Subsonic Solutions to a One-Dimensional Non-isentropic Hydrodynamic Model for Semiconductors

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The one-dimensional stationary full hydrodynamic model for semiconductor devices with non-isentropic pressure is studied. This model consists of the equations for the electron density, electron temperature, and electric field in a bounded domain supplemented with boundary conditions. The existence of a classical subsonic solution with positive particle density and positive temperature is shown in two situations: non-constant and constant heat conductivities. Moreover, we prove uniqueness of a classical solution in the latter case. The existence proofs are based on elliptic estimates, Stampacchia truncation methods, and fixed-point arguments. © 2001 Academic Press

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1. INTRODUCTION

For the simulation of semiconductor devices usually drift-diffusion models are used. These models consist of the continuity equations expressing the conservation of mass and a drift-diffusion relation for the electron current density [M]. In order to model modern submicron devices and hot electron effects, however, more complicated model equations have to be considered, like energy-transport or hydrodynamic equations [Ju]. In this paper, we study the full hydrodynamic model consisting of the continuity equations expressing the conservation of mass, momentum, and energy, coupled self-consistently to the Poisson equation for the electric field. The steady-state equations for the electron density n, the electron temperature T, and the electric field E read as

(1)
$$\left(\frac{mj^2}{n} + P(n,T)\right)_x = -qnE - \frac{mj}{\tau_p},$$

(2)
$$(a(n,T)T_x)_x = qjE + \frac{w-w_0}{\tau_w} + \left(\frac{mj^3}{2n^2} + \frac{5}{2}jT\right)_x$$

(3)
$$E_x = -\frac{q}{\epsilon_s}(n-C(x))$$

in the bounded domain (0, 1). Here, *j* denotes the (constant) electron current density, P(n, T) the pressure, a(n, T) the heat conductivity, and C(x) the doping profile. The physical constants are the effective electron mass *m*, the elementary charge *q*, the momentum and energy relaxation times τ_p and τ_w , respectively, and the semiconductor permittivity ϵ_s . The energy w = w(n, T) is written as $w = w_0 + \tau_w \tilde{w}(n, T - T_L)$, where T_L is the lattice temperature and \tilde{w} satisfies $\tilde{w}(n, 0) = 0$ for all n > 0. We recall that the energy cannot be determined from the state equation [FW, R]. Equations (1)–(3) are supplemented by the boundary conditions

(4)
$$E(0) = E_0$$
, $n(0) = n_0$, $T(0) = T_0$, $T(1) = T_1$.

Notice that we allow *general* pressure functions and heat conductivities. Often the energy equation (3) is replaced by the relation $P = n^{\gamma}$ with $\gamma > 1$. The corresponding model is referred to as the *isentropic* hydrodynamic model. The existence of solutions to this model has been studied in the mathematical literature for several years. Degond and Markowich proved the existence of steady-state solutions in the subsonic case [DM1, DM2]. Gamba showed existence of steady-state solutions in the transonic case by means of the vanishing viscosity method [G]. The transient equa-

tions are studied by several authors; see, e.g., Fang and Ito [FI], Jochmann [Jo], and Marcati and Natalini [MN] for $\gamma > 1$ and Poupaud *et al.* [PRV] for $\gamma = 1$.

For the full hydrodynamic model (1)–(3), usually the polytropic gas ansatz is used to get explicit expressions for the pressure and the energy:

(5)
$$P(n,T) = nT, \quad w = \frac{3}{2}nT + \frac{j^2}{2n}.$$

The system of equations (1)–(3) with the relations (5) has been studied only recently. Yeh showed the existence of a unique strong solution in several space dimensions if the flow is subsonic, the ambient temperature T_L is large enough, and the vorticity on the inflow boundary and the variation of the electron density on the boundary are sufficiently small [Y2]. Zhu and Hattori proved the existence of classical subsonic solutions in one space dimension for the whole space problem under the additional assumption that the doping profile be close to a constant [ZH]. The transient equations have been considered by Yeh [Y1] and Ito [I]. In the work of Ito, the energy equation has been replaced by an equation for the entropy, assuming the relations (5). No results, however, are available for the hydrodynamic equations with *general* pressure P(n, T). In this paper we prove the existence of classical subsonic solutions to (1)–(4). More precisely, our first main result is as follows:

