Photoinduced phase transition and exciton Fano resonance

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external review on CCS
2014/02/18

Outline of talk

- Introduction

  ⇨ **Photoinduced phenomena in materials**

- Photoinduced dynamics in the one-dimensional two-orbital degenerate Hubbard model

  ⇨ **Photoinduced phase transition**

- Laser-Controlled Fano-Resonance in Semiconductor Superlattices

  ⇨ **Exciton Fano resonance**

Photoinduced phenomena

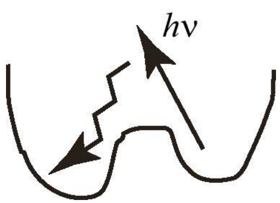
We focus on two topics

- **Photoinduced phase transition**

  (excitation by pulse laser→ phase transition)

  Stable ⇔ Metastable

  ⇒ Non-equilibrium dynamics



- **Optical control of electronic state**

  (excitation by CW laser → Floquet state)

  In particular, electrons in semiconductor superlattices shows dynamical localization, Dynamical Wannier-Stark ladder

Photoinduced dynamics in the one-dimensional two-orbital degenerate Hubbard model

Published papers

“Photoinduced coherent oscillations in the one-dimensional two-orbital Hubbard model”
N. Maeshima, K. Hino and Y. Yonemitsu, Phys. Rev. B **82**, 161105(R) (2010) .

“Photoinduced dynamics of the multi-orbital Hubbard model”,
N. Maeshima, K. Hino, and K. Yonemitsu, physica status solidi (c) 8, (2011).

Photoinduced phase transitions in strongly correlated electron systems

Ex. 1D Ni-Br chain

Photoinduced Metal-insulator transition

Transition metal oxides

Yu *et al.*, PRL **67**, 2581 (1991)

Fiebig, et al., Science **280**, 1925 (1998)

Cavalleri, et al., PRL **87**, 237401 (2001)

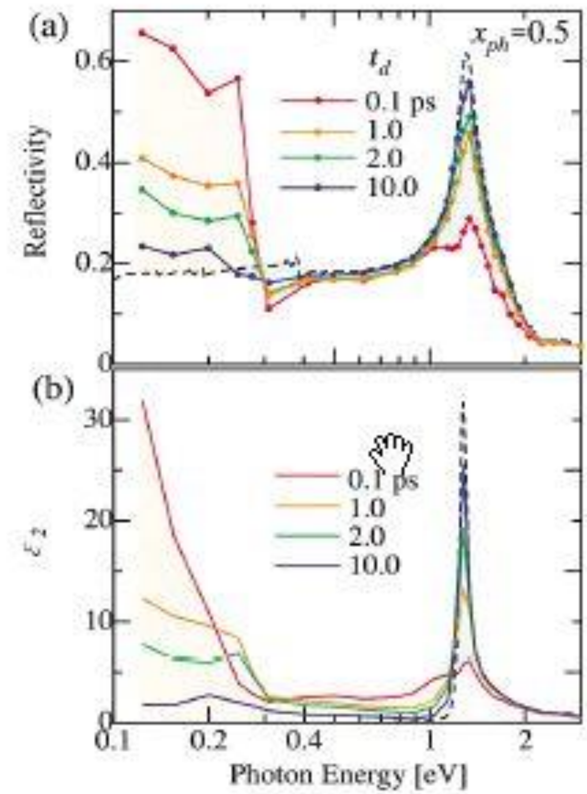
Organic materials

Koshihara, *et.al*. PRB **42**, 6853 (1990)

Iwai, *et.al*. PRL **91**, 057401 (2003)

Chollet *et al.* Science **307**, 86 (2005)

Okamoto *et al.* PRL **98**, 037401 (2007)



Iwai, *et.al*. PRL **91**, 057401 (2003) より

Recent experimental study: photoinduced coherent oscillation

Mn oxides($Pr_{0.7}Ca_{0.3}MnO_3$)

