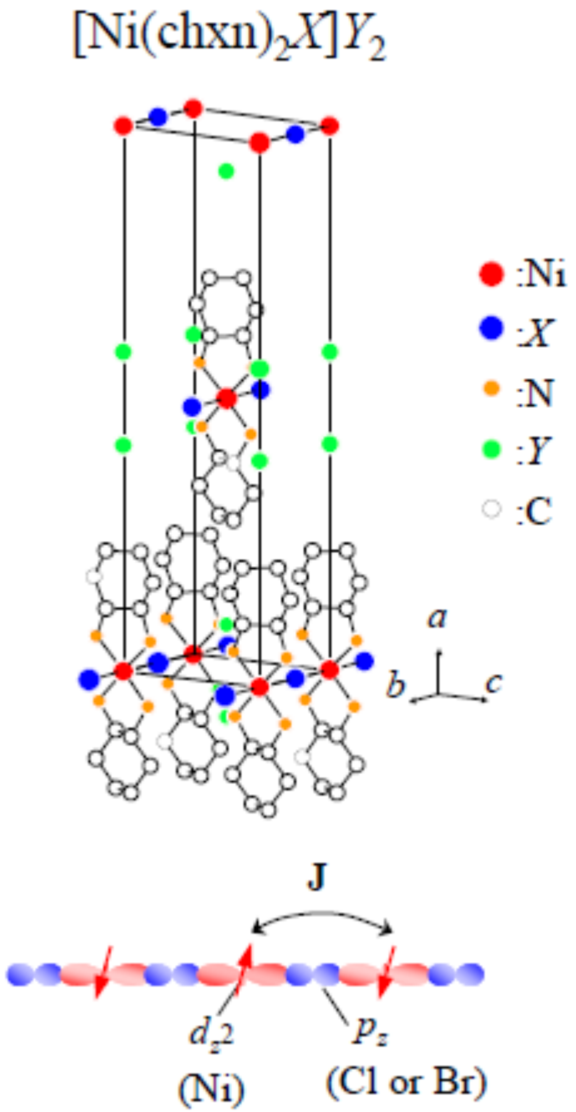
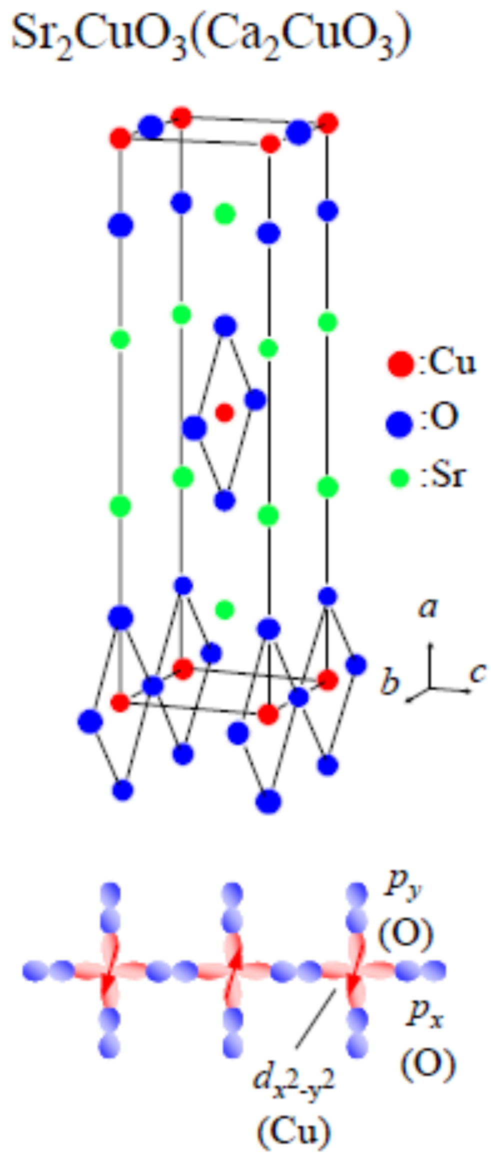
New Development of Numerical Simulations in Low-Dimensional Quamtum Systems:
From Density Matrix Renormalization Group to Tensor Network Formulations
Oct. 27-29, 2010 YITP, Kyoto

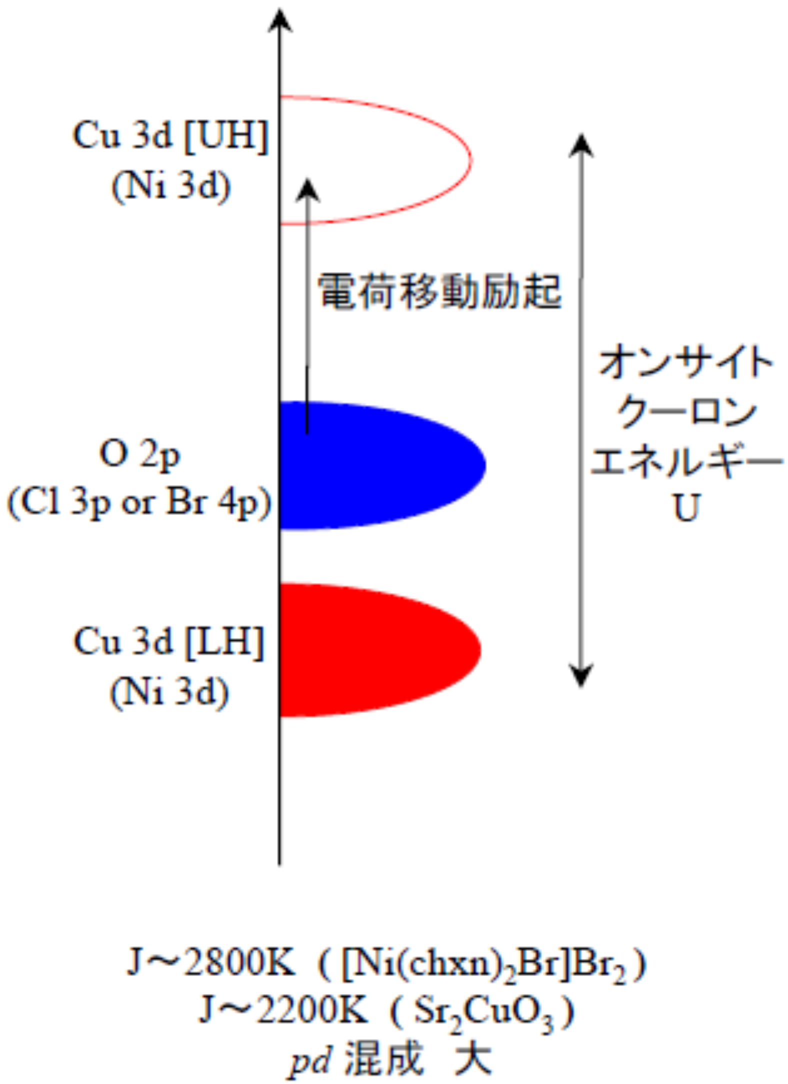
Dynamics of Photoexcited Correlated Electrons
- DMRG Study and MPS viewpoint -

Hiroaki Matsueda
Sendai Nat'l College of Tech. (SNCT)

