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Full Length Article

Quantum-relativistic velocities in nano-transport

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A R T I C L E I N F O

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A B S T R A C T

In this paper I present an interesting analysis focused on the hypothesis of relativistic velocities and quantum aspects inside a nanostructure. A new analytical model is considered, able to well describe the conductors in nanostructured form. Considering appropriate scattering times, it is possible to mimic the infrared properties of oxides and semiconductors in the nano-form. The new presented result concerns the analytical form of the quantum-relativistic velocities correlation function, and how it works with experimental data of carbon nanotube films.

1. Introduction

The creation of new theoretical models and the generalization of existing ones are mandatory for the development of pure and applied science. The theory of relativity and quantum mechanics are the two pillars of the world's understanding, the basis of our description of Nature in its most intimate mechanisms.

The Drude-Lorentz model, well used at nano-level for the description of carriers dynamics, has been partially modified during years for accommodating observed departures. Recently an interesting generalization gives an accurate description of the dynamic response of carriers and includes important previous generalizations. It allows to provide the analytical formulation of the most important dynamics variables, i.e. the velocities correlation function $\langle \vec{v}(0) \cdot \vec{v}(t) \rangle_T$ of a system at the temperature T, the mean square deviation of position $R^2(t)$ and the diffusion coefficient $D(t) = (1/2)(dR^2(t)/dt)$.

Charge transport can be influenced by particles dimensions and presents different characteristics with respect to those of bulk. In mesoscopic systems the mean free path of charges can become larger than the particle dimensions and corrections of the transport bulk theories are possible.

At experimental level, one of the most important technique for the study of the frequency-dependent complex-valued far-infrared photoconductivity $\sigma(\omega)$ is the Time-resolved THz Spectroscopy (TRTS), an ultrafast non-contact optical probe; experimental data are usually fitted via Drude-Lorentz, Drude-Smith and Effective Medium Models [1]. The new considered model fits very well with existing data and encompasses the previous models as subsets.

The imaging technique PINEM (photon-induced near-field electron microscopy) [2] can represent nano-objects with temporal resolution of the femtosecond. It can be used to display ultra-fast events for representing nanostructures in more precise details. Illuminating the nanostructure with a laser pulse at the femtosecond, an evanescent wave is created near the surface that effectively interacts with surface electrons. The electrons used in this microscopy technique travel to 70% of the speed of light with times of order of the femtosecond. Using shorter impulses should allow to track ultra-fast processes that occur, for example, in photonic and plasmonic devices. Further improvement of such techniques could lead to a new way of studying the nanoworld. The inclusion of relativistic effects in nanometric quantum theories is therefore of great help in the process of the deep understanding of nanoscale reality.

In the following the essential lines of the model will be showed, and the new analytical expression of the quantum-relativistic velocities correlation function; then the application to SWCNs will be considered.

2. The new model

The new model extends the Drude-Lorentz relation involving the complex conductivity and is based on the inversion of the complete Fourier transform in the complex plane [3–5] in such a way that the whole time axis occurs:

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$$\langle \vec{v}^{\alpha}(0)\vec{v}^{\beta}(t)\rangle_T = \frac{k_B T V}{\pi e^2}\int_{-\infty}^{+\infty} d\omega Re\sigma_{\beta\alpha}(\omega)e^{i\omega t} \quad (1)$$

The form of the velocities correlation function in quantum (Q) and relativistic (R) case is respectively:

$$Q : \langle \vec{v}(0)\cdot\vec{v}(t)\rangle = \frac{1}{2}\left(\frac{KT}{m}\right)\sum_i\left(\left(\frac{f_i}{\alpha_{il}}\right)\left[(1+\alpha_{il})\exp\left(-\frac{(1+\alpha_{il})}{2}\frac{t}{\tau_i}\right) - \left(1-\alpha_{il}\right)\exp\left(-\frac{(1-\alpha_{il})}{2}\frac{t}{\tau_i}\right)\right]\right)$$

with

$$\alpha_{il} = \sqrt{1-4\tau_i^2\omega_i^2}, \quad \alpha_{il} = \sqrt{\Delta_{quant}}, \quad \Delta_{quant} < 0 \quad (\Delta_{quant} = 4\tau_i^2\omega_i^2 - 1 > 0). \quad (2\text{-}5)$$

