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Generalization of the Drude model

Eldakli Mohsan, Muna M Aoneas2
University of Zawia, Faculty of Science, Physics department, Az Zawiyah, Libya.
University of Zawia, Faculty of Science, Physics department, Al Ajaylat, Libya.
E-mail address: m.amara@zu.edu.ly

الملخص
في هذه الورقة البحثية نقدم تعميماً جزئياً جديداً لصيغة سميث للتعميم الكلاسيكي لمعادلة درود. تم تعميم صيغة درود الموصوفة في الأصل لمراعاة السلوك غير المعتاد للخصائص البصرية للزئبق ومخاليطه، كما يمكن استخدامها للتيلوريوم السائل وبعض المركبات شبه البلورية.

Abstract
In this paper we introduce a new fractional generalization of the Smith's formula for the classical generalization of the Drude equation. The generalized Drude formula described was proposed originally to account for the unusual behavior of the optical properties of mercury and its amalgams, it can be used for liquid tellurium and some quasicrystals.

Keywords: Smith's formula, Drude model, AC conductivity, DC conductivity.

1.Introduction
At the turn of the century, Einstein had not yet explained the photoelectric effect, Rutherford had not determined the size of the nucleus, Bohr had not speculated on the discrete nature of electronic "shells" in atoms, and the formulation of quantum mechanics was still decades away. Although the structure of the atom was not known, Thomson had discovered the electron (1897), enabling Drude (1900) and Lorentz (1905) to formulate a model to explain two of the most striking properties of the metallic

state, namely the conduction of electricity and heat [1] and [2]. Drude attributed conduction in the metallic or similar state to the most loosely bound electrons in atoms somehow becoming mobile. In the fact these "conduction electrons" were assumed to move freely through space apart from collisions, not with each other but rather with the much larger atomic cores. The assumptions of the Drude model are

(1) A metal contains free electrons which form an ideal electron gas; a collision indicates the scattering of an electron by (and only by) an ionic core; i.e. the electrons do not "collide" with anything else (the free electron approximation and independent electron approximation).

(2) Collisions are instantaneous and result in a change in electron velocity. The electrons have some average thermal (kinetic) energy $E = \frac{3}{2}k_B T = \left\langle \frac{1}{2} m_e v_T^2 \right\rangle$ (i.e. obeys of the Maxwell-Boltzmann statistics, T is absolute temperature) [3] . They achieve thermal equilibrium with their surroundings only through collisions.

(3) Because the ions have a very large mass, they are essentially immovable (adiabatic approximation).

(4) An electron suffers a collision with probability per unit time τ (the relaxation-time approximation), i.e. is the scattering rate $\gamma = 1/\tau$ (τ - relaxation time, is the mean time between collisions; τ is independent on the electron position or momentum).

In this work we described a new fractional generalization of the Smith's formula for the classical generalization of the Drude equation. The rest of the paper includes the following: section 2 discusses the Drude model, followed by the failures of the Drude model in section 3. Smith's Classical generalization of the Drude formula for the optical conductivity and Fractional generalization of the Smith's classical generalization of the Drude formula are provided in section 4 and 5 respectively. Finally, a conclusion drawn in section 6.

2. The Drude model

Equation of motion for electrons is obtained on the following assumptions:

(1) Electrons collisions: momentum $\vec{\mathbf{p}}_c(t+dt)=\vec{0}$, the probability for collisions is $P_c = dt/\tau$ [4].

(2) For no collisions holds:

$\vec{\mathbf{p}}_{nc}(t+dt)=\vec{\mathbf{p}}(t)+\vec{\mathbf{F}}(t)dt$ and $P_{nc}=1-P_c$

(3) Average momentum is:

$\vec{\mathbf{p}}(t+dt)=P_c\cdot\vec{\mathbf{p}}_{\mathbf{c}}(t+dt)+P_{nc}\cdot\vec{\mathbf{p}}_{nc}(t+dt)$, *and valid:*

$$\frac{d\vec{\mathbf{p}}(t)}{dt}=-\frac{\vec{\mathbf{p}}(t)}{\tau}+\vec{\mathbf{F}}(t) \tag{1}$$

In uniform DC electric field for electrons (e - elementary charge) is:

$$\frac{d\vec{\mathbf{p}}(t)}{dt}=\vec{0}\wedge\vec{\mathbf{p}}(t)=m_e\vec{\mathbf{v}}_d \Rightarrow \vec{\mathbf{v}}_d=-\frac{e\tau}{m_e}\vec{\mathbf{E}}. \tag{2}$$