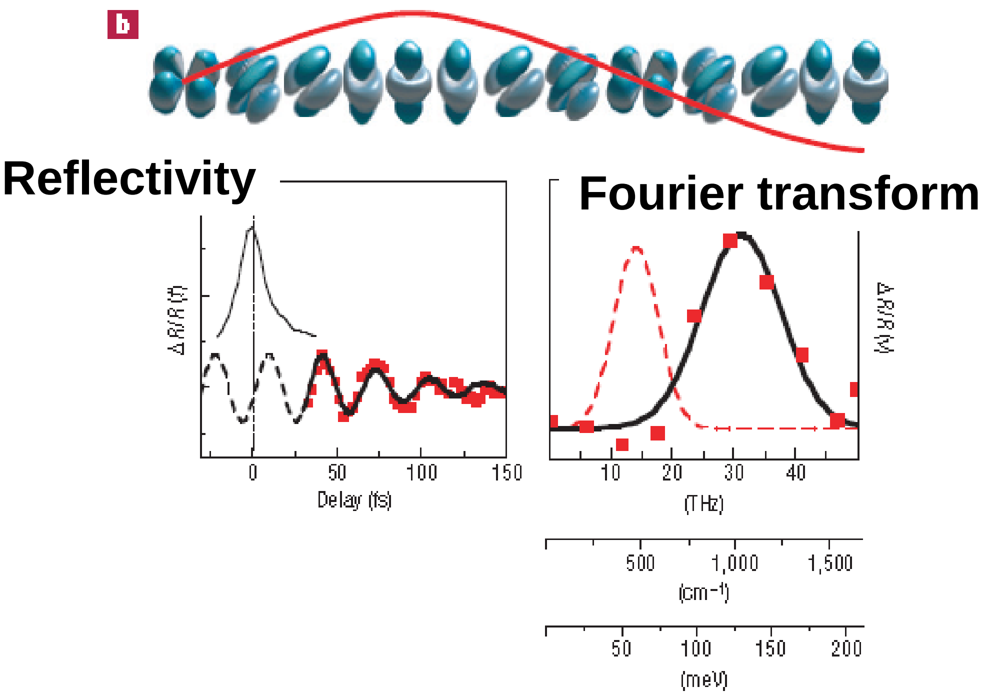


Photo-irradiation

Coherent oscillation

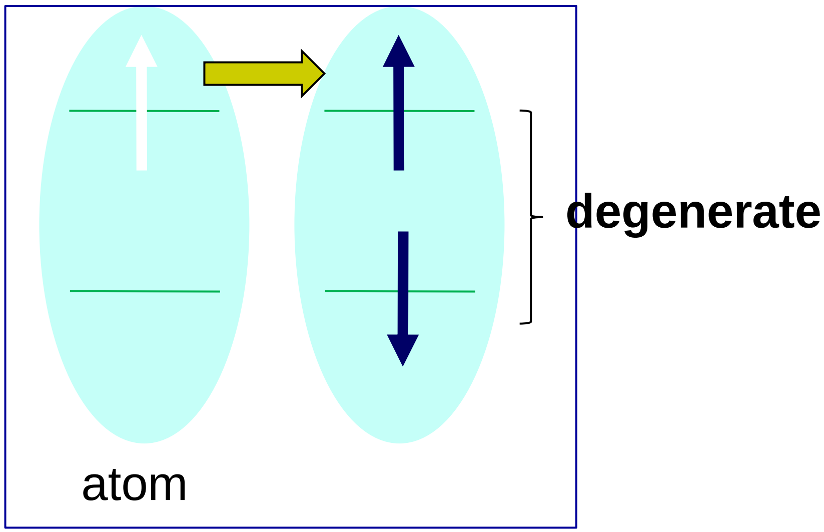
Why does the oscillation occur?

orbiton?

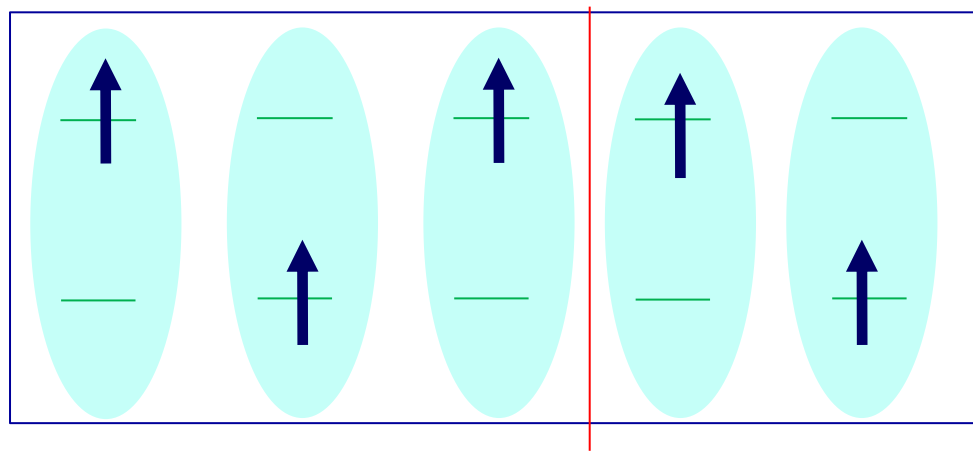
D. Polli, M. Rini, S. Wall, R. W. Schoenlein, Y. Tomioka, Y. Tokura, G. Cerullo, and A. Cavalleri, Nature Mater. **6**, 643 (2007).

Orbiton elementary excitation in orbital-degenerate systems

Charge excitation



Orbital excitation (orbiton)



Domain wall =orbiton

Orbiton can be observed in

Orbital-degenerate systems

Mn oxides, V oxides, ….