Crystal and electronic structures of 1D Mott insulators



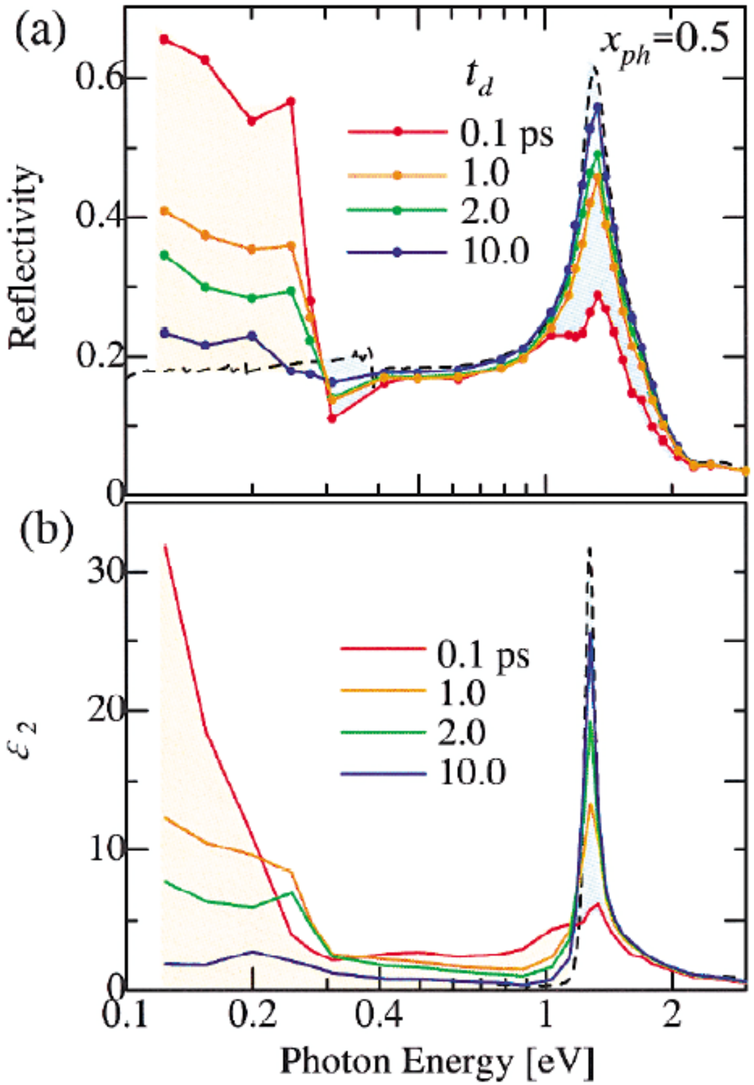


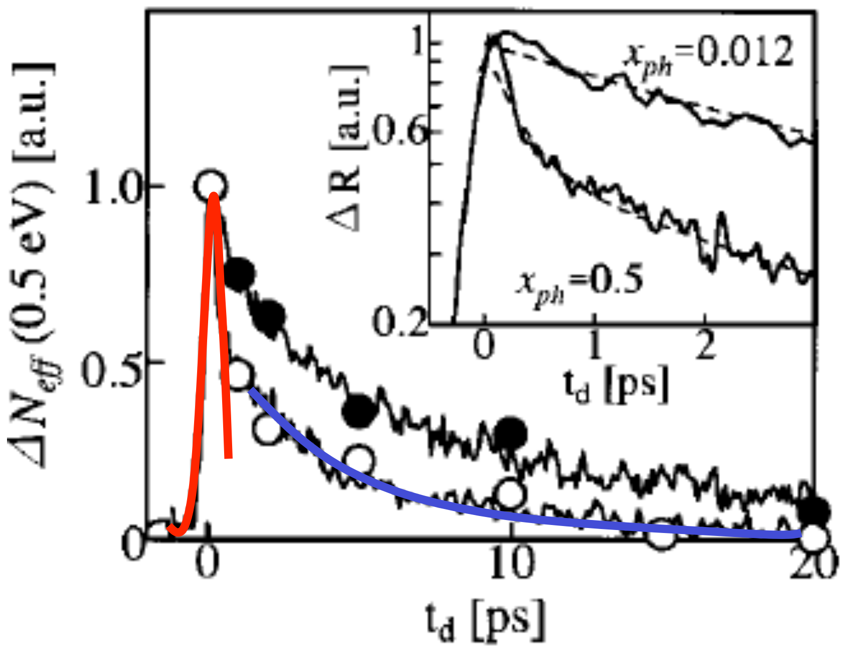


Okamoto G. HP (Tokyo Univ.)

Optical gap～U → effect of U on optical properties

Ultrafast relaxation dynamics in Halogen-bridged Ni compound





(a) Two time scales:

(a-1) instantaneous response

(< pulse width ～ 100fs)

