Theoretical analysis for photoexcited states of a 1D 1/2-filled Hubbard model by many-body Wannier functions method

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Background

Methods for understanding photoexcited states in strongly correlated electron systems

	Precise theoretical method		Our novel method
	exact diagonalization	DMRG / DDMRG	many-body Wannier functions method (MBWFs)
N (1D calculatable size)	$N \lesssim 20$	$N \lesssim 1000$	$N \lesssim 1000$
Extracting physical properties from wave functions (state vectors)	easy	hard	easy

Formulation

Hamiltonian (extended Hubbard model) and optical conductivity

$\hbar = c = e = 1$, lattice constant=1, 0 K

N sites, one-dimension (1D), PBC, 1/2-filling ($N_\uparrow = N_\downarrow = N/2$), total momentum=0

$$H = -T\sum_{j=1}^{N}\sum_{\sigma}[c^\dagger_{j+1,\sigma}c_{j,\sigma} + c^\dagger_{j,\sigma}c_{j+1,\sigma}] + U\sum_{j=1}^{N} n_{j,\uparrow}n_{j,\downarrow}$$

Charge current operator:

$$\hat{J} = iT\sum_{j=1}^{N}\sum_{\sigma}[c^\dagger_{j+1,\sigma}c_{j,\sigma} - c^\dagger_{j,\sigma}c_{j+1,\sigma}]$$

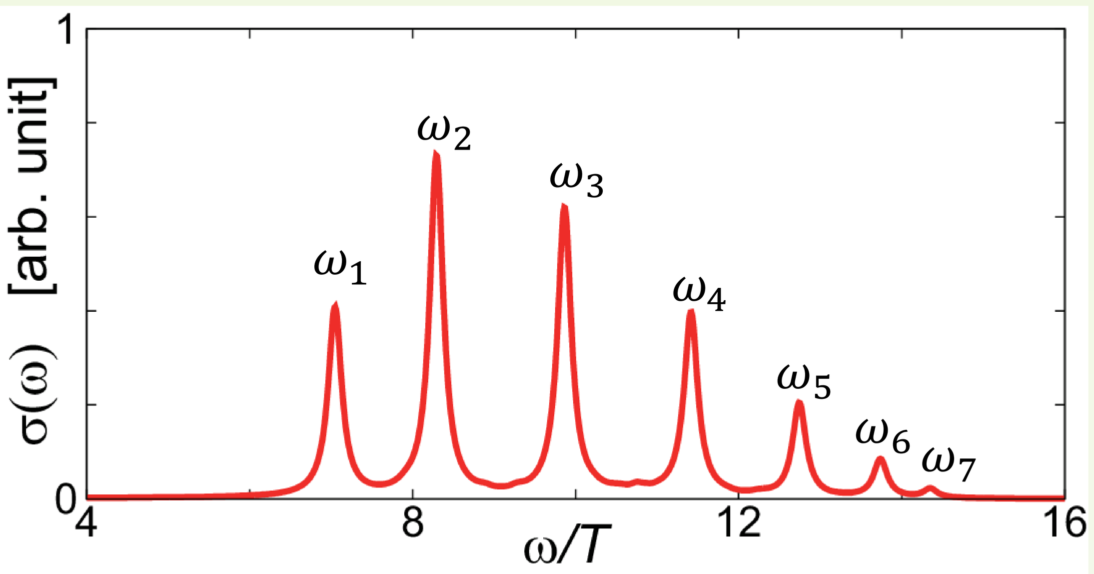
Optical conductivity (peak energies: $\omega = \omega_\mu$ ($\mu = 1,2,\cdots$)):

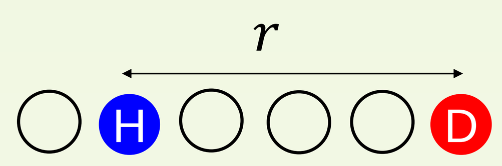
$$\sigma(\omega) = -\frac{1}{N\omega}\mathrm{Im}\langle g|\hat{J}\frac{1}{\omega + i\gamma + E_g - H}\hat{J}|g\rangle$$

