# Photo-induced electron dynamics in one-dimensional extended Hubbard model


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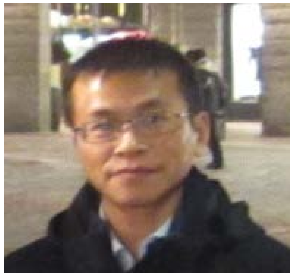


Shigetoshi Sota
(RIKEN)

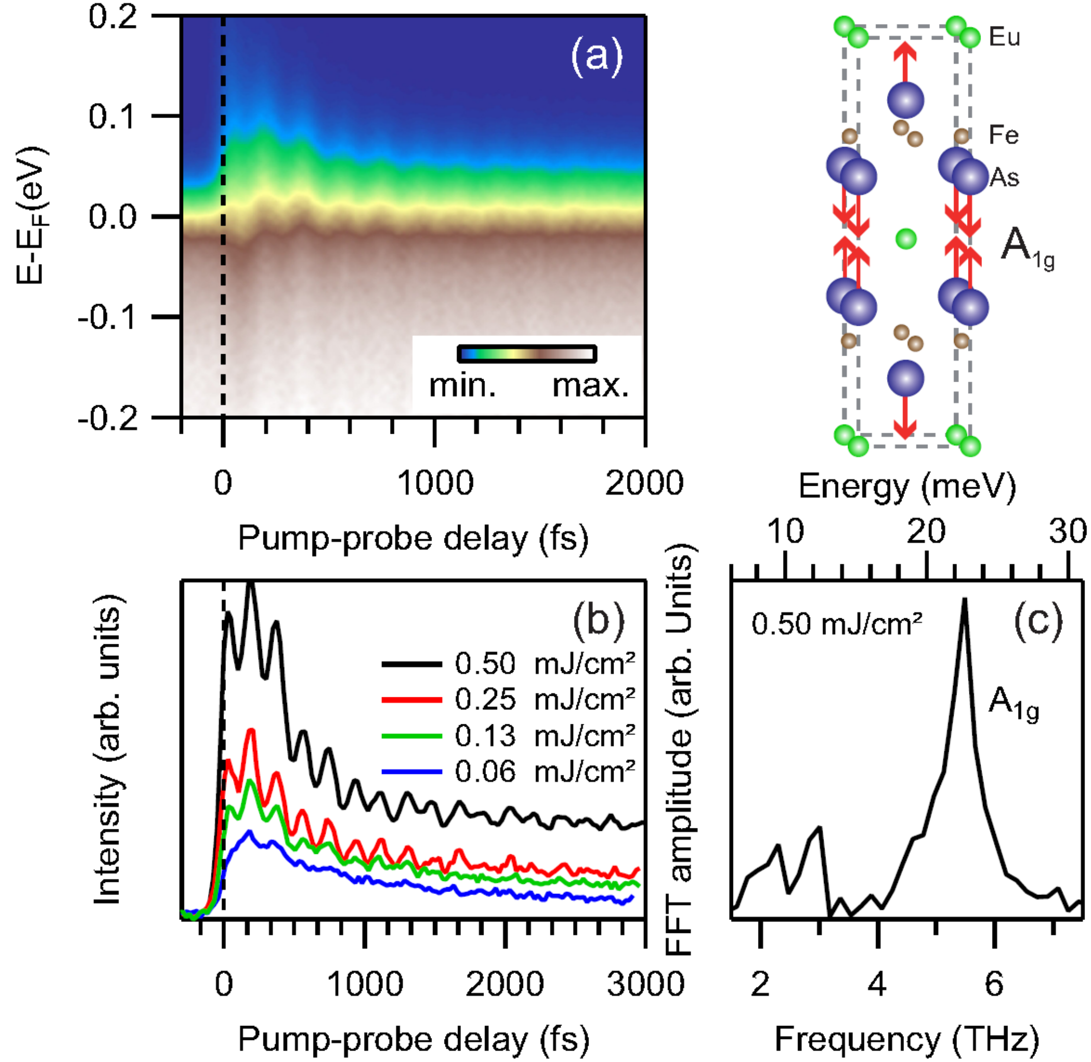
Hiroaki Matsueda
(Sendai Inst. Tech.)

Janez Bonca
(Josef Stephan Inst.)

# Recent experimental development of nonequilibrium dynamics

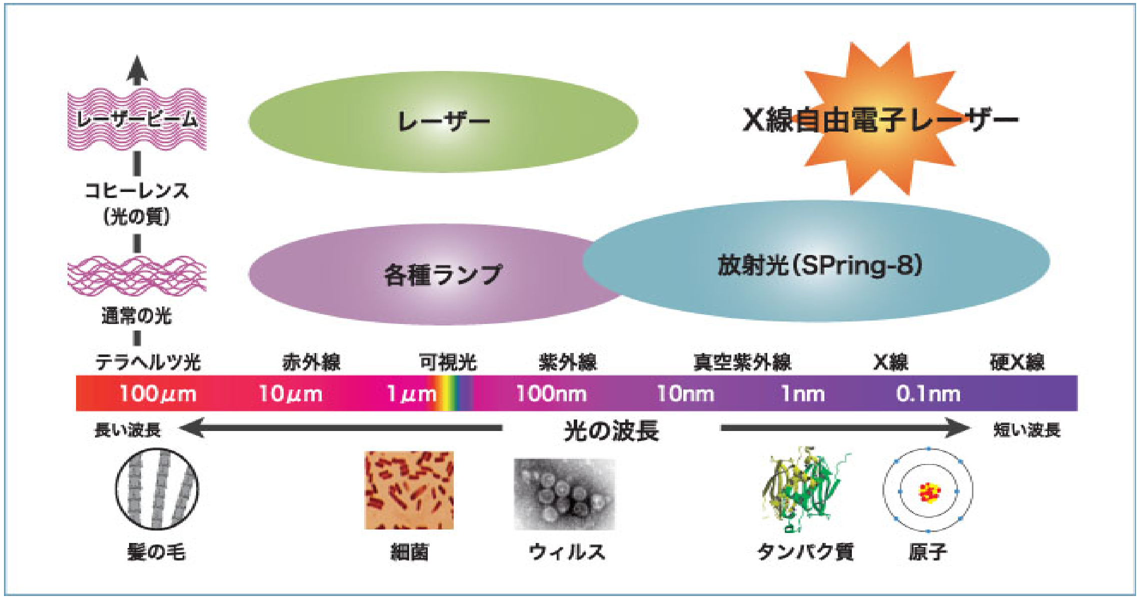
Time-dependent angle-resolved photoemission

Coherent phonon of Iron-pnictide superconductor $EuFe_2As_2$




PRL **108**, 097002 (2012)

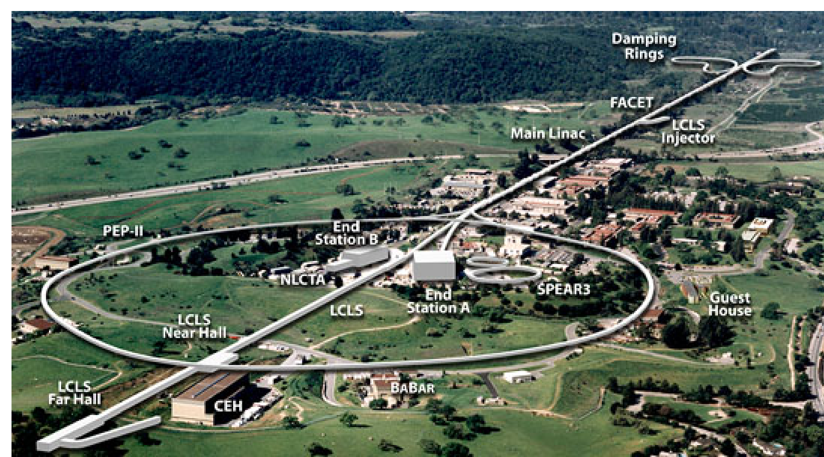
# X-ray Free Electron Laser : XFEL




http://xfel.riken.jp/sacla/

**S**Pring-8 **A**ngstrom **C**ompact Free Electron **La**ser (SACLA) (2012~)

SLAC **L**inac **C**oherent **L**ight **S**ource (LCLS) (2011~)



# Recent development of pump and probe techniques

- Femotosecond time-resolved THz spectroscopy

- Time-resolved angle-resolved photoemission

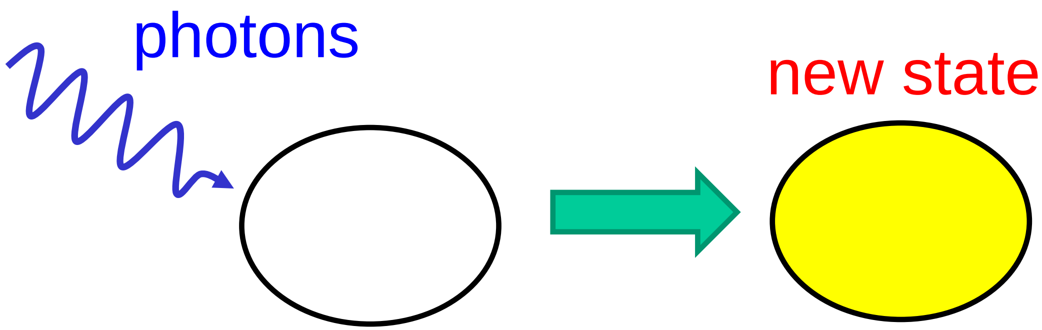
- Time-resolved Raman scattering

- Time-resolved soft X-ray scattering by XFEL

- …….

