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Exact Solutions of a Spherically Symmetric Energy–Transport Model for Semiconductors

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Abstract

The symmetry classification and reduction of a non–stationary spherically symmetric energy–transport model for semiconductors was investigated by Molati and Wafo Soh (2005). In this work the exact solutions of the reduced model in the stationary case are constructed.

1 Introduction

Semiconductors are solid-state materials which possess the properties of both insulators and conductors. They have conductivities lying between those of insulators and conductors. Semiconductors can be elemental, compound and alloy. They have a number of applications which dominate our every day life in electrical, electronic and information engineering. Recently a technology of spherically shaped semiconductor integrated circuit [1, 16] has been discovered and has some advantages over the commonly known semiconductor devices. The main advantage is that of having a larger available surface area which leads to a device being used for longer periods before it gets overheated.

The motion of charge carriers (negatively charged particles, *electrons* and positively charged particles, *holes*) in semiconductors under the effect of an electric field and a carrier concentration gradient is an important phenomenon. This introduces an important parameter, *mobility*, which characterizes the motion of the charge carriers due to *drift* (charged-particle motion under the influence of the electric field) and also the efficiency of many devices. The numerical value of the mobility depends on a given *doping* (addition of controlled amounts of specific impurity atoms with the aim of increasing the concentration of the charge carriers) and temperature for the charge carriers [12, 15].

The energy-transport (ET) model is a macroscopic model derived from the Boltzmann equation [2]. This model comprises a system of diffusion equations for the electron density and temperature, together with the Poisson equation for electric potential.

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In the ET model for semiconductors, there are two groups of unknowns. The first group is made of the electron density, the electron temperature and the electric potential. The second group is formed by the energy production, the mobilities and the doping profile. Traditionally, the latter is obtained experimentally. This work employs the symmetry principle [3, 5, 6, 9, 10, 11] to obtain the elements of the second group of the unknowns, that is, the forms of the energy production, the mobilities and the doping profile are obtained for which the model is maximally symmetric. The stationary solutions are constructed after obtaining the unknown parameters and the symmetries of the governing system of ET model for semiconductors.

A symmetry analysis approach to the ET model was first performed on a non–stationary one dimensional ET model in [13]. The complete symmetry classification was performed and classes of exact solutions were obtained. The work done in [13] was extended in [8] by considering the non–stationary spherically symmetric case and two dimensional case. The complete symmetry classification and reduction was performed, but since the reduced systems were still highly non–linear and difficult to solve analytically, the exact solutions were not constructed.

The outline of this work is as follows. In Section 2 the model to be investigated is presented. In Section 3 the symmetry classification of the model is performed. In Section 4 the exact solutions of the model are constructed.

2 ET model for semiconductors

On coupling the Poisson's equation for the electric potential to the diffusion equations for the electron density and temperature, we have the following equations [13, 14]

$$\begin{aligned}&\frac{\partial n}{\partial t} + \nabla \cdot \boldsymbol{J} = 0,\\ &\frac{\partial (nW)}{\partial t} + \nabla \cdot \boldsymbol{S} - \boldsymbol{J} \cdot \nabla \phi - nC_W = 0,\\ &\lambda^2 \nabla^2 \phi - n + c(\boldsymbol{x}) = 0,\end{aligned} \tag{2.1}$$

where n is the electron density, $\boldsymbol{J}$ the electron momentum density, W the electron energy, $\boldsymbol{S}$ the energy flux density, nC_W the energy production, λ^2 the dielectric constant, ϕ the electric potential, $c(\boldsymbol{x})$ the doping profile that is a given function of the position $\boldsymbol{x}$ and the nabla symbol

$$\nabla = \left(\frac{\partial}{\partial x_1}, \frac{\partial}{\partial x_2}, \cdots, \frac{\partial}{\partial x_n} \right). \tag{2.2}$$

