Development of Dynamical DMRG Method using Regulated Polynomial Expansion and its Application to One-Dimensional Correlated Electron Systems

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Outline

1. Introduction

   Dynamical DMRG method, Target states

2. Kernel polynomial method

   Gibbs phenomena, calculating method for target states

3. Applications

   Temperature dependence of spin chiral order in spin-1/2 zigzag XY chain,

   Optical conductivity in one-dimensional Mott insulator Sr_2CuO_3

4. Summary

Introduction

Arbitrary dynamical correlation function at zero temperature,

$$\chi_A(\omega) \equiv \frac{1}{2\pi N_s} \mathrm{Im} \langle 0 | \hat{A} \frac{1}{\omega - \hat{H} + \varepsilon_0 - i\gamma} \hat{A} | 0 \rangle$$

($\hat{A}$: arbitrary operator)

$$\hat{H}|0\rangle = \varepsilon_0 |0\rangle$$

↑

In low-dimensional systems,

Dynamical DMRG method

Target states

$$|0\rangle, \quad \hat{A}|0\rangle, \quad \frac{1}{\omega - \hat{H} + \varepsilon_0 - i\gamma} \hat{A}|0\rangle$$

Multi target procedure

Calculating target states ← Lanczos method, Conjugate gradient method, ･･･

↑

Kernel polynomial method (KPM)

Motivation

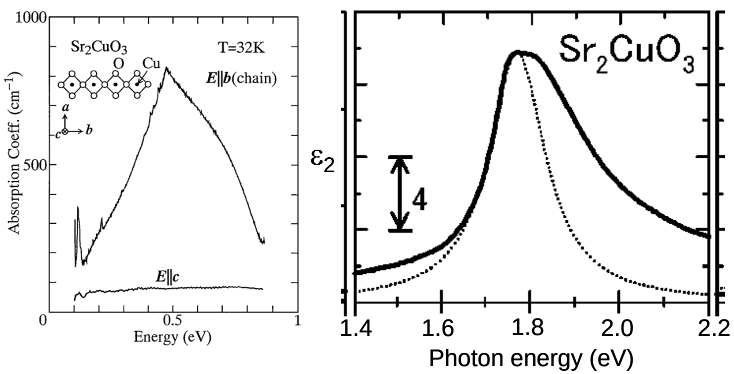
1. Optical response in one dimensional Mott insulator Sr_2CuO_3

- Calculating the correction vector by KPM

$$\frac{1}{\omega - \hat{H} + \varepsilon_0 - i\gamma} \hat{A} |0\rangle$$

Lanczos method, conjugate gradient method: small γ → Lorenzian

Ex. Optical responce of Sr_2CuO_3



The intensity of the spectral function in the charge transfer energy region is several hundreds larger than that in the spin excited energy region.

Our Kernel polynomial method → Gaussian

2. Temperature dependence of spin chirality in spin-1/2 zigzag XY chain

- Finite temperature calculation

$$|0\rangle, \quad \hat{A}|0\rangle, \quad \frac{1}{\omega - \hat{H} + \varepsilon_0 - i\gamma} \hat{A} |0\rangle \qquad (T=0)$$

$$\to \sum_n e^{-\beta\varepsilon_n/2} |n\rangle, \quad \sum_n e^{-\beta\varepsilon_n/2} \hat{A}|n\rangle, \quad \sum_n e^{-\beta\varepsilon_n/2} \frac{1}{\omega - \hat{H} + \varepsilon_n - i\gamma} \hat{A}|n\rangle \quad \text{(finite temperatures)}$$

Kernel Polynomial Method (KPM)

$$\delta(x'-x) = w(x)\sum_{l=0}^{\infty} w_l^{-1}\varphi_l(x')\varphi_l(x)$$

$$G(\omega - i\gamma) \equiv \frac{1}{\omega - \hat{H} - i\gamma} = \sum_{l=0}^{\infty} w_l^{-1}\tilde{\varphi}_l(\omega - i\gamma)\varphi_l(\hat{H})$$

$$\tilde{\varphi}_l(\omega - i\gamma) \equiv \int_a^b dx \frac{w(x)}{\omega - x - i\gamma}\varphi_l(x)$$

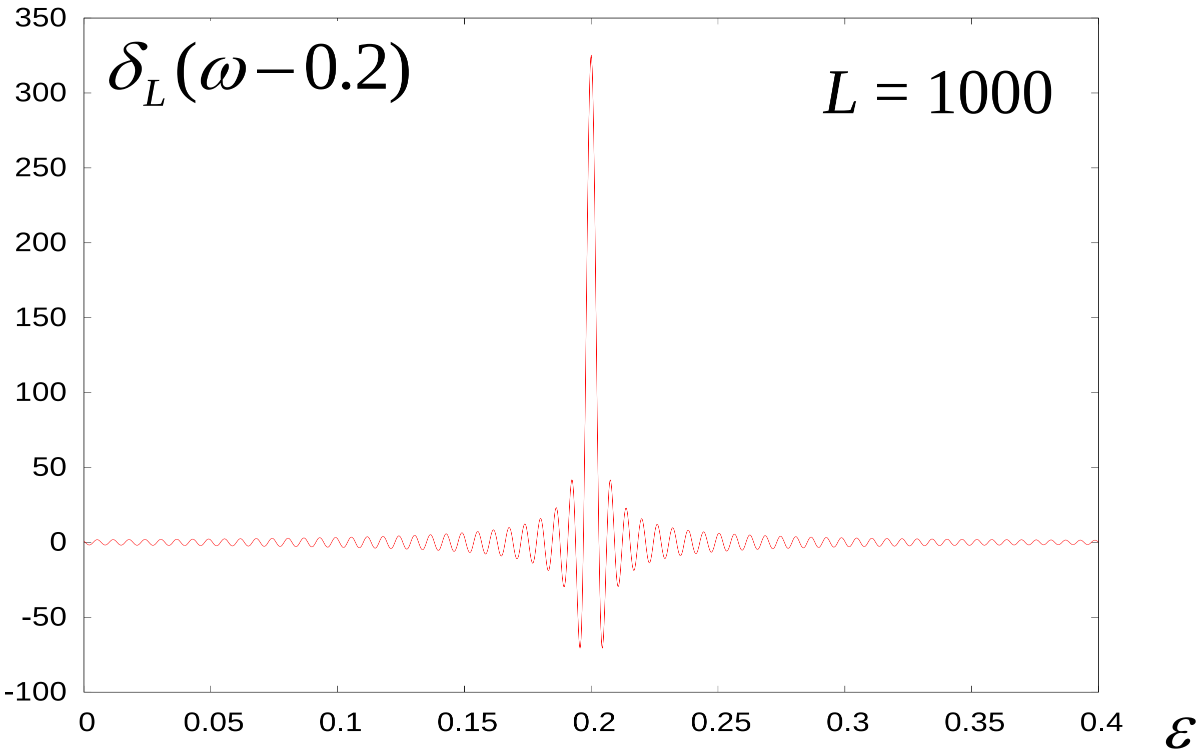
Legendre : $\tilde{P}_l(\omega \pm i\gamma) = 2Q_l(\omega) \mp i\pi P_l(\omega)$

$$\Rightarrow \quad \frac{1}{\omega - \hat{H} - i\gamma} = \sum_{l=0}^{\infty} w_l^{-1}\{2Q_l(\omega) + iP_l(\omega)\}P_l(\hat{H})$$