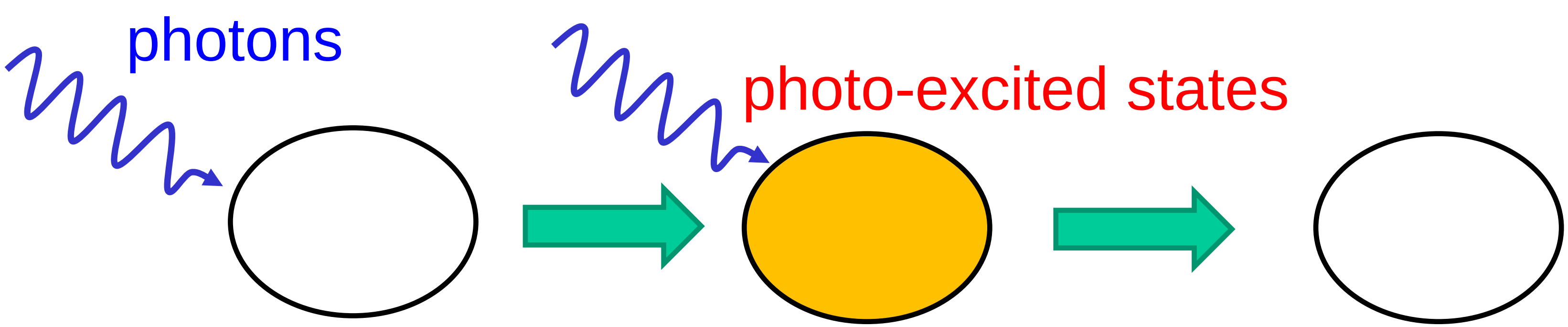
Physics of nonequilibrium photo dynamics
in strongly correlated electron systems

# Nonequilibrium photo-induced dynamics in strongly correlated electron systems




What is the condition for the change of states?

H. Lu, S. Sota, H. Matsueda, J. Bonca, and T.T., PRL **109**, 197401 (2012)




Is it possible to detect quantum interference?

H. Lu, J. Bonca, and T.T., EPL **103**, 57005 (2013)

# Extended Hubbard Model

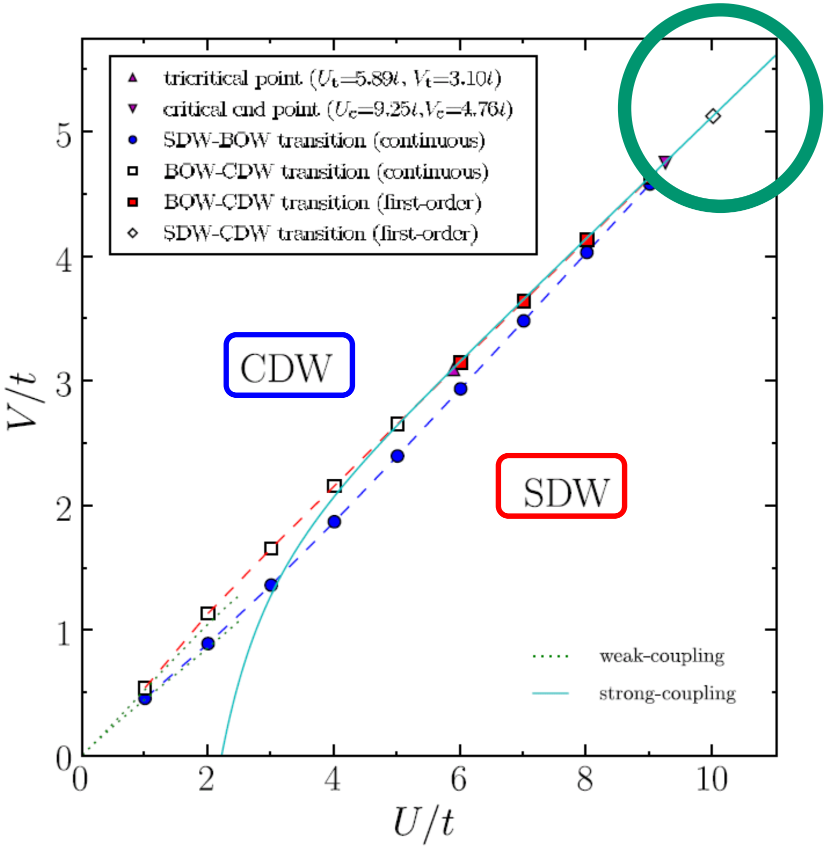
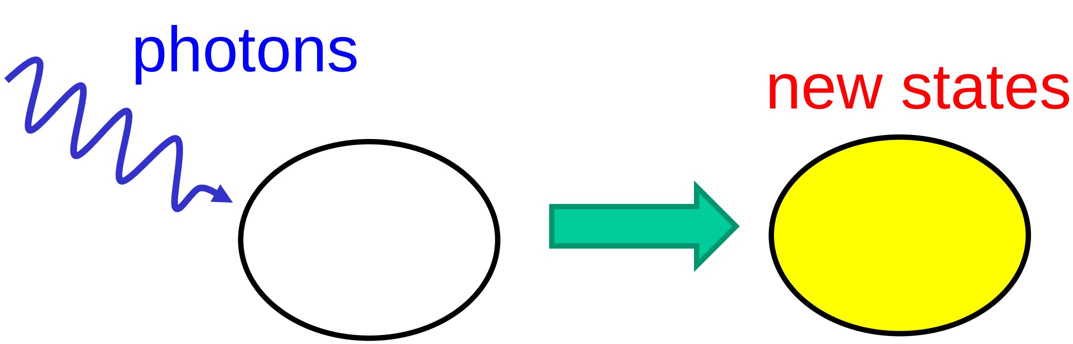
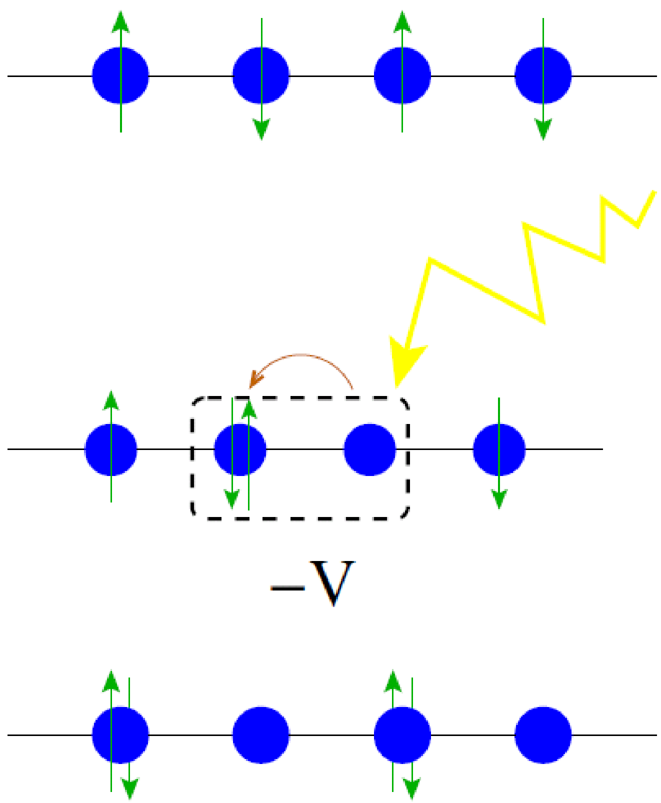



Figure: Phase diagram of the 1D half-filled EHM. Source: S. Ejima and S. Nishimoto, *Phys. Rev. Lett.* **99**, 216403 (2007).

$$H_{\text{EHM}} = -t_h \sum_{i,\sigma} \left( c_{i,\sigma}^{\dagger} c_{i+1,\sigma} + \text{H.c.} \right) + U \sum_i \left( n_{i,\uparrow} - \frac{1}{2} \right) \left( n_{i,\downarrow} - \frac{1}{2} \right) + V \sum_i (n_i - 1)(n_{i+1} - 1)$$

First order phase transition in equilibrium happens around $U \approx 2V$ between spin-density-wave (SDW) and charge-density-wave (CDW), driven by the competition between energy cost for doublon generation and energy reward due to the attraction between doublon-holon pairs.