(a-2) picosecond response

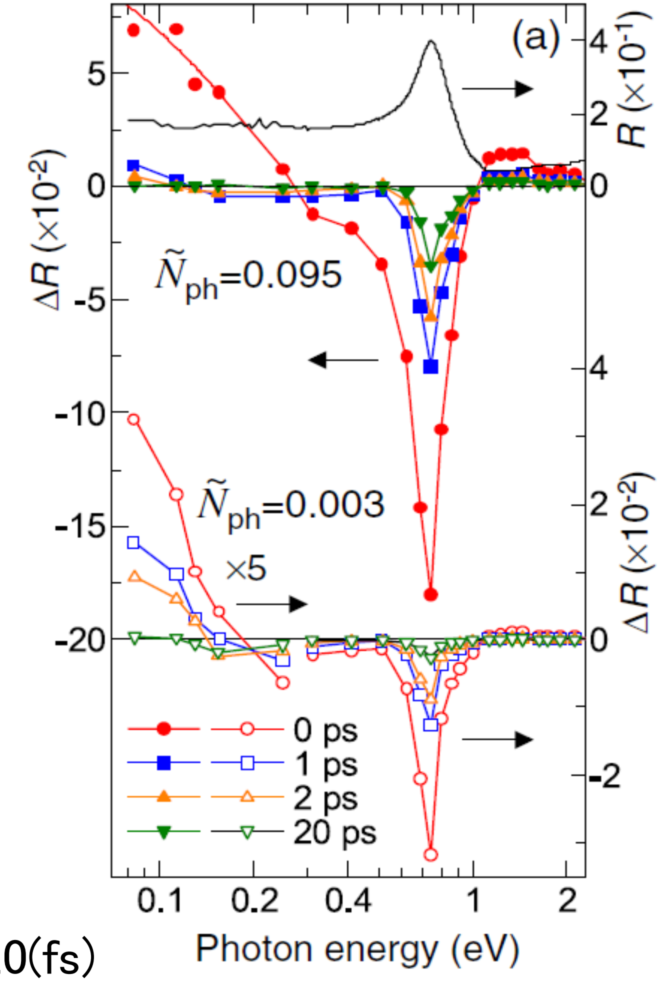
(b) x_{ph} dependence

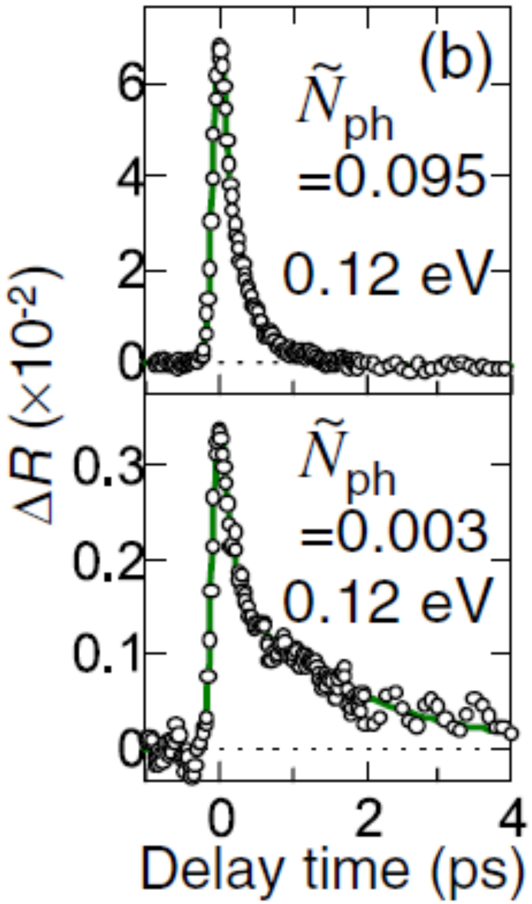
$$\omega_{pump} = 1.55(\text{eV})$$

S. Iwai et al., PRL91, 057401 (2003)

Ultrafast dynamics in ET-F_2TCNQ

H. Okamoto et al., PRL98 037401 (2007)





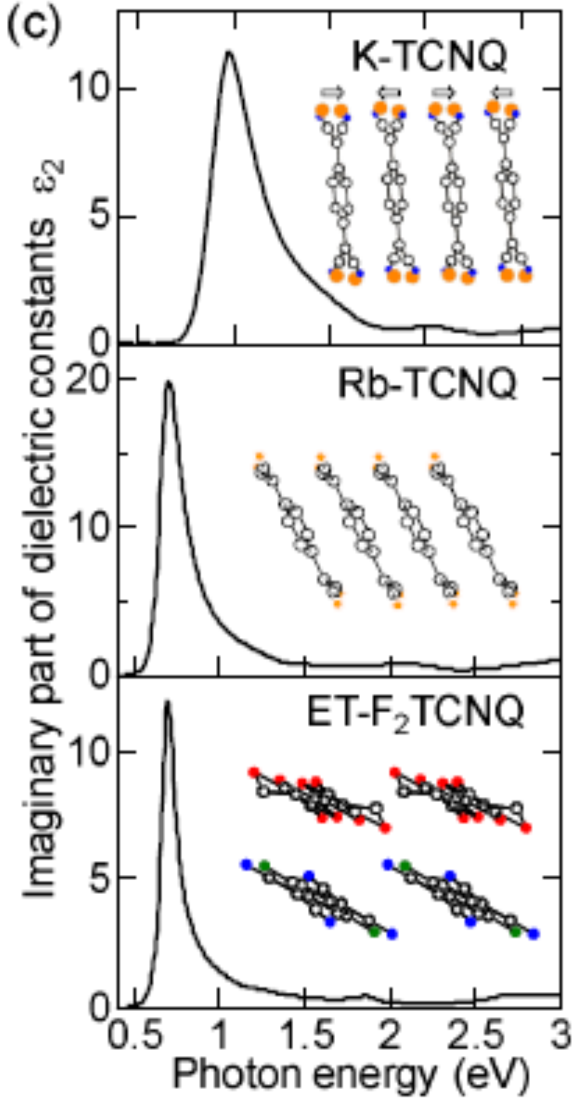
T_N=30(K)

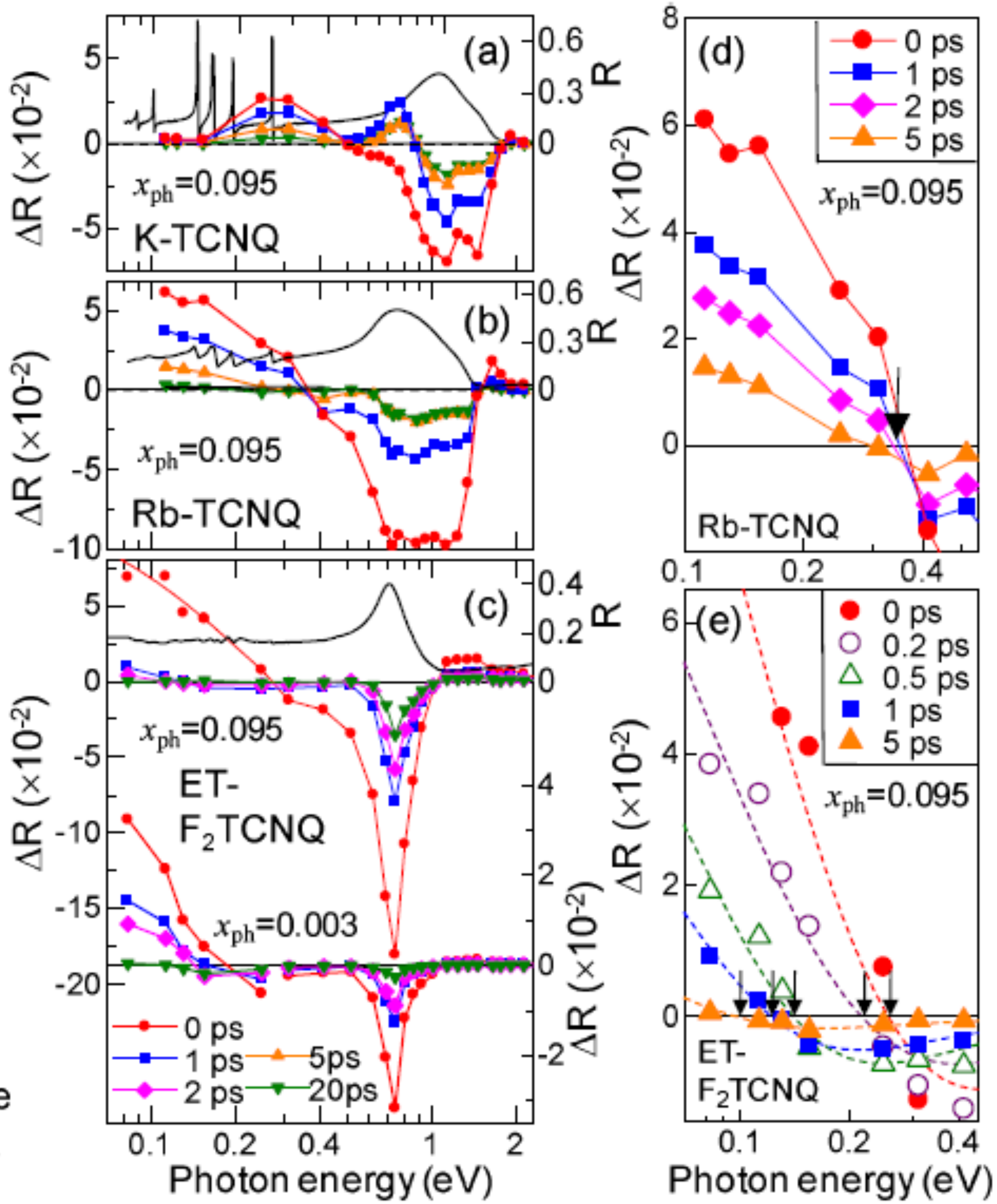
$\tau_{dulation}$=20(fs)

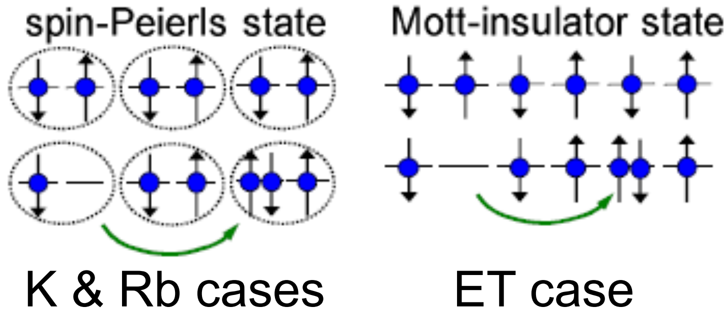
(a) No spin-Peierls dimerization → Weak electron-lattice interaction

