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Beyond Drude-Lorentz-like Models: the Analytical Quantum-Relativistic Diffusion Function

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ABSTRACT

In this paper I present the complete technical analysis of the diffusion function $D(t)$ in the hypothesis of quantum-relativistic effects inside a nanostructure. The calculation is carried out through the use of a recently appeared analytical model, known as DS model, that have a wide scale range of applicability and is able to describe every oscillating process in nature. The nanoscale is considered in the paper, but the presence of a gauge term inside the model allows its application from sub-pico-level to macro-level. In addition to the theoretical framework, the graphical behavior of the function $D(t)$ is considered and an example of application is performed.

***Keywords*:** Drude-Lorentz-like models, Mathematical modeling, Quantum-relativistic effects, Nanophysics, Diffusion, Charge/Carrier transport, Nanomaterials, DS model.

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1. INTRODUCTION

One of the most important aspects at the nanoscale affects the charge transport, which can be influenced by particles dimensions and takes different characteristics with respect to those of bulk. In particular, if the mean free path of charges, from scattering phenomena, is larger than the particle dimensions, we have a mesoscopic system, in which the transport depends on dimensions and as criterion it is possible to correct the transport bulk theories by considering this phenomenon.

A similar situation occurs also in a thin film, in which the smallest nanostructure dimension can be less than the free displacement and then needs variations for existing theoretical transport bulk models. Therefore, a rigorous and deep knowledge of transport properties is significant and fruitful.

From a theoretical point of view, various techniques can be used for the comprehension of transport phenomena, both numerical and analytical descriptions based on transport equations. The numerical approaches result in general not able to provide an overall vision, instead typical of analytical approaches; these latter are of high mathematical interest and lead to newsworthy results and predictions, implemented through the experimental data existing in literature and continuously obtained by experiments.

In the will to create an analytical model that generalizes the Drude-Lorentz-like models, in last years it has appeared a new theoretical approach, based on correlation functions obtained by the complete Fourier transform of the frequency-dependent complex-valued far-infrared photo-conductivity $\sigma(\omega)$ of a system. With this model it is possible to exactly calculate the expressions of the velocities correlation function, the mean square deviation of position and the diffusion coefficient.

Among the most important experimental techniques for the study of $\sigma(\omega)$, there is the Time-resolved THz Spectroscopy (TRTS), an ultrafast non-contact optical probe; data are normally fitted via Drude-Lorentz, Drude-Smith or effective medium models [1].

The recent analytical generalization has been performed at classical [2], quantum [3], and relativistic level [4]; the final step concerns the case of quantum-relativistic effects inside a nanostructure. The complete technical analysis of the function $D(t)$ is considered in this paper, completing the quantum-relativistic study together with what has already been calculated for the velocities correlation function $\langle \vec{v}(t) \cdot \vec{v}(0) \rangle_T$ [5] and the mean square deviation of position $R^2(t)$ [6].

The paper summarizes the key elements of this analytical generalization (§2), presents the general expressions of the quantum-relativistic diffusion function $D(t)$ (§3), and ends with an example of application (§4) and the conclusions (§5).

2. A POWERFUL ANALYTICAL GENERALIZATION OF THE DRUDE-LORENTZ-LIKE MODELS

A recent analytical generalization of the Drude-Lorentz-like models for transport processes is showing to fit very well with experimental data and gives interesting new predictions of various peculiarities in nanostructures.

The model studies the dynamics of processes from sub-pico-level to macro-level; it is based on the complete Fourier transform of the frequency-dependent complex-valued far-infrared photo-conductivity $\sigma(\omega)$, as deduced by the linear response theory [7,8], considering the Cauchy integration and the use of the residue theorem in the complex plane [9].