Mott insulator
(SDW state)

$\Downarrow$

Attraction
between doublons and holes
$V \sum_i n_i n_{i+1}$

$\Downarrow$

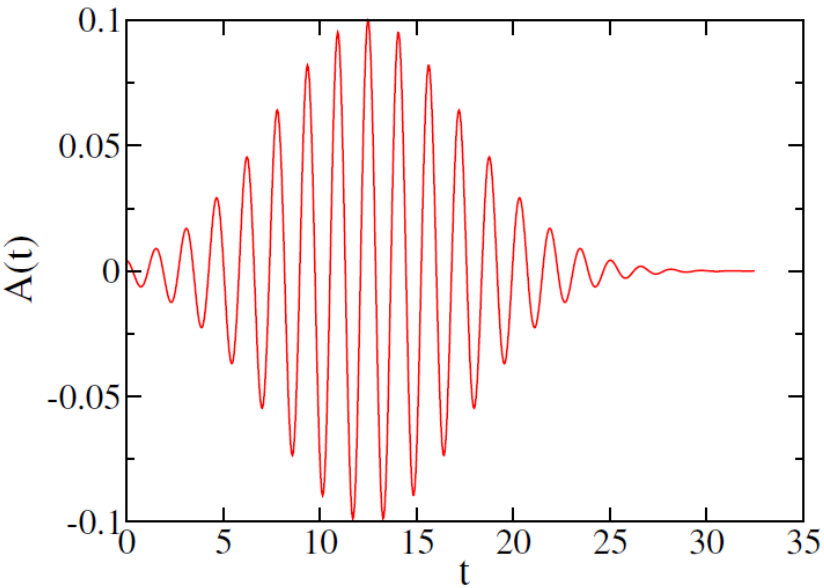
CDW state?

# Laser Added

In the 1D extended Hubbard model with laser pulse applied, the external field is incorporated by means of the Peierls substitution:

$$c^{\dagger}_{i,\sigma} c_{i+1,\sigma} + \mathrm{H.c.} \quad \rightarrow \quad e^{iA(t)} c^{\dagger}_{i,\sigma} c_{i+1,\sigma} + \mathrm{H.c.}$$

$$A(t) = A_0 e^{-(t-t_0)^2/2t_d^2} \cos\left[\omega_{\mathrm{pump}} (t - t_0)\right],$$




An illustration of the vector potential $A(t)$ with parameters as:

$$A_0 = 0.10, \quad \omega_{\mathrm{pump}} = 4,$$
$$t_0 = 12.5, \quad t_d = 5$$

# Time-dependent Lanczos method

[T. J. Park and J. C. Light, J. Chem. Phys. **85**, 5870 (1986)]

$$i\frac{\partial\psi(t)}{\partial t} = H(t)\psi(t)$$

We approximate the time evolution of $|\psi(t)\rangle$ by step-vise change of time $t$ in small increment $\delta t$. At each step, Lanczos basis with dimension $M$ are generated to follow the evolution

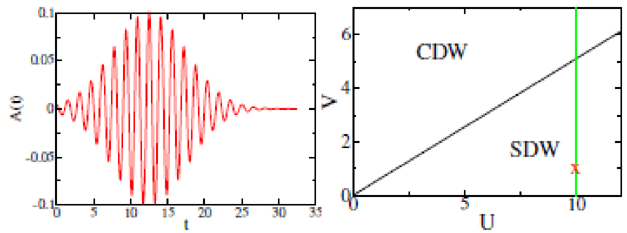
$$|\psi(t+\delta t)\rangle \simeq e^{-iH(t)\delta t}|\psi(t)\rangle$$

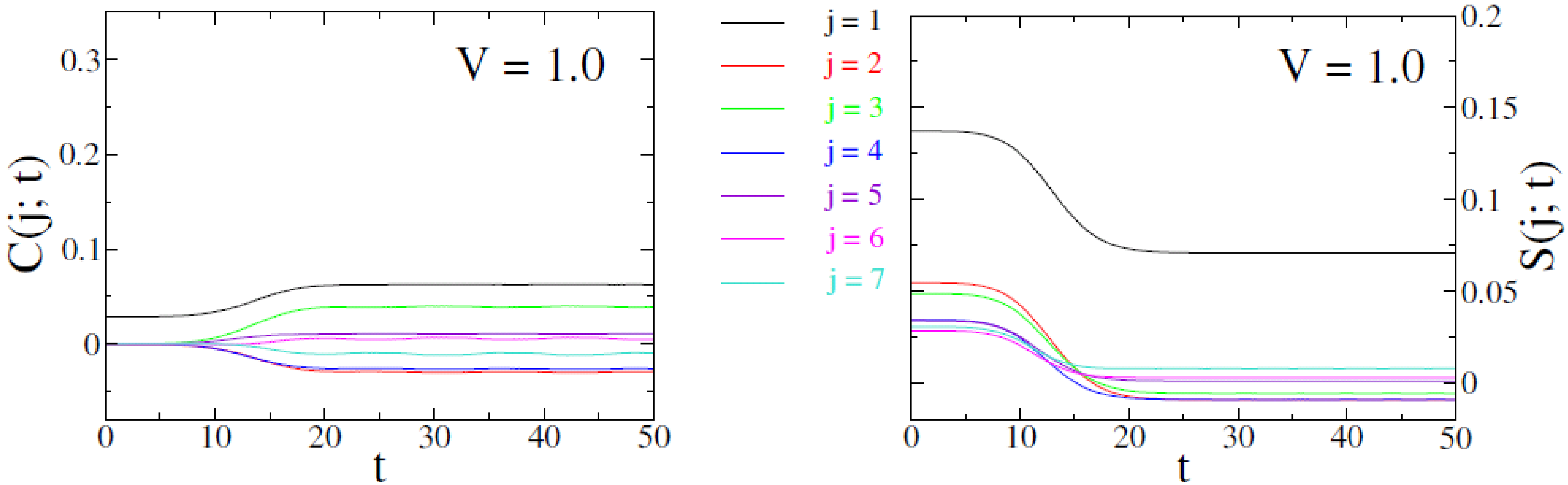
$$\simeq \sum_{l=1}^{M} e^{-i\epsilon_l \delta t}|\phi_l\rangle\langle\phi_l|\psi(t)\rangle$$

# Correlations (14 sites)

$$C(j;t) = \frac{(-1)^j}{L}\sum_{i=0}^{L-1}\langle\psi(t)|(n_{i+j}-1)(n_i-1)|\psi(t)\rangle,$$

$$S(j;t) = \frac{(-1)^j}{L}\sum_{i=0}^{L-1}\langle\psi(t)|\mathbf{S}_{i+j}\cdot\mathbf{S}_i|\psi(t)\rangle.$$



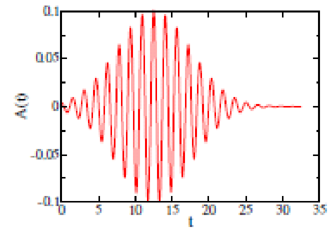

$V = 1.0$, $\omega_{\text{pump}} = 7.1$, $A_0 = 0.10$

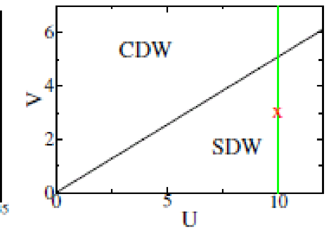
Hantao Lu *et al.* PRL **109**, 197401 (2012); arXiv:1211.1749.