The known quantities in (2.1) are

$$\boldsymbol{J} = -\nabla(\mu^{(1)} T n) + \mu^{(1)} n \nabla \phi, \tag{2.3a}$$

$$\boldsymbol{S} = -\nabla(\mu^{(2)} T^2 n) + \mu^{(2)} T n \nabla \phi, \tag{2.3b}$$

$$W = \frac{3}{2} T, \tag{2.3c}$$

$$C_W = \frac{-\frac{3}{2}(T - T_L)}{\tau_W(T)}, \tag{2.3d}$$

where T is the electron temperature, T_L is the lattice temperature (taken as constant), $\mu^{(i)}$ are the electron mobilities and τ_W is the energy relaxation time. In general the mobilities are temperature-dependent. The system (2.1) and (2.3a–2.3d) must be solved subject to appropriate initial and boundary conditions.

Some special cases considered in the literature are:

• the Chen *et al* [4] model with

$$\boldsymbol{J} = -\mu_0 \left(\nabla n - \frac{n}{T}\nabla\phi\right), \tag{2.4a}$$

$$\boldsymbol{S} = -\frac{3}{2}\mu_0 \left[\nabla(nT) - n\nabla\phi\right], \tag{2.4b}$$

$$C_W = \frac{-\frac{3}{2}(T - T_L)}{\tau_0}\ , \tag{2.4c}$$

where μ_0 and τ_0 are positive constants,

• the Lyumkis *et al* [7] model in which

$$\boldsymbol{J} = -\frac{2\mu_0}{\sqrt{\pi}}\left[\nabla(nT^{\frac{1}{2}}) - \frac{n}{T^{\frac{1}{2}}}\nabla\phi\right], \tag{2.5a}$$

$$\boldsymbol{S} = -\frac{4\mu_0}{\sqrt{\pi}}\left[\nabla(nT^{\frac{3}{2}}) - nT^{\frac{1}{2}}\nabla\phi\right], \tag{2.5b}$$

$$C_W = -\frac{2}{\sqrt{\pi}}\frac{(T - T_L)}{\tau_0 T^{\frac{1}{2}}}. \tag{2.5c}$$

3 Symmetry classification of the spherically symmetric ET model for semiconductors

In this section we focus on the symmetry analysis of the spherically symmetric ET model for semiconductors in the stationary case. By spherically symmetric we mean that the spatial dependence of the model is through the radial coordinate

$$r = \sqrt{(x^1)^2 + (x^2)^2 + \cdots (x^d)^2}\ ,$$

where d is the spatial dimension. We arrive at the following spherically symmetric equations for $r \neq 0$

$$\begin{aligned} J_r + \frac{k}{r}J = 0, \\ S_r + \frac{k}{r}S - J\phi_r + \frac{3}{2}n\frac{(T - T_L)}{\tau_W(T)} = 0, \\ \lambda^2(\phi_{rr} + \frac{k}{r}\phi_r) - n + c(r) = 0, \end{aligned} \tag{3.1}$$

where $k = d - 1$ and the subscript denotes differentiation with respect to r:

$$\begin{aligned} J &= -\left(\mu^{(1)}Tn\right)_r + \mu^{(1)}n\phi_r, \\ S &= -\left(\mu^{(2)}T^2 n\right)_r + \mu^{(2)}Tn\phi_r. \end{aligned}$$

The cases of interest are $d = 1, 2, 3$; i.e. $k = 0, 1, 2$. In the case $k = 0$ one would expect to recover the stationary solutions of the one–dimensional model obtained in [13]. But this is yet to be proved. For instance, the three dimensional model in the stationary case cannot be recovered by simply substituting $k = 2$ in the model (3.1).