One of the new introduced key ideas has been to perform the integration on the entire time axis (-∞, +∞) and not on the half time axis (0, +∞), as ordinarily considered in literature [10]; with this procedure we arrived to write the following expression:

$$<\vec{v}^{\alpha}(0)\,\vec{v}^{\beta}(t)>_T = \frac{k_B T V}{\pi e^2}\int_{-\infty}^{+\infty} d\omega\ \mathrm{Re}\,\sigma_{\beta\alpha}(\omega)\,e^{i\omega t}\,. \tag{1}$$

The carrier dynamics is studied considering, in addition to the velocities correlation function $\langle \vec{v}(t)\cdot\vec{v}(0)\rangle_T$, the mean square deviation of position of particles $R^2(t)$ and the diffusion function $D(t)$. $R^2(t)$ is defined as:

$$R^2(t) = \left\langle [\vec{R}(t) - \vec{R}(0)]^2 \right\rangle. \tag{2}$$

Eq. (2) is connected to Eq. (1) by the relation:

$$R^2(t) = 2\int_0^t dt'(t-t')\langle \vec{v}(t')\cdot\vec{v}(0)\rangle\,. \tag{3}$$

With the residue theorem it is possible to obtain the analytical expressions of $\langle \vec{v}(t)\cdot\vec{v}(0)\rangle_T$, $R^2(t)$ and of the diffusion function $D(t)$, defined as [2,3]:

$$D(t) = \frac{1}{2}\frac{dR^2(t)}{dt}. \tag{4}$$

3. GENERAL ANALYTICAL EXPRESSIONS OF THE QUANTUM-RELATIVISTIC DIFFUSION FUNCTION *D(t)*

About the *quantum behavior*, we considered a frequency-dependent electric field of the form $\vec{E} = \vec{E}_0\, e^{-i\omega t}$ in the contest of the time-dependent perturbation theory, with the factor $e\,\vec{E}\cdot\vec{r}$ as perturbing potential.

Written the matrix elements of the dipole moment of the charge in the direction of the electric field as:

$$x_{j0} = \int \Phi_j^* \, e\, x \, \Phi_0 \, dr, \tag{5}$$

defining the oscillator strength of the *j*-th transition as:

$$f_j = \frac{2m}{\hbar^2} \sum_j \hbar \omega_j \left| x_{0j} \right|^2, \tag{6}$$

and keeping into account the relation between permittivity and conductivity of a system, we obtained the relation:

$$\frac{i\sigma(\omega)}{\omega} = \frac{1}{4\pi} \sum_i \frac{\omega_{p_i}^2}{(\omega_i^2 - \omega^2) - i\omega\Gamma_i}, \tag{7}$$

with:

$$\omega_{p_i}{}^2 = \frac{4\pi N e^2}{m} f_i \tag{8}$$

and:

- $\omega_i = (E_i - E_0)/\hbar$;
- E_i, E_0 energies of the excited and the ground states respectively;
- $\Gamma_i = 1/\tau_i$ inverse of the decay time of every mode;
- N density of carriers.

Unlike the classical case, the real part of conductivity is calculated at quantum level through the weights f_i. The relaxation times can be obtained by $\tau_i = 1/\Gamma_i$ and weights f_i. The calculation of N can be exactly obtained by Eq. (8), considering that it holds: $\sum_i f_i = 1$.

About the *relativistic behavior*, we considered the possibility of relativistic velocities of carriers inside a nanostructure through the study of the condition of relativistic variation of the mass along an *x*-axis on which a nanostructure is placed, in the fixed ground reference frame. About the forces acting on the carrier (electrons, but this is not restrictive), we considered the following outer forces:

- a passive elastic-type force of the form $F_{el} = K\, x$;
- a passive friction-type force of the form $F_{fr} = \lambda \dot{x}$, with $\lambda = m_{part}/\tau$;
- the force deriving by an oscillating electric field $E = e\, E_0\, e^{-i\omega t}$.

Performing the calculation as for the velocities correlation function $\langle \vec{v}(t)\cdot\vec{v}(0)\rangle_T$ [5] and the mean square deviation of position $R^2(t)$ [6], the quantum-relativistic analytical expressions of $D(t)$ are as follows:

Q-R$_1$) Case $\Delta_{iR_{Q-R}}>0$

$$D(t)=2\left(\frac{k_B T}{m_0}\right)\left(\frac{1}{\gamma}\right)\sum_i\left\{\left(\frac{f_i\tau_i}{\alpha_{iR_{Q-R}}}\right)\left[\exp\left(-\frac{1}{2\rho}\frac{t}{\tau_i}\right)\sin\left(\frac{\alpha_{iR_{Q-R}}}{2\rho}\frac{t}{\tau_i}\right)\right]\right\} \tag{9}$$

with:

$\alpha_{iR_{Q-R}}=\sqrt{4\gamma\omega_i^2\tau_i^2-1}\ \in\Re^+$ (positive real numbers);