(b) No mid-gap state → Spin-charge separation

N_{ph} dependence of ω_{plasma}







H. Uemura et al., JPSJ77, 113714 (2008)

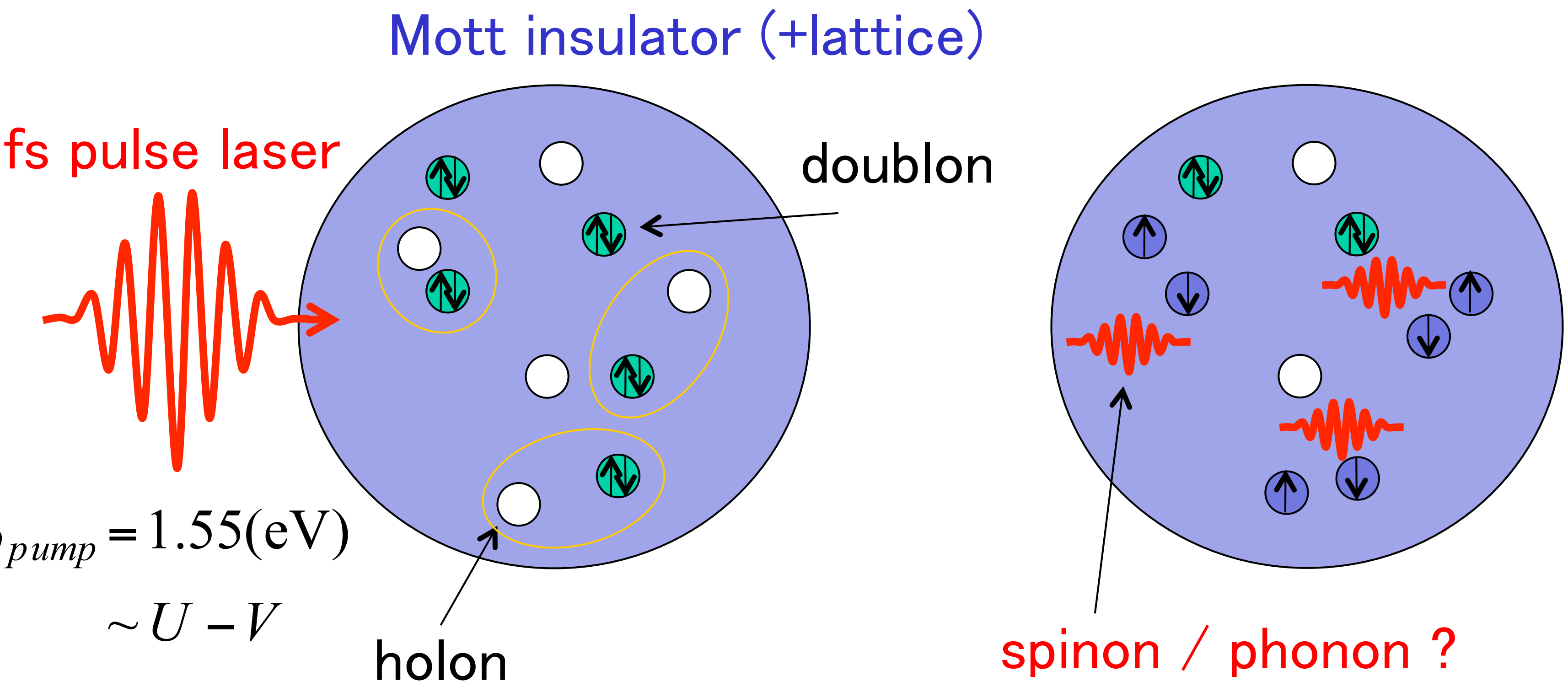
Purpose of this research

(1) Driving force of (instantaneous & ps scale) relaxation

* Both of spin & phonon only weakly couple with holon & doublon.

(2) lattice relaxation

→ difference between Mott insulators and semiconductors



$\omega_{pump} = 1.55(\mathrm{eV})$

$\sim U - V$

Spin degree: large J (3000K) but spin-charge separation

Lattice: large coupling leads to localization, 100K × 100 phonons

Hubbard-Holstein Model

Electrons coupled with (quantum) phonon degrees of freedom
& (classical) vector potential of pulsed laser light

$$H(\tau) = -t\sum_{i,\sigma}\left(e^{iA(\tau)}c_{i,\sigma}^{+}c_{i+1,\sigma} + e^{-iA(\tau)}c_{i+1,\sigma}^{+}c_{i,\sigma}\right)$$
$$+U\sum_{i}n_{i,\uparrow}n_{i,\downarrow} + V\sum_{i}(n_i - 1)(n_{i+1} - 1)$$
$$+\omega_0\sum_{i}b_{i+1/2}^{+}b_{i+1/2} - g\sum_{i}(n_i - n_{i+1})(b_{i+1/2}^{+} + b_{i+1/2})$$

$$A(\tau) = A_0\exp\left(-(\tau-\tau_s)^2/2\tau_d^{\,2}\right)\cos\left(\omega_{pump}(\tau-\tau_s)\right)$$

Strong electron correlation
Bosonic degrees of freedom
Time dependence → non-equillibrium

Time-dependent quantities

(1) Total energy $E(\tau) = \langle \tau | H(\tau) | \tau \rangle$ $\delta = \left(E(\infty) - E_0 \right) / L \omega_{pump}$

(2) Doublon number $D(\tau) = \langle \tau | \sum_i n_{i,\uparrow} n_{i,\downarrow} | \tau \rangle$

(3) Phonon number $N_{phonon}(\tau) = \langle \tau | \sum_i b^{+}_{i+1/2} b_{i+1/2} | \tau \rangle$

(4) Spin energy $S(\tau) = \langle \tau | \sum_i \vec{S}_i \cdot \vec{S}_{i+1} | \tau \rangle$

$$|\tau\rangle = T \exp\left(-i \int_0^{\tau} H(t) dt \right) |0\rangle \qquad \rho = \sum_{i=1}^{m} p_i Tr |\psi_i\rangle\langle\psi_i|, \sum_i p_i = 1$$