From now on we will use $\tau(T)$ to mean $\tau_W(T)$. According to Lie's algorithm, the vector field

$$X = \xi(r,n,T,\phi)\frac{\partial}{\partial r} + \eta^1(r,n,T,\phi)\frac{\partial}{\partial n} + \eta^2(r,n,T,\phi)\frac{\partial}{\partial T} + \eta^3(r,n,T,\phi)\frac{\partial}{\partial \phi}$$

is a symmetry generator of (3.1) if and only if

$$\begin{aligned} X^{[2]}\left(J_r + \frac{k}{r}J\right)\Big|_{(3.1)} &= 0, \\ X^{[2]}\left(S_r + \frac{k}{r}S - J\phi_r + \frac{3}{2}n\frac{(T-T_L)}{\tau(T)}\right)\Big|_{(3.1)} &= 0, \\ X^{[2]}\left(\lambda^2\left[\phi_{rr} + \frac{k}{r}\phi_r\right] + c(r) - n\right)\Big|_{(3.1)} &= 0, \end{aligned} \tag{3.2}$$

where

$$X^{[2]} = X + \zeta_1^1\frac{\partial}{\partial n_r} + \zeta_1^2\frac{\partial}{\partial T_r} + \zeta_1^3\frac{\partial}{\partial \phi_r} + \zeta_2^1\frac{\partial}{\partial n_{rr}} + \zeta_2^2\frac{\partial}{\partial T_{rr}} + \zeta_2^3\frac{\partial}{\partial \phi_{rr}}$$

is the second prolongation of X. The coefficients ζ_j^i $(i = 1,2,3;\ j = 1,2)$ are given by the prolongation formulae

$$\zeta_1^i = D_r(\eta^i) - u_r^i D_r(\xi), \tag{3.3a}$$

$$\zeta_2^i = D_r(\zeta_1^i) - u_{rr}^i D_r(\xi), \tag{3.3b}$$

where

$$(u^1, u^2, u^3) \equiv (n, T, \phi),$$

$$D_r = \frac{\partial}{\partial r} + n_r\frac{\partial}{\partial n} + T_r\frac{\partial}{\partial T} + \phi_r\frac{\partial}{\partial \phi}.$$

When expanded and separated, the determining equations (3.2) span many pages, hence only the final step in the analysis of the determining equations is presented. The symmetry analysis is performed for cases $k = 0$ and $k \neq 0$.

Case (i) $k = 0$

$$\xi = \frac{a_1 q}{2}r + a_0, \tag{3.4a}$$

$$\eta^1 = a_1(1-q)n, \tag{3.4b}$$

$$\eta^2 = a_1 T, \tag{3.4c}$$

$$\eta^3 = a_1\phi, \tag{3.4d}$$

$$\mu^{(1)}(T) = \mu_0^{(1)} T^{q-1}, \tag{3.4e}$$

$$\mu^{(2)}(T) = \mu_0^{(2)} T^{q-1}, \tag{3.4f}$$

$$T(T - T_L)\tau_T - T_L \tau = 0, \tag{3.4g}$$

$$(2a_0 + a_1 q\, r)c_r + 2a_1(q-1)c = 0. \tag{3.4h}$$

In the above equations (3.4a)–(3.4h), a_0, a_1, $\mu_0^{(1)}$, $\mu_0^{(2)}$ and q are the arbitrary constants. The case $k \neq 0$ corresponds to $a_0 = 0$.

Equations (3.4g) and (3.4h) give the forms of the energy relaxation time $\tau(T)$ and the doping profile $c(r)$ respectively.
Since equation (3.4g) does not contain the constants a_0 and/or a_1, its solution is the same for both cases and is given by

$$\tau(T) = \tau_0 (T - T_L) T^{-1}, \tag{3.5}$$

where τ_0 is an arbitrary constant.