Q-R$_2$) Case $\Delta_{iI_{Q-R}}<0$

$$D(t)=\left(\frac{k_B T}{m_0}\right)\left(\frac{1}{\gamma}\right)\sum_i\left\{\left(\frac{f_i\tau_i}{\alpha_{iI_{Q-R}}}\right)\left[\exp\left(-\frac{(1-\alpha_{iI_{Q-R}})}{2\rho}\frac{t}{\tau_i}\right)-\exp\left(-\frac{(1+\alpha_{iI_{Q-R}})}{2\rho}\frac{t}{\tau_i}\right)\right]\right\} \tag{10}$$

with:

$\alpha_{iI_{Q-R}}=\sqrt{1-4\gamma\omega_i^2\tau_i^2}\ \in(0,1)\subset\Re$

It holds: $\alpha_{iI_{Q-R}}=\sqrt{\Delta_{iI_{Q-R}}}$, $\alpha_{iR_{Q-R}}=\sqrt{\Delta_{iR_{Q-R}}}$, $\gamma=1/\sqrt{1-\beta^2}$, $\beta=v/c$, $\rho=1+\beta^2\gamma^2=\gamma^2$ [5,6].

4. EXAMPLE OF APPLICATION

As example of application, I considered experimental data from international literature, by which three states have been extracted through a personal elaboration (Table 1). Data are related to single-walled carbon nanotube films at the temperature of 300 K [11-14].

Table 1. Values of parameters for each considered state.

States	ω_i (× 10 $^{-12}$ Hz)	τ_i (× 10 ^{12} Hz)	f_i
1	6.59	0.0042	0.312
2	1166.01	0.0037	0.176
3	2000.05	0.0014	0.512

The corresponding values of α_{I-R}, calculated for each considered velocity, are resumed in Table 2.

Table 2. Values of each considered state.

States	$\alpha_{I\text{-}R}$ (v_1)	$\alpha_{I\text{-}R}$ (v_2)	$\alpha_{I\text{-}R}$ (v_3)
1	0.998	0.998	0.997
2	8.57	8.83	11.52
3	5.51	5.68	7.44

Figures 1-3 show the behavior of each single weight f_i (i = 1,2,3) considering $v = v_1$; in Figure 4 the graph represents their sum. In this last one, the presence of both α_I and α_R implies that the D function is a mix of Eq. (9) and Eq. (10), with a damped oscillating increased behavior.

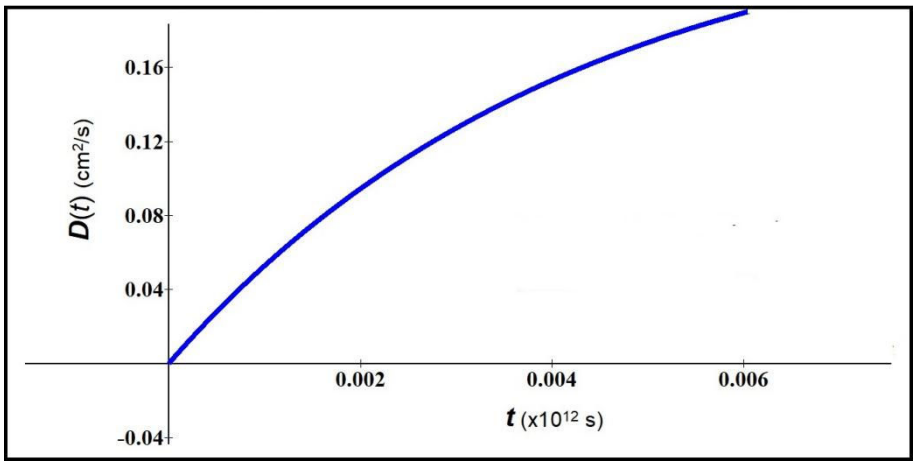

Figure 1. $D(t)$ vs t for f_1 with $v = v_1$.