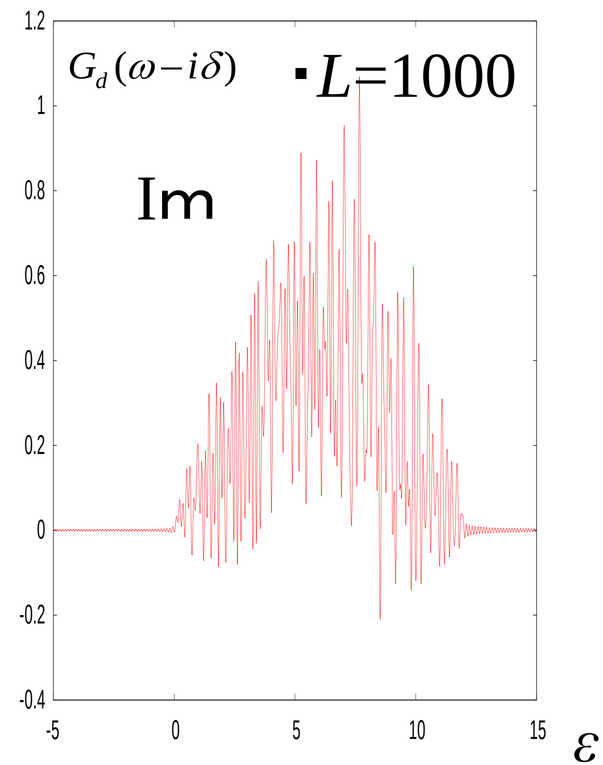
Kernel function

$$D(\omega) = \sum_{\mu} \delta(\omega - \varepsilon_{\mu}) \quad \text{(DOS)}$$

$$\delta_L(\omega - \varepsilon_{\mu}) \equiv \sum_{l=0}^{L} w_l^{-1} P_l(\omega) P_l(\varepsilon_{\mu})$$



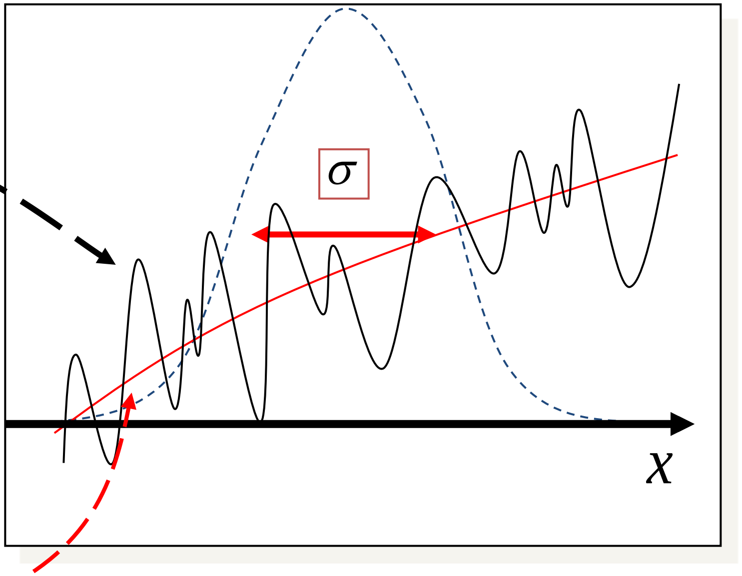
S.C. lattice (19^3 atoms)



Regulated Polynomial Expansion (RPE)

- Regulation ≡ Smearing an oscillating function by Gaussian distribution

$f(x)$



Regulated function

$$\langle f(x) \rangle_{\sigma} \equiv \int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi\sigma^2}} e^{(x'-x)^2/2\sigma^2} \cdot f(x')dx' \quad (7)$$

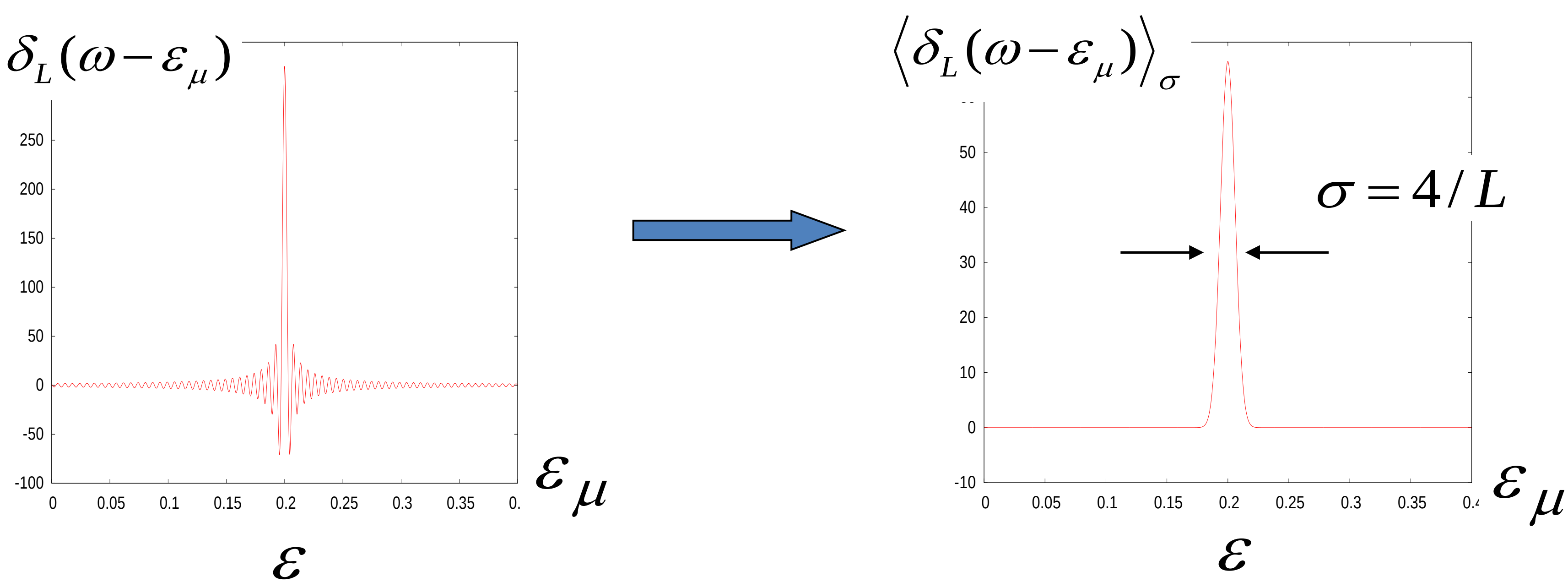
Smoothing Kernel polynomial

$$\delta_L(\omega - \varepsilon_\mu) = \sum_{l=0}^{L} w_l^{-1} P_l(\omega) P_l(\varepsilon_\mu)$$

↓ Regulation

$$\left\langle \delta_L(\omega - \varepsilon_\mu) \right\rangle_\sigma = \sum_{l=0}^{L} w_l^{-1} P_l(\omega) \left\langle P_l(\varepsilon_\mu) \right\rangle_\sigma$$

Regulated Polynomial



<u>Regulated Polynomial Expansion (RPE) of Green function</u>

$$\hat{G}(z) = \sum_{l=0}^{L} w_l^{-1} \widetilde{P}_l(z) \left\langle P_l(\hat{H}) \right\rangle_\sigma \qquad \left\langle P_l(\hat{H}) \right\rangle_\sigma \equiv \frac{1}{\sqrt{2\pi\sigma^2}} \int_{-\infty}^{\infty} e^{(x'-\hat{H})^2/2\sigma^2} P_l(x') dx'$$

Coalitional 3-term recursive formula

$$\left\langle P_{l+1}(\hat{H}) \right\rangle_\sigma = \frac{2l+1}{l+1} \hat{H} \left\langle P_l(\hat{H}) \right\rangle_\sigma - \frac{l}{l-1} \left\langle P_{l-1}(\hat{H}) \right\rangle_\sigma + \frac{2l+1}{l+1} \sigma^2 \left\langle P_l'(\hat{H}) \right\rangle_\sigma$$

$$\left\langle P_{l+1}'(\hat{H}) \right\rangle_\sigma = (2n+1) \left\langle P_l(\hat{H}) \right\rangle_\sigma + \left\langle P_{l-1}'(\hat{H}) \right\rangle_\sigma$$

$$\left. \begin{aligned} P_{l+1}(\hat{H}) &= \frac{2l+1}{l+1} \hat{H} P_l(\hat{H}) - \frac{l}{l-1} P_{l-1}(\hat{H}) \\ P_{l+1}'(\hat{H}) &= (2l+1) P_l(\hat{H}) + P_{l-1}'(\hat{H}) \end{aligned} \right\}$$

Simultaneous recursive equations of Legendre polynomial

For an arbitrary vector $|\xi\rangle$, $\left\langle P_l(\hat{H}) \right\rangle_\sigma |\xi\rangle$ can be calculated recursively!