The time-dependent wave function is optimized by DMRG

$$U = 10t, V = 2t, \omega_0 = 0.1t (< J), L = 8 \sim 12$$

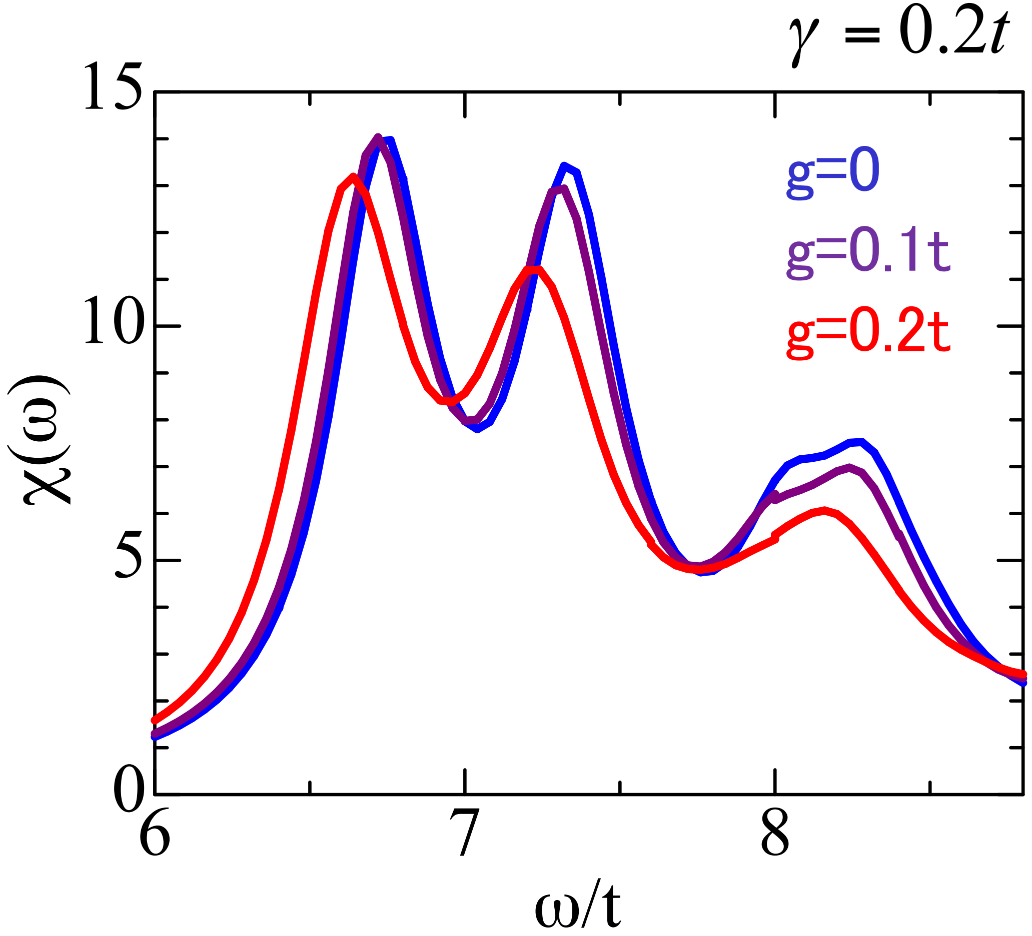
Optical absorption spectra

$$\omega_{pump} = U - V$$

$$\tau_s = 15/t$$

$$\tau_d = 5/t$$

$$1/t \sim fs$$



$$\lambda = \frac{g^2}{4t\,\omega_0}$$

$$\lambda(g = 0.1t) = 0.025$$

$$\lambda(g = 0.2t) = 0.1$$

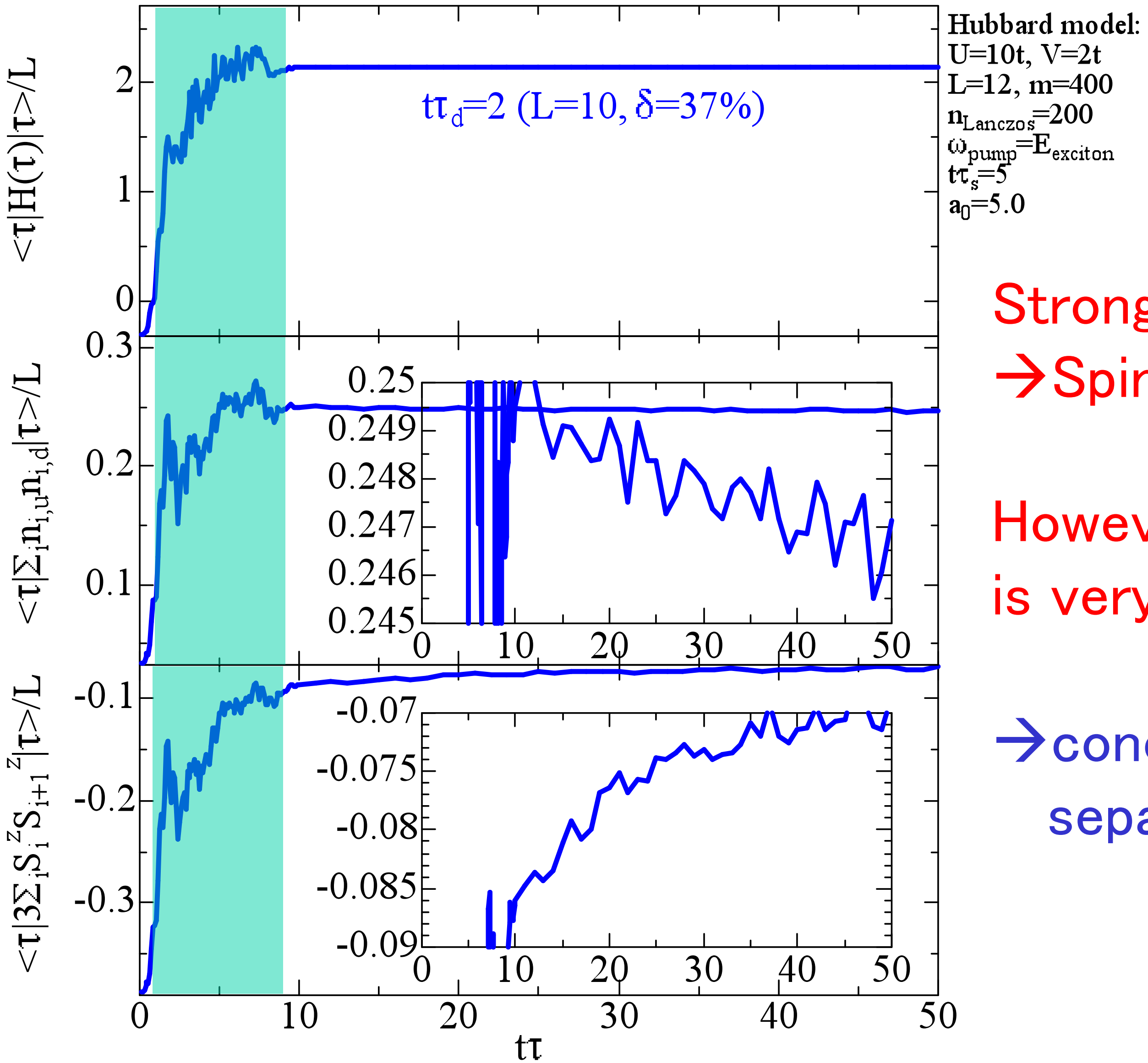
g=0.1t, 0.2t → χ(ω) is not modified strongly by g in comparison with χ(ω) for g=0.

Numerical results for Hubbard model (g=0)

