Space homogeneous solutions of the linear Boltzmann equation for semiconductors: a semigroup approach

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1 Introduction

In a recent paper Majorana and Milazzo [7] considered the linear Boltzmann equation describing electron flow in a semiconductor. The electron-phonon interactions are simulated by a version of the $\delta-$like kernel, first mathematically investigated in ref. 8, that in the setting of this paper may be unbounded for large energies. The initial value problem for the linear Boltzmann equation reads as follows

$$\begin{cases} \dfrac{\partial f}{\partial t}(t,\mathbf{k}) = Kf(t,\mathbf{k}) - \nu(\mathbf{k})f(t,\mathbf{k})\,, \\ \\ f(0,\mathbf{k}) = f_0(\mathbf{k})\,, \end{cases} \tag{1.1}$$

with the gain collision operator K and the collision frequency ν defined by

$$Kf(t,\mathbf{k}) = \int_{\mathbb{R}^3} S(\mathbf{k}',\mathbf{k})f(t,\mathbf{k}')\,d\mathbf{k}', \qquad \nu(\mathbf{k}) = \int_{\mathbb{R}^3} S(\mathbf{k},\mathbf{k}')\,d\mathbf{k}'\,.$$

The kernel $S(\mathbf{k},\mathbf{k}')$ which accounts for the scattering processes between electrons and the background takes the following form

$$\begin{aligned} S(\mathbf{k},\mathbf{k}') = {} & \mathcal{G}(\mathbf{k},\mathbf{k}')[(n_q+1)\delta(\varepsilon(\mathbf{k}')-\varepsilon(\mathbf{k})+\hbar\omega) + n_q\delta(\varepsilon(\mathbf{k}')-\varepsilon(\mathbf{k})-\hbar\omega)] \\ & + \mathcal{G}_0(\mathbf{k},\mathbf{k}')\delta(\varepsilon(\mathbf{k}')-\varepsilon(\mathbf{k}))\,. \end{aligned}$$

$\mathcal{G}(\mathbf{k},\mathbf{k}')$ and $\mathcal{G}_0(\mathbf{k},\mathbf{k}')$ denote symmetric continuous functions on $\mathbb{R}^3 \times \mathbb{R}^3$ characterizing inelastic collisions with optical phonons and elastic collisions with acoustic phonons and impurities, respectively. The constant positive parameter n_q is given by $n_q = \left[\exp\left(\frac{\hbar\omega}{k_B T_L}\right) - 1\right]^{-1}$, where $\hbar$ is the Planck constant divided by 2π, ω is the positive constant phonon frequency, k_B is the Boltzmann constant and T_L is the lattice temperature. $\delta(\varepsilon(\mathbf{k}))$ denotes the Dirac function composed with the electron energy function $\varepsilon(\mathbf{k})$:

$$\varepsilon(\mathbf{k}) = \frac{\hbar^2|\mathbf{k}|^2}{m^* + \sqrt{m^*(m^* + 2|\mathbf{k}|^2\alpha\hbar^2)}} \tag{1.2}$$

where m^* is the effective mass. Note that for $\alpha = 0$, eq. (1.2) gives the mass parabolic approximation.

In ref. 7 the Cauchy problem for eq. (1.1) is investigated in the Banach space of summable functions, without requiring the boundedness of the collision frequency, and the existence of the solution is established. The uniqueness of the solution can be recovered adding suitable conditions on the growth speed of the collision frequency $\nu(\mathbf{k})$ (ref. 7, Th. 7).

In this paper we shall study the initial value problem (1.1) by semigroups. Problems of this form fall into the general framework of the theory of substochastic semigroups (see ref. 1, 2, 4 and references therein). This approach gives almost immediately the existence of the semigroup, however the full characterization of the generator is usually obtained by some other means. This creates the possibility that the class of solutions obtained in this theory may not coincide with the solutions obtained by e.g. the approximation approach as in ref. 7. A more detailed analysis of the problem of multiple solutions is given ref. 5.

