A new analytical transport model for (nano) physics

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Abstract - ***In this paper we focus on a new analytical transport Drude-Lorentz-like model, able to adjust previous unresolved problems and to present new interesting peculiarities. It works from sub-pico-scale to macro-scale and has a wide range of applications.***

Key Words: *Mathematical Modelling, Analytical Calculus, Applied Analysis, Theoretical Physics, Nano-science, Nano-Bio-Technology.*

1. INTRODUCTION

In these years it has been performed a new generalization of the Drude-Lorentz model, based on the complete Fourier transform of the frequency-dependent complex conductivity $\sigma(\omega)$ of a system, which provides analytical expressions of the three most important quantities related to transport phenomena, i.e. the velocities correlation function $\langle \vec{v}(t) \cdot \vec{v}(0) \rangle_T$ at the temperature T, the mean squared deviation of position $R^2(t)$ and the diffusion coefficient $D(t)$ [1]. The model avoids time-consuming numerical and/or simulation procedures and, in the case of nano-scale, it has been well tested and is useful both "a priori", for searching new characteristics and peculiarities at nano-level, and "a posteriori", for testing existing experimental data. It considers also quantum [2] and relativistic [3] effects. The comparison with existing models, like Drude-Lorentz and Smith models [4,5], has demonstrated a very good fit with current knowledge and is giving also interesting information's about new behaviors at nano-scale, as damped oscillations at beginning of processes [6-11].

2. TECHNICAL DETAILS

The diffusion coefficients for nano-scale, of great importance for their connection with the sensitivity of nano-bio-devices, present the following analytical expressions.

(a) Case: $\Delta < 0$

Classical expression

$$D(t) = \left(\frac{k_B T}{m^*}\right)\left(\frac{\tau}{\alpha_I}\right) \cdot$$

$$\cdot \left[\exp\left(-\frac{(1-\alpha_I)}{2}\frac{t}{\tau}\right) - \exp\left(-\frac{(1+\alpha_I)}{2}\frac{t}{\tau}\right)\right] \quad (1)$$

with: $\alpha_I = \sqrt{1 - 4\tau^2 \omega_0^2}$ (2)

Quantum expression

$$D(t) = \left(\frac{k_B T}{m^*}\right) \cdot$$

$$\cdot\sum_{i=0}^{n}\left(\left(\frac{f_i\,\tau_i}{\alpha_{iI}}\right)\left[\exp\left(-\frac{(1-\alpha_{iI})}{2}\frac{t}{\tau_i}\right)-\exp\left(-\frac{(1+\alpha_{iI})}{2}\frac{t}{\tau_i}\right)\right]\right) \quad (3)$$

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

Relativistic expression

$$D(t)=\left(\frac{k_B\,T}{m_0}\right)(\tau)\left(\frac{1}{\gamma}\right)\left(\frac{1}{\alpha_{I_{rel}}}\right)\cdot$$

$$\cdot\left[\exp\left(-\frac{(1-\alpha_{I_{rel}})}{2\,\rho}\frac{t}{\tau}\right)-\exp\left(-\frac{(1+\alpha_{I_{rel}})}{2\,\rho}\frac{t}{\tau}\right)\right] \quad (5)$$

With $\alpha_{I_{rel}}=\sqrt{1-4\gamma\,\omega_0^2\,\tau^2}\in(0,1)\subset$ □ (6)

(b) Case: $\Delta>0$

Classical expression

$$D=2\left(\frac{K_B\,T}{m^*}\right)\left[\frac{\tau}{\alpha_R}\sin\left(\frac{\alpha_R}{2}\frac{t}{\tau}\right)\exp\left(-\frac{t}{2\,\tau}\right)\right] \quad (7)$$

With: $\alpha_R=\sqrt{4\,\tau^2\,\omega_0^{\,2}-1}$ (8)

Quantum expression

$$D=2\left(\frac{K_B\,T}{m^*}\right)\cdot$$

$$\cdot\sum_i\left(\left[\frac{f_i\,\tau_i}{\alpha_{iR}}\sin\left(\frac{\alpha_{iR}}{2}\frac{t}{\tau_i}\right)\exp\left(-\frac{t}{2\,\tau_i}\right)\right]\right) \quad (9)$$

with: $\alpha_{iR}=\sqrt{4\,\tau_i^{\,2}\,\omega_i^{\,2}-1}$ (10)

Relativistic expression

$$D(t)=2\left(\frac{k_B\,T}{m_0}\right)\left(\frac{1}{\gamma}\right)\left(\frac{\tau}{\alpha_{R_{rel}}}\right)\cdot$$

$$\cdot\left[\exp\left(-\frac{t}{2\,\tau\,\rho}\right)\sin\left(\frac{\alpha_{R_{rel}}}{2\,\rho}\frac{t}{\tau}\right)\right] \quad (11)$$

with $\alpha_{R_{rel}}=\sqrt{4\,\gamma\,\omega_0^2\,\tau^2-1}\in$ □+ (12)

We have also:

$\alpha_{I_{rel}} = \sqrt{\Delta_{I_{rel}}}$ (13)

$\alpha_{R_{rel}} = \sqrt{\Delta_{R_{rel}}}$ (14)

$\gamma = 1/\sqrt{1-\beta^2}$ (15)

$\beta = v/c$ (16)

$\rho = \gamma^2$ (17)

For $<\vec{v}(t)\cdot\vec{v}(0)>_T$ [1,2,12] and $R^2(t)$ [1,2,13] we obtained similar analytical expressions.
The case $\Delta_{rel} = 0$ reduces to Drude model.

Moreover v is the speed of carriers, c the speed of light, k_B the Boltzmann's constant, T the temperature of the system, m_0 and m^* rest and effective mass respectively, τ_i and ω_i relaxation time and frequency of the i-th state respectively, ω_0 center frequency.

Equations (1-6), governed by parameter α_I, are a superposition of exponentials; the behaviour of curves is similar to typical Drude-Lotentz behaviour. Equations (7-12), governed by parameter α_R, are a product of an exponential with a sinusoidal function; the behaviour of curves is a typical damped oscillation in time.

The model contains also a gauge factor, which allows its use from sub-pico-level to macro-level. Interesting applications have been performed for economics [14], neuro-science and brain processes [15,16], nano-medicine [17,18].

3. CONCLUSIONS

In this paper we considered the main informations 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.
Acting on all chemical, physical, structural and model-intrinsic parameters, i.e.:

1) the temperature T of the system,

2) the parameters α_I and α_R,

3) the values of τ_i and ω_i,

4) the variation of the effective mass m^*,

5) the variation of the chiral vector,

6) the quantum weights of each mode in the quantum case,

7) the carrier density N,

8) the velocity of carriers,

it is possible to perform a fine and accurate tuning of the quantities $<\vec{v}(t)\cdot\vec{v}(0)>_T$, $R^2(t)$ and $D(t)$ and consequently to calibrate the performance of nano-bio-devices.
Also from an aesthetic point of view, the model is mathematically very elegant, because it presents analytical expressions of results.
It is giving new interesting information's, very useful in the design phase of new nano-bio-devices with particular distinctive attributes [19,20].

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BIOGRAPHY

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