今後の将来展望: HΦ

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目標: 実験データから有効ハミルトニアンの推定
新しい機能: Finite-T linear response

Computational Science Alliance
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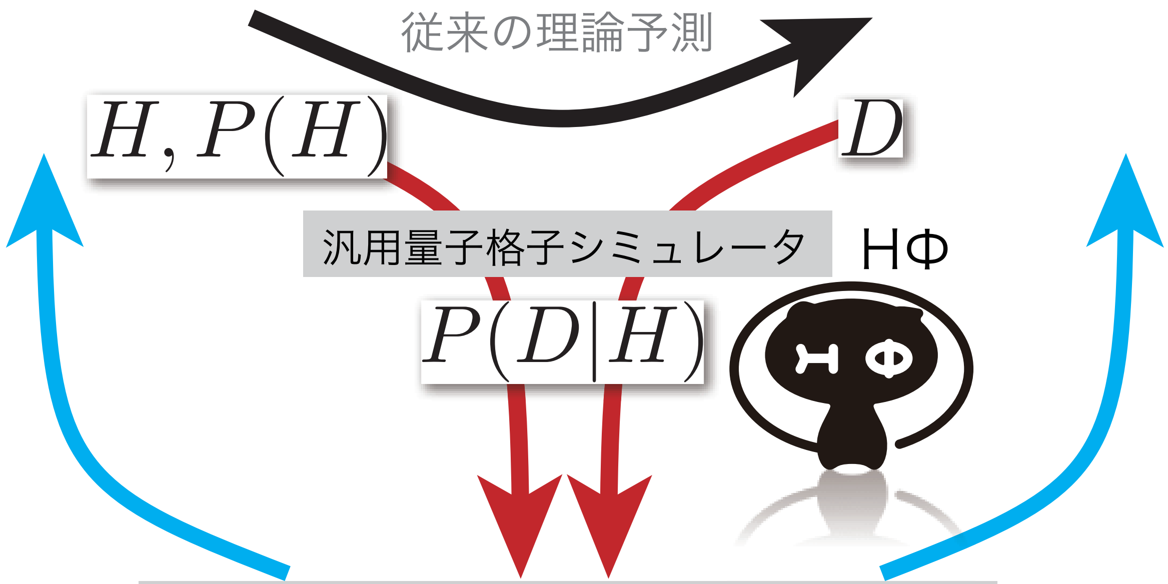
Future Perspective of HΦ

理論・計算科学による
有効ハミルトニアン H

ハバード模型, ハイゼンベルグ模型,
第一原理ハミルトニアン, …

実験データ D

比熱, 磁化過程,
中性子散乱, X線散乱,
光電子分光, …



ベイズの定理による有効ハミルトニアン推定

$$P(H|D) \propto P(D|H)P(H)$$

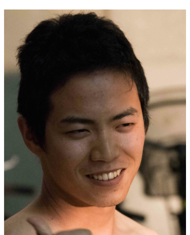
RESPACK
https://sites.google.com/view/kazuma7k6r

combo
https://github.com/tsudalab/combo

計算可能な物理量を増やしていく: 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

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

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

Shifted Krylov Subspace Method

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

Liner equations

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

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

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

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

←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

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

-Shifted equations

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

Seed switch

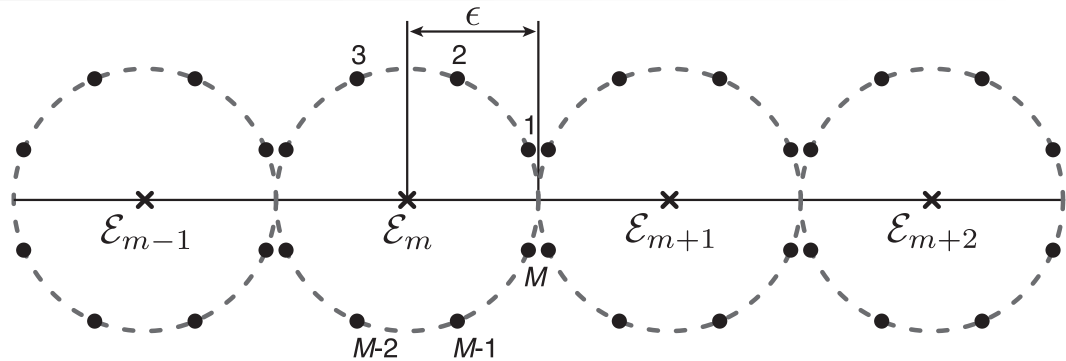
S. Yamamoto, *et al.*,
J. Phys. Soc. Jpn. 77, 114713 (2008).