Here we prove that the generator of the evolution semigroup is the closure of the physical operator, following the same lines of the results obtained by J.Banasiak for the Spiga model (that have similar mathematical structure to the Majorana model). For more details and discussions on the uniqueness and non-uniqueness see the papers quoted in the references.

2 Abstract semigroup approach

Consider the abstract formulation of the Cauchy problem for eq. (1.1):

$$\begin{cases} \dfrac{df}{dt} = Af + Bf \,, \\ f(0) = f_0 \ , \end{cases} \tag{2.3}$$

where A and B are in general unbounded operators in a Banach space X and f is, say, a distribution of particles. For problems of this type the most suitable seems to be the method developed by Kato [6] for Kolmogorov's system. His results were extended to a more general situation and applied to kinetic theory by Voigt, Myiadera, van der Mee, Protopopescu, Desch, Mokhtar-Kharroubi, Banasiak and many others. In the general case, one can only prove that the generator T of the semigroup $\{G(t), t \geq 0\}$ solving the Cauchy problem (2.3) is an extension of the operator $A + B$ and such a result is usually insufficient for applications. The reason for this is that the semigroup G solving eq. (2.3) should be a *transition (stochastic) semigroup*, i.e. one should have

$$\|G(t)f\| = \|f\|, \quad \forall t \geq 0, \ \forall f \geq 0\,;$$

this condition expresses the fact that the total number of particles in conserved through time. A sufficient condition for G to be stochastic is $T = \overline{A + B}$.

Three situations are possible: i) $T = A + B$ or ii) $T = \overline{A + B}$, $T \neq A + B$, whereby G is stochastic, and iii) T is a proper extension of $\overline{A + B}$, in which case G may be not stochastic. The total number of particles is preserved only if G is stochastic, so only in the first case we can claim that the obtained semigroup has physical relevance [4].

The following is an extension of the Kato-Voigt perturbation theorem that generalizes theorem by L. Arlotti [1,4].

Theorem 2.1 *Let A, B operators in $X = L^1(\Omega, \mu)$. Suppose*

i) $(A, \mathcal{D}(A))$ generates substochastic semigroup $\{G_A(t),\ t \geq 0\}$;

ii) $\mathcal{D}(B) \supseteq \mathcal{D}(A)$ and $Bf \geq 0$, $\forall f \in \mathcal{D}(B), f \geq 0$;

iii) $$\int_\Omega (Af + Bf)\, d\mu \leq 0\,, \quad \forall f \in \mathcal{D}(A), f \geq 0. \tag{2.4}$$

Then, there exists a smallest substochastic semigroup $\{G(t), t \geq 0\}$ generated by an extension T of $A + B$ and satisfying the integral equation

$$G(t)f = G_A(t)f + \int_0^t G(t-s)BG_A(s)f\, ds, \qquad \forall f \in \mathcal{D}(A),\ \forall t \geq 0\ .$$

It can also obtained by the Philips-Dyson expansion $G(t)f = \sum_{n=0}^{\infty} S_n(t)f$, $f \in X$ where $S_0(t)f = G_A(t)f$, $S_n(t)f = \int_0^t S_{n-1}(t-s)BG_A(s)f\, ds$.

Note that theorem 2.1 *does not* give any characterization of the domain of the generator T.

3 Existence of Solutions by Semigroup Theory

Let $X = L^1(\mathbb{R}^3)$. The multiplication operator by $-\nu(\mathbf{k})$ plays the role of A in the abstract problem (2.3), with domain $\mathcal{D}(A) = \{f \in X : \nu(\mathbf{k})f \in X\}$, under the assumption that $\nu(\mathbf{k})$ is non-negative and belonging to $L^1_{loc}(\mathbb{R}^3)$. The role of B is played by the positive gain integral operator with symmetric kernel $S(\mathbf{k},\mathbf{k}') \geq 0$, with domain $\mathcal{D}(B) = \{f \in X : Kf \in X\}$. The kernel is such that $\int_{\mathbb{R}^3} S(\mathbf{k},\mathbf{k}'))\, d\mathbf{k}' \notin L^1(\mathbb{R}^3)$ but is only $L^1_{loc}(\mathbb{R}^3)$.