THEOREM 1. Let the regularity assumptions (A1)–(A4) for a, P, \tilde{w} , and C hold (see Section 2) and let $n_0, T_0, T_1 > 0$. Then there exist positive constants $j_0, \delta, K, \underline{n}, \overline{n}, \underline{T}$, and \overline{T} such that if

(6)
$$|j| \le j_0, \quad |T_0 - T_L| + |T_1 - T_L| \le \delta$$

and

(7)
$$\partial_n P(\rho, \theta) \ge K \quad \text{for all } \underline{n} \le \rho \le \overline{n}, \underline{T} \le \theta \le \overline{T},$$

there is a classical solution (n, T, E) of (1)–(4) satisfying

(8)
$$0 \le \underline{n} \le n(x) \le \overline{n}, \quad 0 < \underline{T} \le T(x) \le \overline{T} \text{ for } x \in [0,1].$$

The proof of this theorem is based on the Schauder fixed point theorem and on the following reformulation of (1):

(9)
$$\left(\partial_n P(n,T) - \frac{mj^2}{n^2}\right)n_x = -\left(\partial_T P(n,T) + qnE + \frac{mj}{\tau_p}\right).$$

The first condition in (6) corresponds to a subsonic condition. Indeed, subsonic flow is characterized by

$$\left|\frac{j}{n}\right| < \sqrt{\partial_n P/m} \,.$$

In the proof of Theorem 1 it is shown that $j_0 < n\sqrt{K/m}$. Thus

$$\left|\frac{j}{n}\right| \leq \frac{j_0}{\underline{n}} < \sqrt{K/m} \leq \sqrt{\partial_n P/m} \,.$$

In particular, the bracket on the left-hand side of (9) is positive.

The second condition in (6) is needed to estimate T_x in the space $L^{\infty}(0, 1)$. This bound is used in (9) in order to control the L^{∞} bound on n_x . Together with the assumption (7), for given bounds for the right-hand side of (9), $|n_x|$ can be controlled. Indeed, for sufficiently large K, the variation of the electron density is small enough to get positivity of the variable.

In the case P(n,T) = nT, the condition (7) is equivalent to the hypothesis of sufficiently large ambient temperature which has been assumed by Yeh [Y2]. Hence, the case P(n,T) = nT is included in condition (7) if T_L is sufficiently large.

In the case of constant heat conductivity a(n, T), the assumption of sufficiently small differences $|T_0 - T_L|, |T_1 - T_L|$ can be dropped. Our second main result reads:

THEOREM 2. Let the assumptions (A1)–(A4) hold and let $n_0, T_0, T_1 > 0$. Furthermore, let a = const. Then there exist positive constants $j_0, K, \underline{n}, \overline{n}, \underline{T}, \overline{T} > 0$ such that if $0 < j \le j_0$ hold, there is a classical solution (n, T, E) of (1)–(4) satisfying (8). Moreover, under the additional condition (A.5), this solution is unique in the class of classical solutions satisfying (8).

This paper is organized as follows. In Section 2, we make precise the assumptions (A1)-(A5) and prove Theorem 1. Theorem 2 is proved in Section 3.

2. ASSUMPTIONS AND PROOF OF THEOREM 1

For Theorems 1 and 2 we have supposed the following assumptions:

(A1) P(n,T) is continuously differentiable in $(n,T) \in (0,\infty)^2$.

(A2) a(n,T) is continuously differentiable and a(n,T) > 0 in $(n,T) \in (0,\infty)^2$.

(A3) \tilde{w} is continuous in both arguments, Lipschitz continuous in T, and

$$\tilde{w}(n, T - T_L)(T - T_L) \ge 0$$

for all $(n, T) \in (0, \infty)^2$ and some $T_L > 0$.

(A4) $C \in L^1(0, 1).$

For the uniqueness result (see Theorem 2) we also need the assumption

(A5) $\tilde{w}(n,T)$ is Lipschitz continuous in *n* and

$$\left(\tilde{w}(\rho,\theta_1-T_L)-\tilde{w}(\rho,\theta_2-T_L)\right)(\theta_1-\theta_2)\geq 0 \quad \text{for all } \rho,\theta_1,\theta_2>0.$$

The monotonicity of \tilde{w} imposed in (A5) (and in a weaker form in (A3)) is reasonable from physical considerations. Notice that, due to assumption (A2), the equation for the temperature is allowed to be of degenerate type.

