筑波大学 University of Tsukuba

PACS-CS

Quantum Dynamics in Few-Body System

K. Hino and X. M. Tong

Division of Materials and Life Sciences

Outlines

- Introduction
  - What we are working on
  - Why we belong to the Center
- What we have done
  - Wannier Stark Ladder
  - Intense Laser-Material Interactions
- What we plan to do
  - Develop new numerical tools
  - Investigate dynamics in few-body system

What we are working on

Study the dynamical processes in few-body system by solving

$$i\frac{\partial}{\partial t}\Psi(t) = H(t)\Psi(t)$$ non-perturbative

$$H\Psi = E\Psi$$ perturbative

numerically.

Particles: nuclei, electrons, photons etc.

Processes: electrons, atoms, molecules in the external fields
collisions between electrons, ions, atoms, molecules
ionic, atomic, molecular structures (excited states)

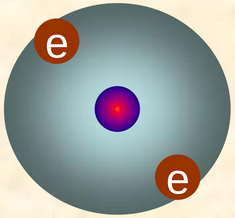
Objects: *Understand* the processes;
Provide the data;
Control the quantum dynamical processes.

Why we belong to the Center

Characteristics of the Study:

- The number of particles involved is accountable with the finger
- Interactions between the particles are well known
- Most of the dynamical processes cannot be solved analytically

Example: Helium atoms (® + 2 e),
The transition from quantum to classic physics (~ $\rightarrow$ 0).



To do the simulation, we need a big computer.

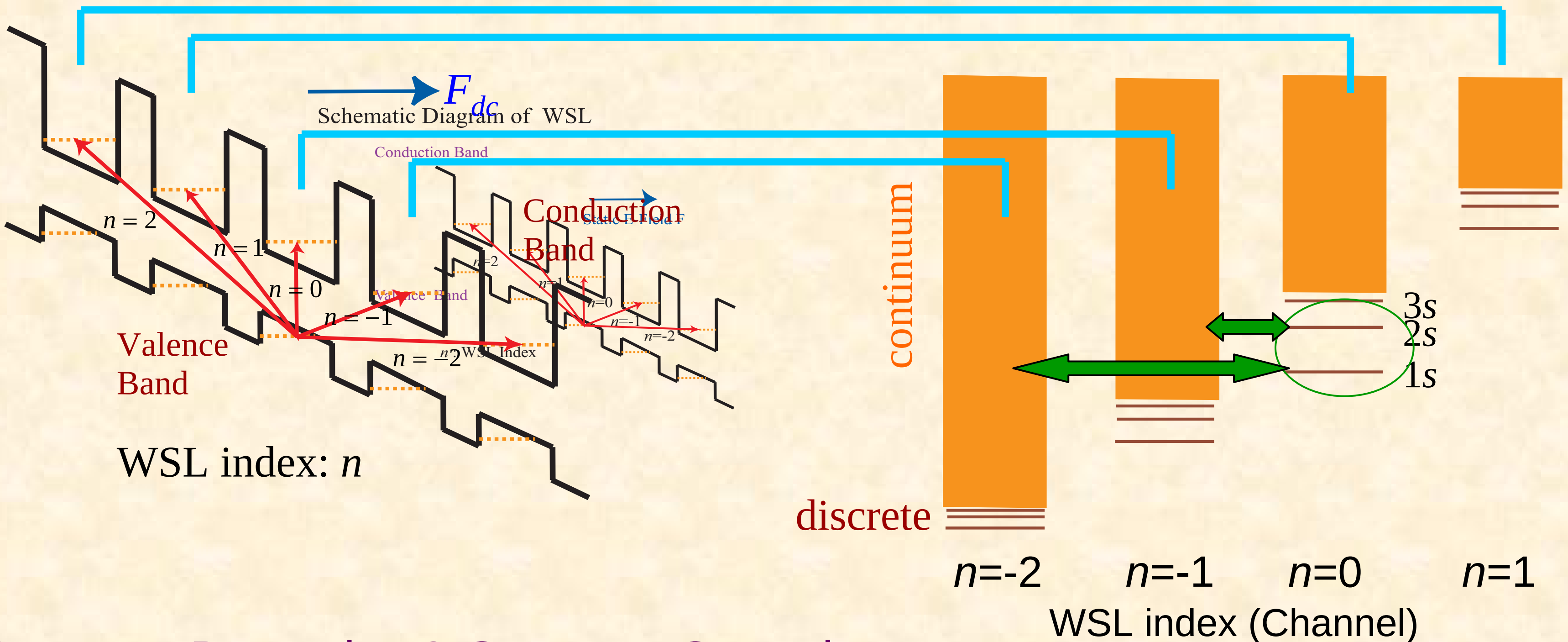
To learn things, we have to discuss with our colleagues