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

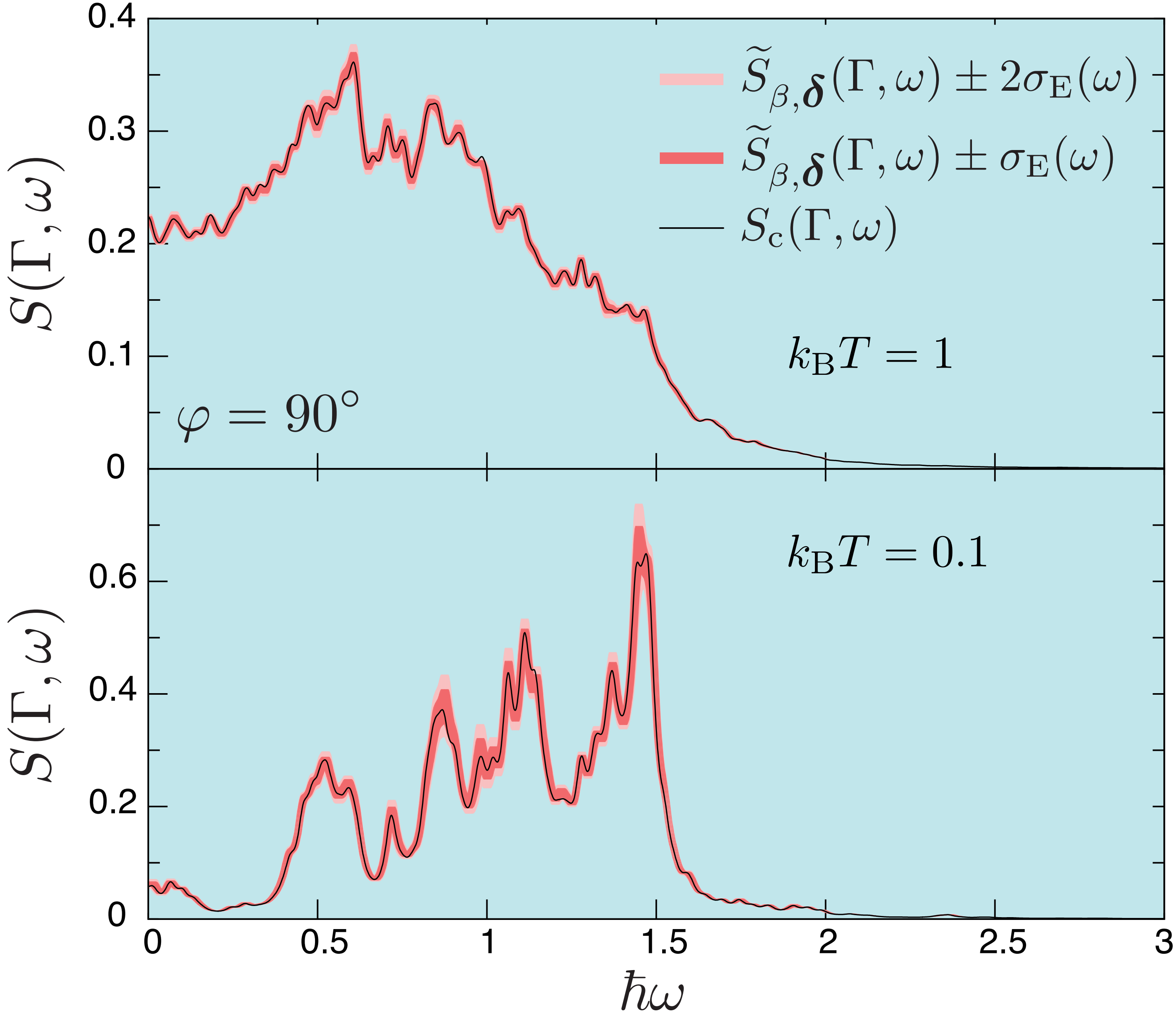
$$\widetilde{\mathcal{G}}^{AB}_{\beta,\boldsymbol{\delta}}(\zeta) = \sum_{m\geq 0} \langle\psi^m_{\beta,\boldsymbol{\delta}}|\hat{A}^\dagger \frac{1}{\zeta + \mathcal{E}_m - \hat{H}} \hat{B}|\psi^m_{\beta,\boldsymbol{\delta}}\rangle$$