$$\omega_{pump} = E_{exciton}, g = 0.2t$$

$$\tau_s = 5/t$$

$$\tau_d = 2/t$$



Strong excitation

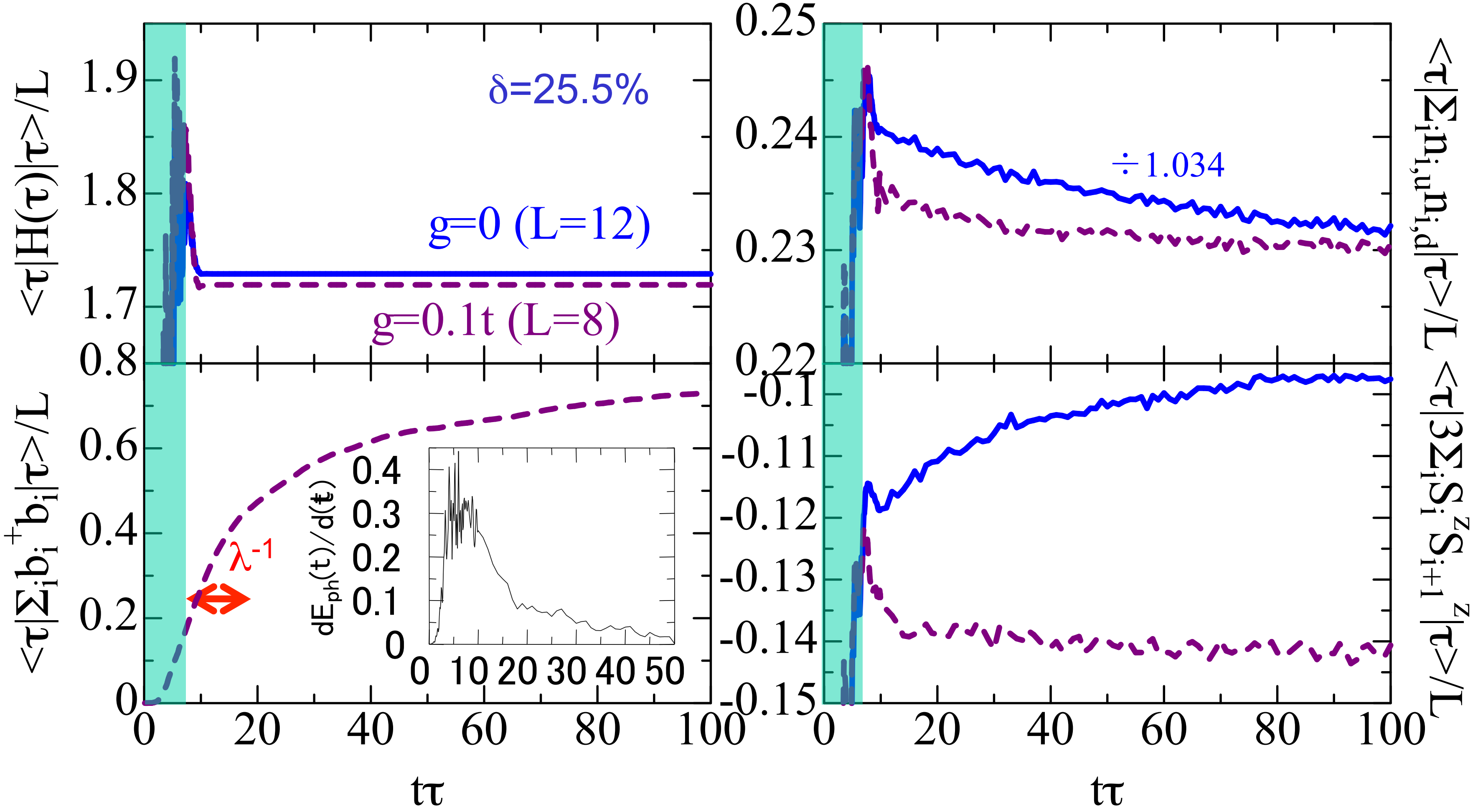
→Spin relaxation

However the decay of D(τ) is very weak

→conceptually spin-charge separation

Effect of g on time evolution

$\omega_{pump} = U - V$



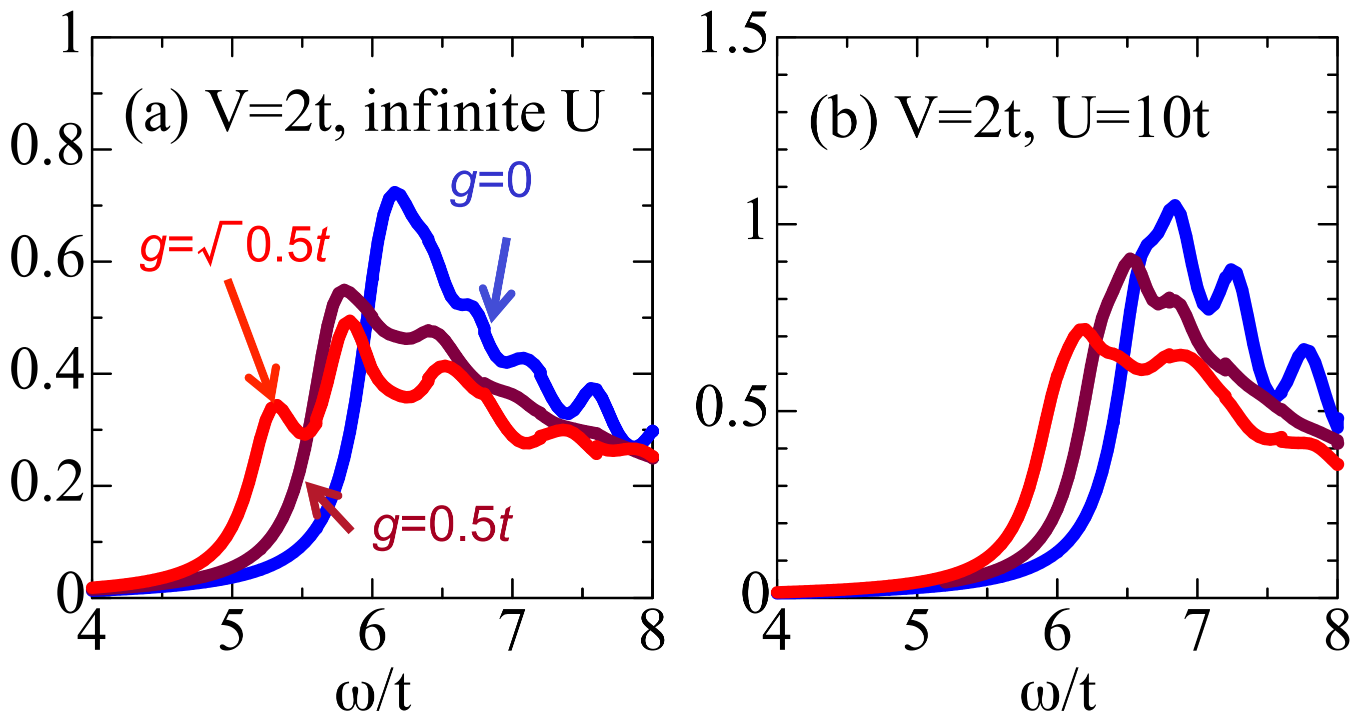
Phonon dominates initial dynamics (spin relaxation is suppressed).

Two time scales: λ^{-1} & long time

λ^{-1}: polaron formation, long time: recombination of holon & doublon

U dependence of phonon effect on the exciton

Hubbard–Holstein model: U=10t, V=2t
(the lowest–energy peak → exciton)
Holon–Doublon model: U→∞



The effect of the EP interaction on the exciton is enhanced, when U increases.

H. Matsueda et al., PRB77, 193112 (2008)

Discussion & Conclusion

* Holon-Doublon model → spin degrees of freedom are traced out.
  (exchange between holon & doublon → ×)

* Spinless carriers (→ weakly correlated carriers) are affected by phonons more strongly than carriers in a case of U=10t.
* Strong EP coupling would accerete localized polaron formation, leading to slow relaxation dynamics.