CPU time practically unchanged!

Calculating the correction vector

$$\frac{1}{\omega-\hat{H}+\varepsilon_0-i\gamma}\hat{A}|0\rangle=\lim_{L\to\infty}\sum_{l=0}^{L} w_l^{-1}\{2Q_l(\omega)+iP_l(\omega)\}\left\langle P_l(\hat{H})\right\rangle_\sigma \hat{A}|0\rangle$$

Coalitional 3-term recursive formula

$$\begin{cases}\left\langle P_{l+1}(\hat{H})\right\rangle_\sigma \hat{A}|0\rangle=\dfrac{2l+1}{l+1}\hat{H}\left\langle P_l(\hat{H})\right\rangle_\sigma \hat{A}|0\rangle-\dfrac{l}{l-1}\left\langle P_{l-1}(\hat{H})\right\rangle_\sigma \hat{A}|0\rangle+\dfrac{2l+1}{l+1}\sigma^2\left\langle P_l'(\hat{H})\right\rangle_\sigma \hat{A}|0\rangle \\ \left\langle P_{l+1}'(\hat{H})\right\rangle_\sigma \hat{A}|0\rangle=(2n+1)\left\langle P_l(\hat{H})\right\rangle_\sigma \hat{A}|0\rangle+\left\langle P_{l-1}'(\hat{H})\right\rangle_\sigma \hat{A}|0\rangle\end{cases}$$

Initial terms

$$\left\langle P_0(\hat{H})\right\rangle_\sigma \hat{A}|0\rangle=\hat{A}|0\rangle,\quad \left\langle P_1(\hat{H})\right\rangle_\sigma \hat{A}|0\rangle=\hat{H}\hat{A}|0\rangle,$$

$$\left\langle P_0'(\hat{H})\right\rangle_\sigma \hat{A}|0\rangle=0,\quad \left\langle P_1'(\hat{H})\right\rangle_\sigma \hat{A}|0\rangle=\hat{A}|0\rangle$$

Finite temperature DDMRG

$$\left|\ \tilde{\xi}\ \right\rangle \equiv \sum_{n=1}^{N} e^{-\beta \hat{H}/2} \left|\xi\right\rangle = \sum_{n} e^{-\beta\varepsilon_n/2} a_n \left|n\right\rangle$$

: Target state

$$\left|\xi\right\rangle \equiv \sum_{n=1}^{N} a_n \left|n\right\rangle$$

: Arbitrary vector

$$\hat{H}\left|n\right\rangle = \varepsilon_n \left|n\right\rangle$$

$$a_n \equiv \left\langle n \middle| \xi \right\rangle$$

: coefficient

In the case of $a_1{}^2 = a_2{}^2 = a_3{}^2 = \cdots = a_N{}^2 = 1$,

the linear product of $\left|\ \tilde{\xi}\ \right\rangle$ gives

$$\left\langle\ \tilde{\xi}\ \middle|\ \tilde{\xi}\ \right\rangle = \sum_{n} e^{-\beta\varepsilon_n} = Z(\beta)$$

: Partition function

But, all eigenstates are required.

Calculation of the target state

$$\left|\,\tilde{\xi}\,\right\rangle = \sum_{n=1}^{N} e^{-\beta\varepsilon_n/2} a_n |n\rangle$$ (definition)

$$= \int_{-\infty}^{\infty} d\varepsilon'\, e^{-\beta\varepsilon'/2} \sum_{n=1}^{N} \delta(\varepsilon' - \varepsilon_n) a_n |n\rangle$$

$$\hat{H}|n\rangle = \varepsilon_n |n\rangle,\ |\xi\rangle \equiv \sum_{n=1}^{N} a_n |n\rangle$$

$$= \int_{-\infty}^{\infty} d\varepsilon'\, e^{-\beta\varepsilon'/2} \delta(\varepsilon' - \hat{H}) |\xi\rangle$$

Kernel polynomial method

$$= \int_{-1}^{1} d\varepsilon\, e^{-\beta\varepsilon/2} \lim_{L\to\infty} \sum_{l=0}^{L} w_l^{-1} P_l(\varepsilon) P_l(\hat{H}_s) |\xi\rangle$$

$P_l(\varepsilon)$: Legendre polynomial, $\hat{H}_s \equiv (\hat{H} - b)/d$ (d, b: rescaling parametar)

Regulated delta function

$$\left\langle \delta_L(\varepsilon - \hat{H}_s) \right\rangle_\sigma |\xi\rangle = \sum_{l=0}^{L} w_l^{-1} P_l(\varepsilon) \left\langle P_l(\hat{H}_s) \right\rangle_\sigma |\xi\rangle$$

$\Updownarrow$

Regulated polynomial: $\left\langle P_l(\hat{H}_s) \right\rangle_\sigma \equiv \frac{1}{\sqrt{2\pi\sigma^2}} \int_{-\infty}^{\infty} e^{-(x'-\hat{H}_s)^2/2\sigma^2} P_l(x') dx'$

3-term recursive formula for regulated polynomials

$$\begin{cases} \left\langle P_{l+1}(\hat{H}_s) \right\rangle_\sigma = \frac{2l+1}{l+1} \hat{H}_s \left\langle P_l(\hat{H}_s) \right\rangle_\sigma - \frac{l}{l-1} \left\langle P_{l-1}(\hat{H}_s) \right\rangle_\sigma + \frac{2l+1}{l+1} \sigma^2 \left\langle P_l'(\hat{H}_s) \right\rangle_\sigma \\ \left\langle P_{l+1}'(\hat{H}_s) \right\rangle_\sigma = (2l+1) \left\langle P_l(\hat{H}_s) \right\rangle_\sigma + \left\langle P_{l-1}'(\hat{H}_s) \right\rangle_\sigma \end{cases}$$

Target state

$$|\tilde{\xi}\rangle = \lim_{L\to\infty} \sum_{l=0}^{L} w_l^{-1} \int_{-\infty}^{\infty} d\varepsilon' e^{-\beta\varepsilon'/2} P_n(\varepsilon') \left\langle P_l(\hat{H}_s) \right\rangle_\sigma |\xi\rangle$$

$\propto i_l(-\beta/2)$: modified spherical Bessel function

$$|\tilde{\xi}\rangle \propto \lim_{L\to\infty} \sum_{l=0}^{L} w_l^{-1} i_l(-\beta/2) \left\langle P_l(\hat{H}_s) \right\rangle_\sigma |\xi\rangle$$

$\longleftarrow$ Recursive calculation

Applications

1. Temperature dependence of the chirality in Spin-1/2 zigzag XY mode

The target state corresponding to finite temperature calculation is calculated by KPM