Purpose

We present a theoretical study of the photoinduced ultrafast coherent oscillations of the one-dimensional (1D) two-orbital Hubbard model (1D analogue of transition metal oxides with orbital degrees of freedom)

simple qualitative picture for the photoinduced ultrafast coherent oscillations

Model

1D orbital-degenerate Hubbard model coupled with static lattice distortion

$$H_e = H_t(\tau) + H_U + H_J + H_{el} + H_l$$

$$H_t = -\sum_i \sum_m \sum_\sigma [t(\tau) c^\dagger_{im\sigma} c_{i+1m\sigma} + H.c.]$$

$$H_U = U \sum_{im} n_{im\uparrow} n_{im\downarrow} + U' \sum_i n_{i1} n_{i2}$$

$$H_J = J \sum_{i\sigma\rho} c^\dagger_{i1\sigma} c_{i2\sigma} c^\dagger_{i2\rho} c_{i1\sigma} + J' \sum_{i,m\neq n} c^\dagger_{im\uparrow} c_{in\uparrow} c^\dagger_{im\downarrow} c_{in\downarrow}$$

$$H_{el} = -g \sum_i Q_i (n_{i1} - n_{i2})$$

U=U'+2J, J=J'

Numerical calculation

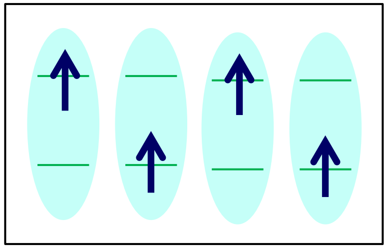
Electron:

$$i\frac{\partial}{\partial \tau}|\psi\rangle = H_e|\psi\rangle$$

solve the time-dependent Schrödinger equation

Peierls phase: $$t(\tau) = te^{iA(\tau)}$$

Spin: ferro
Orbital: antiferro



Laser pulse:

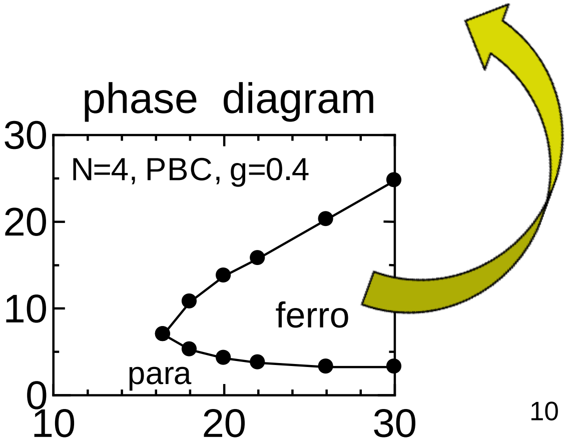
$$A(\tau) = \frac{F}{\omega_{\rm p}}\cos(\omega_{\rm p}\tau)\frac{1}{\sqrt{\pi}\sigma}\exp(-\tau^2/\sigma^2)$$

σ (pulse width) =2 (~13fs for t=0.1eV)

$\omega_{\rm p}$= optical gap

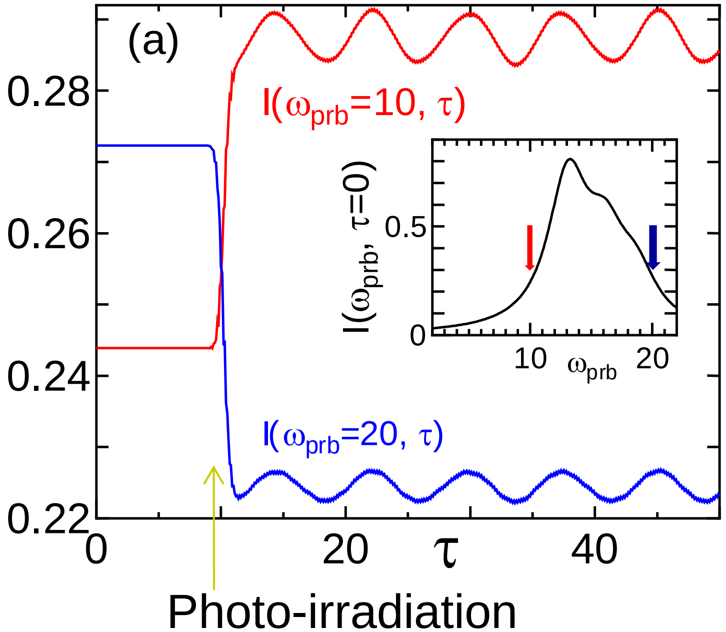
Parameters:

t=1, U'=20, J=5
(ferromagnetic phase)
F=1, g=0.4, K=1, N=4



Results

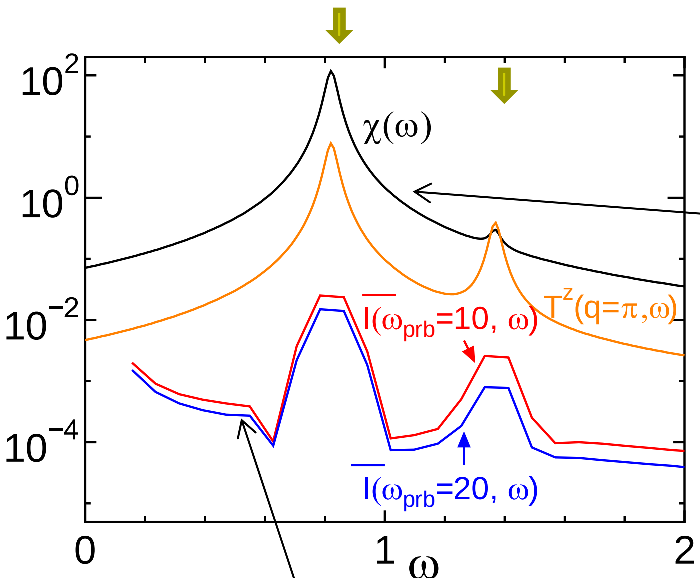
transient optical response function of 1D two-orbital degenerate Hubbard model