For the current density $\vec{\mathbf{j}}=-ne\vec{\mathbf{v}}_d$ (n is an effective number concentration of electrons, $\vec{\mathbf{v}}_d$ - so-called drift velocity)

$$\vec{\mathbf{j}}=\frac{ne^2\tau}{m_e}\vec{\mathbf{E}}, \tag{3}$$

Then valid Ohm's law in the simplest form $\vec{\mathbf{j}}=\sigma\vec{\mathbf{E}}$

(the conductivity $\sigma=\sigma_0=ne^2\tau/m_e$, σ_0-"static", DC conductivity). If we turn off electric field, then the drift velocity relaxing:

$$\vec{\mathbf{v}}_d(t)=\vec{\mathbf{v}}_d(0)\cdot\exp(-t/\tau).$$

For weak fields (in most cases) the $\vec{\mathbf{v}}_d$ is much smaller than average thermal speed

$v_d << \sqrt{\langle v_T^2 \rangle}$.

AC conductivity from (1), using $\vec{\mathbf{E}}(t) = \mathrm{Re}[\vec{\mathbf{E}}(\omega)\cdot e^{-i\omega t}]$ and $\vec{\mathbf{j}}(\omega) = \sigma(\omega)\cdot\vec{\mathbf{E}}(\omega)$:

$$\sigma(\omega) = \frac{\sigma_0}{1 - i\omega\tau} \qquad (4)$$

For the charge's induced electric dipole moment $\vec{\mathbf{d}} = e\cdot\vec{\mathbf{r}}(t)$ ($d\vec{\mathbf{r}}/dt = \vec{\mathbf{v}}_d$), then the net dipole moment per unit volume is the electric polarization $\vec{\mathbf{P}} = n\cdot\vec{\mathbf{d}}$. The total electric displacement can then be found to get the dielectric function, $\vec{\mathbf{D}} = \varepsilon_0\cdot\vec{\mathbf{E}} + \vec{\mathbf{P}} = \varepsilon_0\cdot\varepsilon_r\cdot\vec{\mathbf{E}}$ (ε_0 is the permittivity of vacuum), and $\vec{\mathbf{P}} = \varepsilon_0\cdot(\varepsilon_r - 1)\cdot\vec{\mathbf{E}}$ [5].

In the case of AC conductivity, frequency dispersion of the relative permittivity is:

$$\varepsilon_r(\omega) = 1 - \frac{\omega_p^2}{\omega(\omega + i\cdot\gamma)} \qquad (5)$$

Where is $\omega_p^2 = n\cdot e^2/(m_e\cdot\varepsilon_0)$ the plasma frequency.

For non-magnetic medium the index of refraction is $n(\omega) = \sqrt{\varepsilon_r(\omega)}$, $n(\omega)$ describes the response of the environment when broadcasting electromagnetic waves on it) [6].

In general case, for the equation (1) at one point of the conductor, Ohm's law follows:

$$\vec{\mathbf{j}}(t) + \tau\frac{d\vec{\mathbf{j}}(t)}{dt} = \sigma_0\vec{\mathbf{E}}(t) \qquad (6)$$

3. The failures of the Drude model

The Drude model predicts the electronic heat capacity per unit volume to be the classical "equipartition of energy" result

$C_V = \frac{3}{2} n \cdot k_B$ (i.e., C_{el}). This is independent of temperature. Experimentally, the low-temperature heat capacity of metals follows the relationship $C_V = AT + BT^3$. The second term is obviously the phonon (Debye) component, leading us to suspect that $C_{el} = AT$. Indeed, even at room temperature, the electronic component of the heat capacity of metals is much smaller than the Drude prediction.

The thermal conductivity κ is defined by the equation:

$$\vec{\mathbf{J}}_q = -\kappa \cdot \nabla T \qquad (7)$$

where $\vec{\mathbf{J}}_q$ is the flux of heat (i.e. energy per second per unit area). Kinetic theory of ideal gas expression for κ is $\kappa = \langle v_T^2 \rangle \tau C_{el} / 3$ [7].

The fortuitous success of this approach came with the prediction of the Wiedemann-Franz ratio, $L = \kappa / (\sigma_0 T)$. However, in spite of this apparent success, the individual components of the model are very wrong; e.g. C_{el} in the Drude model is at least two orders of magnitude bigger than the experimental values at room temperature. Furthermore, experimentally L drops away from its constant value at temperatures below room temperature; the Drude model cannot explain this behavior.

4. Smith's Classical generalization of the Drude formula for the optical conductivity

Let us suppose that an electron experiences collisions that are randomly distributed in time but with an average time interval between collision events [8].

