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ON THE HELP OF MATHEMATICAL (ANALYTICAL) MODELING FOR PRESENT AND FUTURE ADVANCES IN (QUANTUM) SCIENCE AND (NANO) TECHNOLOGY

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Abstract:

The challenges that science and technology, in particular engineering, have to face in the present and near future are increasingly linked to nano-bio-technologies, one of the most important mainstreams of current world research. Improvements in devices performance are a primary objective of pure research and applied technology. The devices sensitivity, directly correlated to the diffusion process at the (micro-)nano-level, is an essential characteristic for a high increase in their quality. In this direction, mathematical modeling plays a fundamental role both at experimental and theoretical level, not only from the numerical viewpoint, but also and above all from the analytical one. Developments in this direction are desirable and fruitful.

Key Words: (Quantum) Science, Advances, Quantum Physics, Nanotechnology, Devices Performance, Mathematical (Analytical) Modeling, DS Model.

1. Introduction:

In last years the ability to manipulate matter, combined with advances and discoveries in synthesis and assembly of structures at micro- and nano-scale, brought to significant advances in scientific and technological areas. In order to exploit the nano-scale phenomena in devices, a better understanding of the electronic, magnetic and photonic interactions at this size scale is needed, through experiments, phenomenology, theory and modeling [1,2].

The use of innovative methodologies, based on advanced bottom-up and top-down approaches, is allowing to design and synthesize new organic, organic/inorganic hybrid and inorganic materials, aimed at a controlled assembly in active (micro-)nano-structured devices with applications in all technological sectors of benefit for human being [3].

Through the study and development of new technologies and methodologies, the functionalities of innovative devices can be explored for an ever-increasing range of applications. All fundamental studies are making possible the exploration of new techniques and methodologies in the most diverse engineering fields.

Among present and new technological challenges, carried forward by engineering, we remember problems typical of the construction of large infrastructures, related to the principles of structural modeling and the most advanced digital tools [4-6], renewable energy technologies, micro- and macro-conversion (energy harvesting and controlled nuclear fusion) [7-9], the light technology for bio-medicine and human health, the new frontiers of digital twin, "learning by doing", also through advanced software tools used for modeling and simulation [10-22], the computer security, advances in programming for mobile devices, visual programming of applications for IoT [23-25], the soil ecosystem, rich in biodiversity, in which a wide range of biochemical and biophysical processes occur [26-28].

2. Discussion:

These challenges have as common denominator nano-bio-technologies, which allow the creation of miniaturized devices on a micro- and nanometric scale and, integrated with electronics, become intelligent nano-devices with multiple capabilities and surprising functionalities.

One of the most crucial 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. From a theoretical viewpoint, several techniques can be used for the comprehension of transport phenomena, both numerical and analytical descriptions based on transport equations.

The numerical approaches are important, but not able to provide global solutions, instead typical of the analytical ones; these latter use a fine mathematics and lead to newsworthy results and predictions, when implemented through experimental data existing in literature and continuously obtained by experiments [29].

Among the most used formulations, we underline:

- The "Tight-Binding" Method (T-BM) [30]
- The "ab-initio" formulations:
  - The "Density Functional" Theory (DFT) [31]
  - The "Local Density Functional" Theory (LDFT)
- The "Non-Local Functional" Approach (N-LFA)
- The "Car-Parrinello Molecular Dynamic" Method (C-PMDM) [32]
- The "Conjugate-Gradient" Method (C-GM) [33]

- The "Augmented Plane Wave" Method (APWM) [34]
- The "Korringa-Kohn-Rostoker" Method (K-K-RM) [35]
- The "Linearized-Muffin-Thin-Orbital" Method (L-M-T-OM) [36]
- The "Full Potential Linearized Augmented Plane Wave" Method (FPLAPWM) [37]
- The "Drude-Lorentz-type" Models

About the last indicated ones, they are mainly improvements of Drude model [38]. In the Smith model appears a parameter c_n accounting for the anisotropy of scattering upon the first scattering event [39]. The "Effective Medium Theories" (EMTs) are variations in which the electromagnetic interactions between pure materials and host matrixes are approximately taken into account. Among EMTs, particular consideration is given to the Maxwell-Garnett model (MG) and the Bruggeman model (BR) [40,41].

