MODIFIED SCHRÖDINGER EQUATION FOR ATTOSECOND LASER PULSE INTERACTION WITH MATTER

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Abstract

Recently the measurement of X-ray pulses approaching the attosecond frontier was published (M. Drescher et al., *Science* **291** (2001) p. 1923). The attosecond laser pulse allows the study and control the motion of electrons inside atoms. In this paper we develop and solve the modified Schrödinger equation (MSE) which describes the interaction of electrons with its surroundings in atom. This interaction can be detected only with attosecond laser pulse, for the relaxation time of the interaction is of the order of 10 as.

Key words: Attosecond laser pulses, quantum heat transport, modified Schrödinger equation.

1 Introduction

Physicists and engineers can now take snapshots of evolving atomic systems with pinpoint accuracy using femtosecond laser pulses to both trigger the dynamics and illuminate the system. This can be done by splitting each laser pulse with a partially transmitting mirror and delaying the less energetic"probe" pulse with respect to the stronger excitation or "pump" pulse. In this way a powerful femtosecond laser pulse can initiate the same microscopic process in millions of molecules or sites in a crystal lattice. A weaker portion of the pulse (or a frequency - shifted replica) can than probe the dynamics by measuring changes in the optical properties of the system at a later instant.

It is possible to replay the atomic or molecular dynamics in slow motion by using a series of femtosecond pulses and increasing the delay between successive pump and probe pulses. This method, pump-probe spectroscopy allows the study of microscopic dynamics. The time resolution is only limited by the duration of the pump and probe pulses.

The pulses shorter than 10 fs can be routinely generate using self-mode locking lasers. Femtosecond laser pulses allow physicist and chemists to follow these femtosecond processes by tracing the displacements of atoms, as demonstrated for the first time in the late 1980's by Ahmed Zewail [1]. These displacements include changes in the optical properties of the weakly bound valence electrons that can be revealed instantly by visible-light probe. In complex systems, however, the atomic motion can be more accurately determined by studying core electrons close to the atomic nucleus but this requires X-ray wavelengths.

To the study processes inside atoms the sub-femtosecond laser pulses are needed. In paper [2] the results of the production of the single soft X-ray pulses by high-order harmonic generation with 7-femtoseconds (fs) laser pulses are presented. The techniques developed in paper [2] offer the potential for generating and measuring single attosecond X-ray pulses. Bohr's simple model of the hydrogen atom predicts that the electron takes about 140 attoseconds (as) to orbit around the proton:

$$T_{\text{orbit}} = \frac{2\pi a_{\text{Bohr}}}{v_{\text{orbit}}} = \frac{2\pi a_{\text{Bofhr}}}{\alpha c} = 140\,\text{as}. \tag{1}$$

In formula (1) a_{Bohr} is the Bohr radius of the atom, $a_{\text{Bohr}} = 0.5\,10^{-10}\,\text{m}$, α is the fine structure constant for electromagnetic interaction $\alpha = 137^{-1}$, c is the vacuum light velocity.

The thermal processes generated inside the atom with attosecond laser pulses were investigated in paper [3]. It was shown that for attosecond laser pulses the master thermal equation has the form of hyperbolic quantum heat transport equation (QHT):

$$\tau \frac{\partial^2 T}{\partial t^2} + \frac{\partial T}{\partial t} = \frac{\hbar}{m_e} \nabla^2 T, \tag{2}$$

where T is the temperature, τ is the relaxation time and m_e denotes the electron mass. The relaxation time is defined as follows

$$\tau = \frac{\hbar}{m_e \alpha^2 c^2} \tag{3}$$

and is of the order of 10 as for the hydrogen atom. The quantum heat transport equation (QHT) describes the quantum limit of heat transport when the pulse duration Δt is of the order or smaller than the relaxation time. As was shown in paper [3] for $\Delta t < \tau$ the QHT has the form of the quantum wave equation

$$\frac{1}{v_h^2}\frac{\partial^2 T}{\partial t^2} = \nabla^2 T, \tag{4}$$

where $v_h = \alpha c$ is the velocity of the thermal wave. The thermal wave has the wave length $\lambda\!\!\!^{-}_{th}$:

$$\lambda\!\!\!^{-}_{th} = \frac{1}{\omega} v_{th} = \tau v_{th} = \frac{\hbar}{m v_{th}} = \lambda_B, \tag{5}$$

where $\lambda_B = \hbar/p$ denotes the de Broglie wave length. We can conclude that for laser pulses with $\Delta t < \tau$ the thermal processes inside the atoms can be visualized as the thermal waves, in complete agreement with quantum mechanics.