- Ground state energy and the state: E_g, $|g\rangle$
- Photoexcited states at the peaks of $\sigma(\omega)$, $|\phi_\mu\rangle$, are calculated by solving correction vectors (artificial broadening=10^{-4})
- Assume spin-charge separation
- Parameter values: $U = 10T, V = 0, \gamma = 0.1T$

Details of application of MBWFs to optical conductivity

(1) Exact diagonalization (e.g. *N*=16, *V*=0)





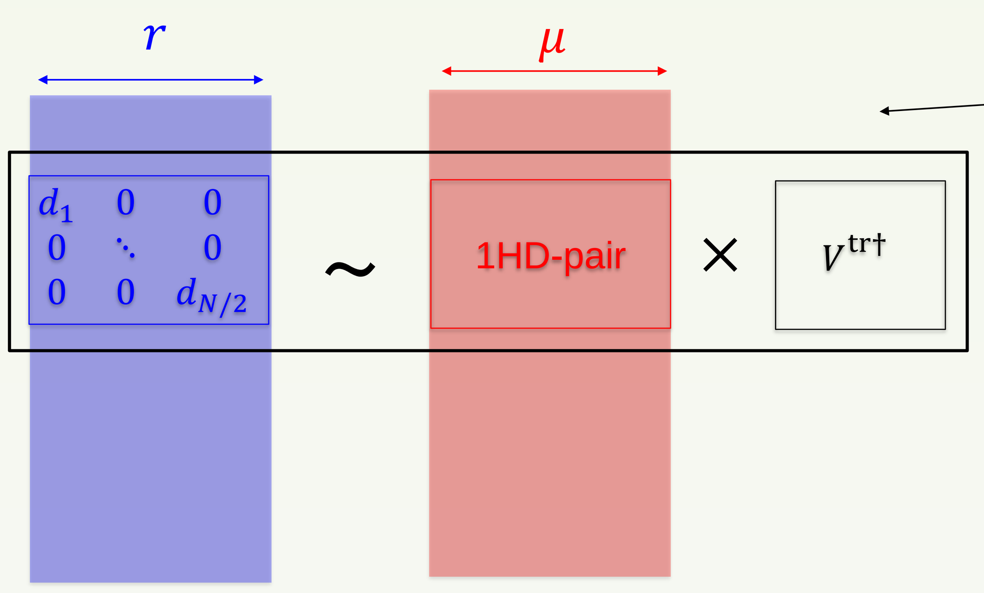
$1 \le r \le I := N/2 - 1$

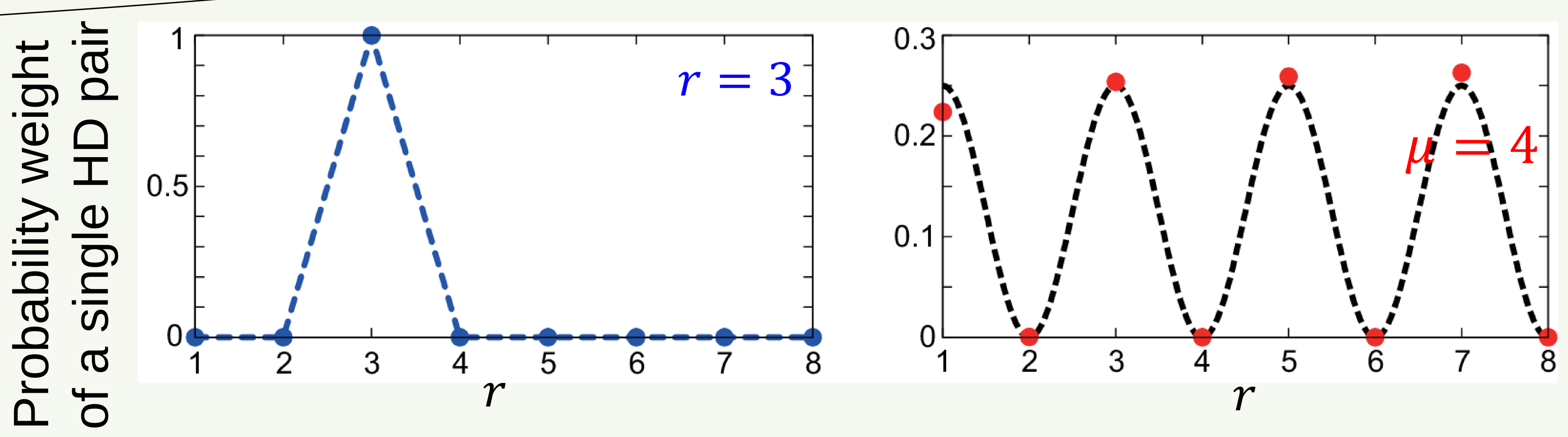
The number of the main peaks are corresponding to localized quantity, r (holon-doublon (HD) distance of a single HD pair)

