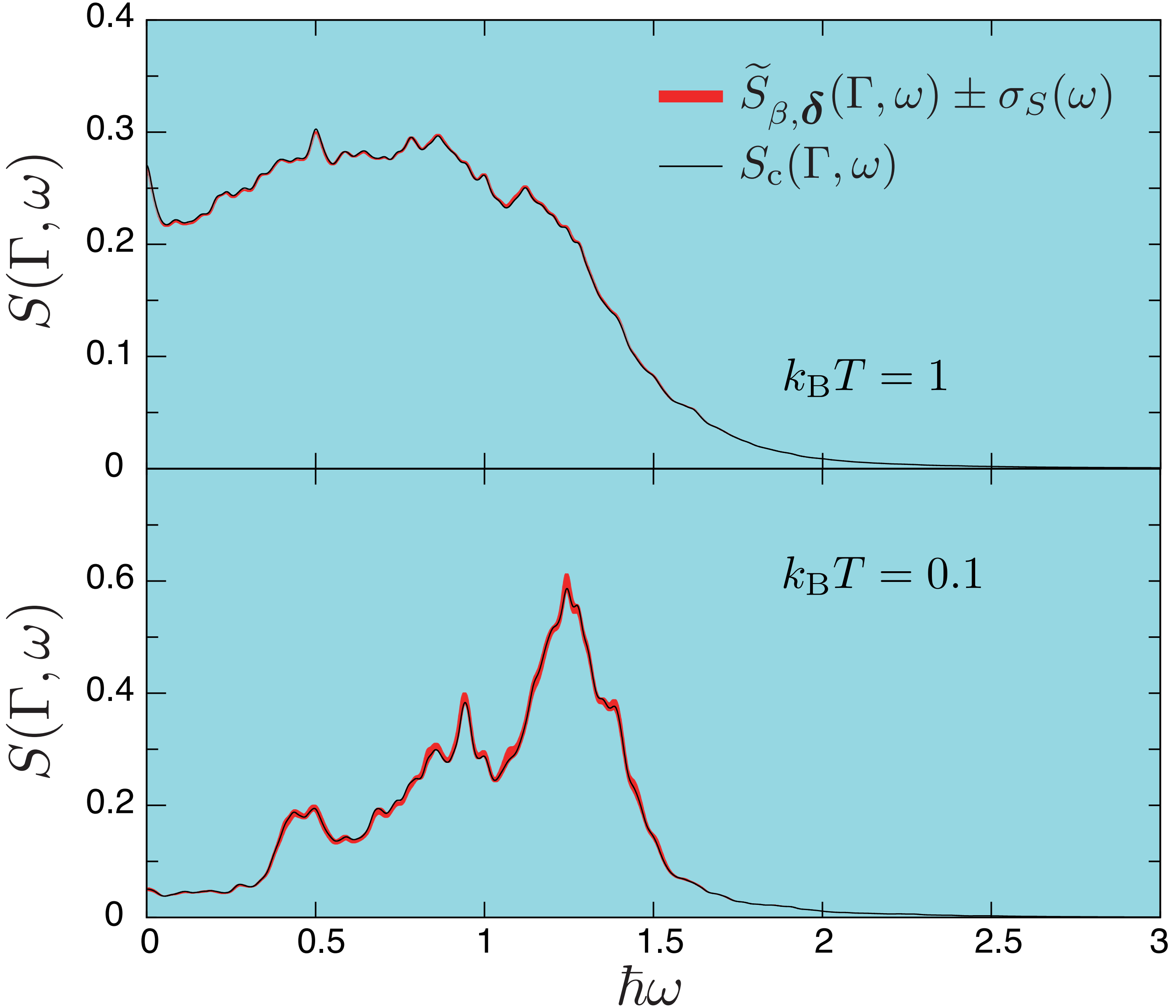
cf.) N. Shimizu, Y. Utsuno, Y. Futamura, T. Sakurai,T. Mizusaki, and T. Otsuka, Physics Letters B 753, 13 (2016).