Proof of Theorem 1. Introduced the closed convex set

$$B = \{ (\rho, \theta) \in C^0([0,1]) \times C^1([0,1]) : \underline{n} \le \rho(x) \le \overline{n}, \underline{T} \le \theta(x) \le \overline{T}, \\ |(\theta - \varphi)_x(x)| \le M \text{ for } x \in [0,1] \},$$

where $\varphi(x) = T_1 + (T_0 - T_1)(1 - x)$ and the positive constants $\underline{n}, \overline{n}, \underline{T}, \overline{T}$, and M are defined below. Now let $(\rho, \theta) \in B$ and define

$$E(x) = E_0 + \frac{q}{\varepsilon} \int_0^x (C - \rho) \, ds.$$

Further, let $n \in C^{1}([0, 1])$ be the unique solution of the linear problem

(10)
$$\left(\partial_n P(\rho,\theta) - \frac{mj^2}{\rho^2}\right) n_x = -\left(\partial_T P(\rho,\theta) \theta_x + q \rho E + \frac{jm}{\tau_p}\right),$$

$$(11) n(0) = n_0,$$

where we take $0 < j < \underline{n}\sqrt{K/m}$, K > 0 being defined below. This implies by (7) that the bracket on the left-hand side of (10) is positive. Finally, let $T \in C^2([0,1])$ be the unique solution of the monotone

Finally, let $T \in C^2([0, 1])$ be the unique solution of the monotone problem

(12)
$$(a(n,\theta)T_x)_x = qjE + \tilde{w}(\rho,T-T_L) + \frac{5}{2}jT_x - \frac{mj^3}{\rho^3}n_x$$

(13)
$$T(0) = T_0, \quad T(1) = T_1.$$

The existence and uniqueness of a solution to (12)-(13) follow from standard arguments (see, e.g., [Tr]). This defines the fixed-point operator

$$S: B \to C^0[(0,1)] \times C^1([0,1]), \quad S(\rho,\theta) = (n,T).$$

Since $(n, T) \in C^1([0, 1]) \times C^2([0, 1])$, it is easy to see that S(B) is precompact. Moreover, using standard arguments, S is continuous. In order to

apply the Schauder fixed-point theorem (see [GT, Tr]), it remains to prove that $S(B) \subset B$.

First we show that there exist constants $\underline{n}, \overline{n} > 0$ such that $\underline{n} \le n(x) \le \overline{n}$ for $x \in [0, 1]$. Fix $0 < j \le j_1$ with arbitrary $j_1 > 0, 0 < N < n_0$ and

$$C_{1} = \left(|T_{1} - T_{0}| + M \right) \max \left\{ \left| \partial_{T} P(\rho, \theta) \right| : \underline{n} \le \rho \le \overline{n}, \underline{T} \le \theta \le \overline{T} \right\} + qjE_{\infty} + j_{1}m/\tau_{p},$$

where $E_{\infty} = |E_0| + (q/\varepsilon_s)(||C||_1 + \overline{n})$. Here and in the following, the norm of $L^p(0,1)$ is denoted by $\|\cdot\|_p$. Then, by Assumption (7), taking $K = 2C_1/N$ and $0 < j \le j_2 := \underline{n}\sqrt{K/2m}$, we have

$$\partial_n P(\rho,\theta) - \frac{mj^2}{\rho^2} \ge K - \frac{mj_2^2}{\underline{n}^2} = \frac{K}{2}$$

and from Eq. (10) we obtain the estimate

$$|n_{x}| \leq \frac{2}{K} \left| \partial_{T} P(\rho, \theta) \theta_{x} + q \rho E + \frac{jm}{\tau_{p}} \right| \leq \frac{2}{K} C_{1} = N.$$

Defining $\underline{n} = n_0 - N$, $\overline{n} = n_0 + N$, this implies that $\underline{n} \le n(x) \le \overline{n}$ for $x \in [0, 1]$. Notice that $\underline{n} > 0$ since $N < n_0$.