T. Sugimoto, SS, T. Tohyama, Phys. Rev. B **82**, 035437 (2010)

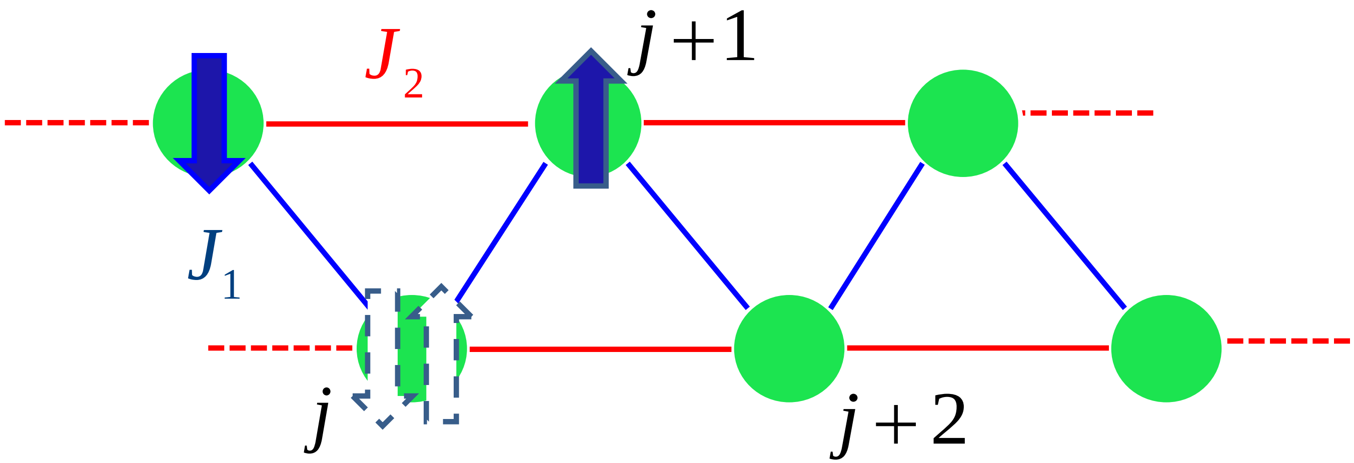
2. Optical response in one-dimensional Mott insulator Sr_2CuO_3

Correction vector (dynamical correlation function) is calculated by KPM

SS, T. Tohyama, arXiv: 1007.5166

Spin-1/2 zigzag model

Hamiltonian: $H = \sum_j [J_1(S_j^x S_{j+1}^x + S_j^y S_{j+1}^y + \Delta S_j^z S_{j+1}^z) + J_2(S_j^x S_{j+2}^x + S_j^y S_{j+2}^y + \Delta S_j^z S_{j+2}^z)]$



In this study, we assume $J_1 > 0, \quad J_2 > 0$

spin frustrated system ⟶ spin chiral order appears

Vector spin chirality: $\kappa_j^z \equiv (\mathbf{S}_j \times \mathbf{S}_{j+1})_z$

$LiCu_2O_2$, LiCuVO…

Spin chirality

At zero-temperature,

	Chiral oder	Chiral excitation
$J_1/J_2<0.8$	✓ (chiral phase)	gapless
$J_1/J_2>0.8$	(dimer phase)	gapful

Bosonization and meanfild theory: A. A. Nersesyan, A. O. Gogolin, and F. H. L. Esseler, Phys. Rev. Lett. **81**, 910(1998)

DMRG study: K. Okunishi, J. Phys. Soc. Jpn. **77**, 114004(2008)

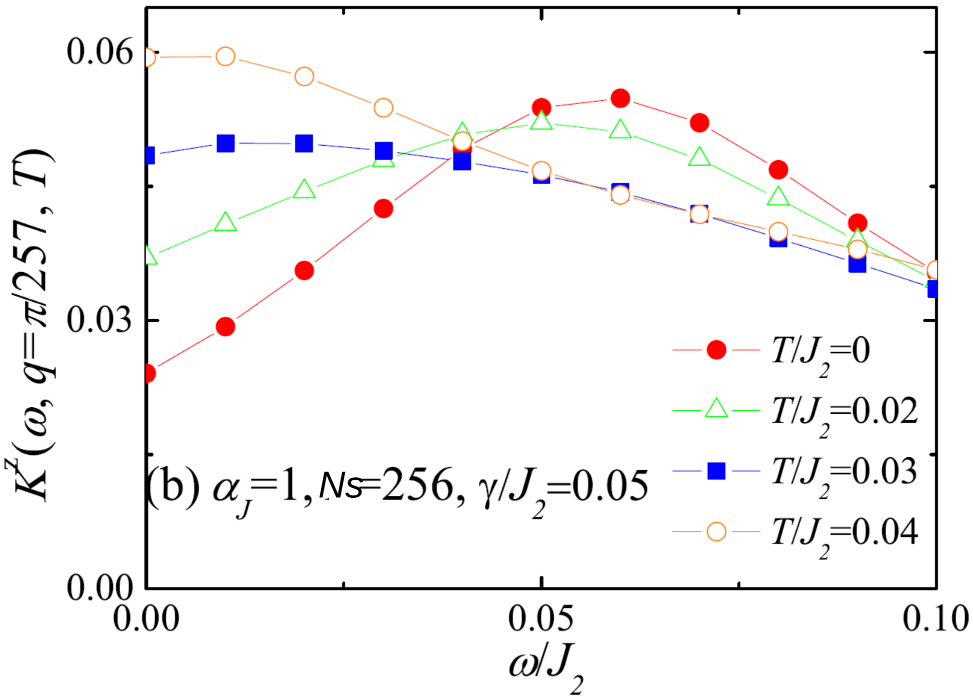
Dynamical chirality correlation function:

$$K^z(q,\omega,T)\equiv\frac{1}{\pi Z L_s}\sum_n e^{-\varepsilon_n/T}\,\mathrm{Im}\langle n|\hat{O}^z_\kappa(q)\frac{1}{\omega-\hat{H}+\varepsilon_n-i\gamma}\hat{O}^z_\kappa(q)|n\rangle$$

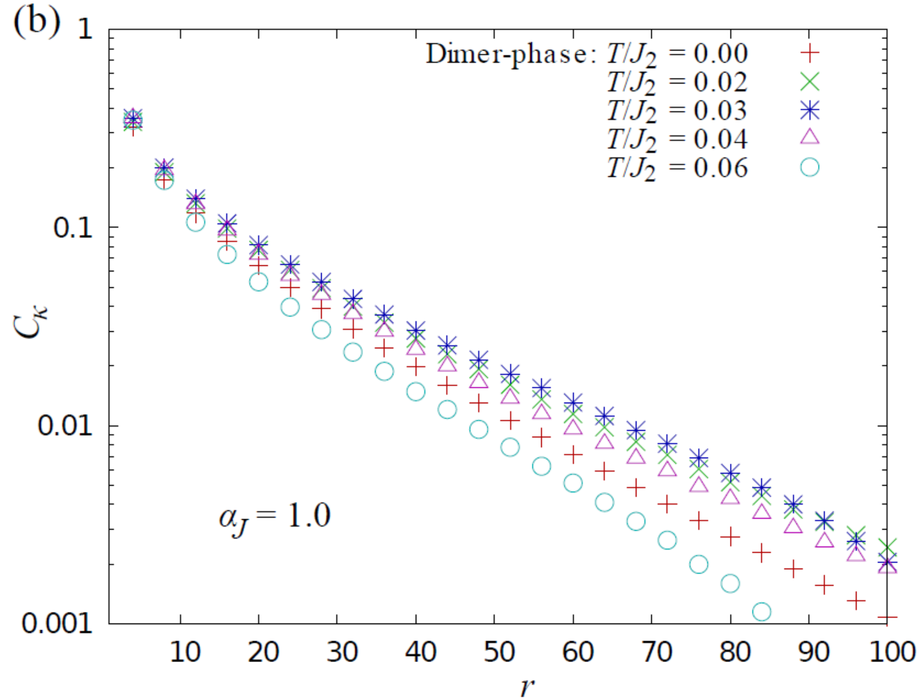
$$\left(\hat{H}|n\rangle=\varepsilon_n|n\rangle,\quad \hat{O}^z_\kappa(q)\equiv\sqrt{2/(L_s+1)}\sum_j \sin(q\,j)(\mathbf{S}_j\times\mathbf{S}_{j+1})_z\right)$$