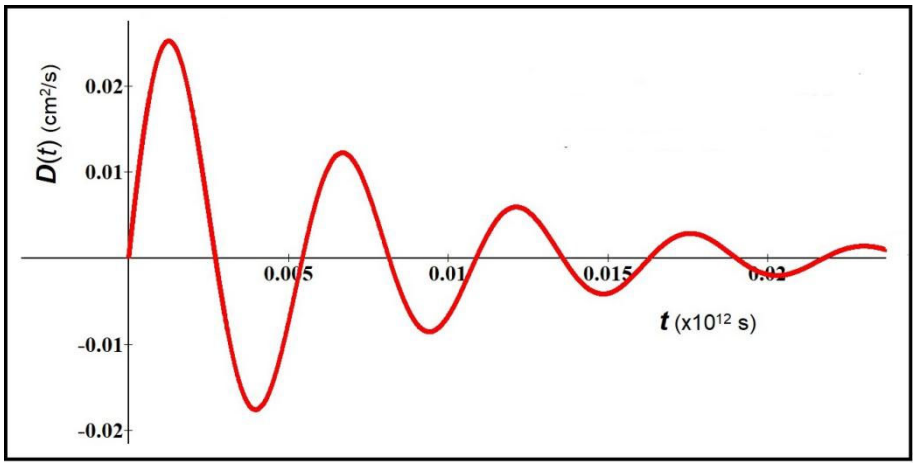

Figure 2. $D(t)$ vs t for f_2 with $v = v_1$.

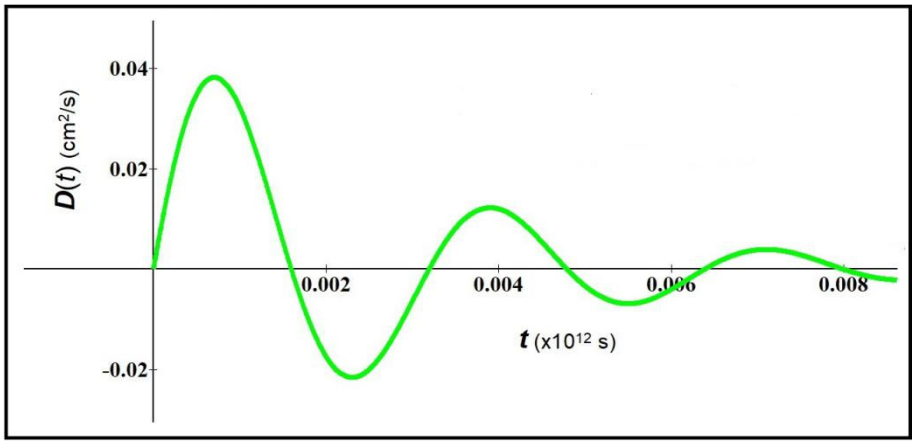

Figure 3. $D(t)$ vs t for f_3 with $v = v_1$.

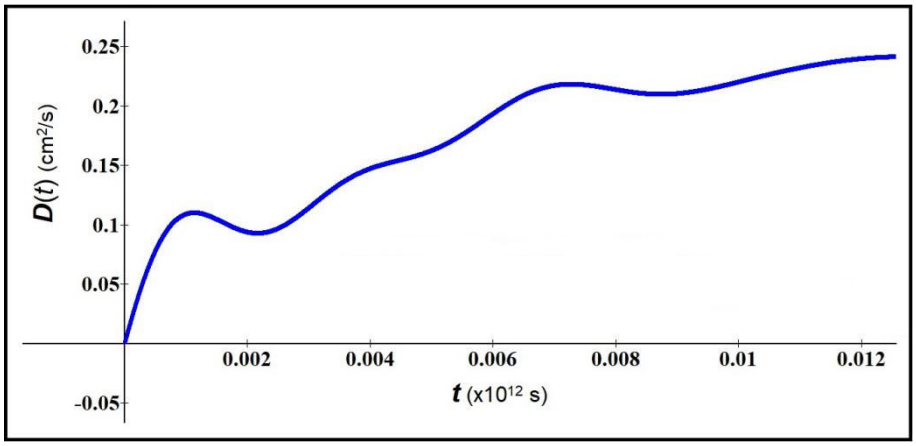

Figure 4. $D(t)$ vs t for the sum of the previous three states.

Figure 5 shows the general quantum-relativistic case, i.e. considering the quantum-relativistic behavior related to the presence of all considered states, with the variation of velocity.