K is the Boltzmann's constant, T the temperature of the system, ω_i and τ_i frequencies and decaying times of each mode respectively. A similar expression is given for $\Delta_{quant} > 0$.

$$R : \langle \vec{v}(0)\cdot\vec{v}(t)\rangle = \frac{1}{2}\left(\frac{k_B T}{m_0}\right)\left(\frac{1}{\gamma\rho}\right)\left(\frac{1}{\alpha_{I_{rel}}}\right)\left[(1+\alpha_{I_{rel}})\exp\left(-\frac{(1+\alpha_{il})}{2\rho}\frac{t}{\tau}\right) - (1-\alpha_{I_{rel}})\exp\left(-\frac{(1-\alpha_{il})}{2\rho}\frac{t}{\tau}\right)\right]$$

with

$$\alpha_{I_{rel}} = \sqrt{1-4\gamma\omega_0^2\tau^2}, \quad \alpha_{I_{rel}} = \sqrt{\Delta_{rel}}, \quad \Delta_{rel} < 0. \quad (6\text{-}9)$$

A similar expression is given for $\Delta_{rel} > 0$. It also holds: $\beta = v/c$, $\gamma = 1/\sqrt{1-\beta^2}$, $\rho = 1+\beta^2\gamma^2 = \gamma^2$. With these expressions we obtain R^2 and D.

In the quantum-relativistic case (Q-R), the analytical relations of $\langle \vec{v}(0)\cdot\vec{v}(t)\rangle_T$ are as follows:

$$Q-R : \langle \vec{v}(0)\cdot\vec{v}(t)\rangle = \frac{1}{2}\left(\frac{k_B T}{m_0}\right)\left(\frac{1}{\gamma\rho}\right)\sum_i\left(\left(\frac{f_i}{\alpha_{il_{Q-R}}}\right)\times\left[(1+\alpha_{il_{Q-R}})\exp\left(-\frac{(1+\alpha_{il_{Q-R}})}{2\rho}\frac{t}{\tau_i}\right) - \left(1-\alpha_{il_{Q-R}}\right)\exp\left(-\frac{(1-\alpha_{il_{Q-R}})}{2\rho}\frac{t}{\tau_i}\right)\right]\right)$$

with

$$\alpha_{il_{Q-R}} = \sqrt{1-4\gamma\omega_i^2\tau_i^2} \in (0,1) \subset R\,(real\ numbers),$$
$$\alpha_{il_{Q-R}} = \sqrt{\Delta_{Q-R}}, \quad \Delta_{Q-R} < 0. \quad (10\text{-}13)$$

$$Q-R : \langle \vec{v}(0)\cdot\vec{v}(t)\rangle = \left(\frac{k_B T}{m_0}\right)\left(\frac{1}{\gamma\rho}\right)\sum_i\left(\left(f_i\exp\left(-\frac{t}{2\rho\tau_i}\right)\right)\times\left[\cos\left(-\frac{\alpha_{iR_{Q-R}}}{2\rho}\frac{t}{\tau_i}\right) - \frac{1}{\alpha_{iR_{Q-R}}}\sin\left(-\frac{\alpha_{iR_{Q-R}}}{2\rho}\frac{t}{\tau_i}\right)\right]\right)$$

with

$$\alpha_{iR_{Q-R}} = \sqrt{4\gamma\omega_i^2\tau_i^2 - 1} \in R^+\,(positive\ real\ numbers),$$
$$\alpha_{iR_{Q-R}} = \sqrt{\Delta_{Q-R}}, \ \Delta_{Q-R} > 0. \quad (14\text{-}17)$$

3. Results and discussion

The obtained results in the classical case gave an explanation of ultra-short times and high mobilities, with which charges spread in mesoporous systems, of wide interest in photocatalitic and photovoltaic systems. The relative short times of few τ indicate easy charge diffusion inside the nanoparticles. The unexplained experimental fact of ultrashort injection of charge carriers, in particular in Grätzel's cells, can be related to this phenomenon. Deviations by the Drude model become strong in nanostructured materials, such as photoexcited TiO_2 nanoparticles, ZnO films, InP nanoparticles, semiconducting polymer molecules and carbon nanotubes [6].