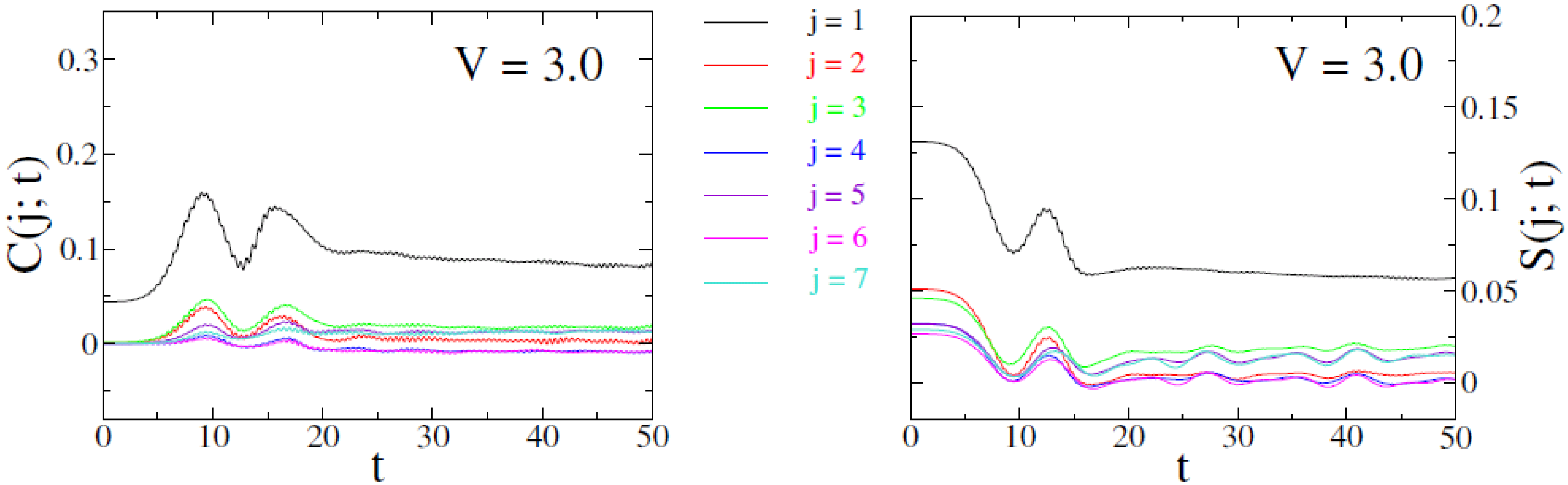
# Correlations (14 sites)

$$C(j;t) = \frac{(-1)^j}{L}\sum_{i=0}^{L-1}\langle\psi(t)|(n_{i+j}-1)(n_i-1)|\psi(t)\rangle,$$

$$S(j;t) = \frac{(-1)^j}{L}\sum_{i=0}^{L-1}\langle\psi(t)|\mathbf{S}_{i+j}\cdot\mathbf{S}_i|\psi(t)\rangle.$$



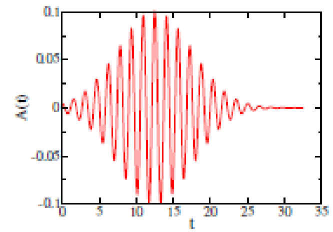

$V = 3.0$, $\omega_{\text{pump}} = 6.1$, $A_0 = 0.30$

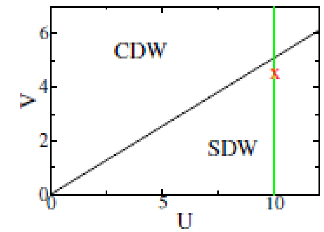
Hantao Lu *et al.* PRL **109**, 197401 (2012); arXiv:1211.1749.

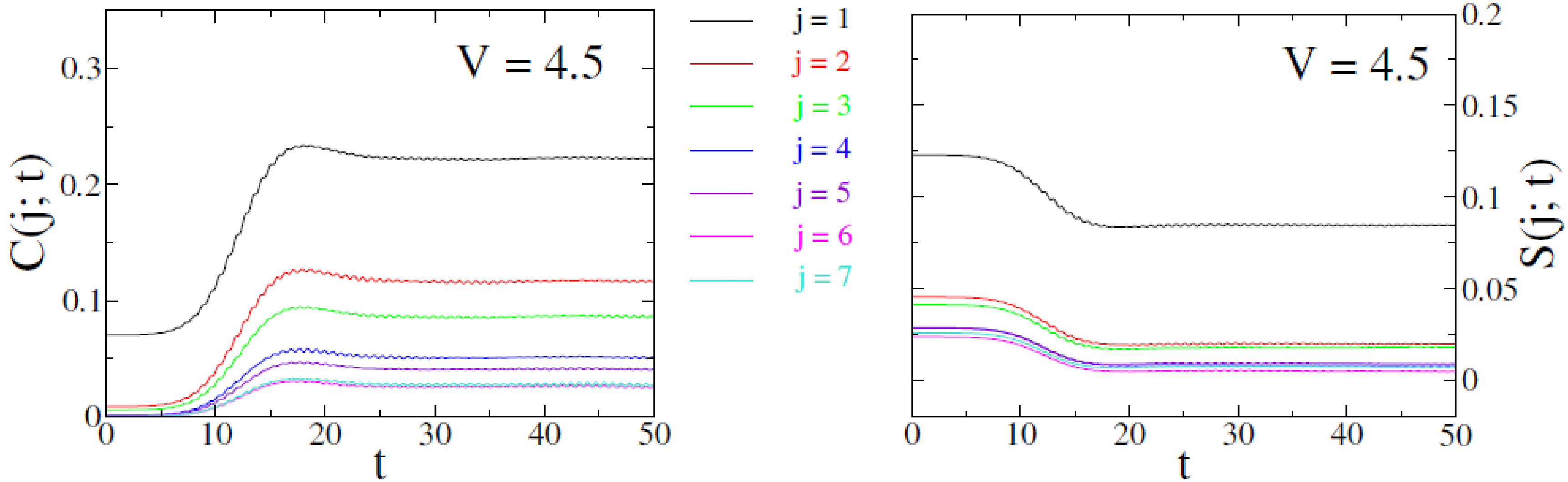
# Correlations (14 sites)

$$C(j;t) = \frac{(-1)^j}{L}\sum_{i=0}^{L-1}\langle\psi(t)|(n_{i+j}-1)(n_i-1)|\psi(t)\rangle,$$

$$S(j;t) = \frac{(-1)^j}{L}\sum_{i=0}^{L-1}\langle\psi(t)|\mathbf{S}_{i+j}\cdot\mathbf{S}_i|\psi(t)\rangle.$$