Quantum mechanics based on the Schrödinger equation has been remarkably successful in all realms of atoms, molecules and solids. In this paper we develop and solve the modified Schrödinger equation which describes the structure of matter as observed by attosecond laser pulses, i.e. for time periods shorter than the characteristic atomic relaxation $\tau \sim 10$ as.

2 The solution of the modified Schrödinger equation

In paper [4] the modified Schrödinger equation MSE was obtained:

$$i\hbar\frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m_e}\nabla^2\Psi + V\Psi - 2\tau\hbar\frac{\partial^2\Psi}{\partial t^2}, \tag{6}$$

where the relaxation time τ is described by formula (3). For equation (6) the probability density ρ fulfils the continuity equation [5]

$$\frac{\partial \rho}{\partial t} + \mathrm{div}\vec{S} = 0, \tag{7}$$

where ρ equals

$$\rho = \Psi\Psi^* - 2i\tau\left(\Psi^*\frac{\partial\Psi}{\partial t} - \Psi\frac{\partial\Psi^*}{\partial t}\right) \tag{8}$$

and $\vec{S}$ is the probability flow vector. By restricting the solution space we may keep $\rho \geq 0$ [6].

The eigenvalue problem for one dimensional MSE

$$i\hbar\frac{\partial\Psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m_e}\frac{\partial^2\Psi}{\partial x^2} + V(x)\Psi(x,t) - 2\tau\hbar\frac{\partial^2\Psi}{\partial t^2} \tag{9}$$

gives for $\Psi(x,t)$ in the form:

$$\Psi(x,t) = u(x)\varphi(t), \tag{10}$$

$$-\frac{\hbar^2}{2m_e}\frac{d^2u(x)}{dx^2} + V(x)u(x) = Eu(x). \tag{11}$$

For time dependent function $\varphi(t)$ we obtain the equation

$$\frac{d^2\varphi(t)}{dt^2} + \frac{i}{2\tau}\frac{d\varphi}{dt} - \frac{E}{2\tau\hbar}\varphi(t) = 0. \tag{12}$$

The solutions of equation (12) have the form:

$$\varphi_1(t) = e^{-\frac{E_i}{\hbar}t}, \qquad \varphi_2(t) = e^{i\left(\frac{Et}{\hbar} - \frac{i}{2\tau}t\right)}. \tag{13}$$

Considering formulae (10) and (13) one obtains the general solution of the MSE in the form:

$$\Psi(x,t) = u(x)e^{-\frac{it}{2\tau}}\left[Ae^{-\left(\frac{Et}{\hbar} - \frac{t}{2\tau}\right)} + Be^{\frac{iE}{\hbar}t}\right]. \tag{14}$$

The additional term (in comparison to Schrödinger equation, $\exp(-\frac{it}{2\tau})$ describes the interaction of the electron with its surrounding in atom, i.e. frictional force. It is worthwhile to recognize that this real frictional force is described by the real relaxation time, formula (3). It can be imagined that in the atom electron is moving in highly viscous medium which is not observable for long time pulses, $\Delta t \gg \tau$.

Considering the formula (14) which describes the wave function for stationary state of the electron as "observed" by attosecond laser pulse, the following *scenario* of the electron motion can be formulated. In hydrogen - like atoms due to frictional force electron moves with constant velocity $v = \alpha c$. The background viscous medium can be discovered and observed only with attosecond laser pulses.

For obtaining the Schrödiger equation we are forced to assure $\tau \to 0$ in MSE. Considering formula (3), $\tau = 0$, means for $m \neq 0,\ c \to \infty$. This is in accord with the non-relativistic nature of the Schrödinger equation. It means that Schrödinger equation allows for propagation of the information with infinite velocity. On the other hand with MSE, Eq. (6) the information can be transferred with finite velocity $v = \alpha c,\ v < c$.

3 Conclusions

Attosecond flashes of light allow us to take snapshots of electrons in atom and let us reconstruct their motion. In this paper we developed and solved the modified Schrödinger equation (MSE) which takes into account the interaction of electron in atom with its surroundings. This interaction is described by the relaxation time $\tau = \hbar/m\alpha^2c^2$ which is of the order of 10 attoseconds (as) for the hydrogen like atoms. With attosecond laser pulse one's can observe the wavy motion of electrons in the atoms. This wavy motion can be well described by modified Schrödinger equation.

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