Coherent oscillation appears around the charge-transfer peak

Results

U'=20, J=5 (ferromagnetic phase), F=1



Response function for Raman-active excitations

$$\chi(\omega) = -\frac{1}{\pi}\mathrm{Im}[\langle JJ|\frac{1}{\omega + E_0 - H_e + i\varepsilon}|JJ\rangle]$$

$$|JJ\rangle \equiv JJ|0\rangle - |0\rangle\langle 0|JJ|0\rangle$$

J: current operator

$|0\rangle$: ground state

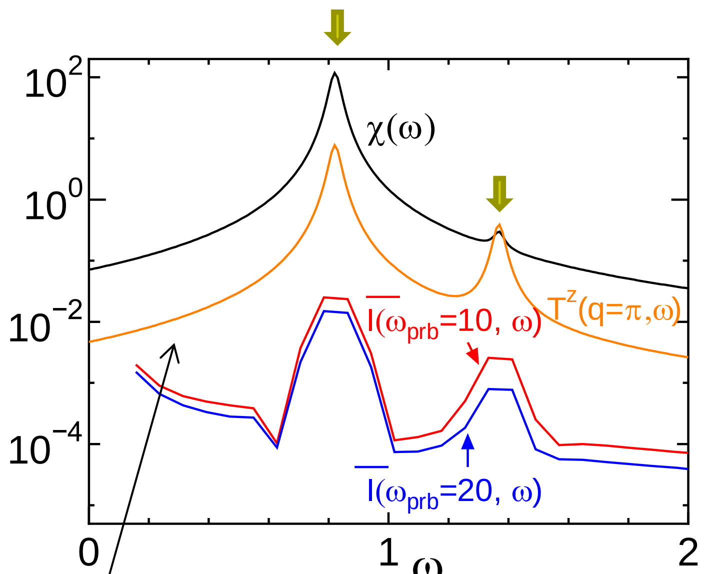
Fourier transform

$$\bar{I}(\omega_{prb}, \omega) = \frac{1}{\sqrt{2\pi}} \int d\tau I(\omega_{prb}, \tau) e^{i\omega\tau}$$

Coherent oscillation is related to Raman-active excitations

Results

U'=20, J=5, N=4 (ferromagnetic phase)

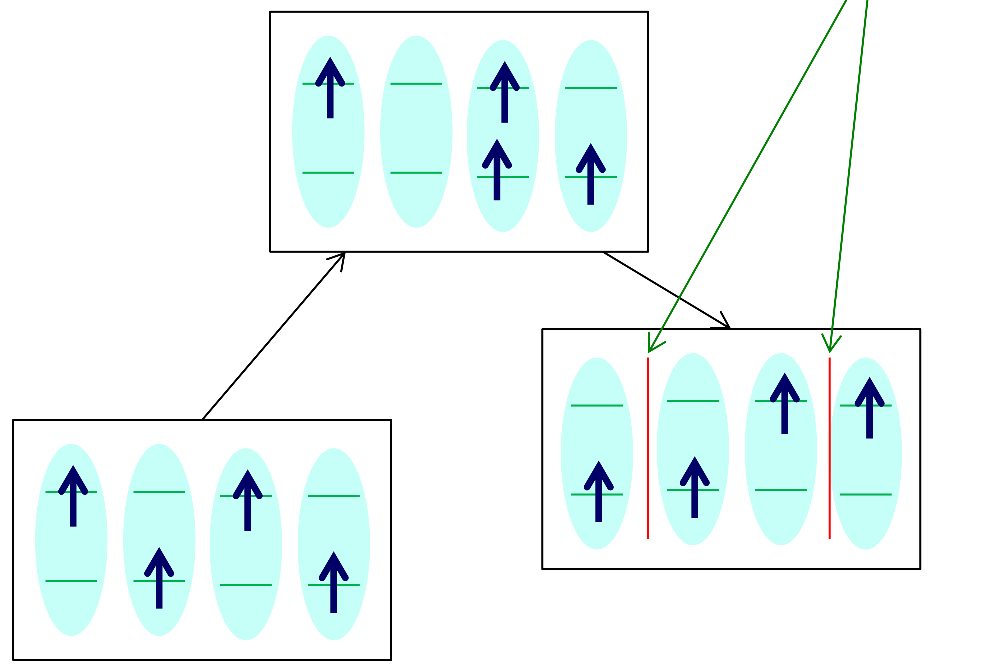


Dynamical structure factor for orbital excitations

$$T(q,\omega) = -\mathrm{Im}[\langle 0 | T_{-q}^{z} \frac{1}{\omega + E_0 - H_e + i\delta} T_q^z | 0 \rangle]$$