When $k = 0$, equation (3.4h) prompts the consideration of the cases $a_1 q = 0$ and $a_1 q \neq 0$. In the first case, Eq. (3.4h) simplifies to

$$a_0 c_r - a_1 c = 0;\; a_0 \neq 0. \tag{3.6}$$

Solving Eq. (3.6) we obtain

$$c(r) = c_0\, e^{\alpha r}, \tag{3.7}$$

where $\alpha = \dfrac{a_1}{a_0}$ and c_0 are the arbitrary constants. Thus,

$$X = \frac{\partial}{\partial r} + \alpha n \frac{\partial}{\partial n} + \alpha T \frac{\partial}{\partial T} + \alpha \phi \frac{\partial}{\partial \phi}\cdot \tag{3.8}$$

In the second case, we obtain

$$c(r) = \bar{c}_0 (2 + \alpha q r)^{\frac{2(1-q)}{q}};\; q \neq 0, \tag{3.9}$$

where $\bar{c}_0$ and $\alpha = \dfrac{a_1}{a_0}$ are the arbitrary constants. Hence,

$$X = \frac{1}{2}(2 + \alpha q r)\frac{\partial}{\partial r} + \alpha(1-q) n \frac{\partial}{\partial n} + \alpha T \frac{\partial}{\partial T} + \alpha \phi \frac{\partial}{\partial \phi}\cdot \tag{3.10}$$

Case (ii) $k \neq 0$
Then $a_0 = 0$ and equations (3.4a)–(3.4h) hold with $a_0 = 0$. Equation (3.4h) reduces to

$$a_1 q\, r c_r + 2a_1(q-1)c = 0. \tag{3.11}$$

Equation (3.11) prompts the consideration of the cases $a_1 = 0$ and $a_1 \neq 0$. In the first case there are no symmetries and the second case gives rise to the subcases: $q = 0$ and $q \neq 0$. In the first subcase there is no doping profile, that is $c(r) = 0$ and the second subcase yields

$$c(r) = c_1\, r^{\frac{2(1-q)}{q}};\; q \neq 0, \tag{3.12}$$

for arbitrary constant c_1. Therefore,

$$X = \frac{q\,r}{2}\frac{\partial}{\partial r} + (1-q)n\frac{\partial}{\partial n} + T\frac{\partial}{\partial T} + \phi\frac{\partial}{\partial \phi}\cdot \tag{3.13}$$

Remark 1: For $q = 0$ and $q = \frac{1}{2}$ we obtain the forms of $\boldsymbol{J}$ and $\boldsymbol{S}$ for the Chen *et al* [4] model and the Lyumkis *et al* [7] model respectively.

4 Exact solutions of the spherically symmetric ET model for semiconductors in the stationary case

Case (a) $k = 0$

(i) $\mu^{(1)}(T) = \mu_0^{(1)}T^{q-1}$, $\mu^{(2)}(T) = \mu_0^{(2)}T^{q-1}$, $\tau(T) = \tau_0(T - T_L)T^{-1}$, $c(r) = c_0\,e^{\alpha r}$,

$$X = \frac{\partial}{\partial r} + \alpha n\frac{\partial}{\partial n} + \alpha T\frac{\partial}{\partial T} + \alpha\phi\frac{\partial}{\partial \phi}\cdot$$

The characteristic equations for the invariants of X are

$$\frac{dr}{1} = \frac{dn}{\alpha n} = \frac{dT}{\alpha T} = \frac{d\phi}{\alpha\phi}\cdot \tag{4.1}$$

The invariant solutions for $\alpha \neq 0$ assume the form

$$n = n_0\,e^{\alpha r}, \tag{4.2a}$$
$$T = T_0\,e^{\alpha r}, \tag{4.2b}$$
$$\phi = \phi_0\,e^{\alpha r}, \tag{4.2c}$$

where n_0, T_0 and ϕ_0 are the arbitrary constants. Substituting the invariant solutions (4.2a)–(4.2c) into the governing system (3.1) yields the reduced system which is solved for the arbitrary constants. Thus, the exact solutions are

