Microscopic analysis on light-induced nonequilibrium electron dynamics

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1. Project Purpose

The research aims to control material properties using light and explore new physical phenomena through advanced computational simulations utilizing supercomputers. The present project is structured around three key themes: (1) employing attosecond light pulses to investigate ultrafast electron dynamics and develop theoretical frameworks for controlling quantum transitions in semiconductor materials; (2) analyzing dissipative effects in light-driven systems by refining quantum master equation models to better capture non-equilibrium steady states; and (3) optimizing quantum master equation computations for GPU platforms to enhance simulation efficiency and accuracy. The project seeks to advance the understanding of light-matter interactions and establish methods for manipulating material properties using intense light fields.

2. Results

We performed electron dynamics simulations using two light pulses. One is a strong pulse that induces dynamics in the material, and the other is a weak and very short pulse that observes the dynamics induced by the first pulse. The first pulse is referred to as the pump pulse, while the second pulse is called the probe pulse. Thus, this scheme is known as the pump-probe method, a widely used experimental technique in the optics community.

In the present work, we numerically implemented the pump-probe method to investigate the roles of light-induced intraband and interband transitions and their coupling in the transient optical properties. As the target system, we employed GaAs, a prototypical semiconductor. Through the pump-probe simulation, we found that the coupling between intraband and interband transitions plays an essential role, in addition to the individual contributions from the intraband and interband transitions. This coupling effect has been largely overlooked in the optics community, despite extensive investigations of each contribution individually. Therefore, the coupling between intraband and interband transitions may open a new avenue for controlling the state of matter via light. Currently, we are conducting further analysis and will soon finalize the results and write a paper.

In addition to the pump-probe analysis, we have theoretically developed a novel approach to address dissipative and relaxation phenomena in driven systems. In the optics community, the relaxation time approximation is commonly used to describe the relaxation process of driven quantum systems. However, in this approximation, field-induced effects are not considered in the relaxation process, even though the relaxation path itself should be modified by the driving field. In this project, we developed a new basis to determine the correct relaxation path, effectively suppressing spurious relaxation effects in the relaxation time approximation. This proper relaxation approach enables the investigation of longer-time dynamics of the system. Thus, it may provide a pathway to exploring novel methods for controlling driven quantum systems and realizing the control of the state of matter via light.

3. Roles of the MCRP and its significance

The MCRP offers high-performance supercomputers equipped with both CPUs and GPUs. Therefore, it is a highly valuable program for both product execution and the development of code and methodologies.

4. Future plan

We are currently summarizing the results obtained from the MCRP projects and preparing academic papers for submission to journals.

5. Publications and conference presentations

(1) Journal papers

(2) Presentations

(3) Others

Supercomputer	Use	Allocated resources*		
		Initial resources	Transferred resources**	Additional resources
Cygnus	Yes/No	1000		
Pegasus	Yes/No			
Wisteria/BDEC-01	Yes/No	189260		
	*in units of node-hour product ** If the budget transfer was performed, fill in here, such as “+2000” and “−1000”.			