$$T_q^z = \sum_{l=0}^{N-1} T_l^z e^{-iql}$$

Coherent oscillations are induced by the Raman-active 2-orbiton excitations



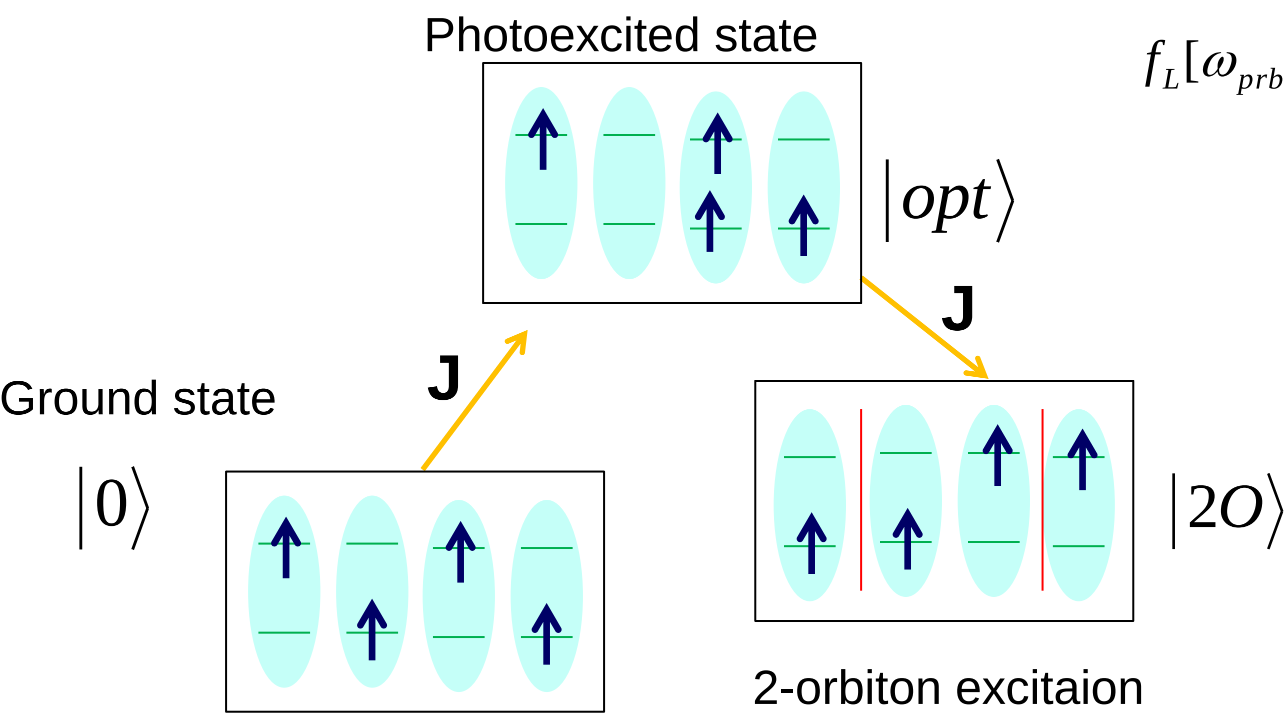
S. Miyasaka *et al.*, Phys. Rev. Lett. **85**, 5388 (2005).

Origin of the coherent oscillation

For $\omega_{prb} \approx \Delta_{opt} \equiv \varepsilon_{opt} - \varepsilon_0$

$$I(\omega_{prb}, \tau) \approx \langle 2O \,|\, j \,|\, opt \rangle \langle opt \,|\, j \,|\, 0 \rangle e^{i(\varepsilon_{2O} - \varepsilon_0)\tau} f_L[\omega_{prb} - (\varepsilon_{opt} - \varepsilon_0)] + c.c.$$

$$f_L[\omega_{prb} - \Delta] = \frac{\delta}{(\omega_{prb} - \Delta)^2 + \delta^2}$$



The oscillations observed in the optical responses are caused by the quantum interference

Summary

We present a quantum-mechanical treatment for the photoinduced ultrafast coherent oscillations of the one-dimensional (1D) two-orbital Hubbard model .

The oscillations observed in the optical responses are caused by the quantum interference between the eigenstates included in the photoexcited state. These oscillations around the CT peak result from the Raman-active two-orbiton state.

Published papers

- "Photoinduced coherent oscillations in the one-dimensional two-orbital Hubbard model", N. Maeshima, K. Hino and Y. Yonemitsu, Phys. Rev. B **82**, 161105(R) (2010) .
- "Photoinduced dynamics of the multi-orbital Hubbard model", N. Maeshima, K. Hino, and K. Yonemitsu, physica status solidi (c) 8, (2011).

