THERMAL TRANSPORT

INDUCED BY ULTRA-SHORT LASER PULSES IN MOLECULAR NANOMATERIALS

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Abstract

In this paper the thermal transport in molecular electronics materials is described. Within the quantum heat transport equation (developed in our monograph: *From Quarks to Bulk Matter*) we investigate the heat transport induced by ultra-short laser pulses. As the molecular electronics materials example the heat transport in DNA strands is described and the formula for relaxation time is obtained.

Keywords: DNA strands; Quantum heat transport; Ultra-short laser pulses.

1 Introduction

Electronic transport through molecules was first described theoretically in 1970's [1, 2]. Since then numerous experiments have been investigated where electrical current was driven through single - layer molecular films between two metallic electrodes [3]-[5]. Transport through single or at most a few molecules on a gold surface has been observed with scanning tunnelling microscopes (STM), where the tip serves as a counter electrode [6, 7]. A few experiments have been realized which target current through a single molecule while the connection to both electrodes is symmetrically realized by a well defined chemical bond, which allows mechanical stability of the function even at room temperature [8, 9]. Very recently transport phenomena in single organic molecule [10] and hydrogen molecules [11] were reported.

Processes on the atomic scale can be imaged with ultrafast laser pulses. Ultrafast spectroscopy has now produced the first measurements of dynamic processes deep inside an atom. In this experiment [12] a krypton atom is excited by a short X-ray pulse to create a hole in its inner shell. Electron rearrangement in the excited atom is tracked with attosecond (10^{-18} s) resolution with a synchronized laser beam.

Contemporary electronics is the *molecular scale electronics* in which the electronic properties of single molecule are investigated and applied. For a short we will use the term *molecular electronics* (ME). Very recently it was shown that DNA (deoxyribonucleic acid) - mediated assembly of nano - and micrometer scale structures can have a profound impact in the fields of nanoelectronics and nanotechnology. Such structures can also find applications in microelectromechanical systems, hybrid biosensors and switches [13].

Several issues involving the fundamentals of charge and heat transport in ME elements remain unclear. Among other fundamental question include: (a) How are electrostatic potential (in ME) determined, (b) What energy dissipation mechanism occurs, where is heat generated, and can that heat be managed. (c) Can dissipative processes be controlled by choice of molecular structures and interfaces.

In this paper we will describe the application of the quantum heat transport equation (QHT) [14] to the investigation of heat generation and transport induced in ME structures by ultra-short laser pulses.

2 The model

There are no active device concepts using single DNA molecule itself, but the electronic properties are being studied. Even though there are contradictory measurements of DNA conductivity [15] recent reports show that DNA measured between two electrodes behaves like a large band-gap semiconductor [16]. Resistance in the conductive regime is of the order of $4\,10^{10}$ $\Omega/100$ Å long molecule. The idea assuming that DNA behaves as a conductor in specific voltage / current regimes is presented in [13]. It was suggested that two complementary strands of DNA can be used to make a DNA-based switch. If the heating of the DNA-based switch is induced by current flow through the DNA strands a negative differential resistance device may be possible. Such a device could also be used to form an oscillator.

When a DNA-based switch is heated with attosecond laser pulses the

heat transport is described by QHT [14], (in 1D case)

$$\frac{1}{v^2}\frac{\partial^2 T}{\partial t^2} + \frac{m_e}{\hbar}\frac{\partial T}{\partial t} + \frac{2Vm_e}{\hbar^2}T - \frac{\partial^2 T}{\partial x^2} = 0. \tag{1}$$

In Eq. (1) T denotes temperature, m_e is the mass of heat carrier in DNA (electrons), v is the velocity of heat propagation and V is the potential carrier created by interfaces. As was shown in [14]

$$v = \alpha \left(\frac{m_e}{m_{\rm mol}}\right)^{1/2} c, \tag{2}$$

where α is the fine structure constant for electromagnetic interaction: $\alpha = 137^{-1}$, $m_{\rm mol}$ is the molecular mass of the DNA-strand and c – light velocity.