(2) Produce MBWFs by unitary transformation

$$|\tilde{\phi}_r\rangle := \sum_\mu V^{\mathrm{tr}}_{r\mu}|\phi_\mu\rangle \qquad V^{\mathrm{tr}}_{r\mu} := \frac{2}{\sqrt{N}}\sin\left(\frac{\pi}{N/2}r\mu\right)$$

Wannier — Bloch



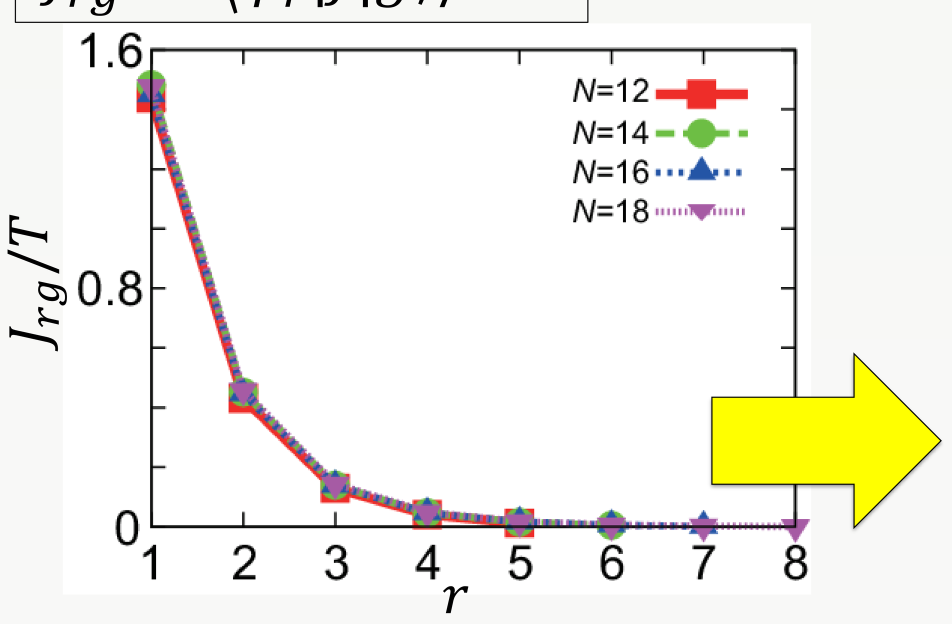


(3) Extrapolation and size extension $|Jg\rangle := [J_{1g}, J_{2g}, \dots, J_{(N/2-1)g}]^t$

$$\sigma(\omega) \sim \frac{\gamma}{\omega N}\sum_{\mu=1}^{I}\frac{|\langle\phi_\mu|\hat{J}|g\rangle|^2}{(\omega-\omega_\mu)^2+\gamma^2} = \frac{\gamma}{\omega}\sum_{\lambda=1}^{I}\frac{|\langle\tilde{\Phi}_\lambda|Jg\rangle|^2}{(\omega-\varepsilon_\lambda)^2+\gamma^2} \quad (N := 2I+2) \quad \tilde{h}|\tilde{\Phi}_\lambda\rangle = \varepsilon_\lambda|\tilde{\Phi}_\lambda\rangle$$