Dimer phase $\alpha_J \equiv J_1 / J_2 = 1$

- Dynamical chiral correlation function

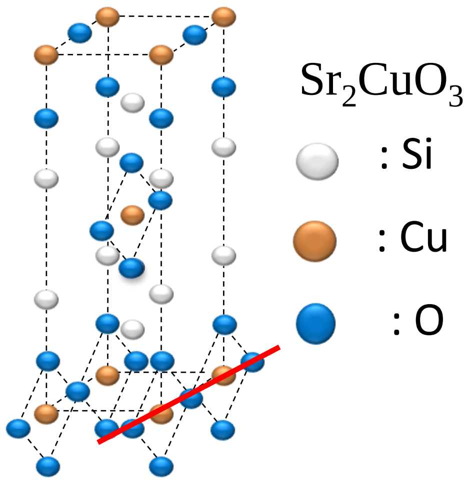


- Static chiral correlation function



Chiral low-energy fluctuation increases.

Optical conductivity of one-dimensional Mott insulatar Sr_2CuO_3

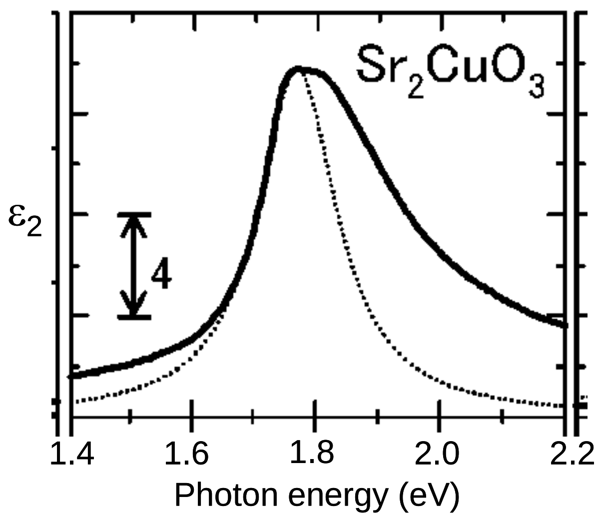


- Giant non-linear optical response
- Ultra fast relaxation time

⟺ New optical switching device

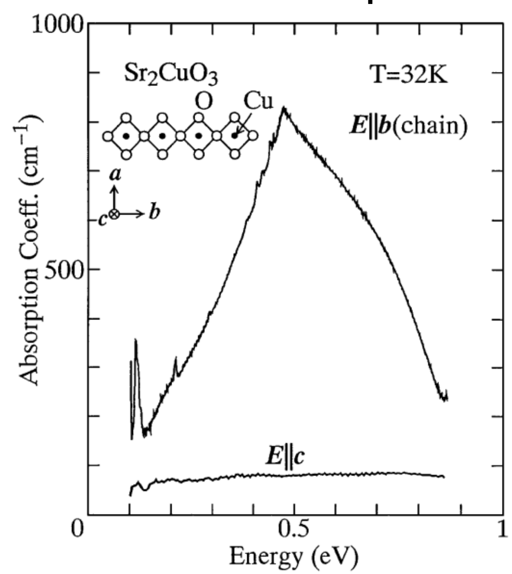
Experimental data

- Charge-transfer excitation



M. Ono *et al*, Phys. Rev. B. **70**, 085101 (2004)

- Phonon-assisted spin excitation



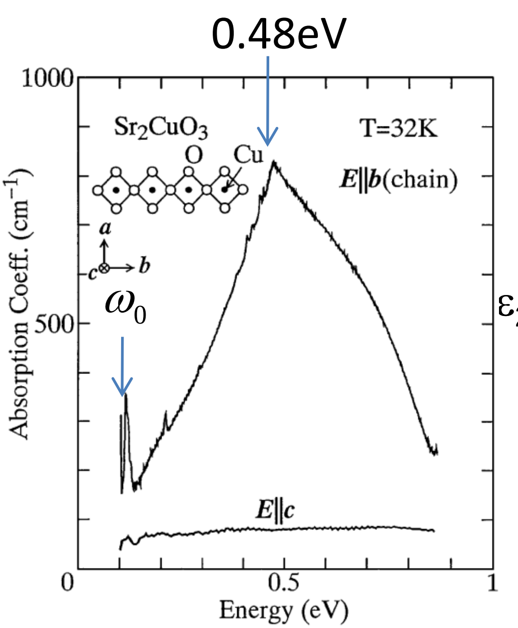
H. Suzuura *et al*, Phys. Rev. Lett. **76**, 2579 (1996)

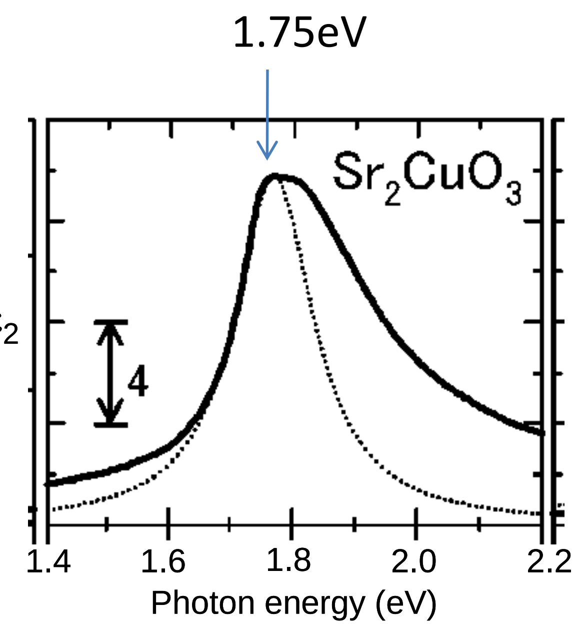
Hubbard-Holstein model

$$H = H_{ex-hubbard} + H_{phonon} + H_{el-ph}$$

$$H_{ex-hubbard} = -t\sum_{i,\sigma}(c^{\dagger}_{i+1,\sigma}c_{i,\sigma} + h.c.) + U\sum_{i} n_{i,\downarrow}n_{i,\uparrow} + V\sum_{i}(n_i - 1)(n_{i+1} - 1)$$

$$H_{phonon} = \omega_0 \sum_{i} b^{\dagger}_{i+1/2} b_{i+1/2} \qquad H_{el-ph} = -g\sum_{i}(b^{\dagger}_{i+1/2} + b_{i+1/2})(n_i - n_{i+1})$$





