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Concerning exact analytical STFT solutions to some families of inverse problems in engineering material theory

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ABSTRACT

The problem of finding the exact analytical closed-form solution of some families of transcendental equations, which describe two different physical phenomenon, thermionic emission and electrical conductivity in semiconductors, is studied, in some detail, by the Special Trans Functions Theory (STFT). The mathematical genesis of the analytical closed-form solution is presented, and the structure of the theoretical derivation, proofs and numerical results confirm the validity and base principle of the STFT. Undoubtedly, the proposed analytical approach implies the qualitative improvement of the conventional analytical and numerical methods.

1. Introduction

In any solid metal, some electrons are free to move from atom to atom in material. This is sometimes collectively referred to as a "sea of electrons". Their velocities follow a statistical distribution, rather than being uniform, and occasionally an electron will have enough velocity to exit the metal without being pulled back in.

In 1901, Richardson published the results of his research in domain of the thermionic emission. The modern formulae (demonstrated by Saul Dushman in 1923 and hence sometimes called the Richardson–Dushman equations) take the following form [1,2]

$$J(W,T) = AT^2 \exp\left(-\frac{W}{kT}\right), \tag{1}$$

where $J(W,T)$ is the emission current density [A/m^2], T is the thermodynamic temperature of the metal [Kelvin (K)], W is the work function of the metal, k is the Boltzmann constant, and A is Richardson–Dushman constant. Note that in the period 1911 to 1930, as physical understanding of the behavior of electrons in metals increased, Richardson put various different theoretical expressions (based on different physical assumptions) for A. Over 60 years later, there is still no consensus amongst interested theoreticians as to what the precise form of the expression for A should be, but the subject matter of this manuscript is invariant of the theoretical precise form of constant A, and for our analysis A is an universal constant (Richardson constant) given by

$$A = ((4\pi mk^2e)/(h^3)) = 1.20173 \times 10^6\ [(\mathrm{A}/(\mathrm{m}^2\ \mathrm{K}^2))], \tag{2}$$

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where m and e are the mass and charge of an electron, respectively, and h is Planck's constant.

Let us note that experimental values for the coefficient A are generally of the order of magnitude of A given in Eq. (2), but do differ significantly as between different emitting materials, and can differ as between different crystallographic faces of the same material.

After simple modification, Eq. (1) takes the form

$$\Psi(W,J) = \beta(W,J)\exp(-\Psi(W,J)), \tag{3}$$

where

$$\begin{aligned}&\Psi(W,J) = \frac{W}{2kT}, \quad \beta(W,J) = \frac{W}{2k}\sqrt{\frac{A}{J}},\\ &\Psi(W,J) \in R^+, \quad \beta(W,J) \in R^+.\end{aligned} \tag{4}$$

Let us note that after simple modification Eq. (3) takes the form

$$-\Psi(W,J) = -\beta(W,J)\exp(-\Psi(W,J))$$

or form

$$Z(W,J) = B(W,J)\exp(Z(W,J)) \tag{4a}$$

since $Z(W,J) = -\Psi(W,J)$, $B(W,J) = -\beta(W,J)$.

Thus, Eq. (3) is transformed in Eq. (4a).

In addition, we study the electrical conductivity in polycrystalline semiconductors for an arbitrary temperature range. Thus, according to the Arrhenius relationship we have:

$$\sigma_{DC} = \frac{A_0}{T}\exp\left(-\frac{E_a}{kT}\right)$$

where A_0 and E_a represent the preexponential factor and activation energy, respectively, k is the Boltzmann's constant. The calculated values of activation energy and preexponential factor are given in [3].

At lower temperature range, Mott has proposed that DC conductivity in this case is given by [3–5]:

$$\sigma_{DC} = \frac{\sigma_0}{T^{2\gamma}}\exp\left(-\left(\frac{T_0}{T}\right)^{\gamma}\right),$$

where σ_0 and T_0 are parameters of Mott model and the values of γ are 1/2, 1/3, or 1/4. Of course, the above equations, for some temperature range, takes the following general form

$$\sigma_{DC} = \frac{\sigma_0}{T^p}\exp\left(-\left(\frac{T_0}{T}\right)^{q}\right), \tag{5}$$

where σ_0 and T_0 are parameters for corresponding temperature range, and where p and q are integers or the inverse of integers.

After simple modification Eq. (5) takes the form

$$\left(\frac{T_0}{T}\right)^q = \left(\frac{\sigma_{DC}T_0^p}{\sigma_0}\right)^{\frac{q}{p}}\exp\left(\frac{q}{p}\left(\frac{T_0}{T}\right)^q\right). \tag{6}$$

Thus, we have

$$\begin{aligned}&Z = B\exp(Z), \quad Z = \frac{q}{p}\left(\frac{T_0}{T}\right)^q, \quad B = \frac{q}{p}\left(\frac{\sigma_{DC}T_0^p}{\sigma_0}\right)^{\frac{q}{p}},\\ &T = \frac{T_o}{(Zp/q)^{\frac{1}{q}}}, \quad 0 < B < \frac{1}{\exp(1)}, \quad Z > 1.\end{aligned} \tag{7}$$

2. Obtaining the exact analytical closed form solution to the transcendental Eq. (3) (inverse thermionic emission equation) by using the Special Trans Functions Theory – STFT

The Special Trans Functions Theory [6–15] (S.M. Perovich), for Eq. (3), gives an exact analytical closed form solution

$$\Psi(W,J) = \mathrm{tran}_+(\beta(W,J)), \tag{8}$$

where $\mathrm{tran}_+(\beta(W,J))$ is a special tran function defined as

$$\mathrm{tran}_+(\beta(W,J)) = \lim_{x\to\infty}\left[\ln\left(\frac{\varphi(x+1,\beta(W,J))}{\varphi(x,\beta(W,J))}\right)\right], \tag{9}$$