Laser-Controlled Fano-Resonance in Semiconductor Superlattices

Published papers

"Parallelization of the R-matrix propagation method for the study of intense-laser-driven semiconductor superlattices"

N. Maeshima and K. Hino, Comput. Phys. Commun. **183**, 8-14 (2012)

"Dynamical Fano resonance of an exciton in laser-driven semiconductor superlattices"

N. Maeshima and K. Hino, Phys. Rev. B **85**, 205305 (2012)

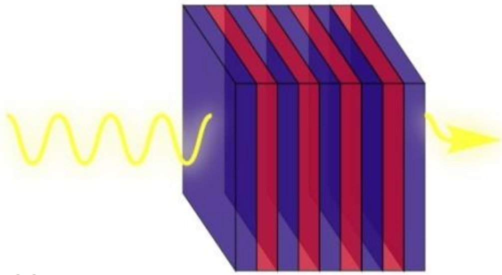
"Laser-Controlled Exciton Fano-Resonance in Semiconductor Superlattices"

N. Maeshima, K. Yamada, and K. Hino, J. Phys.: Condens. Matter 25, 435801 (2013)

Photodressed Electron-Hole System

Strong Interactions of Semiconductor Nanostructures with Intense CW laser

(~ 200-300 kV/cm)



➡ Strongly Coupled Light-Electron/Hole System

⟶ "Temporal Periodicity" in Hamiltonian

Floquet's Theorem

$$H(t) = H(t+T), \quad \left[H(t) - i\frac{\partial}{\partial t} \right] \Psi(t) = 0$$

$$\Psi(t) = \exp\left(-iEt\right)\psi(t), \quad \psi(t) = \psi(t+T)$$

$$\left[H(t) - i\frac{\partial}{\partial t} \right] \psi(t) = E\psi(t)$$

E : Quasienergy (Good Quantum Number)

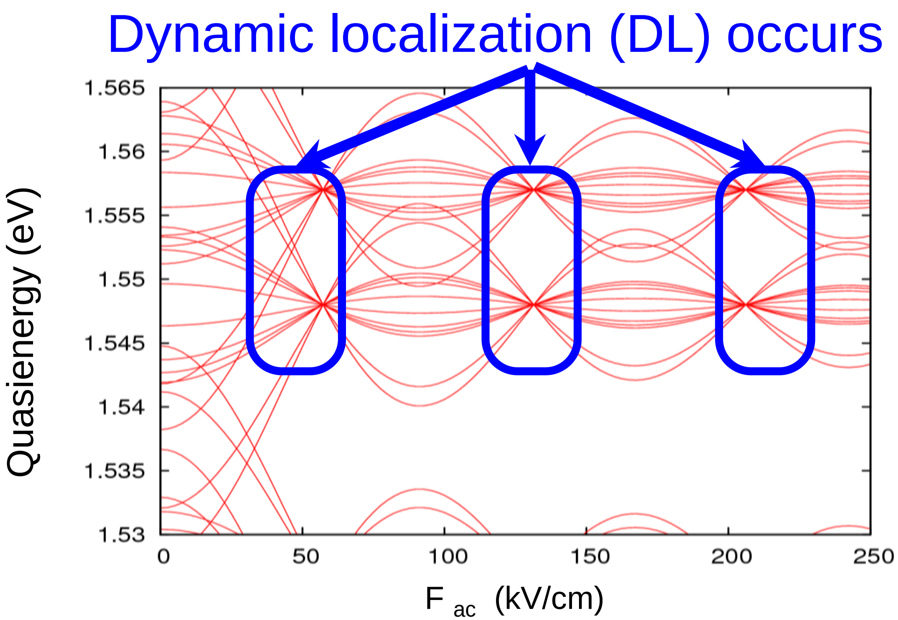
$\Psi(t)$: Floquet State

Photodressed State

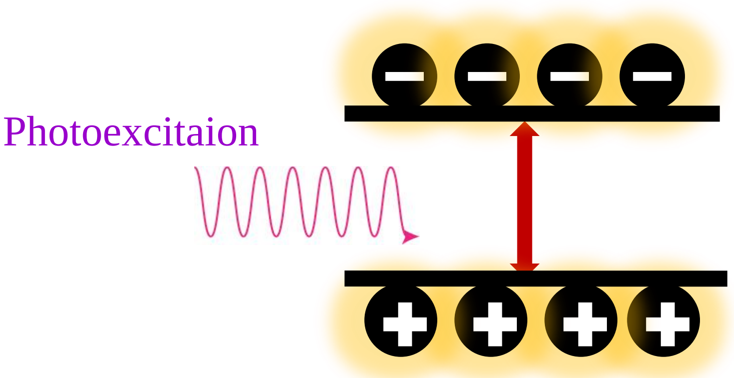
purpose

Free electorn

Electron-hole pair



K. Yashima *et al.*, Phys. Rev. B 68, 235325 (2003)



Photon-dressed exciton?
(excitonic Floquet state)

Investigate electron-hole pairs states in GaAs/GaAlAs superlattices driven by a THz laser, In particular, we focus on properties of Photon-dressed exciton state.