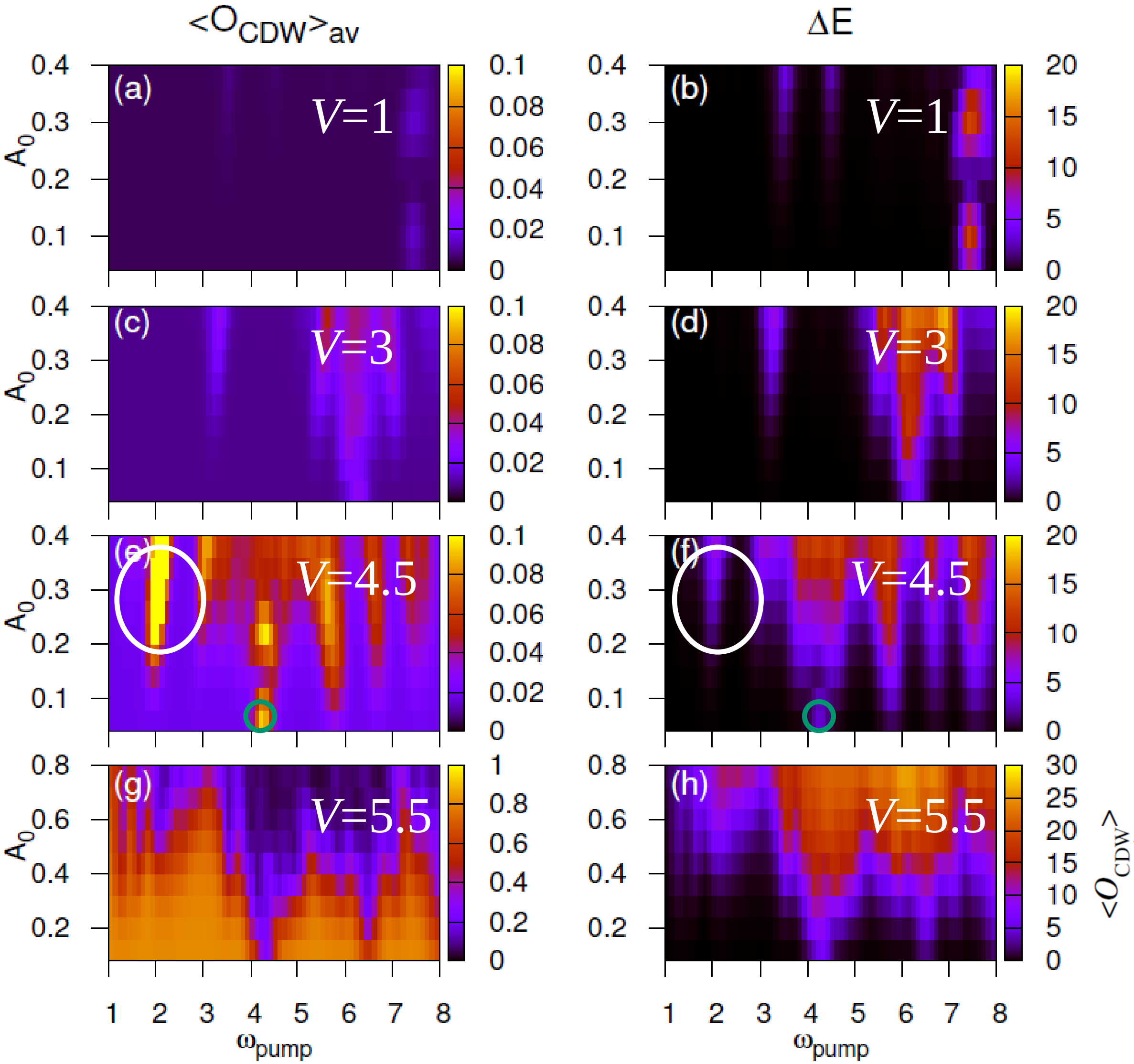



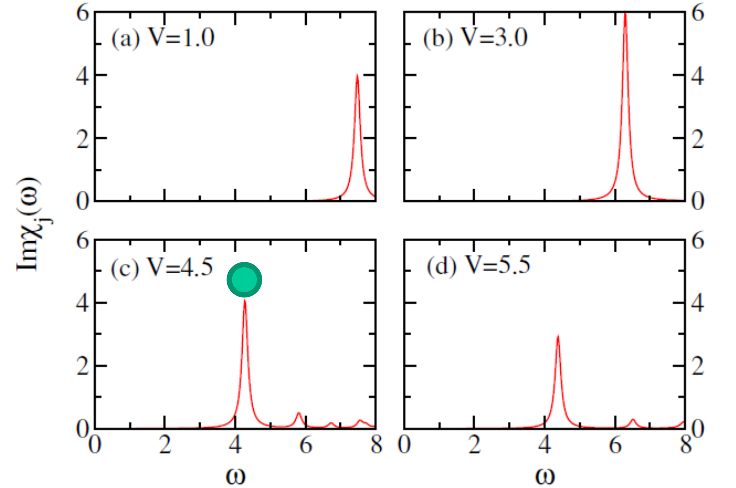

$V = 4.5,\ \omega_{\text{pump}} = 4.0,\ A_0 = 0.07$

Hantao Lu *et al.* PRL **109**, 197401 (2012); arXiv:1211.1749.

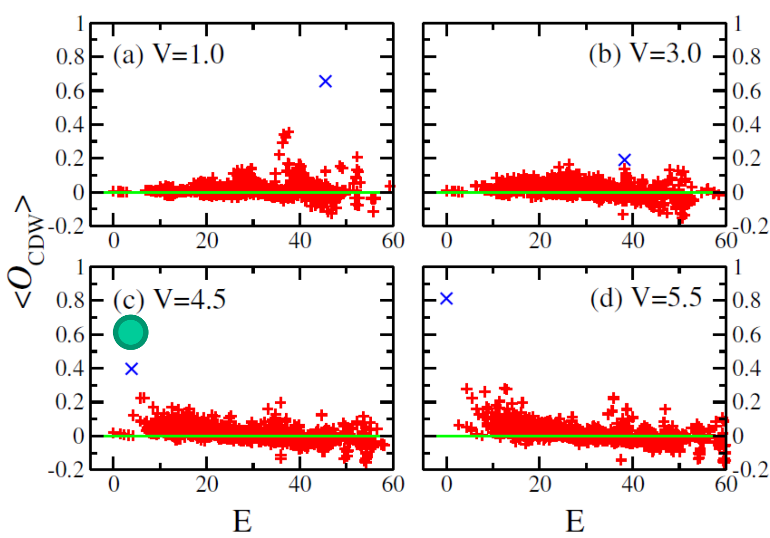
# Parameter Sweeping (10 Sites)




## Optical spectra




$$\mathcal{O}_{\text{CDW}} := \frac{1}{LL_c}\sum_{i=0}^{L-1}\sum_{j=1}^{L_c}(-1)^j\,(n_{i+j}-1)\,(n_i-1)$$



# Summary (1)

Starting from SDW side, we find a possible photo-induced state with significant enhancement of CDW correlation

Conditions:

$\omega_{pump}$ ($2\,\omega_{pump}$) --> matching absorption energy

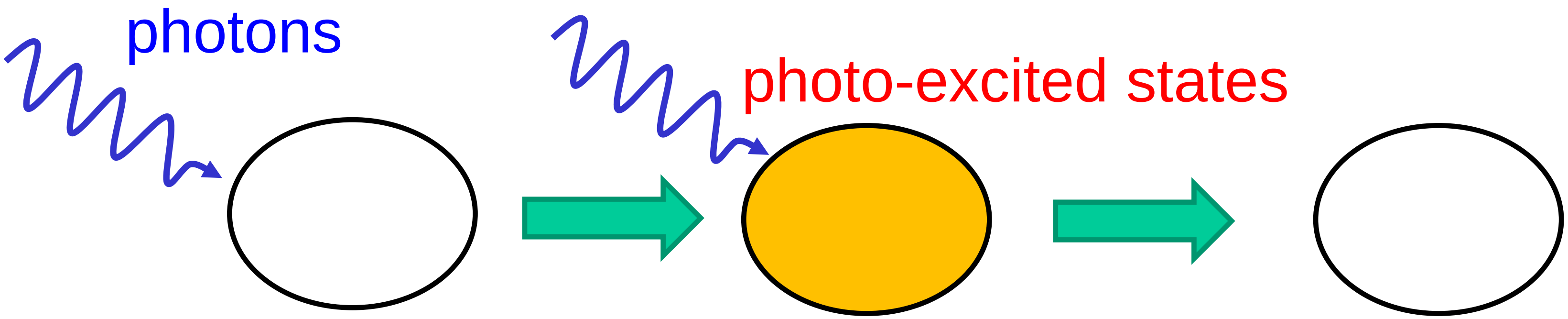
$A_0$ --> giving a proper energy increase reaching a CDW enhanced excited states

Experimental evidence: from CDW to Mott insulator (SDW)

1D organic material: K. Kimura *et al*. PRB 79, 075116 (2009)

No experimental evidence yet: from SDW to CDW

# Double-pulse deexcitations




Is it possible to detect quantum interference by ultrafast optical technique in strongly correlated electron systems?