* Calculation of ARPES spectra for Hubbard-Holstein model
  Phonon Hilbert space for U=0 > that for U=10t
  H. Matsueda et al., PRB74, 241103(R)(2006)

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Conclusion:

(1) g=0 → weak spin relaxation

(2) g>0 → phonon dominates relaxation even for small g

(3) Two time scales, U dependence of relaxation time

Application of MPS to the analysis of PIPT

PIPT → Relaxation dynamics after pulsed-laser irradiation

Electrons coupling with environmental (phonon) degrees of freedom

Prototypical model:

$$H = -t \sum_{i,\sigma} \left(c^{+}_{i,\sigma} c_{i+1,\sigma} + H.c. \right) + U \sum_{i} n_{i,\uparrow} n_{i,\downarrow}$$

$$+ \omega_0 \sum_{i} b^{+}_{i} b_{i} - g \sum_{i} n_i (b^{+}_{i} + b_i)$$

Trial wave function in 1D → MPS

$$|\psi\rangle = \sum_{\{s_1 s_2 \cdots s_n\}} tr\left(A^{s_1}_{1} A^{s_2}_{2} \cdots A^{s_n}_{n} \right) |s_1 s_2 \cdots s_n\rangle$$

Full Hilbert space (DMRG, almost difficult to handle directly)

→ Decomposition to a set of local degrees of freedom

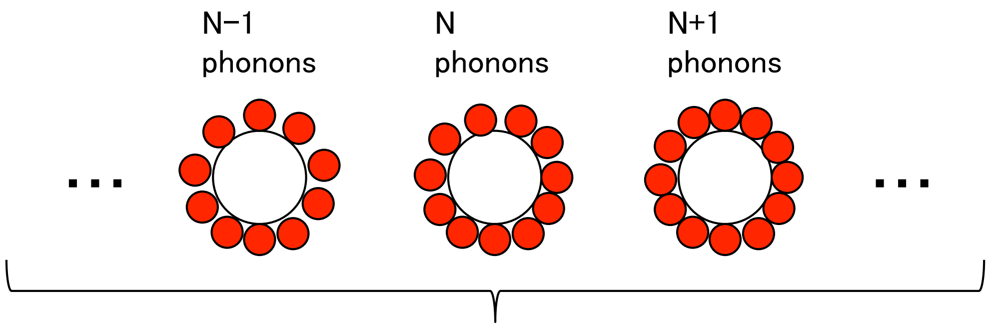
What about the physical meaning of matrix dimension D ?

$$|\psi\rangle = \sum_{\{s_1 s_2 \cdots s_n\}} tr\left(A_1^{s_1} A_2^{s_2} \cdots A_i^{s_i} \cdots A_n^{s_n}\right) |s_1 s_2 \cdots s_n\rangle$$

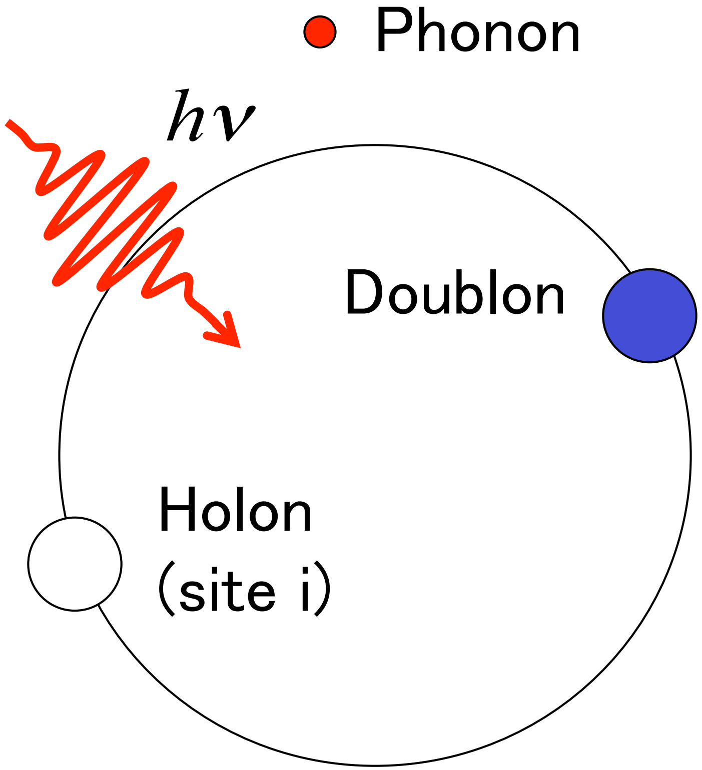
$A_i^{s_i}$: D × D matrix

Meaning of matrix dimension D

$$\langle\psi | b_i^{+} b_i | \psi\rangle = N$$



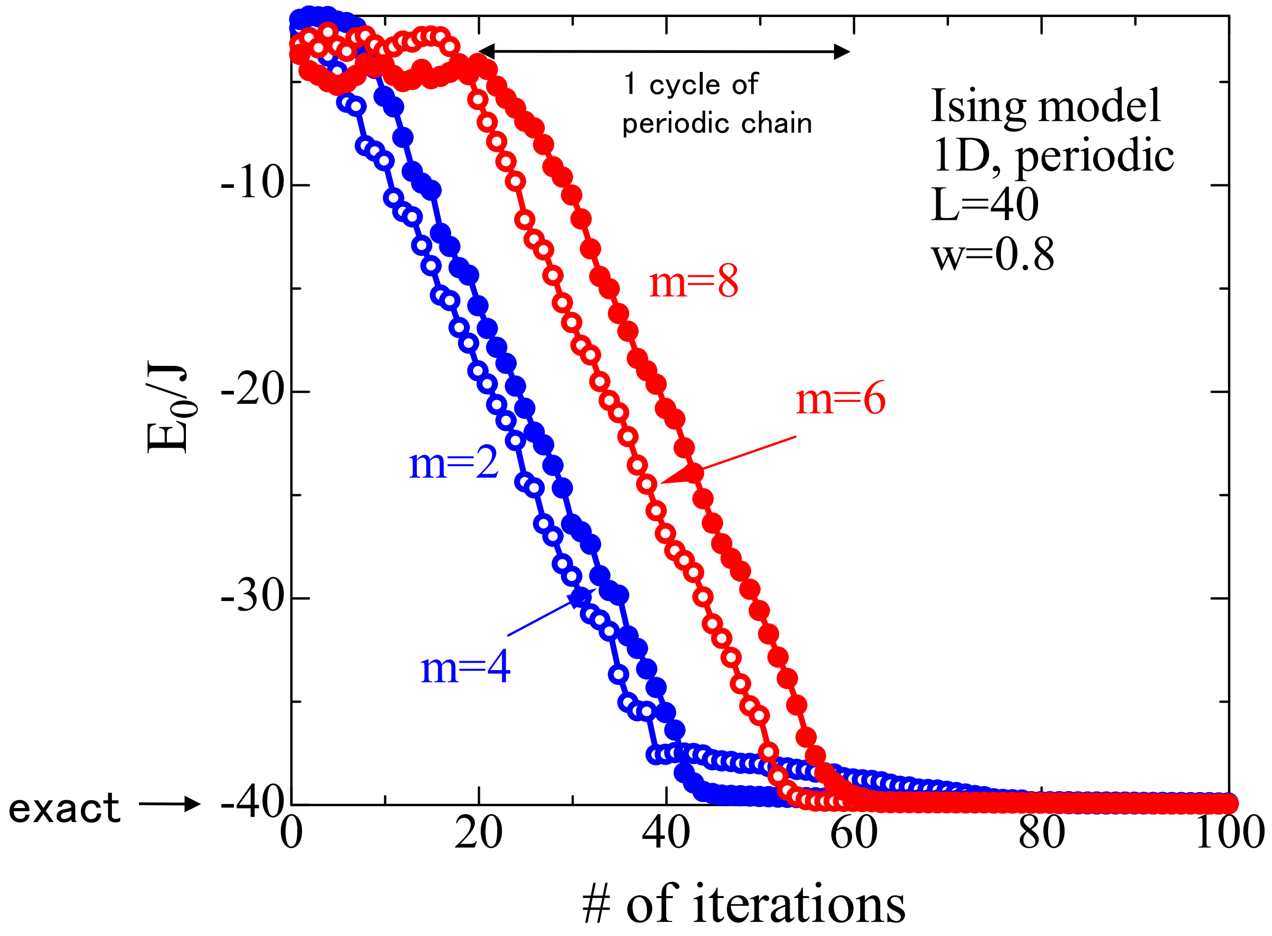
$\sim$ D_1 states $\quad \sqrt{N}$



Electron site → D_2 for Heisenberg spin (large-U case)