Expectation value of $\hat{J}$ in MBWFs

$$J_{rg} := \langle\tilde{\phi}_r|\hat{J}|g\rangle/\sqrt{N}$$

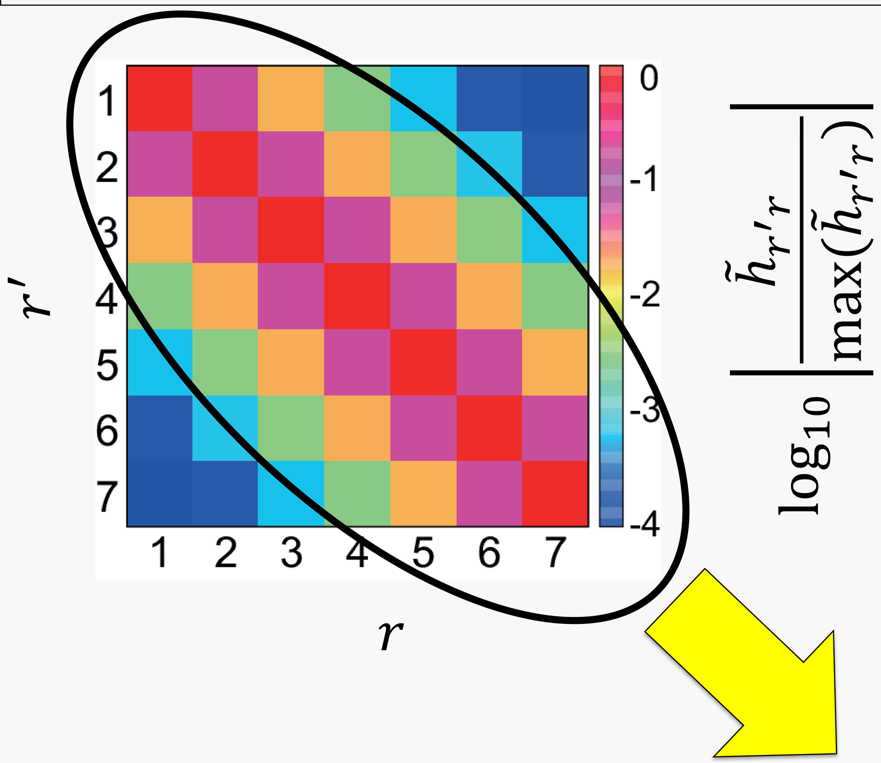


Use values for $I = 8$ ($N = 18$)

$$J_{rg}/\sqrt{N} := \begin{cases} J_{rg}/\sqrt{18} & (1 \le r \le 8) \\ 0 & (9 \le r) \end{cases}$$

Effective Hamiltonian of photoexcited states in MBWFs

$$\tilde{h}_{r'r} := \langle\tilde{\phi}_{r'}|H - E_g|\tilde{\phi}_r\rangle = \sum_\mu V^{\mathrm{tr}*}_{r'\mu}\omega_\mu V^{\mathrm{tr}}_{r\mu}$$