The solution of Eq. (1) can be written as

$$T(x,t) = e^{-t/2\tau}u(x,t), \tag{3}$$

where $\tau = \hbar/m_e v^2$ is the relaxation time for DNA-strand. After substitution formula (3) to Eq. (1) we obtain

$$\frac{1}{v^2}\frac{\partial^2 u}{\partial t^2} - \frac{\partial^2 u}{\partial x^2} + qu(x,t) = 0 \tag{4}$$

and

$$q = \frac{2Vm_e}{\hbar^2} - \left(\frac{mv}{2\hbar}\right)^2. \tag{5}$$

With $q > 0$ Eq. (4) is the Klein-Gordon (K-G) equation. The solution of K-G equation for the initial conditions

$$u(x,0) = f(x), \qquad u_t(x,0) = g(x)$$

has the form [14]:

$$\begin{aligned} u(x,t) &= \frac{f(x-vt)+f(x+vt)}{2} \\ &+ \frac{1}{2v}\int_{x-vt}^{x+vt} g(\zeta) J_0\left[q\sqrt{v^2t^2-(x-\zeta)^2}\right] d\zeta \\ &- \frac{\sqrt{q}vt}{2}\int_{x-vt}^{x+vt} f(\zeta)\frac{J_1\left[q\sqrt{v^2t^2-(x-\zeta)^2}\right]}{\sqrt{v^2t^2-(x-\zeta)^2}} d\zeta. \end{aligned} \tag{6}$$

When $q < 0$, Eq. (4) is the modified Heaviside equation with the solution [14]

$$\begin{aligned} u(x,t) &= \frac{f(x-vt)+f(x+vt)}{2} \\ &+ \frac{1}{2v}\int_{x-vt}^{x+vt} g(\zeta) J_0\left[-q\sqrt{v^2t^2-(x-\zeta)^2}\right] d\zeta \\ &+ \frac{v\sqrt{-q}t}{2}\int_{x-vt}^{x+vt} f(\zeta)\frac{J_1\left[-q\sqrt{v^2t^2-(x-\zeta)^2}\right]}{\sqrt{v^2t^2-(x-\zeta)^2}} d\zeta. \end{aligned} \tag{7}$$

When $q = 0$, Eq. (4) is distortionless wave equation

$$\frac{\partial^2 u}{\partial t^2} - v^2\frac{\partial^2 u}{\partial x^2} = 0. \tag{8}$$

The condition $q = 0$ can be expressed as

$$V = \frac{T_h}{8}, \tag{9}$$

where [14]

$$T_h = \alpha^2 \frac{m_e}{m_{\text{molecular}}} m_e c^2. \tag{10}$$

In equation (10) c is the light velocity in the vacuum.

It can be stated that the distortionless waves can be generated and transported through DNA strands only if $V < T_h$. For $T_h < V$ i.e. when "Heisenberg rule" (9) is broken the shape of the thermal waves is changed.

It occurs that DNA strands behave as the thermal switch for ultra-short laser pulses. For $T_h > V$ DNA strand conducts the heat in the form of distortionless thermal waves. For $T_h < V$ the DNA strand blocks the heat transport.

3 Conclusion

In this paper we describe the heat transport on the molecular scale (DNA strands) induced by ultra-short laser pulse. Considering the quantum heat transport equation we show that for ultra-short laser pulse heating the DNA strands the thermal waves can be generated. The transport of thermal energy through the DNA strands depends on the DNA strands relaxation time. We developed the formula for the relaxation time in DNA structures heated with ultra-short laser pulses. It is shown that when the relaxation time τ and the interface potential V fulfill the Heisenberg type relaxation, $V\tau \sim \hbar$, in the DNA strands the undistorted thermal waves can be generated and transported.

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