Next we prove that there exist constants $\underline{T}, \overline{T} > 0$ such that $\underline{T} \leq T(x) \leq \overline{T}$ for $x \in [0, 1]$ by employing the Stampacchia truncation method. According to Assumption (A2) and the bounds on n and θ , there exists a constant $\alpha > 0$ such that $\alpha(n, \theta) \geq \alpha$. Set $\overline{\theta} = \max(T_0, T_1, T_L)$ and use $(T - \overline{\theta})^+ = \max(0, T - \overline{\theta})$ as a test function in the weak formulation of (12):

$$\alpha \int_0^1 \left| (T - \overline{\theta})_x^+ \right|^2 dx \le \int_0^1 \left(\frac{m j^3}{\rho^3} n_x - q j E \right) (T - \overline{\theta})^+ dx$$
$$- \int_0^1 \tilde{w} (\rho, T - T_L) (T - \overline{\theta})^+ dx$$
$$- \frac{5}{2} j \int_0^1 T_x (T - \overline{\theta})^+ dx.$$

The second term on the right-hand side is non-positive due to Assumption (A3). The last term vanishes since

$$-\frac{5}{2}j\int_{0}^{1}T_{x}(T-\bar{\theta})^{+}dx = -\frac{5}{4}j\int_{0}^{1}\left(\left((T-\bar{\theta})^{+}\right)^{2}\right)_{x}dx$$
$$= -\frac{5}{4}j\left[\left((T-\bar{\theta})^{+}\right)^{2}\right]_{0}^{1} = 0.$$

Therefore, setting

$$C_2 = \frac{mj_2^2}{\alpha \overline{n}^3} N + \frac{q}{\alpha} E_{\infty},$$

we get

$$\int_0^1 \left| (T - \overline{\theta})_x^+ \right|^2 dx \le C_2 j \int_0^1 (T - \overline{\theta})^+ dx$$
$$\le C_2 j \operatorname{meas}(T > \overline{\theta})^{1/2} \left\| (T - \overline{\theta})^+ \right\|_2$$

Using Poincaré's inequality $||(T - \overline{\theta})^+||_2 \le (1/\sqrt{2})||(T - \overline{\theta})^+_x||_2$, we obtain

(14)
$$\left\| (T - \bar{\theta})_x^+ \right\|_2 \le j \frac{C_2}{\sqrt{2}} \operatorname{meas}(T > \bar{\theta})^{1/2}.$$

The imbedding $H^1(0,1) \hookrightarrow L^r(0,1)$ is continuous for any $r \leq \infty$ and it is well known that for $\mathscr{U} > \overline{\theta}$ and r > 2 the inequality

$$\operatorname{meas}(T > \mathscr{U})^{1/r} (\mathscr{U} - \overline{\theta}) \le c \left\| (T - \overline{\theta})^{+} \right\|_{H^{1}}$$

holds [St, Chap. 4]. Therefore we get from (14) and Poincaré's inequality, for another constant c > 0, for $\mathscr{U} > \overline{\theta}$,

$$\operatorname{meas}(T > \mathscr{U}) \leq \frac{c}{\left(\mathscr{U} - \overline{\theta}\right)^r} \operatorname{meas}(T > \overline{\theta})^{r/2}.$$

Choosing r/2 > 1, we can apply Stampacchia's lemma [St, Chap. 4]. Hence, there is a constant C_3 depending only on C_2 such that $T \le \overline{\theta} + jC_3$ in [0, 1]. We set $\overline{T} = \overline{\theta} + j_2C_3$.

For the lower bound we set $\underline{\theta} = \min(T_0, T_1, T_L)$ and use $(-T + \underline{\theta})^+$ as a test function in the weak formulation of (12). A similar estimate as above gives

$$\left\| \left(-T + \underline{\theta} \right)_x^+ \right\|_2 \le jC'_2 \operatorname{meas} \left(-T > -\underline{\theta} \right)^{1/2}$$

and in an analogous way we conclude the existence of a constant C_4 depending only on C'_2 such that $-T \leq -\underline{\theta} + jC_4$ in [0, 1], i.e.,

$$T \ge \underline{\theta} - jC_4$$
 in $[0, 1]$.