Common interests (computation) and common tools (computer) put us together.

Example I: Wannier-Stark Ladder

WSL space structure:

WSL energy structure

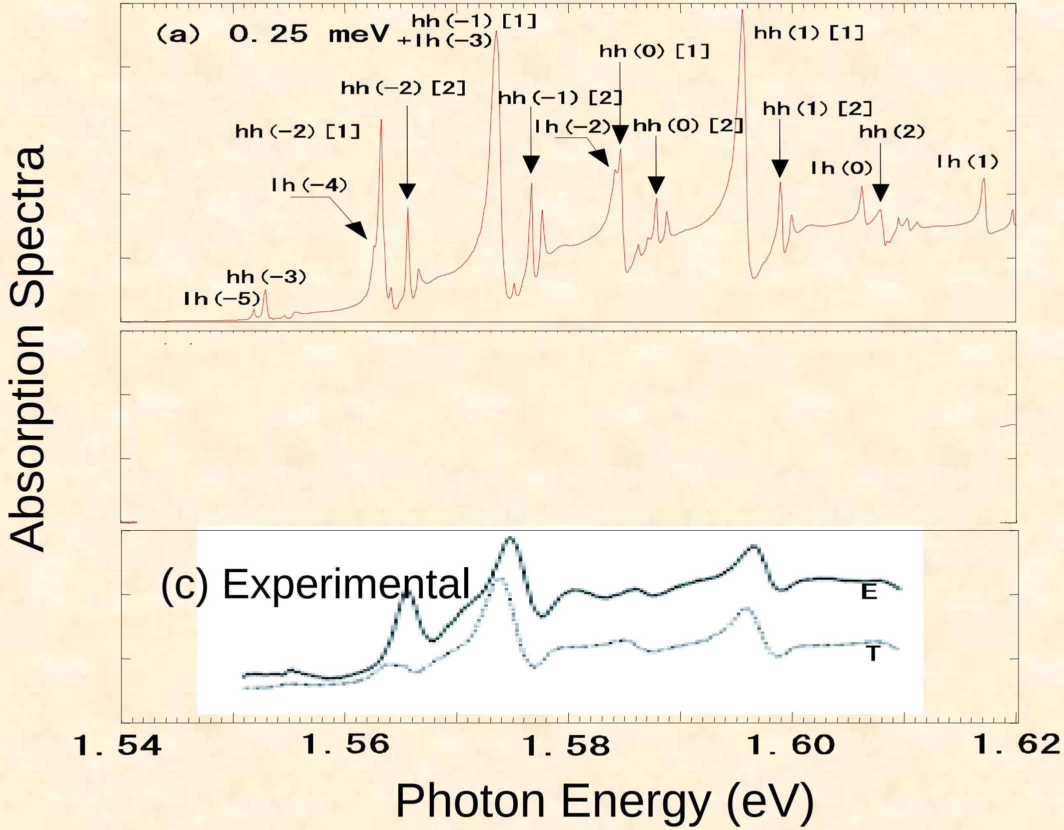


Quantum Dynamics & Quantum Control

Fano Resonance

Linear Optical Response