$$n = c_0\,e^{\alpha r} + \left[\frac{3}{2\alpha^2(q+2)\mu_0^{(2)}\tau_0}\right]^{\frac{1}{q}}, \tag{4.3a}$$
$$T = \left[\frac{3}{2\alpha^2(q+2)\mu_0^{(2)}\tau_0}\right]^{\frac{1}{q}}, \tag{4.3b}$$
$$\phi = (q+1)\left[\frac{3}{2\alpha^2(q+2)\mu_0^{(2)}\tau_0}\right]^{\frac{1}{q}}, \tag{4.3c}$$

provided $q \neq -1, -2, 0$. The case $q = -1$ results in a reduced system which is inconsistent. The reduced system is identically satisfied when $q = -2$.
The case $q = 0$ (corresponding to the Chen *et al* model) yields two sets of solutions:

$$n = c_0, \quad T = \phi = 0$$

and

$$n = 0, \quad T = \phi = -\frac{c_0}{\alpha^2\lambda^2}\cdot$$

These solutions are discarded because we require non–zero solutions for the system under consideration.

$$\text{(ii)}\;\; q \neq 0,\;\; \mu^{(1)}(T) = \mu_0^{(1)} T^{q-1},\;\; \mu^{(2)}(T) = \mu_0^{(2)} T^{q-1},\;\; \tau(T) = \tau_0 (T - T_L) T^{-1},$$

$$c(r) = \bar{c}_0 (2 + \alpha q r)^{\frac{2(1-q)}{q}},\; X = \frac{1}{2}(2 + \alpha q r)\frac{\partial}{\partial r} + \alpha(1-q) n \frac{\partial}{\partial n} + \alpha T \frac{\partial}{\partial T} + \alpha \phi \frac{\partial}{\partial \phi}\cdot$$

The characteristic equations for the invariants of X are

$$\frac{2\,dr}{2 + \alpha q r} = \frac{1}{\alpha(1-q)}\frac{dn}{n} = \frac{dT}{\alpha T} = \frac{d\phi}{\alpha \phi}\cdot \tag{4.4}$$

Solving the above characteristic equations for $q \neq 1$ and $\alpha \neq 0$ yields

$$n = \overline{n}_0 (2 + \alpha q r)^{\frac{2(1-q)}{q}}, \tag{4.5a}$$

$$T = \overline{T}_0 (2 + \alpha q r)^{\frac{2}{q}}, \tag{4.5b}$$

$$\phi = \overline{\phi}_0 (2 + \alpha q r)^{\frac{2}{q}}, \tag{4.5c}$$

where $\overline{n}_0$, $\overline{T}_0$ and $\overline{\phi}_0$ are the arbitrary constants. The invariant solutions (4.5a)–(4.5c) are substituted into the original system (3.1) to yield the reduced system which is solved for the arbitrary constants. Therefore, a class of exact solutions with $q \neq 4$ assumes the form

$$n = \left[\bar{c}_0 - 2\alpha^2 \lambda^2 (q-2)\left(\frac{3}{4\alpha^2 \mu_0^{(2)} \tau_0 (4-q)}\right)^{\frac{1}{q}}\right](2 + \alpha q r)^{\frac{2(1-q)}{q}}, \tag{4.6a}$$

$$T = \left[\frac{3}{4\alpha^2 \mu_0^{(2)} \tau_0 (4-q)}\right]^{\frac{1}{q}} (2 + \alpha q r)^{\frac{2}{q}}, \tag{4.6b}$$

$$\phi = \left[\frac{3}{4\alpha^2 \mu_0^{(2)} \tau_0 (4-q)}\right]^{\frac{1}{q}} (2 + \alpha q r)^{\frac{2}{q}}. \tag{4.6c}$$

The original system (3.1) is not satisfied when $q = 4$. Hence, the case $q \neq 4$ is discarded.