$t = 0.4\text{eV}$

$U = 3.2\text{eV}$

$V = 0.8\text{eV}$

$V = 2t$

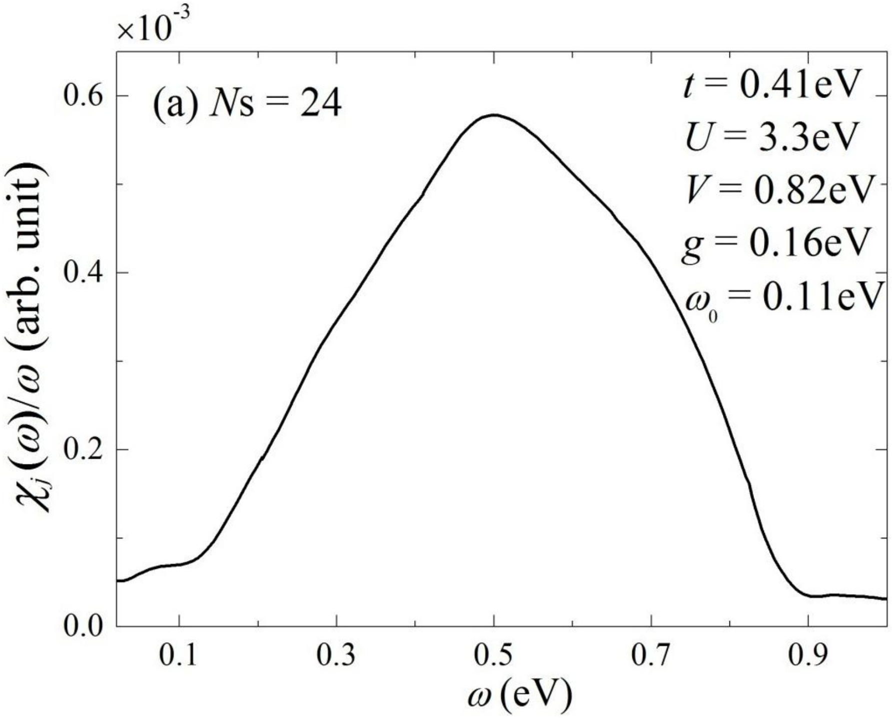
$J = 4t^2/(U - V) = 0.272\text{eV}$

$\omega_0 = 0.11\text{eV}$

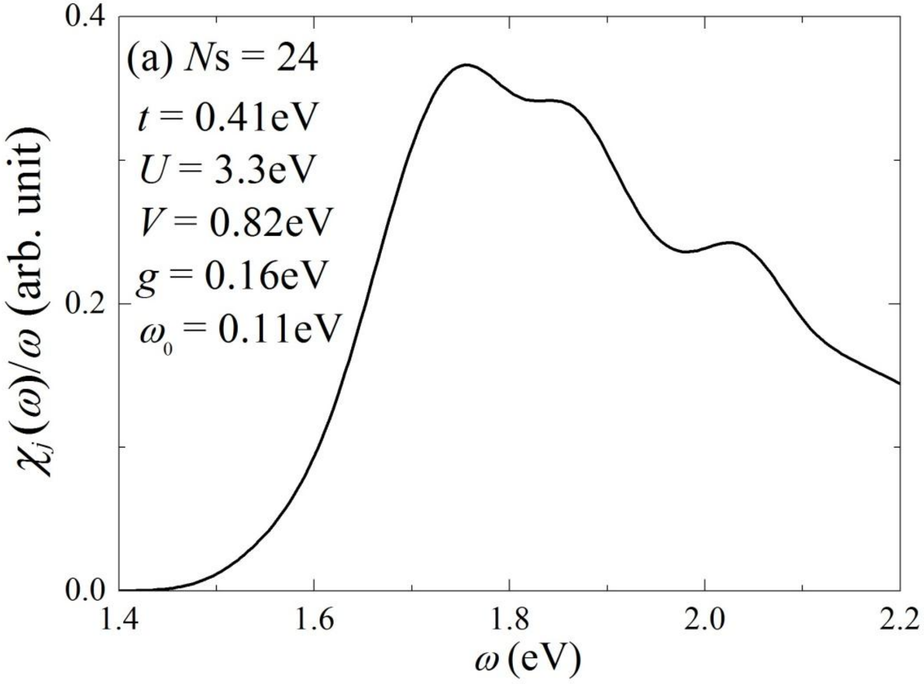
$g = 0.18\text{eV}$

Results

•Phonon-assisted spin excitation



•Charge-transfer excitation



We can reproduce the optical conductivity of Sr2CuO3 in both the spin excited energy region and the charge-transfer energy region at the same time.

summary

Kernel polynomial method ⟹ Dynamical DMRG method

- Correction vector calculation
- Finite temperature calculation

- We investigate the temperature dependence of the spin chirality in the spin-1/2 zigzag XY chain. We find that the chiral correlation is enhanced by the temperature in the dimmer phase.

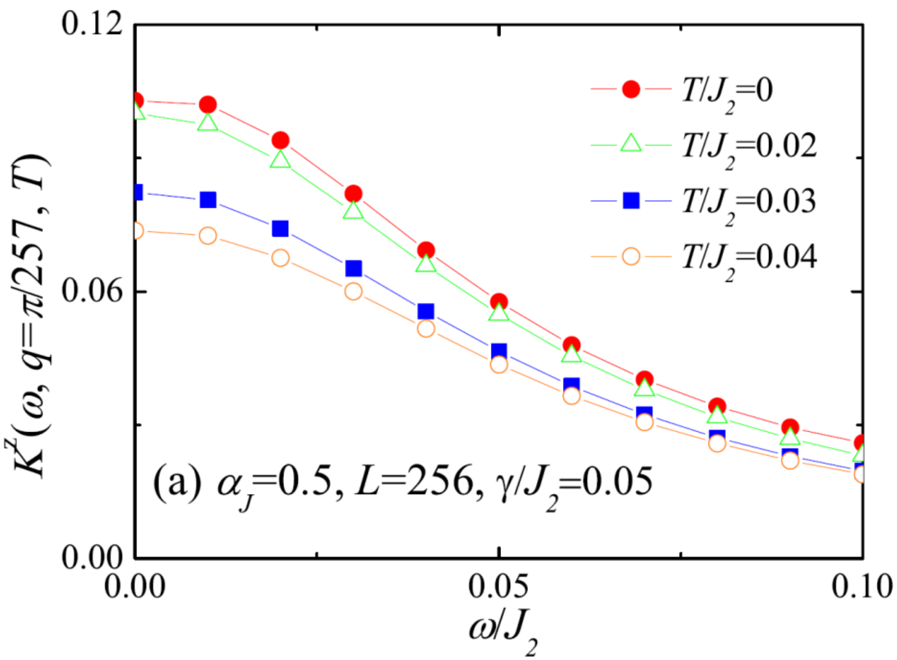
- Using the dynamical DMRG method and the kernel polynomial method, we reproduce the optical conductivity of Sr_2CuO_3.

Appendix

Temperature dependence

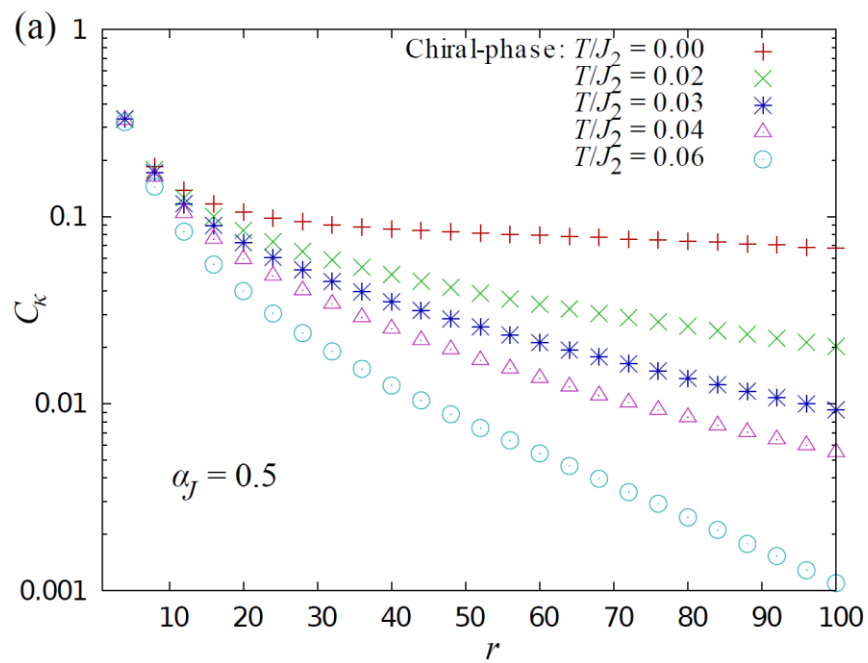
Chiral phase $\alpha_J \equiv J_1 / J_2 = 0.5$