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

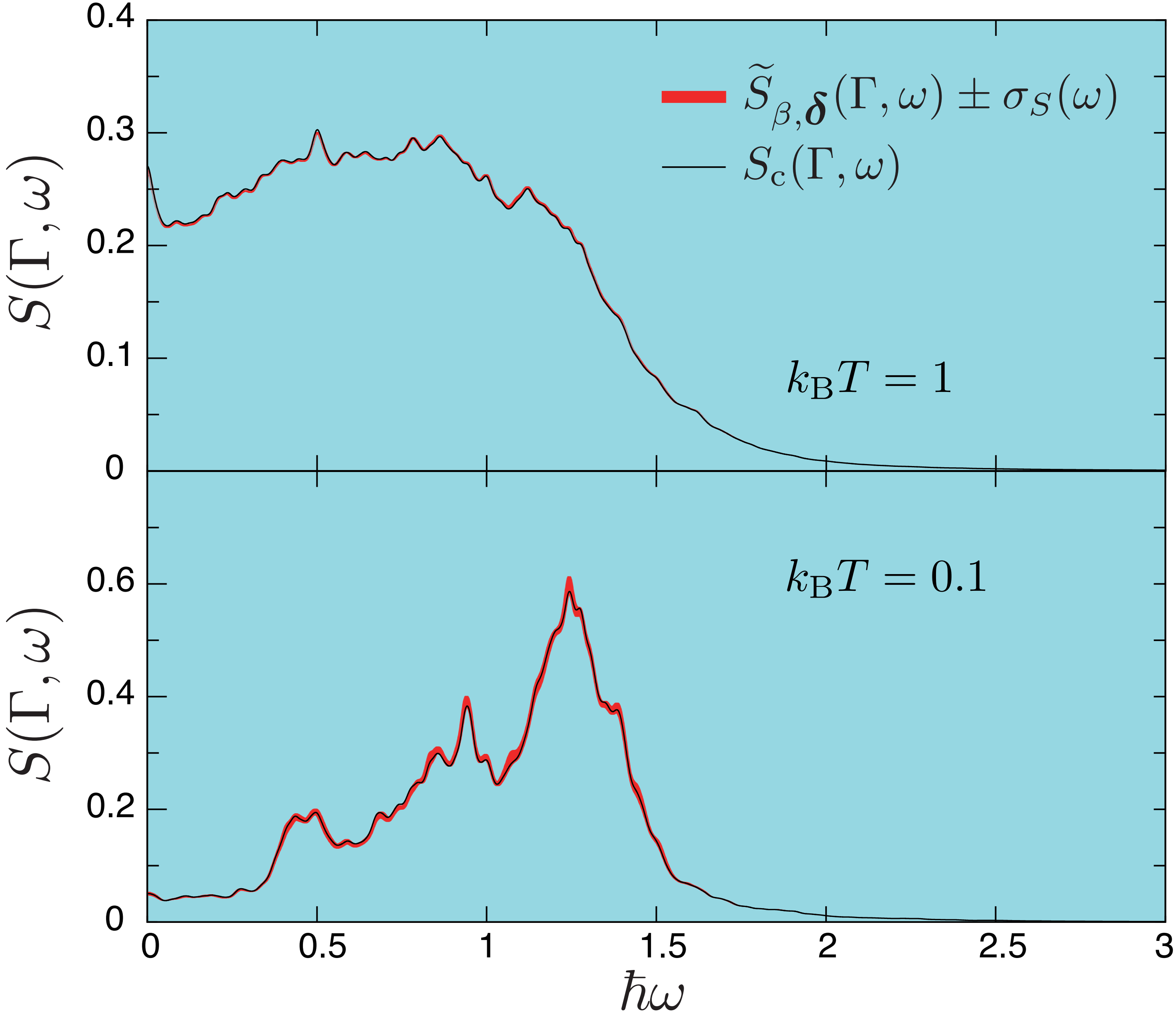
Probability distribution $\widetilde{P}_{\boldsymbol{\delta}}(\mathcal{E}_m) = \langle\psi^m_{\beta,\boldsymbol{\delta}}|\psi^m_{\beta,\boldsymbol{\delta}}\rangle$