Method1

Semiconductor Bloch equation

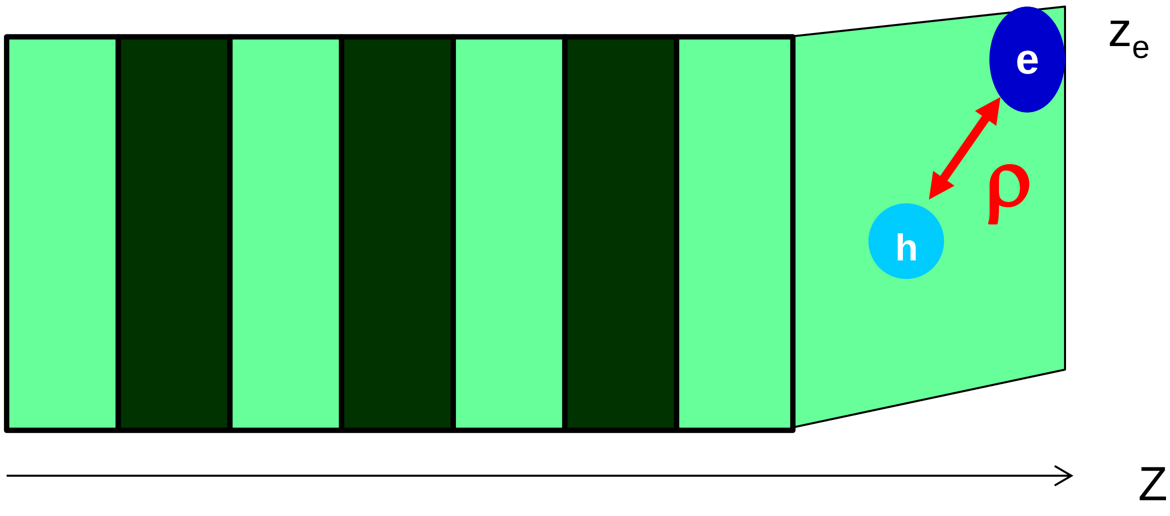
$$i\frac{d}{dt}p(\rho,z_h,z_e,t)=\langle[p(\rho,z_h,z_e,t),H(t)]\rangle$$

$H(t)$ **Hamiltonian**

$p(\rho,z_h,z_e,t)$ **polarization**

z_h Z-coordinate of hole

z_e Z-coordinate of electron



Method2

1. Expand the exciton wave function with respect to the Houston basis

$$\psi(\rho, z_h, z_e, t) = \sum_{\mu} \Phi_{\mu}(z_h, z_c, t) F_{\mu}(\rho)$$

, where $\Phi_{\mu}(z_h, z_c, t)$ is the Houston basis.

W.V. Houston, Phys. Rev. **57**, 184 (1940).

2. Solve the following radial equation

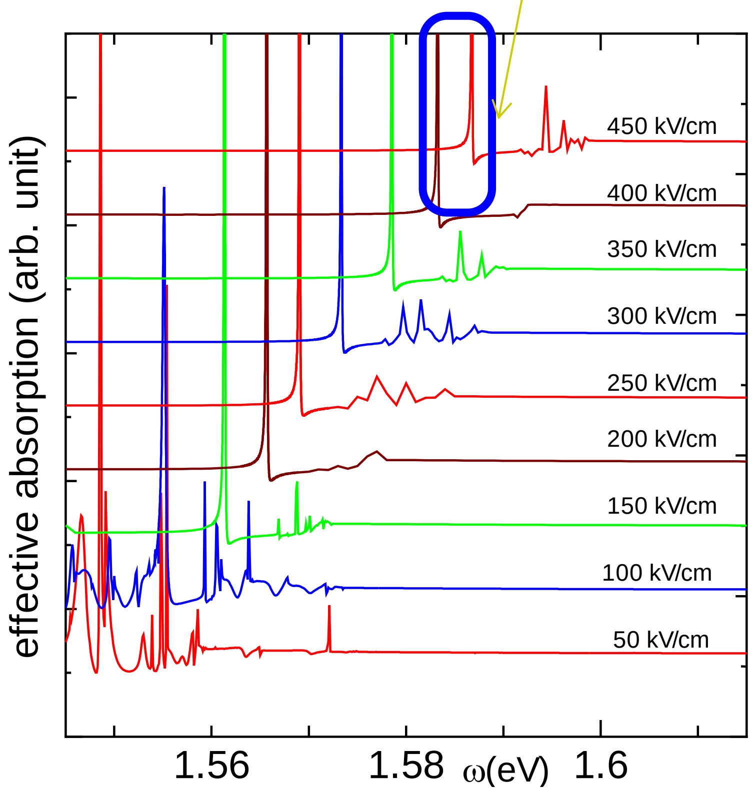
$$\sum_{\nu} L_{\mu\nu}(\rho) F_{\nu}(\rho) = E F_{\nu}(\rho) \qquad L_{\mu\nu}(\rho) = \delta_{\mu\nu}\left[-\frac{1}{2m}\nabla_{\rho}^{2} + \varepsilon_{\mu}\right] + V_{\mu\nu}(\rho)$$

Then, use the R-matrix propagation technique to obtain the wave function Ψ in the whole system (details are omitted in this talk).