- Dynamical chiral correlation function



- Static chiral correlation function

$$C_\kappa(r_l) = \frac{1}{S^4}\langle \kappa_{l_L}\kappa_{l_R}\rangle$$

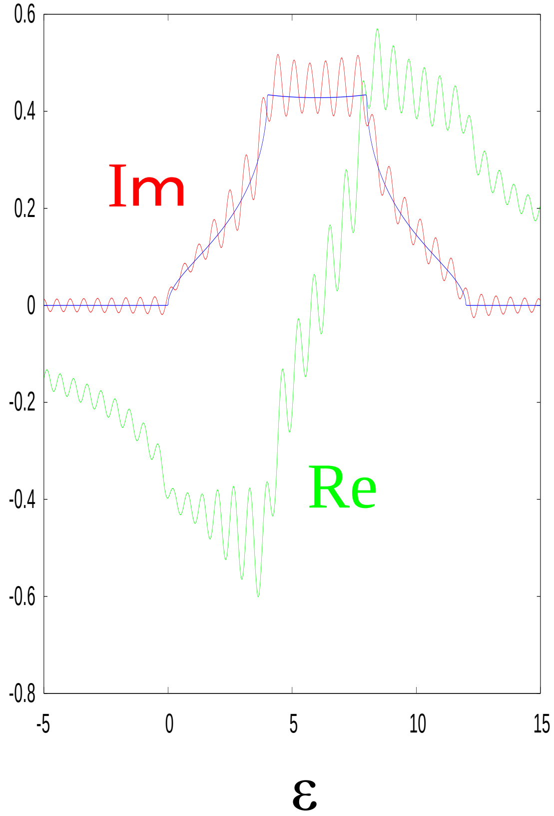


Chiral fructuation decreases with increasing temperature.

Ex.: Simple cubic lattice dynamics（19^3atoms）

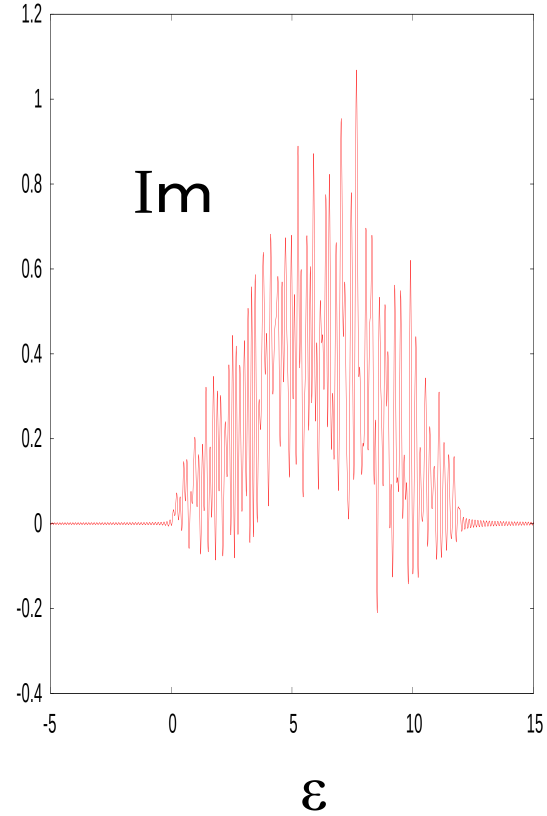
- L=200

$G_d(\omega - i\delta)$



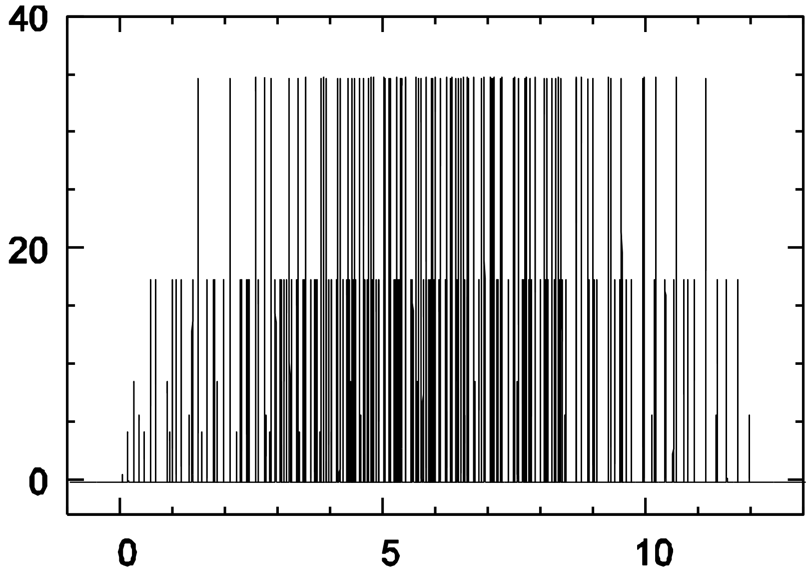
- L=1000

$G_d(\omega - i\delta)$



Example. Eigenvalue spectrum of simple cubic lattice dynamics

Convergence result ($L=5\times10^5$, 19^3atoms)

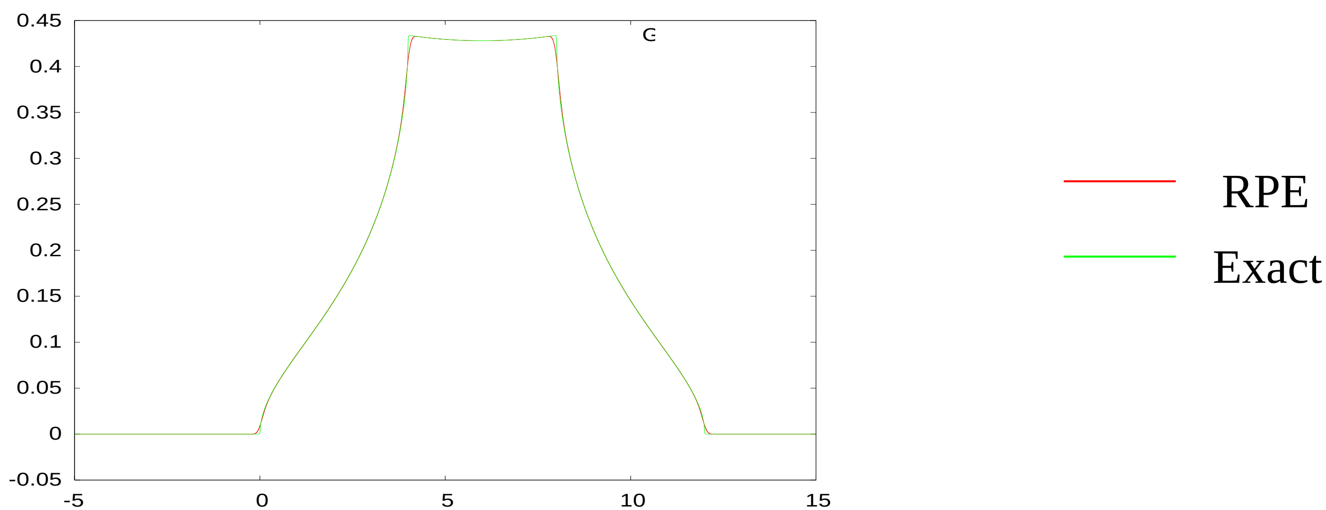


- •220 eigenvalues
- •height $\propto$ degeneracy

Accuracy comparable to diagonalization

(up to six digits)