The quantum and relativistic versions of the model gave interesting other features respectively, including new ones. In the quantum case we keep into account of the weight of different modes with the respective ω_i and τ_i values, the relativistic case deals with ultra-high velocities of carriers inside nanostructures. The quantum-relativistic case associate both features.

Fig. 1 shows the evolution of $\langle \vec{v}(0)\cdot\vec{v}(t)\rangle$ vs t for the fixed value $\alpha_{R_{rel}} = 10$ in the case of one only mode ($m^* = 0.24\ m_e$; $\tau = 0.84 \cdot 10^{-13}$ s) [7]; the considered velocities of carriers are $v = 10^7$ cm/s (blue solid line), $v = 10^{10}$ cm/s (red dashed line) and $v = 2.5\cdot 10^{10}$ cm/s (green dots line). The classical "Drude" velocity $v = 10^7$ cm/s implies a negligible variation in mass for the electrons. We note that the increase in velocity tends to raise the wavelength of the damped oscillation, reducing its amplitude.

With one only mode and considering the parameter $\alpha_{I_{rel}}$, the velocities correlation function has a "Smith behaviour" (Fig. 2) [7].

Afterwards I considered experimental data from literature, in particular the first three weights of samples from the same baked piece of film at the temperature of 300 K. The thermal processing of baking consisted of treating the samples in flowing pure argon at 1000 °C for 12 hours, by removing the nitric acid (used during purification) from sample [8,9]. The elaborated data are resumed in Tables 1–3.

In this case we have both the presence of more modes and the possibility of relativistic velocities of carriers. Fig. 3 shows the

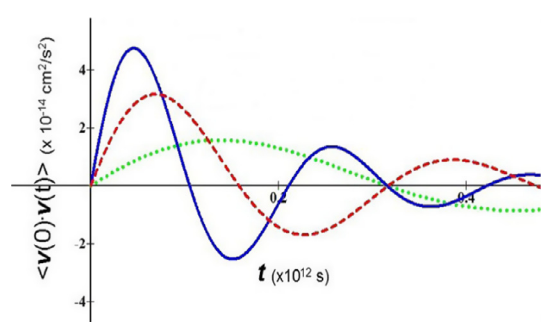

Fig. 1. $\langle \vec{v}(0)\cdot\vec{v}(t)\rangle$ vs t with $\alpha_{R_{rel}} = 10$, T = 300 K; $v = 10^7$ cm/s (blue solid line), $v = 10^{10}$ cm/s (red dashed line) and $v = 2.5\cdot 10^{10}$ cm/s (green dots line). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

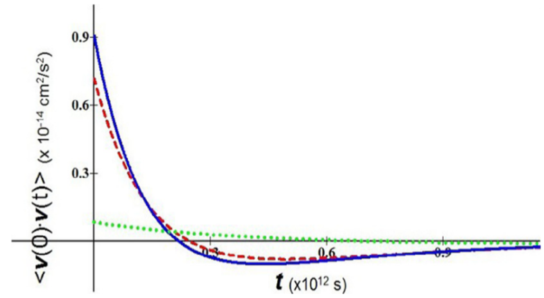

Fig. 2. $\langle \vec{v}(0)\cdot\vec{v}(t)\rangle$ vs t for fixed value $\alpha_{I_{rel}} = 0.5$, T = 300 K; $v = 10^7$ cm/s (blue solid line), $v = 10^{10}$ cm/s (red dashed line) and $v = 2,5\cdot 10^{10}$ cm/s (green dots line). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)