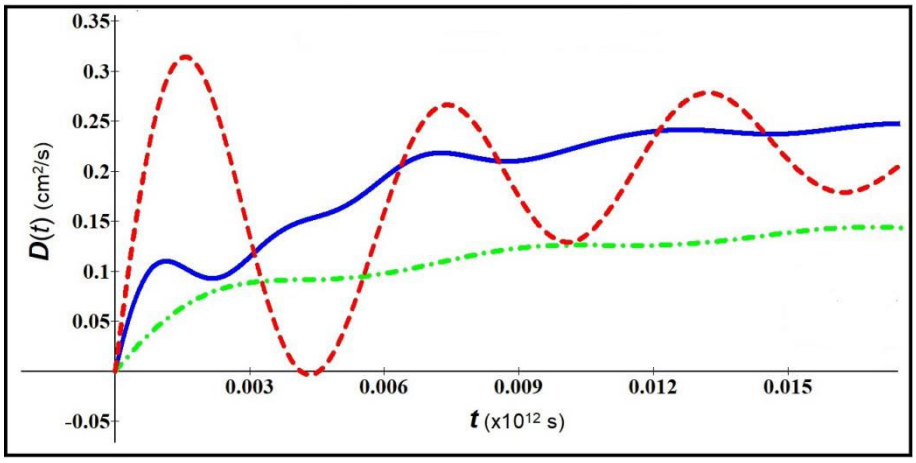

Figure 5. $D(t)$ vs t for the general case given by the sum of the three states; $v=10^7\ cm/s$ (blue solid line), $v=10^{10}\ cm/s$ (red dashed line) and $v=2.5\cdot10^{10}\ cm/s$ (green dot-dashed line).

The example shows that it is possible to perform a general fine-tuned quantum-relativistic study of the charge transport in a nanostructure. The assumption of quantum-relativistic aspects inside it is a globally important feature; quantum processes with ultra-high velocities of carriers are concerning both the current science and technology and the future of theoretical and phenomenological (nano)physics.

What discussed here can be considered as the starting point of an investigation pathway linked to physical assumptions, i.e. how scattering, ballistic transport, influence of temperature [14], size effect, etc., can impact on the studied phenomenon. This research is also a challenge for phenomenologists, whose insights and inspirations could usefully support this theoretical effort, through, but not only, TRTS [15-17], Photon-Induced Near-Field Electron Microscopy [18,19] and Graphene based Plasmonics [20-22].

5. CONCLUSIONS

In this paper it has been presented a new theoretical result: the complete analytical form of the function $D(t)$ considering the possibility of quantum-relativistic effects inside a nanostructure. We have generalized a new analytical model appeared in classical, quantum and relativistic form [2-4], and tested during last years with fine accordance with experimental existing data. Eqs (9,10) become those of the classical case, when the carriers velocity becomes classic and we do not consider quantum effects. The introduced formulae for the diffusion function $D(t)$ complete the quantum-relativistic version of this model, known as DS model [5,6].

The considered extension is mathematically accurate, fine and elegant, because of the analytical approach, which overcomes time-consuming numerical approaches. It is able to give also new interesting information, useful in the design phase of new nano-bio-devices with dedicated and specific features, in particular in the field of sensoristics. This new information may be appropriately tested through current experimental techniques, like TRTS, PINEM, Graphene based Plasmonics.

Considering all parameters influencing the system at chemical, physical, structural and model-intrinsic level, as the system's temperature *T*, the parameters $\alpha_{iI_{Q-R}}$ and $\alpha_{iR_{Q-R}}$, the values of τ_i and ω_i, possible variations of the effective mass m^* [23], variations of the chiral vector, the quantum weights f_i of modes, the carrier density *N*, the velocity of carriers, it is possible to perform a precise tuning of the three fundamental functions related to the dynamics of charge transport, i.e. $\langle \vec{v}(t) \cdot \vec{v}(0) \rangle_T$, $R^2(t)$, and $D(t)$ in the contest of ultrafast carrier dynamics [24-26].

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Biography

Paolo Di Sia (Adj. Prof., Dr., Dr., Dr.) is currently Adjunct Professor by the Universities of Padova and Verona (Italy), already Adj. Prof. by the Universities of Pavia, Bolzano-Bozen (Italy), Visiting Professor by the "National Center for Theoretical Sciences" (National Chiao Tung University, Hsinchu, Taiwan ROC), qualified as Associate Professor in Mathematics Didactics - Mathematics in Norwegian University of Science and Technology (NTNU), Universitetet i Agder, Nord Universitet, Universitetet i Stavanger, Oslo Metropolitan University (Norway) and Head of the "Primordial Dynamic Space" Research in Verona (Italy).
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