# Extended one-dimensional Hubbard model

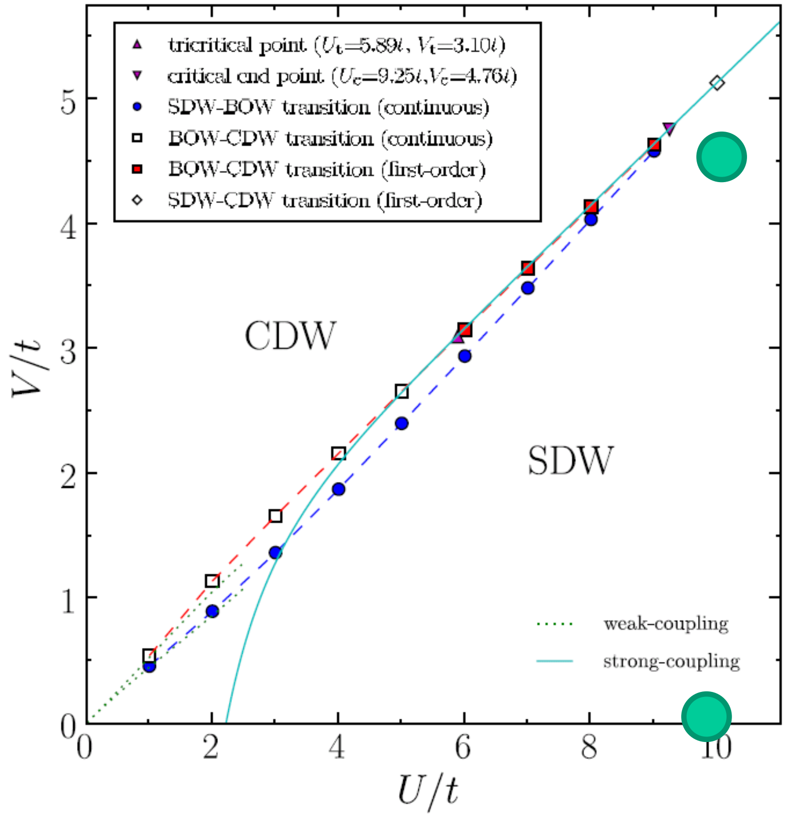



Figure: Phase diagram of the 1D half-filled EHM. Source: S. Ejima and S. Nishimoto, *Phys. Rev. Lett.* **99**, 216403 (2007).

$$
\begin{aligned}
H_{\text{EHM}} &= -t_h \sum_{i,\sigma} \left( c^\dagger_{i,\sigma} c_{i+1,\sigma} + \text{H.c.} \right) \\
&+ U \sum_i \left( n_{i,\uparrow} - \frac{1}{2} \right) \left( n_{i,\downarrow} - \frac{1}{2} \right) \\
&+ V \sum_i \left( n_i - 1 \right) \left( n_{i+1} - 1 \right)
\end{aligned}
$$

First order phase transition in equilibrium happens around $U \approx 2V$ between spin-density-wave (SDW) and charge-density-wave (CDW), driven by the competition between energy cost for doublon generation and energy reward due to the attraction between doublon-holon pairs.

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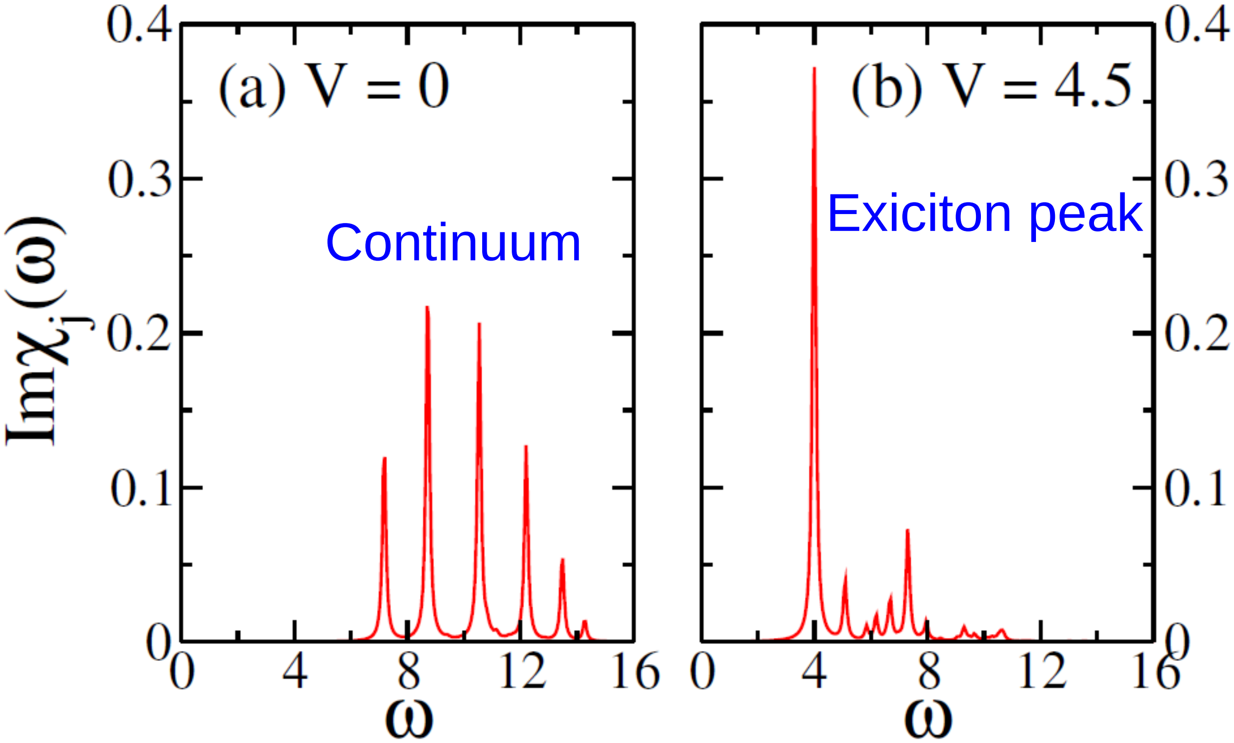
# Optical absorption spectrum

$$\mathrm{Im}\chi_j(\omega) = \frac{1}{L}\sum_n \left|\langle n|\hat{j}|0\rangle\right|^2 \delta\left(\omega - E_n + E_0\right) \sim i\omega\sigma(\omega)$$

$L$=14 ring



# Two external pulses

The vector potential of the external field $A(t)$
→ Peierls phase

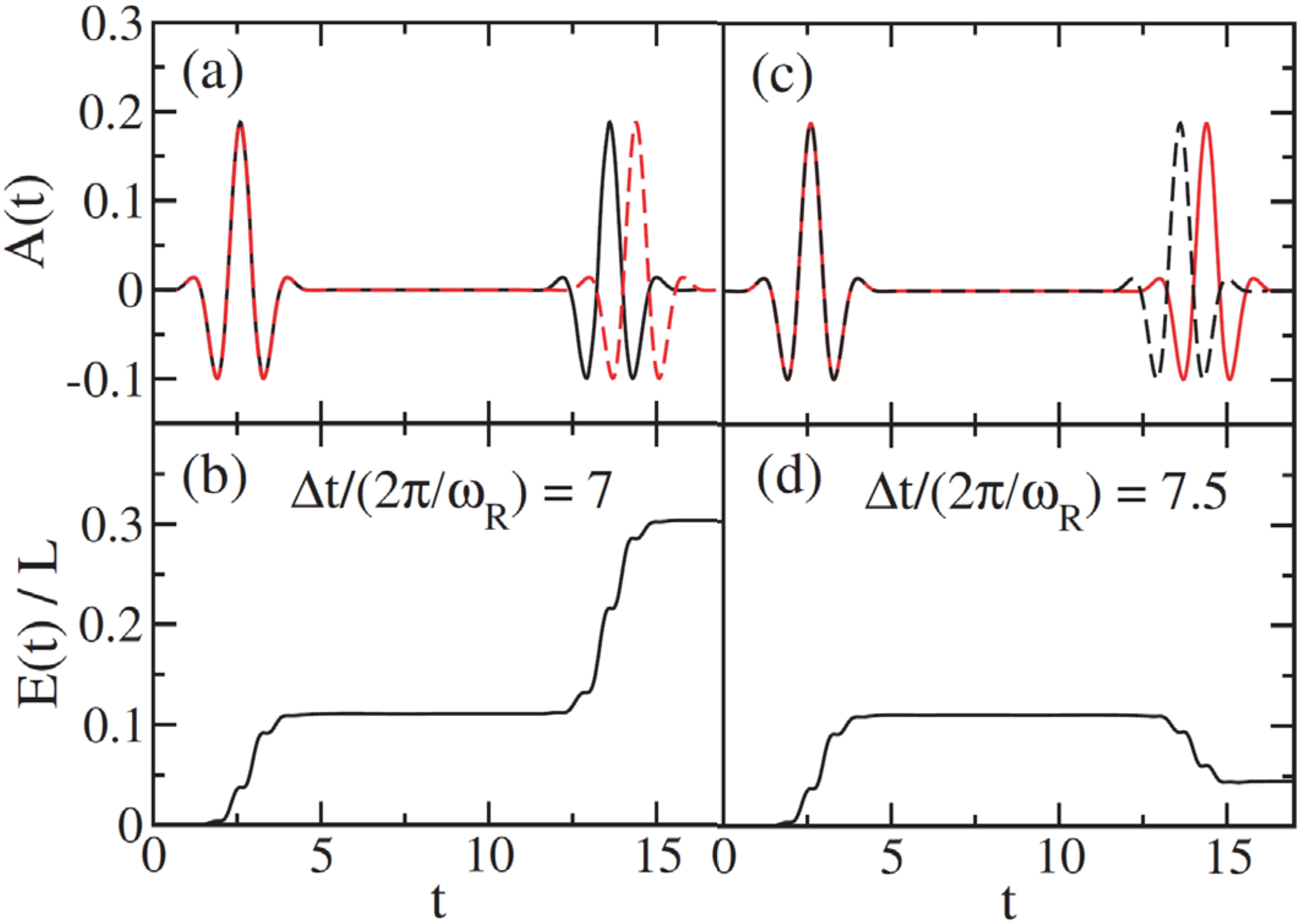
$$c_{i,\sigma}^{\dagger} c_{i+1,\sigma} + \mathrm{H.c.} \rightarrow e^{iA(t)} c_{i,\sigma}^{\dagger} c_{i+1,\sigma} + \mathrm{H.c.}$$