Case (b) $k \neq 0$

$$\text{(i)}\;\; q \neq 0,\;\; \mu^{(1)}(T) = \mu_0^{(1)} T^{q-1},\;\; \mu^{(2)}(T) = \mu_0^{(2)} T^{q-1},\;\; \tau(T) = \tau_0 (T - T_L) T^{-1},$$

$$c(r) = c_1\, r^{\frac{2(1-q)}{q}},\; X = \frac{q\,r}{2}\frac{\partial}{\partial r} + (1-q) n \frac{\partial}{\partial n} + T \frac{\partial}{\partial T} + \phi \frac{\partial}{\partial \phi}\cdot$$

The characteristic equations for the invariants of X are

$$\frac{2}{q}\frac{dr}{r} = \frac{1}{(1-q)}\frac{dn}{n} = \frac{dT}{T} = \frac{d\phi}{\phi}\cdot \tag{4.7}$$

The invariant solutions for $q \neq 1$ assume the form

$$n = n_1\, r^{\frac{2(1-q)}{q}}, \tag{4.8a}$$

$$T = T_1\, r^{\frac{2}{q}}, \tag{4.8b}$$

$$\phi = \phi_1\, r^{\frac{2}{q}}, \tag{4.8c}$$

where n_1, T_1 and ϕ_1 are the arbitrary constants. The substitution of the invariant solutions (4.8a)–(4.8c) into the underlying system (3.1) yields the reduced system from which the arbitrary constants are obtained. Therefore, the exact solutions are

$$n = \left[c_1 + \frac{2\lambda^2[2+(k-1)q]}{q^2}\left(\frac{3q^2}{4\mu_0^{(2)}\tau_0[4+(k-1)q]}\right)^{\frac{1}{q}}\right] r^{\frac{2(1-q)}{q}}, \tag{4.9a}$$

$$T = \left(\frac{3q^2}{4\mu_0^{(2)}\tau_0[4+(k-1)q]}\right)^{\frac{1}{q}} r^{\frac{2}{q}}, \tag{4.9b}$$

$$\phi = \left(\frac{3q^2}{4\mu_0^{(2)}\tau_0[4+(k-1)q]}\right)^{\frac{1}{q}} r^{\frac{2}{q}}, \tag{4.9c}$$

provided $4+(k-1)q \neq 0$.

(ii) The condition $4+(k-1)q = 0$ requires $k \neq 1$. Hence, with $q = \dfrac{4}{1-k}$ in Eq. (4.7) the invariant solutions have the form

$$n = \overline{n}_1\, r^{-\frac{k+3}{2}}, \tag{4.10a}$$

$$T = \overline{T}_1\, r^{\frac{1-k}{2}}, \tag{4.10b}$$

$$\phi = \overline{\phi}_1\, r^{\frac{1-k}{2}}, \tag{4.10c}$$

where $\overline{n}_1$, $\overline{T}_1$ and $\overline{\phi}_1$ are the arbitrary constants. The substitution of the invariant solutions (4.10a)–(4.10c) into the system under consideration, (3.1), yields the exact solutions

$$n = \left[c_1 + \frac{\lambda^2(1+2k-k^2)^{\frac{k+3}{4}}}{4}\left(\frac{\mu_0^{(1)}\tau_0(k+3)}{6(k-1)}\right)^{\frac{k-1}{4}}\right] r^{-\frac{k+3}{2}}, \tag{4.11a}$$

$$T = \left[\frac{\mu_0^{(1)}\tau_0(k+3)(1+2k-k^2)}{6(k-1)}\right]^{\frac{k-1}{4}} r^{\frac{1-k}{2}}, \tag{4.11b}$$

$$\phi = \left[\frac{\mu_0^{(1)}\tau_0(k+3)(1+2k-k^2)}{6(k-1)}\right]^{\frac{k-1}{4}} r^{\frac{1-k}{2}}. \tag{4.11c}$$

Remark 2: The case $k = 1$ corresponding to a two dimensional stationary model does not satisfy the underlying model (3.1). Hence, the two dimensional stationary case treated in [14] cannot be recovered by simply substituting $k = 1$ in the stationary spherically symmetric model (3.1). Now, with $k \neq 1$ the cases of interest are $k = 0$ and $k = 2$.