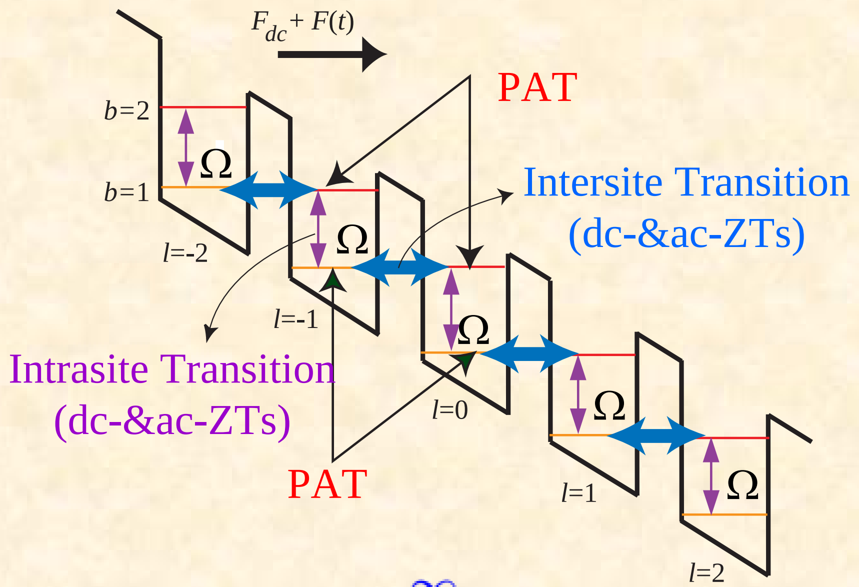
67Å-GaAs / 17Å-$Ga_{0.7}Al_{0.3}As$ (F=13.3kV/cm)

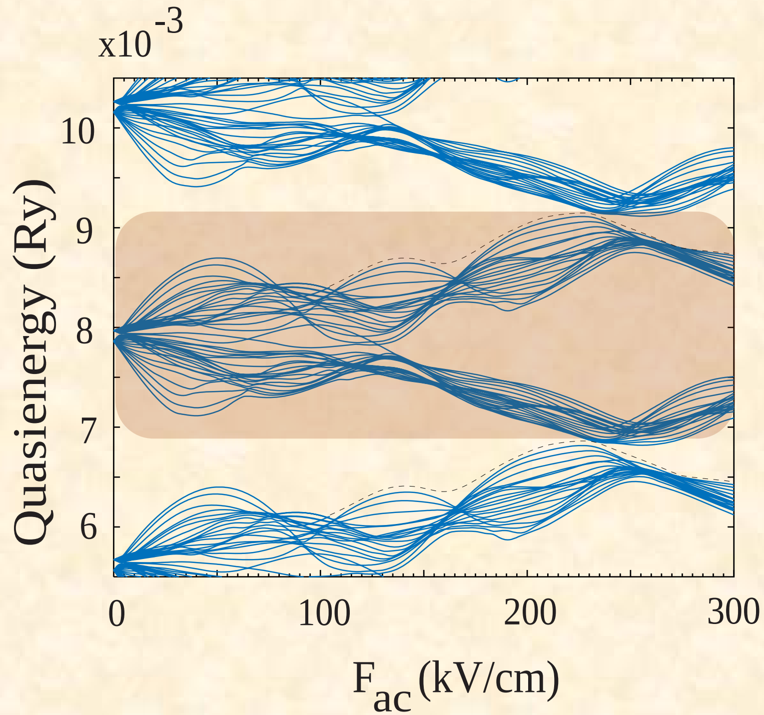


Theory: <u>K. Hino</u> and N. Toshima, *PRB* **71,** 205326 (2005).
Experiment: C. P. Holfeld *et al., PRL* **81**, 874 (1998).