Setting $j_3 = \underline{\theta}/2C_4$ and $\underline{T} = \underline{\theta}/2$, we obtain for all $0 < j \le j_3$:

$$T \ge \underline{\theta} - j_3 C_4 = \underline{T} \quad \text{in } [0, 1].$$

It remains to prove that $||(T - \varphi)_x||_{\infty} \leq M$ for an appropriate constant M > 0. By elliptic estimates (see, e.g., [GT]), there exists a constant $C_5 > 0$ depending on the $W^{1,\infty}$ norms of n and θ (and hence, on \overline{n} , N, \overline{T} , and $|T_1 - T_0| + M$) such that

$$\|T\|_{H^2} \le C_5(M) \|qjE + \tilde{w}(\rho, T - T_L) + \frac{5}{2}jT_x - mj^3\rho^{-3}n_x\|_2.$$

Using the Lipschitz continuity of $\tilde{w}(\rho, \cdot)$ and the above bounds, it is clear that if j and $|T_0 - T_L| + |T_1 - T_L|$ are chosen sufficiently small, the L^2 norm on the right-hand side can be made arbitrarily small.

Thus there exist $j_4 \leq \min(j_1, j_2, j_3)$ and $\delta > 0$ such that for all $0 < j \leq j_4$ and $|T_0 - T_L| + |T_1 - T_L| \leq \delta$,

$$\|(T-\varphi)_x\|_{\infty} \le \|T_x\|_{\infty} + |T_1-T_0| \le c \|T\|_{H^2} + \delta \le M.$$

Here we do not need to impose restrictions on M > 0.

We have shown that $S(B) \subset B$. Hence, Schauder's Theorem applies and we obtain a classical solution to the boundary-value problem (1)–(4).

3. PROOF OF THEOREM 2

The proof of the existence result of Theorem 2 is similar to that of Theorem 1, except the proof of $||(T - \varphi)_x||_{\infty} \le M$. From (12) we get the estimate

$$a\|T_{xx}\|_{2} \le qjE_{\infty} + c|T - T_{L}| + \frac{5}{2}j\|T_{x}\|_{2} + mj^{3}\underline{n}^{-3}N.$$

Since $T - \varphi$ vanishes at x = 0 and x = 1, there exists $x_0 \in (0, 1)$ such that $(T - \varphi)_x(x_0) = 0$. Thus

$$(T-\varphi)_x(x) = \int_{x_0}^x T_{xx} \, ds$$

and

$$||T_x||_2 \le |T_1 - T_0| + ||T_{xx}||_2.$$

We obtain

$$\left(a - \frac{5}{2}j\right) \|T_{xx}\|_{2} \le qjE_{\infty} + c|T - T_{L}| + mj^{3}\underline{n}^{-3}N + \frac{5}{2}j|T_{1} - T_{0}|.$$

Taking $0 < j \le j_5 = \min(j_1, j_2, j_3, \frac{\alpha}{5})$ we can find a constant M > 0 such that

$$\|(T-\varphi)_x\|_{\infty} \le c \|T\|_{H^2} + |T_1 - T_0| \le M.$$

This proves the existence of solutions.

To prove the uniqueness of solutions, let $(n^{(1)}, T^{(1)}, E^{(1)})$ and $(n^{(2)}, T^{(2)}, E^{(2)})$ be two classical solutions of (1)–(4) satisfying (8). Then, taking the difference of Eqs. (2) satisfied by $T^{(1)}, T^{(2)}$, respectively, and using $T^{(1)} - T^{(2)}$ as test function in the difference, we obtain

$$a \int_{0}^{1} (T^{(1)} - T^{(2)})_{x}^{2} dx$$

= $-qj \int_{0}^{1} (E^{(1)} - E^{(2)})(T^{(1)} - T^{(2)}) dx$
 $- \int_{0}^{1} (\tilde{w}(n^{(1)}, T^{(1)} - T_{L}) - \tilde{w}(n^{(2)}, T^{(2)} - T_{L}))(T^{(1)} - T^{(2)}) dx$
 $+ \frac{mj^{3}}{2} \int_{0}^{1} \left(\frac{1}{(n^{(1)})^{2}} - \frac{1}{(n^{(2)})^{2}}\right)(T^{(1)} - T^{(2)})_{x} dx$
 $- \frac{5}{2}j \int_{0}^{1} (T^{(1)} - T^{(2)})_{x}(T^{(1)} - T^{(2)}) dx$
 $= I_{1} + \dots + I_{4}.$