For simplicity, two identical pulses centered at $t=t_1$ and $t=t_2$ are assumed:

$$A(t) = A_0 e^{-(t-t_1)^2/2t_d^2} \cos\left[\omega_{\mathrm{pump}} (t - t_1)\right] + A_0 e^{-(t-t_2)^2/2t_d^2} \cos\left[\omega_{\mathrm{pump}} (t - t_2)\right]$$

# Double-pulse excitation for V=4.5

$A_0 = 0.19$ $\omega_{\rm pump} = 4.0$ $t_d = 0.65$ $E(t) = \langle\psi(t)|H(t)|\psi(t)\rangle - E_{\rm GS}$




$\Delta t = t_2 - t_1$

$\omega_{\rm pump} = \omega_{\rm R}$

$$\Delta t = N \times \frac{2\pi}{\omega_{\rm R}}$$

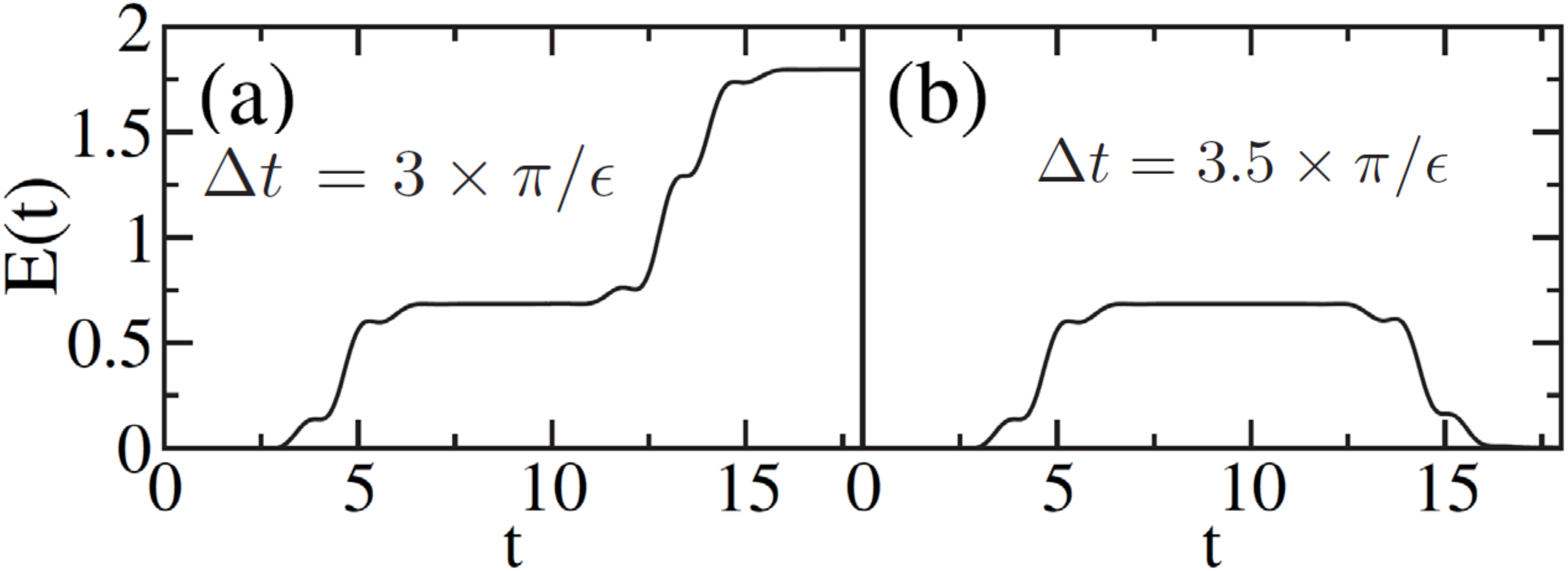
$$\Delta t = (N + \tfrac{1}{2}) \times \frac{2\pi}{\omega_{\rm R}}$$

# Two-level model (Rabi model)

$$H_{\mathrm{R}}(t) = \epsilon\sigma_z + g(t)\sigma_x$$

$$g(t) \longrightarrow A(t) \qquad \omega_{\mathrm{pump}} = 2\epsilon$$

$$A_0 = 0.5,\ \omega_{\mathrm{pump}} = 2\epsilon = 2,\ t_d = 1,\ t_1 = 4t_d$$

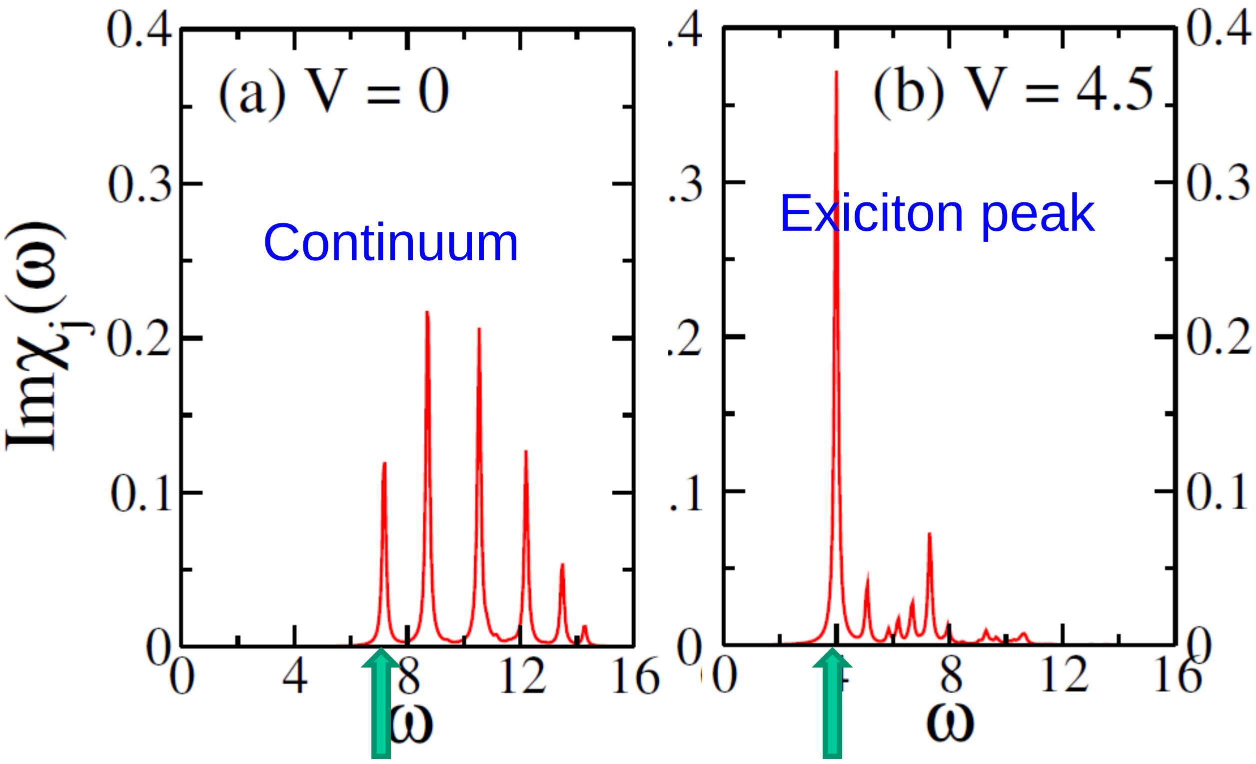



$$\Delta t = N \times \frac{2\pi}{\omega_{\mathrm{R}}} \qquad \Delta t = \left(N + \tfrac{1}{2}\right) \times \frac{2\pi}{\omega_{\mathrm{R}}}$$