Quantum Control: DWSL

Schematic Diagram of the DWSL





$$\Psi(t) = e^{-iEt} \sum_{n=-\infty}^{\infty} e^{-in\Omega t} \psi_n$$

The energy structure can be controlled by F_{ac} and measured by a weak probe field.

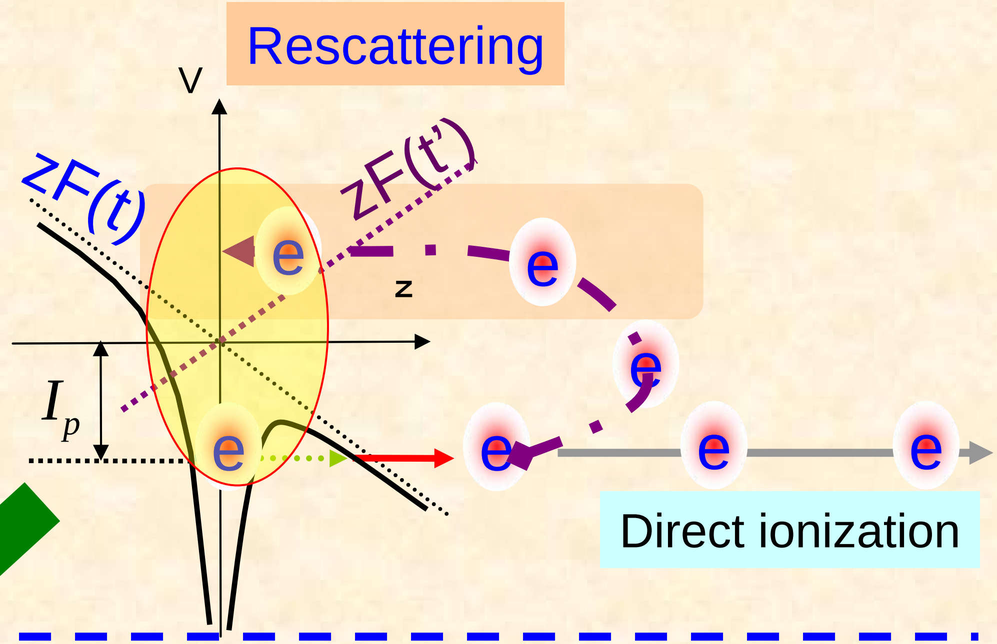
E: quasienergy calculated by Floquet theory

K. Hino, X. M. Tong and N. Toshima, *PRB*, accepted (2007).

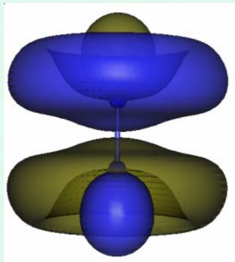
Example II: Laser Material Interactions

1. Tunneling Ionization
2. *Rescattering*
3. Electron-Core Collision

Strong, coherent electron beam



Electron beam

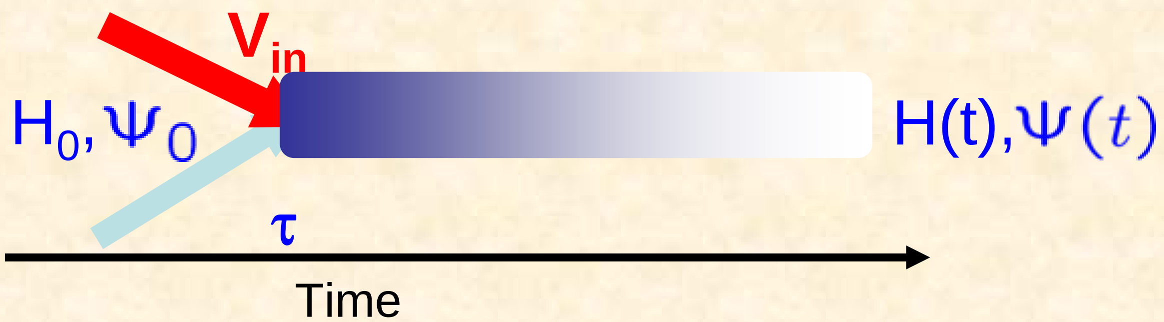


conventional	*rescattering*
non-coherent	*coherent*
• Radiative Rec.	(HHG)
• Ion. or Dis.	(Mol. Clock)
• Scattering	(Imaging)