Result

Optical absorption

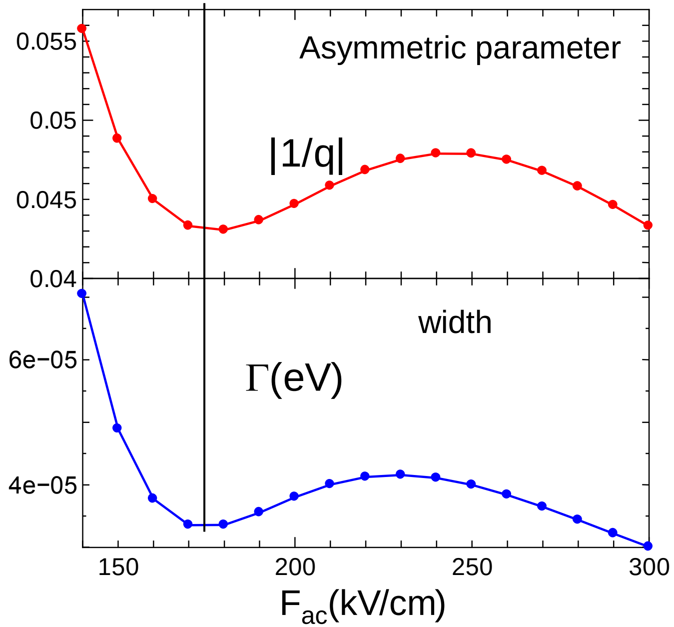
Fano-like spectral peak



$$\sigma(\varepsilon) = A\frac{(q+\varepsilon)^2}{1+\varepsilon^2}$$

$$\varepsilon = \frac{\omega - E_F}{\Gamma/2}$$

Dynamical localization (DL) occurs



Parameters are tunable by F_{ac}

minimum at the point where the DL occurs

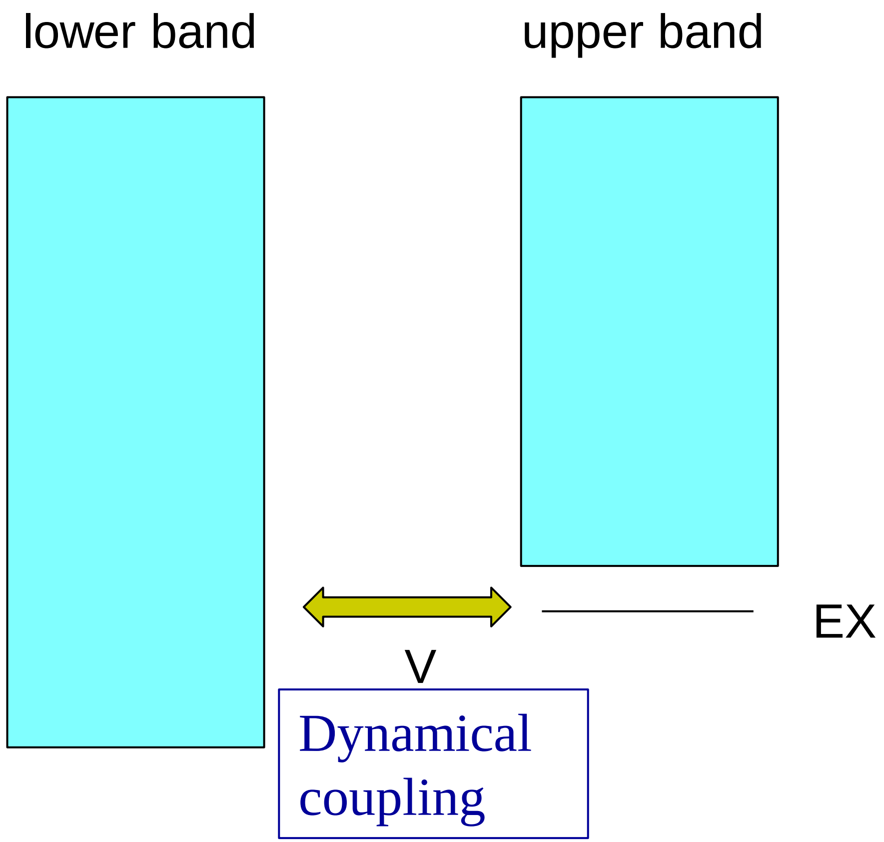
Summary

Properties of the exciton states can be manipulated by the THz-laser.

- spectral width
- parameters of the Fano resonance

➡ **Dynamic Fano resonance**

Dynamic Fano resonance



Publication list

Floquet state, exciton Fano resonance

- N. Meshima and K. Hino, Phys. Rev. B **85**, 205305 (2012).
- N. Maeshima and K. Hino, Comp. Phys. Comm. **183**, 8-14 (2012).
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- K. Yashima, K. Oka, K. Hino, N. Maeshima, X. M. Tong, Solid State Comm. **149**, 823-826 (2009).

Photoinduced phase transition

- N. Maeshima, K. Moriya, and K. Hino, J. Phys. Soc. Jpn. **81**, 104708 (2012).
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- N. Maeshima and K. Yonemitsu, J. Phys. Soc. Jpn. **77,** 074713, (2008)

Other

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