The probability $p_n(0,t)$ of n events in the time interval $(0,t)$ is given by the Poisson distribution $p_n(0,t)=(t/\tau)^n \cdot \exp(-t/\tau)/n!$
The probability of zero collisions is
$\exp(-t/\tau)=v_d(t)/v_d(0)=j(t)/j(0)$.
Taking account of what happens after the first and subsequent collisions we write:

$$\frac{j(t)}{j(0)}=\exp\left(-\frac{t}{\tau}\right)\cdot\left(1+\sum_{n=1}^{\infty}\frac{c_n}{n!}\left(\frac{t}{\tau}\right)^n\right). \tag{8}$$

The coefficient c_n represents that fraction of the electron's original velocity that is retained after the nth collision. It is a memory or persistence of velocity effect. Taking the Laplace-Fourier transform ($s=-i\omega$) : $\sigma(\omega)=\int_0^{\infty} j(t)\cdot\exp(i\omega t)\cdot dt$ (for) yields:

$$\sigma(\omega)=\frac{\sigma_0}{1-i\omega\tau}\cdot\left(1+\sum_{n=1}^{\infty}\frac{c_n}{(1-i\omega\tau)^n}\right). \tag{9}$$

5. Fractional generalization of the Smith's classical generalization of the Drude formula

For these purpose we introduce the fractional generalized Poisson distribution:

$$p_{k,\beta}(0,t)=\frac{(t/\tau)^{k\beta}}{k!}\cdot E_\beta^{(k)}\left(-\left(\frac{t}{\tau}\right)^{\beta}\right),\ k=0,1,2,3,\ldots;\ 0<\beta\le 1, \tag{10}$$

Where $E_\beta^{(k)}\left(-(t/\tau)^\beta\right):=\left(d^k\left(E_\beta(z)\right)/dz^k\right)|_{z=-(t/\tau)^\beta}$

And $E_\beta\left(z^\beta\right):=1+\sum_{n=1}^{\infty} z^{n\beta}/\Gamma(n\beta+1)$ are the Mittag-Leffler functions, $\Gamma(1+\alpha):=\int_0^\infty t^\alpha e^{-t}dt$ is the Gamma function, also valid relation $e^z=E_1(z)$.

Then the probability of zero collisions is:

$$E_\beta\left(-(t/\tau)^\beta\right)=v_{d\beta}(t)/v_{d\beta}(0)=j_\beta(t)/j_\beta(0).$$

Generalization of (8) is:

$$\frac{j_\beta(t)}{j_\beta(0)}=\left(E_\beta\left(-\left(\frac{t}{\tau}\right)^\beta\right)+\sum_{n=1}^{\infty} c_{n\beta}\frac{1}{n!}\cdot\left(\frac{t}{\tau}\right)^{n\beta}E_\beta^{(n)}\left(-\left(\frac{t}{\tau}\right)^\beta\right)\right). \quad (11)$$

For the Laplace-Fourier transform of the equation (11) we need the next Laplace-Fourier transform pair:

$$L\left(\frac{1}{k!}\cdot\left(\frac{t}{\tau}\right)^{k\beta}\cdot E_\beta^{(k)}\left(-\left(\frac{t}{\tau}\right)^\beta\right);s\right)=\frac{(\tau s)^{\beta-1}}{\left(1+(\tau s)^\beta\right)^{k+1}}. \quad (12)$$

Then generalization of the equation (9) is:

$$\sigma_\beta(\omega)=\frac{\sigma_0}{1+(-i\omega\tau)^\beta}\cdot\left(1+\sum_{n=1}^{\infty}\frac{c_{n\beta}\cdot(-i\omega\tau)^{\beta-1}}{\left(1+(-i\omega\tau)^\beta\right)^n}\right). \quad (13)$$

The equation (13) is a new formula. It describes a slow and fractal stochastic processes, rare events with memory. There is still a lot of analysis about this equation. Then, for example, the equation (6) replaced with formula from the Caputo fractional derivative.

6. Conclusions

The characteristic behavior of a Drude metal in the time or frequency domain, i.e. exponential relaxation with time constant τ

or the frequency dependence for $\sigma(\omega)$ stated above, is called Drude response. In a conventional, simple, real metal (e.g. sodium, silver, or gold at room temperature) such behavior is not found experimentally, because the characteristic frequency $1/\tau$ is in the infrared frequency range, where other features that are not considered in the Drude model (such as band structure) play an important role. But for certain other materials with metallic properties, frequency-dependent conductivity were found that closely follows the simple Drude prediction for $\sigma(\omega)$.

These are materials where the relaxation rate $1/\tau$ is at much lower frequencies. This is the case for certain doped semiconductor single crystals, high-mobility two-dimensional electron gases, and heavy-fermion metals.

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