# Optical absorption spectrum

$$\mathrm{Im}\chi_j(\omega) = \frac{1}{L}\sum_n \left|\langle n|\hat{j}|0\rangle\right|^2 \delta\left(\omega - E_n + E_0\right) \sim i\omega\sigma(\omega)$$

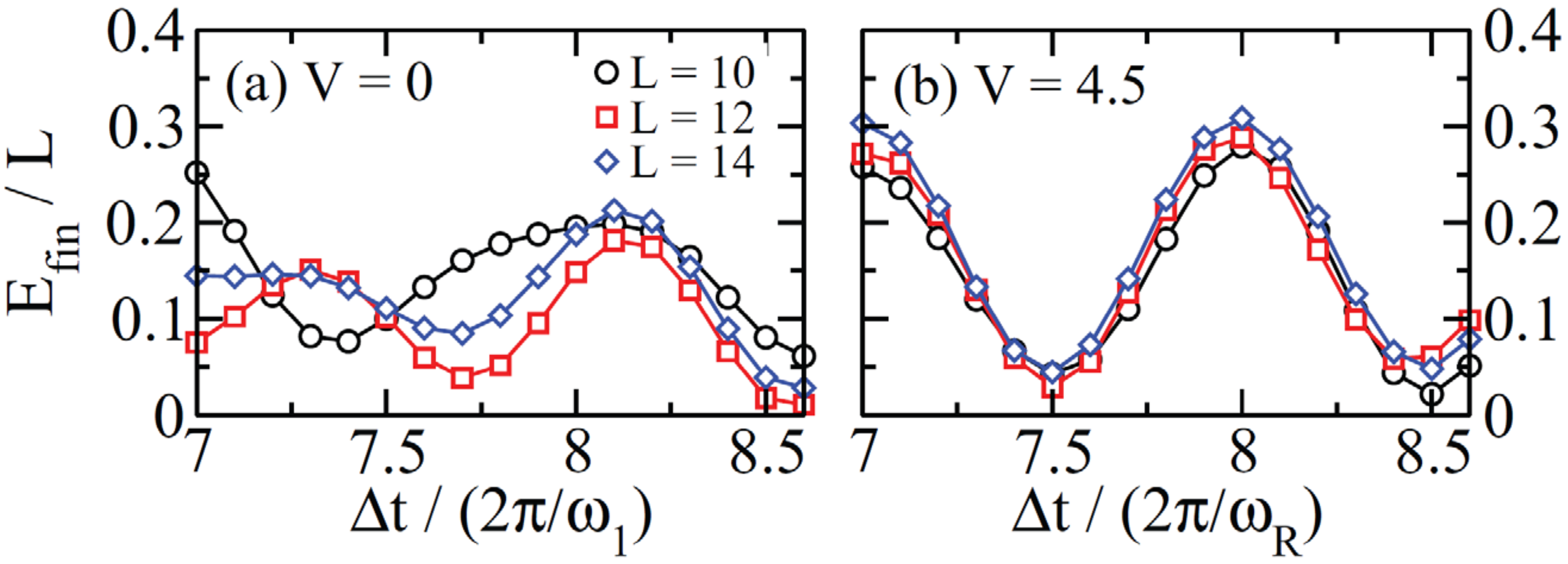
*L*=14 ring




$\omega_{\mathrm{pump}} = \omega_1 \quad \omega_{\mathrm{pump}} = \omega_{\mathrm{R}}$

# Comparison of $E(t)$ between $V$=0 and $V$=4.5

$$\omega_{\mathrm{pump}} = \omega_1 \ (V = 0) \text{ or } \omega_{\mathrm{R}} \ (V = 4.5)$$




No period of $2\pi/\omega_1$ — A period of $2\pi/\omega_R$

Presence of continuum — Analogous to the optical quantum beat in semiconductors

# Summary (2)

**Double-pulse deexcitations in the extended one-dimensional Hubbard model at half-filling**

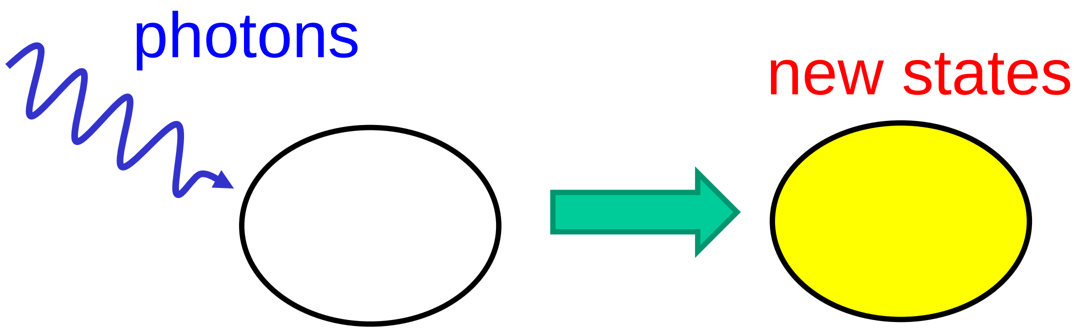
L. Hantao, J. Bonca, and T.T., EPL **103**, 57005 (2013)

- When a precisely selected pulse in a correlated system triggers the excitation, a quantum interference can be realized.

- Coherent control and manipulations on many-body systems

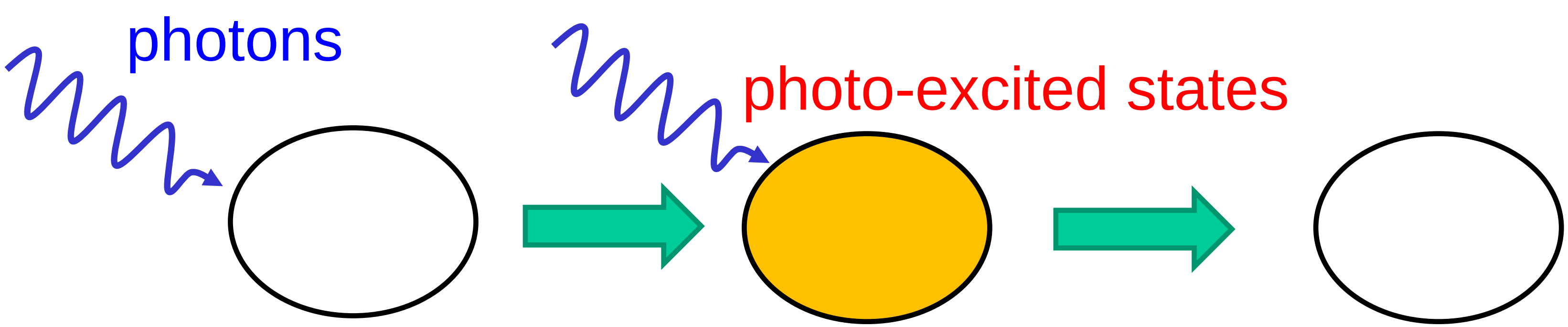
- Materials for 1D Mott insulators: halogen-bridge Ni compounds, etc.
- But $\delta$-like excitonic peak is hard to realize in the Mott insulators.
- Some isolated midgap states?

# Nonequilibrium photo-induced dynamics in strongly correlated electron systems




The condition for the change of states

H. Lu, S. Sota, H. Matsueda, J. Bonca, and T.T., PRL **109**, 197401 (2012)




Possibility of detecting quantum interference

H. Lu, J. Bonca, and T.T., EPL **103**, 57005 (2013)