12 site AF Kitaev

Standard deviation of averaged values

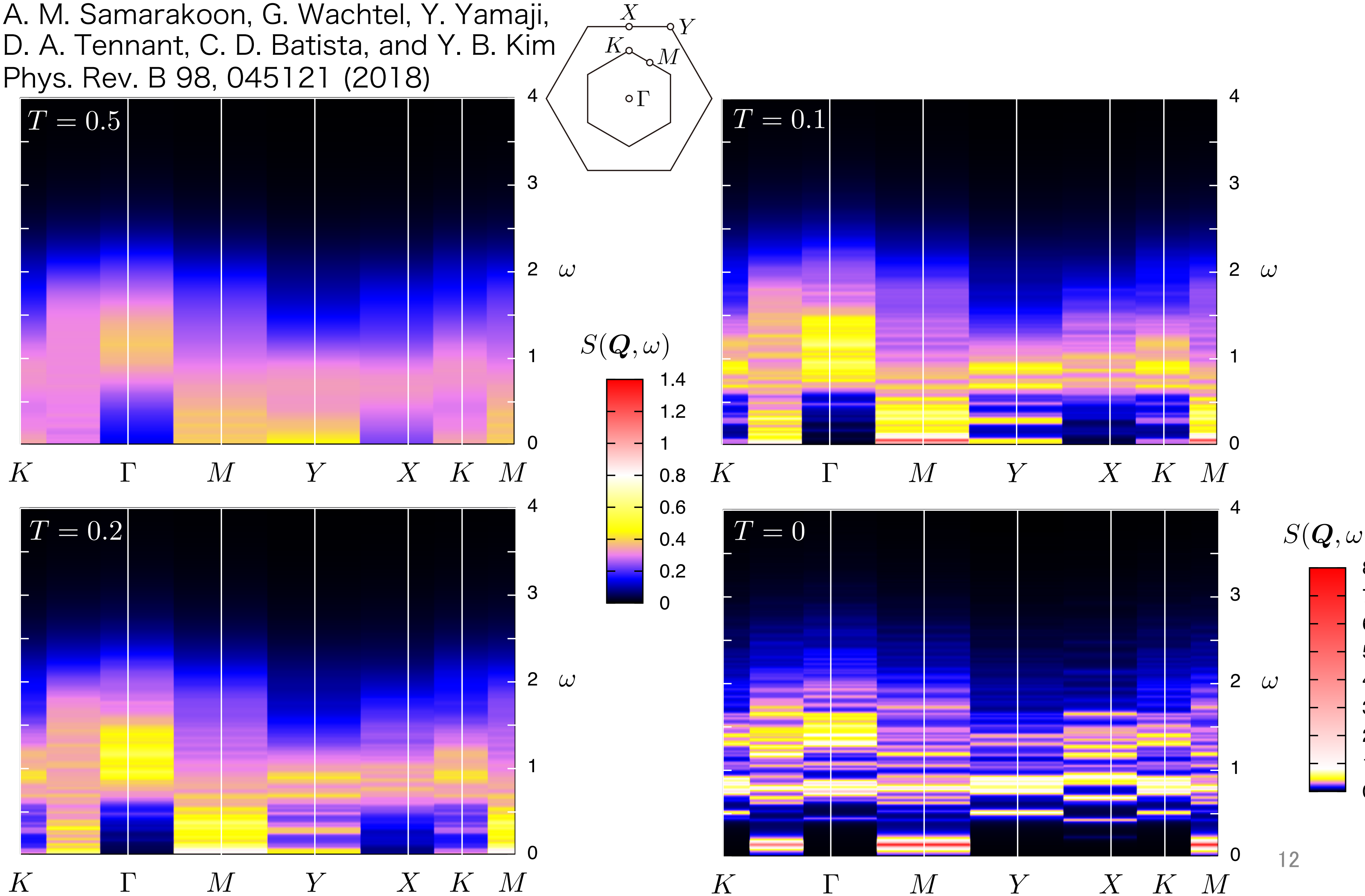


18 site AF Kitaev Standard deviation



Finite-T $S(Q,\omega)$ of a Frustrated Magnets: 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. *N* spin/body interaction and Green's function
3. Tool for optimizing model parameters to
   fit experimental measurements
   -Example: Find an effective spin Hamiltonian that
   reproduces an observed magnetizaion process
4. Symmetry
   -Reduction of dimension of Hilbert space
   -Analysis of wave fucntions