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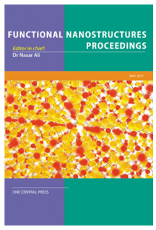

Quantum-Relativistic Carrier Nano-Transport and Plasmonics

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ABSTRACT

In this paper I consider the quantum-relativistic aspects of a recent Drude-Lorentz-like model able to well describe the conductors in nanostructured form. The model is characterized by the assumption of a collective mode at a finite frequency, leading to the occurrence of anomalous charge transport. Considering appropriate scattering times, it is possible to mimic the infrared properties of oxides and semiconductors in the nano-form. The carrier current reverses its direction before decaying to zero and presents also damped oscillation in time, features possibly detectable with femtosecond time resolved techniques. The new presented result concerns the analytical form of the quantum-relativistic velocities correlation function, and how it works with specific examples related to Si, ZnO, TiO_2, GaAs, SWCN.

I. INTRODUCTION

The Drude-Lorentz model for the description of dynamics of carriers, currently well used at nano-level, has been partially modified during years for accomodating observed departures. Recently an interesting generalization has been made, based on linear response theory and resonant plasmonic mode, that gives a detailed description of the dynamic response of the carriers and includes the most important previous generalization, as the Smith model. Among the principal features we have the assumption of a characteristic frequency describing a collective mode and the response evaluation is made in the time domain by the use of the residue theorem in the complex plane. This allows to get the analytical formulation of the most important dynamics variables, i.e. the velocities correlation function $<\vec{v}(0)\cdot\vec{v}(t)>_T$ of the system at the temperature *T*, the mean square deviation of position $R^2(t)$ and the diffusion coefficient $D(t)=(1/2)(dR^2(t)/dt)$. Consequently velocity, travelled space e diffusion of carriers are obtainable. Experimental data have indicated that plasmon models describe nanostructured systems in particularly effective way.

II. THE NEW MODEL

The model has been performed at classical, quantum and relativistic level, the last step refers to quantum-relativistic motion and is in progress. In the paper we present for first time the quantum-relativistic expression for $<\vec{v}(0)\cdot\vec{v}(t)>_T$.
If a collective mode exists at frequency ω_0 with a decay time τ, the complex conductivity can be expressed as:

$$\sigma(\omega)=\frac{i\omega N e^2}{m(\omega^2-\omega_0^2+i\omega/\tau)} \qquad (1)$$

Eq. (1) in the THz range leads to a class of Drude-Lorentz functions. Using the connection between conductivity and velocities correlation function, by inverting the complete Fourier transform in such a way that the whole time axis occurs, after rigorous calculation we obtain [1]:

$$< \vec{v}^{\alpha}(0)\, \vec{v}^{\beta}(t) >_T = \frac{k_B T V}{\pi e^2} \int_{-\infty}^{+\infty} d\omega \, \mathrm{Re}\sigma_{\beta\alpha}(\omega) e^{i\omega t} \qquad (2)$$

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

Q: $$\langle \vec{v}(0)\cdot\vec{v}(t)\rangle = \frac{1}{2}\left(\frac{KT}{m}\right)\sum_i \left(\left(\frac{f_i}{\alpha_{iI}}\right)\left[(1+\alpha_{iI})\exp\left(-\frac{(1+\alpha_{iI})}{2}\frac{t}{\tau_i}\right) - (1-\alpha_{iI})\exp\left(-\frac{(1-\alpha_{iI})}{2}\frac{t}{\tau_i}\right)\right]\right) \qquad (3)$$

with: $\alpha_{iI} = \sqrt{1-4\tau_i^2\omega_i^2}$, $\Delta_{quant} = 4\omega_i^2\tau_i^2 - 1$, $\Delta_{quant} < 0$. (4)

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 $\Delta_{quant} > 0$ [2].

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

with: $\alpha_{I_{rel}} = \sqrt{1-4\gamma\omega_0^2\tau^2}$, $\Delta_{rel} < 0$. (5,6)

It holds: $\beta = v/c$, $\gamma = 1/\sqrt{1-\beta^2}$, $\Delta_{rel} = 4\gamma\omega_0^2\tau^2 - 1$, $\rho = 1+\beta^2\gamma^2 = \gamma^2$. A similar expression is given for $\Delta_{rel} > 0$.

With these expressions we obtain R^2 and D [3].

III. RESULTS AND DISCUSSION

The results so far obtained can give an explanation of the ultra-short times and of high mobilities, with which the charges spread in mesoporous systems, of large interest in photocatalitic and photovoltaic systems. In particular, the relative short times (few τ), with which charges can reach much larger distances than typical dimensions of nanoparticles, indicate easy diffusion of charges 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.

The extension of Drude model proposed by Smith was successfully applied to fit the conductivity in a variety of systems in the frequency domain. A parameter c_1 accounts for the anisotropy of scattering upon the first scattering event. $c_1 = 0$ describes isotropic response, proper to the Drude model; $c_1 \neq 0$ corresponds to a preferential backscattering of charge carriers. This parameter originated main criticism; the model assumes that anisotropic scattering occurs only upon the first scattering event, while all subsequent events are characterized by isotropic scattering, without physical reasons proposed by the author to justify this assumption.

The Smith model with $c_1 = -1$ is obtained as a limit of the new model when $\alpha_I \to 0$. From the other hand, both Smith's and this model reduce to the Drude model in the limit $\omega_o \to 0$. So, although the two models are analytically different, their predictions are expected to be quite similar. The backscattering mechanism invoked by Smith arises in a natural way in this model, without further assumption on successive scattering events.

The quantum and relativistic version offer interesting other features, including new ones.

IV. SUMMARY

The are arriving to the last step (quantum-relativistic case) of a new appeared analytical transport model, able to describe the systems dynamics from sub-pico-level to nano-level, thanks to a gauge factor inside it. The model has been performed at classical, quantum and relativistic level.

Acting on all chemical, physical, structural and model-intrinsic parameters, i.e.:

a) the temperature *T* of the system,
b) the parameters α_I and α_R ,
c) the values of τ_i and ω_i ,
d) the variation of the effective mass m^*,
e) the variation of the chiral vector,
f) the quantum weights of each mode in the quantum case,
g) the carrier density *N*,
h) the velocity of carriers,

it is possible to perform an accurate tuning of the quantities $< \vec{v}(t)\cdot\vec{v}(0) >_T$, $R^2(t)$ and $D(t)$ and then to calibrate the performance of nano-bio-devices.

Also from a mathematical point of view, the model is very elegant, because it gives analytical expressions of the results and all calculus is analytical. It is giving new interesting informations, very useful in the phase of design/creation of new nano-bio-devices with dedicated features and in general for the deep understanding of nano-world.

The quantum-relativistic version will give a global view and will allow the possibility of simultaneously modifying all available variables. Moreover, the “ad hoc” creation of new analytical forms of the conductivity, then implemented in Eq. (2), will lead to further new interesting results.

V. REFERENCES

[1] P. Di Sia, An Analytical Transport Model for Nanomaterials, Journal of Computational and Theoretical Nanoscience 8 (2011) 84-89.

[2] P. Di Sia, An Analytical Transport Model for Nanomaterials: The Quantum Version. Journal of Computational and Theoretical Nanoscience 9(1) (2012) 31-34.

[3] P. Di Sia, Relativistic nano-transport and artificial neural networks: details by a new analytical model, International Journal of Artificial Intelligence and Mechatronics (IJAIM) 3(3) (2014) 96-100.