About further generalizations of Drude-Lorentz-type, Smith models and Effective Medium Theories (EMTs) for transport processes in solid state physics and soft condensed matter, a recent extension, said DS model, is showing to fit very well with experimental data and is also able to give interesting new predictions of various peculiarities at nano-level. It is the most generalized model with respect to the indicated previous ones, and takes into account quantum and relativistic aspects.

As example, Figure 1 shows the velocities correlation function as a function of time compared with experimental data using TiO_2; similar results have been found with various other current used materials. The indicated result is predicted also by the Smith model, but with the DS model it appears without assumptions similar to the transport parameters c_n of the Smith model.

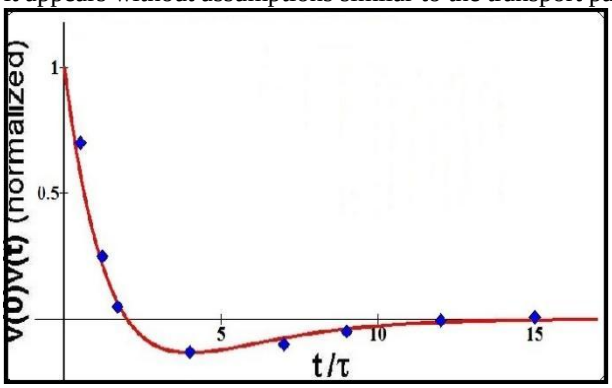

Figure 1: Dots represent experimental data, the curve derives by the DS model (classical case).

The model provides the analytical form of the velocities correlation function $\langle \vec{v}(t)\cdot\vec{v}(0)\rangle_T$, the mean square deviation of position of particles $R^2(t)=\langle[\vec{R}(t)-\vec{R}(0)]^2\rangle$ and the diffusion coefficient $D(t)=\frac{1}{2}\left(dR^2(t)/dt\right)$, involving classical and quantum-relativistic aspects; it studies the dynamics of processes ranging from sub-pico- to macro-level, thanks to an inner gauge factor.

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, considering the Cauchy integration on the entire time axis (-∞, +∞) and the use of the residue theorem in the complex plane. One of the central starting relation is:

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

With which we can perform a complete inversion on temporal scale, considering the entire time axis (-∞, +∞), not the half-time one as usually considered in literature. Eq. (1) allows the analytical calculation of $R^2(t)$ and $D(t)$, considering that it holds:

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

$$D(t)=\int_0^t dt'\langle\vec{v}(t')\cdot\vec{v}(0)\rangle \qquad (3)$$

Eqs (1-3) offer the analytical description of the three most important parameters concerning transport phenomena [42-45].

3. Future Perspectives:

Acting on all chemical, physical, structural and model-intrinsic parameters, on the temperature *T* of the system, on values of relaxation times τ_i and frequencies ω_i, on the carrier density *N*, the effective mass m^*, variations of the chiral vector, on the quantum weights of each mode (in the quantum case), on the velocity of carriers (in the relativistic case), it is possible to perform a fine tuning of $\langle\vec{v}(t)\cdot\vec{v}(0)\rangle_T$, $R^2(t)$ and $D(t)$ and to calibrate the performance of nano-bio-devices, with both an "a-priori" (predictive) and "a-posteriori" (confirmatory) use of the model [46]. In the first case, we use tuned data in consideration to the specific situation, in the second one we can use experimental data from literature.

Drude-Lorentz-type models are very interesting tools from a theoretical and predictive point of view, and the DS model is a powerful generalization that considers also quantum and relativistic effects. These extensions are mathematically elegant, because totally analytical; they are giving confirmations with respect to the previous models, so as new information about the

dynamics of systems at the nano-scale, conveniently tested through experimental time-resolved techniques, like TRTS, Photon-Induced Near-Field Electron Microscopy and Graphene based Plasmonics [47-60].

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