Appropriate dimension : D $\sim$ max(D_1,D_2)

Iterative optimization of MPS and the ground-state energy

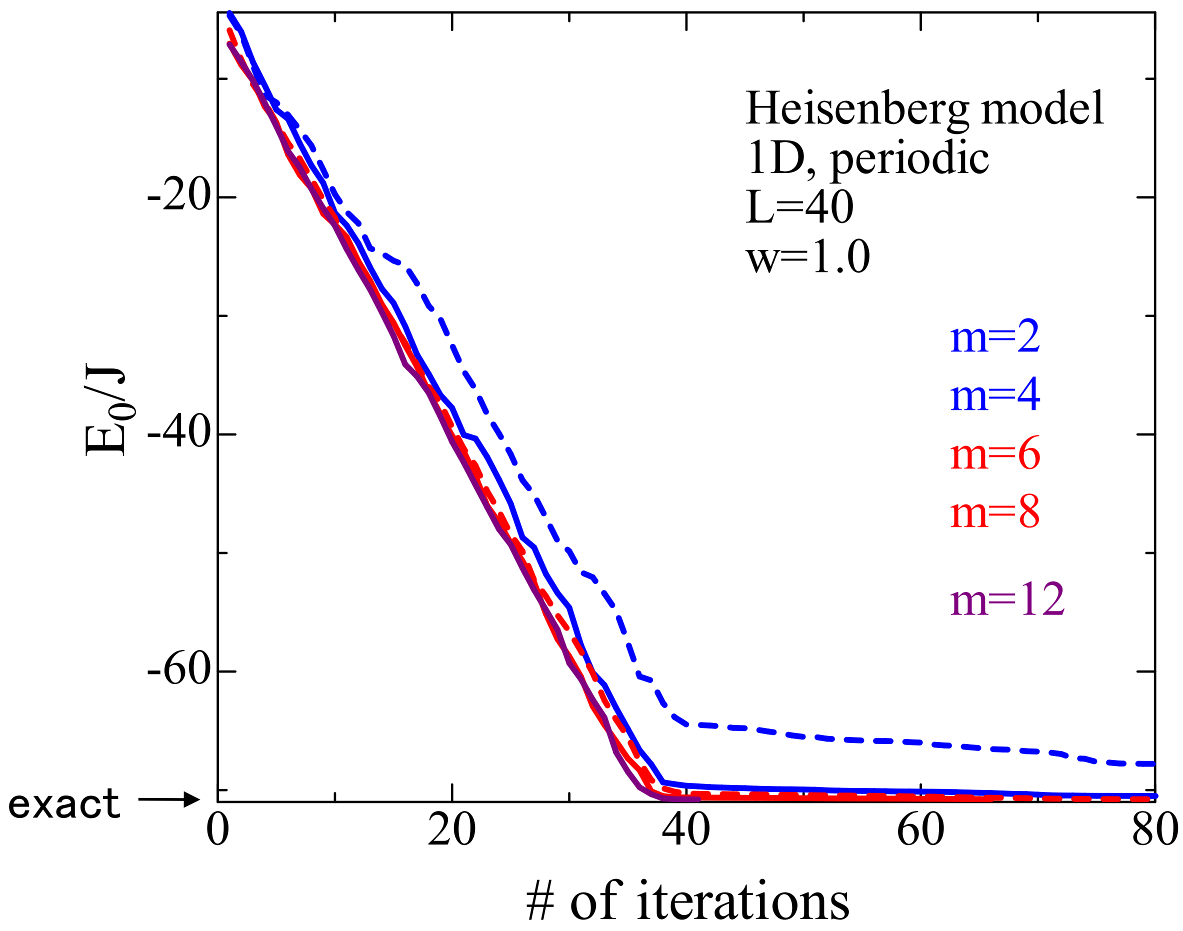


$$w\,A_{new} + (1-w)\,A_{old} \Rightarrow A_{new}$$

Ising model → weak entanglement (best case: m=4～6)

Too many internal degrees do not accelerate convergence

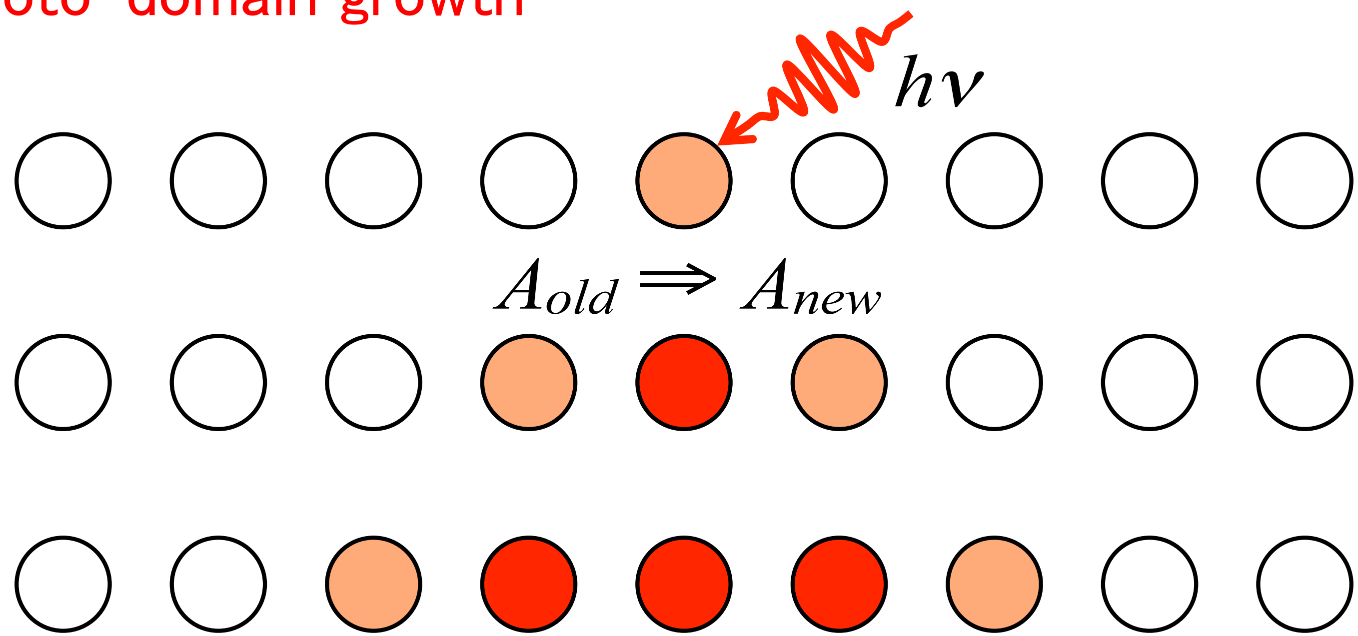
Heisenberg model (critical):
Spin correlation → algebraic decay
(long-range interactions play a role on entanglement)
The numerical convergence becomes better as we increase D.



Future perspective

(a) Hubbard-Holstein, study of PIPT
standard DMRG → MPS

(b) 'surfing' DMRG (named by Nishino-san)
photo-domain growth



Drastic change occurs only at the domain boudaries.
→ More efficient MPS optimization may exist.

Thank you for attention