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

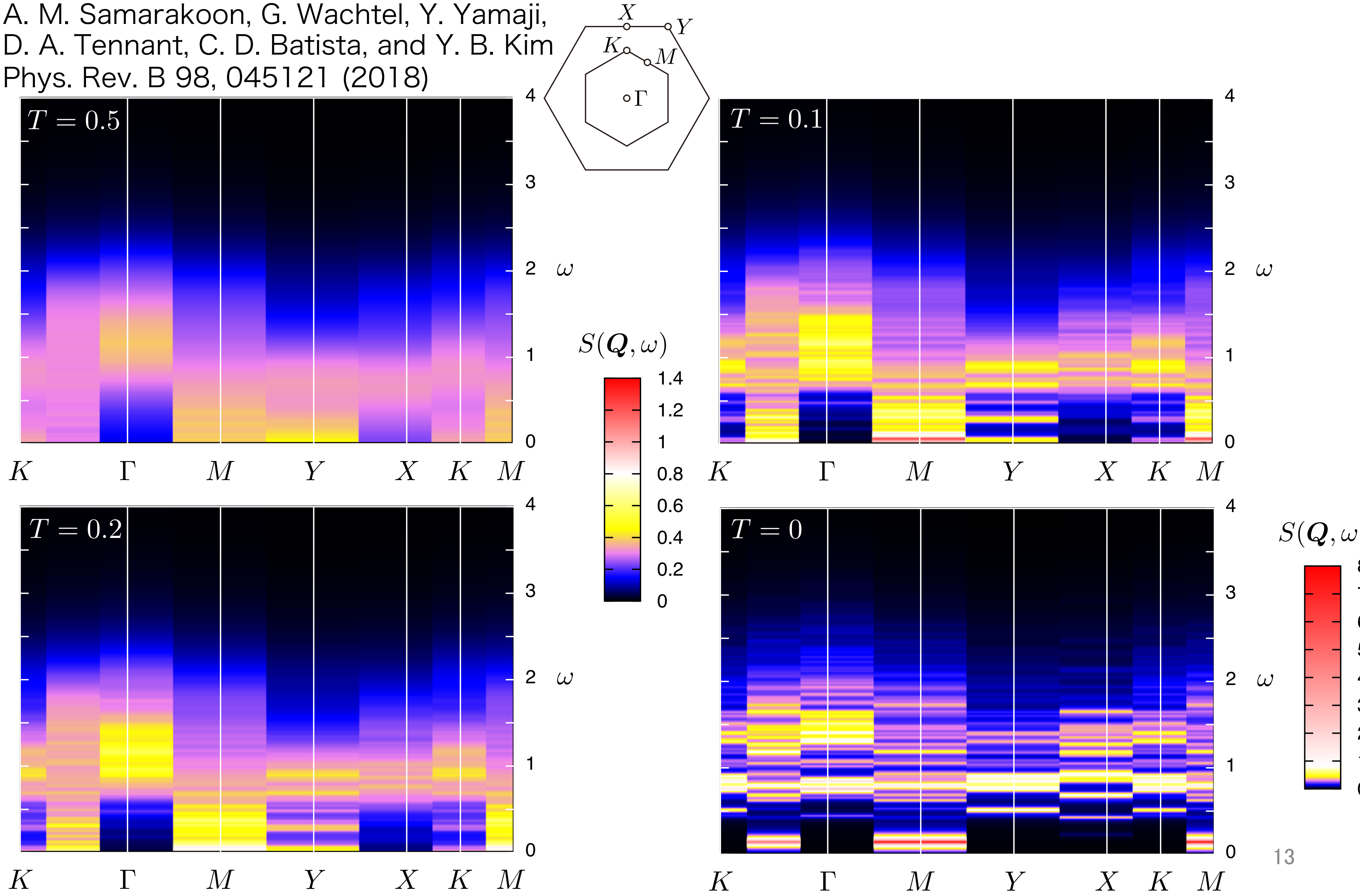


18 site AF Kitaev Standard deviation



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 (now under construction):
   - -Canonical TPQ
   - -Combination of TPQ and Kω
2. N spin/body interaction and Green's function
3. Symmetry
   - -Reduction of dimension of Hilbert space
   - -Analysis of wave fucntions