Computational Scheme

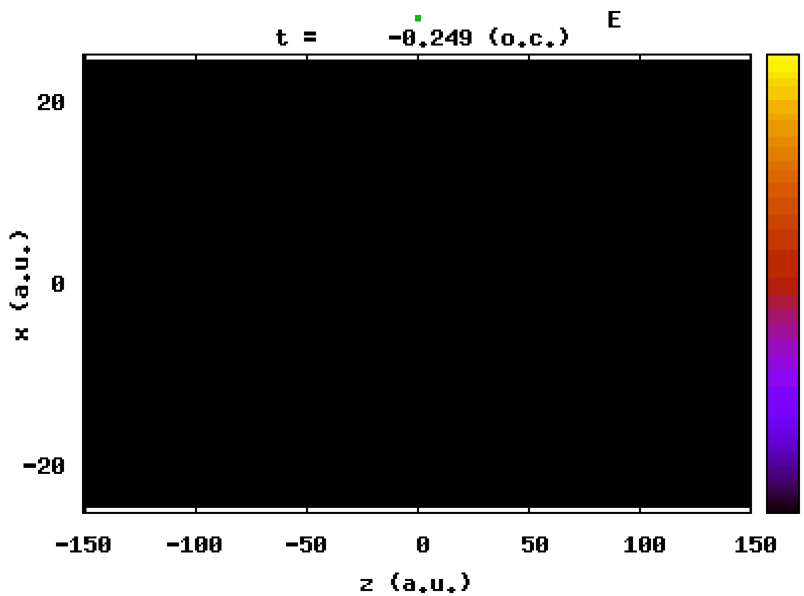
$$i\frac{\partial}{\partial t}\Psi(t) = H(t)\Psi(t) \quad \text{with} \quad \Psi(-\infty) = \Psi_0$$

$$\begin{aligned}\Psi(t) &= -i\int_{-\infty}^{t} e^{-i\int_{\tau}^{t} H(\tau')d\tau'} V_{in} e^{-iE_0\tau}\Psi_0 d\tau + e^{-iE_0 t}\Psi_0 \\ &= -i\int_{-\infty}^{t} U(t,\tau)V_{in}U_0(\tau,-\infty)\Psi_0 d\tau + U_0(t,-\infty)\Psi_0\end{aligned}$$