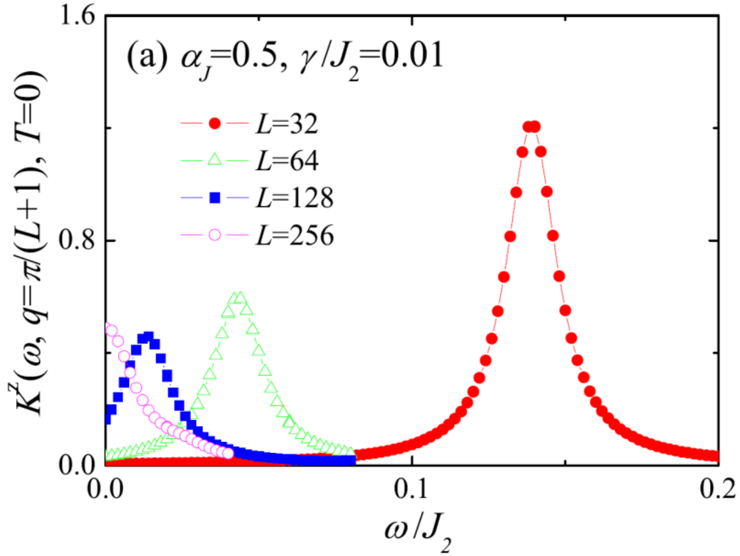
Comparison to bulk spectrum with a larger matrix (151^3 atoms)



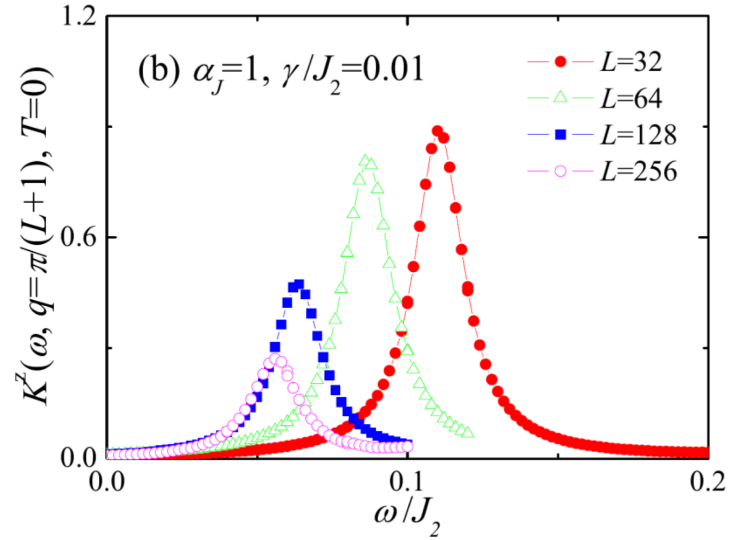
Zero-temperature calculations

DDMRG results ($q = \pi/(L_s + 1)$: smallest momentum in open boundary condition)

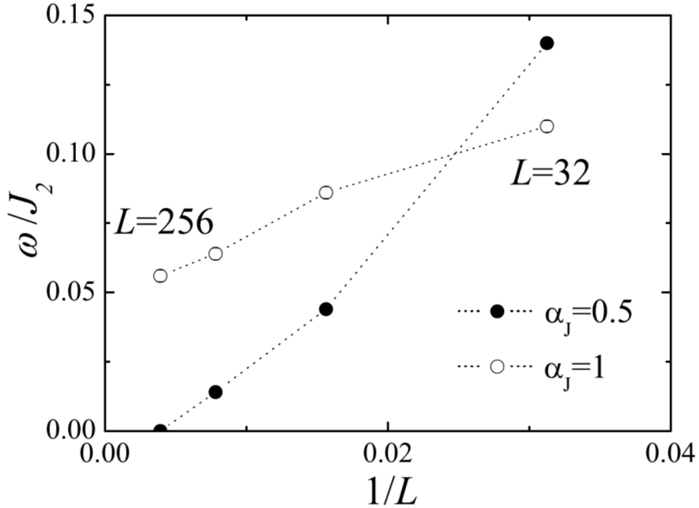
•Chiral phase



•Dimer phase



•Peak position



In the thermo dynamical limit:

•Chiral phase → Gapless

•Dimer phase → Gapful

Calculation of Physical Quantities

Expectation value

$$\langle A \rangle = \frac{1}{Z} \sum_{n=1}^{N} e^{-\beta \varepsilon_n} \langle n | \hat{A} | n \rangle$$

($\hat{A}$: arbitrary operator)

Using $|\tilde{\xi}\rangle$

$$\begin{cases} a_1^2 = a_2^2 = \cdots = a_N^2 = 1 \\ a_n a_m = 0 \quad (n \neq m) \end{cases}$$

$$\frac{\langle \tilde{\xi} | \hat{A} | \tilde{\xi} \rangle}{\langle \tilde{\xi} | \tilde{\xi} \rangle} = \frac{\sum_{n=1}^{N} \sum_{m=1}^{N} a_n a_m e^{-\beta(\varepsilon_n + \varepsilon_m)/2} \langle n | \hat{A} | m \rangle}{\sum_{n=1}^{N} a_n{}^2 e^{-\beta \varepsilon_n}}$$

Random sampling and averaging

- Initial vector of KPM

$$|\xi\rangle = \sum_{n=1}^{N} a_n |n\rangle = \sum_{i=1}^{N} r_i |\xi_i\rangle = \begin{pmatrix} r_1 \\ r_2 \\ \vdots \\ r_n \end{pmatrix}$$

$$\left(|n\rangle = \sum_{i=1}^{N} b_{n,i} |\xi_i\rangle, \ \sum_{i=1}^{N} b_{n,i} b_{m,i} = \delta_{nm} \right)$$

Random number [-α,α]

•Diagonal parts (partition function)

$$a_n^2 = \sum_i r_i^2 b_{n,i}^2 + \sum_{i \neq j} r_i r_j b_{n,i} b_{n,j} \xrightarrow{\text{averaging}} \langle r^2 \rangle$$

$$r_i r_j \to 0$$

$$r_1^2 = r_2^2 = \cdots = r_N^2 \equiv \langle r^2 \rangle, \quad \sum_i b_{n.i}^2 = 1$$

$$\langle \tilde{\xi} | \tilde{\xi} \rangle \longrightarrow \langle r^2 \rangle Z$$

•Off-diagonal parts $([H, \hat{A}] \neq 0)$

$$a_n a_m = \sum_i r_i^2 b_{n,i} b_{m,i} + \sum_{i \neq j} r_i r_j b_{n,i} b_{m,j} \xrightarrow{\text{averaging}} 0$$

$$r_i r_j \to 0$$

$$r_1^2 = r_2^2 = \cdots = r_N^2 \equiv \langle r^2 \rangle, \quad \sum_i b_{n.i} b_{m.i} = 0 \ \ (n \neq m)$$

$$\langle \tilde{\xi} | \hat{A} | \tilde{\xi} \rangle \longrightarrow \langle r^2 \rangle \langle A \rangle$$

Expectation values

$$\frac{\langle \tilde{\xi} | \hat{A} | \tilde{\xi} \rangle}{\langle \tilde{\xi} | \tilde{\xi} \rangle} \xrightarrow{\text{Random sampling and averaging}} \langle A \rangle = \frac{1}{Z} \sum_n e^{-\beta \varepsilon_n} \langle n | \hat{A} | n \rangle$$