In view of Assumption (A5) (see Section 2) and Poincaré's inequality, it holds

$$\begin{split} I_2 &\leq -\int_0^1 \left(\tilde{w} \big(n^{(1)}, T^{(1)} - T_L \big) - \tilde{w} \big(n^{(2)}, T^{(1)} - T_L \big) \big) (T^{(1)} - T^{(2)}) \, dx \\ &\leq c \| n^{(1)} - n^{(2)} \|_2 \| (T^{(1)} - T^{(2)})_x \|_2, \end{split}$$

where c > 0 denotes a positive generic constant. Furthermore, the first and third integral can be estimated as

$$\begin{split} I_1 + I_3 &\leq cj \big(\| E^{(1)} - E^{(2)} \|_2 \| T^{(1)} - T^{(2)} \|_2 + \| n^{(1)} - n^{(2)} \|_2 \| (T^{(1)} - T^{(2)})_x \|_2 \big) \\ &\leq cj \| n^{(1)} - n^{(2)} \|_2 \| (T^{(1)} - T^{(2)})_x \|_2. \end{split}$$

Finally, the fourth term vanishes: $I_4 = 0$. Therefore, we obtain

(15)
$$\|(T^{(1)} - T^{(2)})_x\|_2 \le cj \|n^{(1)} - n^{(2)}\|_2.$$

To derive an estimate for $n^{(1)} - n^{(2)}$, we take the difference of Eqs. (1) for $n^{(1)}$, $n^{(2)}$, respectively, integrate over $0 < \xi < x$ for some $x \in (0, 1]$, and

multiply the resulting equation with $(n^{(1)} - n^{(2)})(x)$:

(16)
$$(P(n^{(1)}, T^{(1)}) - P(n^{(2)}, T^{(2)}))(x)(n^{(1)} - n^{(2)})(x)$$
$$= -\left(\frac{mj^2}{n^{(1)}} - \frac{mj^2}{n^{(2)}}\right)(x)(n^{(1)} - n^{(2)})(x)$$
$$- q \int_0^x (n^{(1)}E^{(1)} - n^{(2)}E^{(2)}) d\xi(n^{(1)} - n^{(2)})(x).$$

We estimate the left-hand side by using the Lipschitz continuity of *P* in $[\underline{n}, \overline{n}] \times [\underline{T}, \overline{T}]$:

$$\begin{aligned} & \left(P(n^{(1)},T^{(1)}) - P(n^{(2)},T^{(2)})\right)(x)(n^{(1)} - n^{(2)})(x) \\ & = \int_0^1 \partial_n P(\lambda n^{(1)} + (1-\lambda)n^{(2)},T^{(1)})(x) \, d\lambda(n^{(1)} - n^{(2)})(x)^2 \\ & + \left(P(n^{(2)},T^{(1)}) - P(n^{(2)},T^{(2)})\right)(x)(n^{(1)} - n^{(2)})(x) \\ & \geq K(n^{(1)} - n^{(2)})(x)^2 - c \left| (T^{(1)} - T^{(2)})(x)(n^{(1)} - n^{(2)})(x) \right|. \end{aligned}$$

The right-hand side of (16) is majorized by

$$cj|(n^{(1)}-n^{(2)})(x)|^2+c||n^{(1)}-n^{(2)}||_1^2.$$

Therefore, we get from (16)

$$K \| n^{(1)} - n^{(2)} \|_{\infty}^{2} \le c \| T^{(1)} - T^{(2)} \|_{\infty} \| n^{(1)} - n^{(2)} \|_{\infty} + c(j+1) \| n^{(1)} - n^{(2)} \|_{\infty}^{2}.$$

Choosing K > 0 large enough, we conclude, using Sobolev's inequality,

$$\|n^{(1)} - n^{(2)}\|_{\infty} \le c \|T^{(1)} - T^{(2)}\|_{\infty} \le c \|(T^{(1)} - T^{(2)})_x\|_2.$$

Hence, by (15),

$$\|(T^{(1)} - T^{(2)})_x\|_2 \le cj \|n^{(1)} - n^{(2)}\|_{\infty} \le cj \|(T^{(1)} - T^{(2)})_x\|_2.$$

Thus, choosing j > 0 small enough, we obtain $T^{(1)} = T^{(2)}$. This implies $n^{(1)} = n^{(2)}$ and $E^{(1)} = E^{(2)}$. The theorem is proved.

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