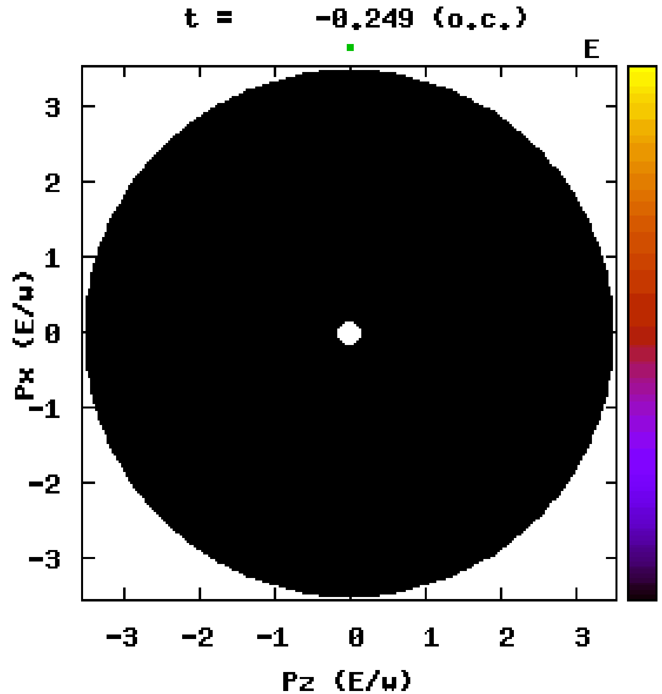
TD-momentum distribution

$I_o = 2x10^{14}$ W/cm^2 λ = 800 nm



TD- Space Distribution

$$|\Psi_j(t)|^2$$



TD- Momentum Distribution

$$\frac{dP(E,\Omega,t)}{dEd\Omega}$$

X. M. Tong, S. Watahiki, K. Hino and N. Toshima, *PRL* **99**, 093001 (2007).

Future Plan

Develop a time-dependent Floquet method:
to study atoms, molecules, clusters or semiconductors in a periodic time-dependent external field.

$$i\frac{\partial}{\partial t}\Psi(t) = H(t)\Psi(t) \quad \text{with} \quad H(t) = H(t+T)$$

$$\Psi(t) = e^{-iEt} \sum_{n=-\infty}^{\infty} e^{-i2n\pi\frac{t}{T}} \psi_n$$

Time-independent method:

a coupled channel eigen-value problem; / n^3

Time-dependent method:

propagate the w.f. for one period and dig out the dynamic information based on the Floquet theory. / n

Future Plan

Develop a time-dependent method: to study the photoionization of many-electron system [DFT + Configuration Interaction (CI)]

Interference

$$h\nu + \mathrm{A} \rightarrow \begin{cases} \mathrm{A}^{+} + e \\ \mathrm{A}^{*} \rightarrow \begin{cases} \mathrm{A}^{+} + e \\ \mathrm{A} + h\nu \end{cases} \end{cases}$$

Difficulties: too many ionization channels and continuum w.f.

Suggested: *Structures* calculated by DFT and CI (well developed);
Dynamics investigated by time-dependent method.

$$\Psi(0) \;=\; -i\int_{-\infty}^{0} e^{-i\int_{\tau}^{0} H d\tau'} V_{in} e^{-iE_0\tau}\Psi_0 d\tau + e^{-iE_0 t}\Psi_0$$

Key step: the continuum w.f. in the outer region will be absorbed.

Future Plan

Study capture processes by our newly developed TD-method [1].

$$\bar{p} + \mathrm{H} \rightarrow \bar{p}p + e$$

Basic research: formation and properties of anti-material

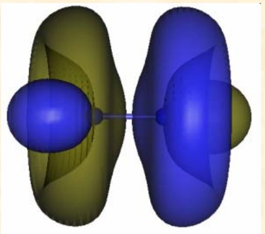
Application: charge capture processes in astrophysics [2]

[1] "State-specified protonium formation in low-energy antiproton-hydrogen-atom collisions", X. M. Tong, K. Hino, and N. Toshima, *PRL* **97**, 243202 (2006).

[2] "X-ray emission from comets", T. E. Cravens, *Science* **296**, 1042 (2002)

Future Plan

Study intense laser material interactions by our TD-method [3].

Laser →  Materials

Steer the rescattering wavepacket by tuning laser parameters;
Study the dynamics in the femto-second (10^{-15}s) time scale [4];
Study the tomographic imaging of molecular orbitals [5].

[3] "Numerical Observation of the Rescattering Wavepacket in Laser-Atom Interactions",
X. M. Tong, S. Watahiki, K. Hino and N. Toshima, *PRL* **99**, 093001 (2007).

[4] "X-ray driven femtosecond molecular dynamics",
E. Gagnon, P. Ranitovic, X. M. Tong, C. L. Cocke *et al*., *Science* **317**, 1374 (2007).

[5] "Tomographic imaging of molecular orbitals",
J. Itatani, J. Levesque, D. Zeidler, H. Niikura, H. Pepin *et al*., *Nature,* **432***,* 867 (2004).

Thank You