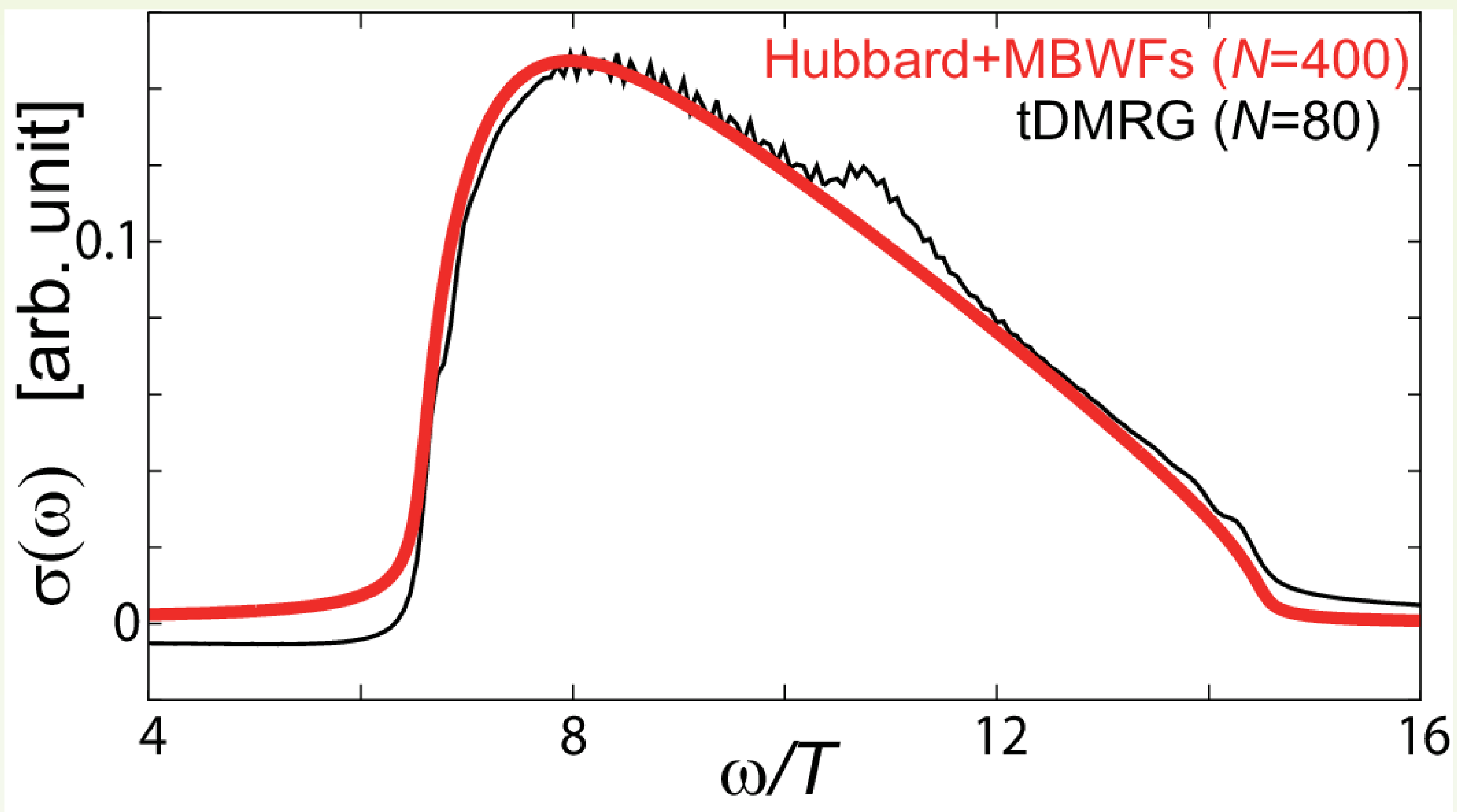


Consider size extension with hepta-diagonal elements

Conclusion

- ➢ We theoretically proposed a novel method, which is called a many-body Wannier functions method (MBWFs), to calculate optical conductivity spectra $\sigma(\omega)$ in strongly correlated electron systems and applied the method to a 1D extended Hubbard model at 1/2-filling.
- ➢ Calculated $\sigma(\omega)$ at 0 K is in good agreement with corresponding tDMRG results.

Results



This method can be extended to perturbatively include finite long-range Coulomb terms, see:

S. Ohmura, *et al.*, PRB **100**, 235134 (2019).
T. Yamaguchi, *et al.*, PRB **103**, 045124 (2021).

Extrapolate in the direction to increasing *r* and achieve size extension