Remark 3: The graphs of the solutions (4.2a)–(4.2c) and (4.10a)–(4.10c) corresponding to $k = 0$ and $k = 2$ respectively are presented below. These are the graphs of the electron density n in cm^{-3}, electron energy W in eV and electric potential ϕ in V/micron against r (micron). After setting $T_0 = \phi_0 = \overline{T}_1 = \overline{\phi}_1 = 1$ and $\alpha = -1$ for $n_0 = \overline{n}_1 = 10^{17}$ cm^{-3}, the following graphs are obtained

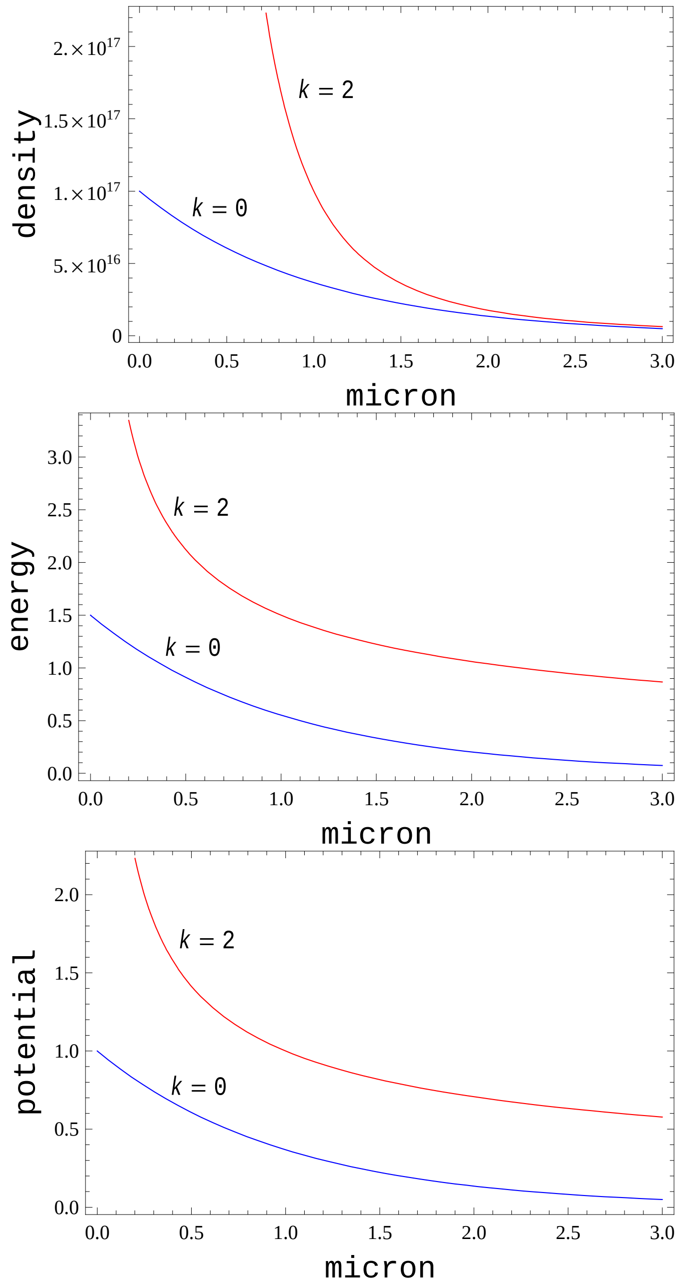

Figure 1: Plot of the solutions (4.2a)–(4.2c) and (4.10a)–(4.10c).

5 Conclusion

Four classes of exact solutions of a spherically symmetric ET model for semiconductors in the stationary case have been constructed. The solutions provide benchmarks useful for testing numerical codes for the stationary spherically symmetric ET models. The graphical solutions of these exact solutions can be constructed provided a relevant data for the model parameters is at hand.

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