Proposition 3.1

$$\|Bf\|_{L^1(\mathbb{R}^3)} \leq \|Af\|_{L^1(\mathbb{R}^3)} \qquad \forall f \in \mathcal{D}(A) \tag{3.5}$$

Proof: Let $f \in L^1(\mathbb{R}^3) \cap \mathcal{D}(A)$. Evaluating the l.h.s of (3.5) and applying triangle inequality, the result follows immediately using the symmetry and the positiveness of the kernel S. ■

From Proposition 3.1 it follows that $\mathcal{D}(B) \supseteq \mathcal{D}(A)$. A generates the substochastic semigroup $G_A(t) = \exp\{-\nu(\mathbf{k})t\}$. Then it is easy to prove that

$$\int_{\mathbb{R}^3} (Af + Bf)\, d\mathbf{k} = 0, \quad \forall f \in \mathcal{D}(A), \quad f \geq 0, \tag{3.6}$$

thus we can apply Theorem 2.1, obtaining the existence of the semigroup of the evolution operator of our process. This semigroup, obtained by the Phillips-Dyson expansion, is substochastic and its generator is an extension of $A + B = -\nu I + K$, where I is the identity operator.

In the present context we can use the method introduced by Arlotti [1] and adapted by Banasiak [3,5], which consists in a suitable extension of the domain of the collision operator. With this understanding, we have

Theorem 3.1 *If for any $f \in X, f \geq 0$, such that the expression $Kf(\mathbf{k})$ is finite almost everywhere and such that $-\nu f + Kf \in X$, we have*

$$\int_{\mathbb{R}^3} (-\nu(\mathbf{k})f(\mathbf{k}) + Kf(\mathbf{k}))\, d\mathbf{k} \geq 0, \tag{3.7}$$

then $T = \overline{-\nu I + K}$.

Before giving the characterization of T, we prove the following technical lemma

Lemma 3.1 *Let $B_n = \{(\varepsilon, \mathbf{u}) : 0 \leq \varepsilon < n\hbar\omega,\ \mathbf{u} \in S^2\}$. Then,*

$$\int_{B_n} (-\nu(\mathbf{k})f(\mathbf{k}) + (Kf)(\mathbf{k}))\, d\mathbf{k} = \tag{3.8}$$

$$= -\, n_q \int_{n\hbar\omega}^{(n+1)\hbar\omega} D(\varepsilon)D(\varepsilon - \hbar\omega) \int_{S^2\times S^2} \mathcal{G}(\varepsilon, \varepsilon - \hbar\omega, \mathbf{u}, \mathbf{u}')f(\varepsilon - \hbar\omega, \mathbf{u}')\, d\mathbf{u}'\, d\mathbf{u}\, d\varepsilon$$

$$+\ (n_q + 1) \int_{n\hbar\omega}^{(n+1)\hbar\omega} D(\varepsilon)D(\varepsilon - \hbar\omega) \int_{S^2\times S^2} \mathcal{G}(\varepsilon, \varepsilon - \hbar\omega, \mathbf{u}', \mathbf{u})f(\varepsilon, \mathbf{u}')\, d\mathbf{u}'\, d\mathbf{u}\, d\varepsilon\,.$$

Proof. Function $\varepsilon(\mathbf{k})$ is invertible on $\mathbb{R}^+$ if considered as function of $k = |\mathbf{k}|$: $k = \sqrt{2\alpha(\varepsilon + a\varepsilon^2)}$, where $a = m^*/\hbar^2$. From now on, we will express quantities in terms of the energy ε instead of $\mathbf{k}$, having $k\,dk = 2\alpha(1+2a\varepsilon)\,d\varepsilon$ and

$$\int_{\mathbb{R}^3} \cdot\, d\mathbf{k} = \int_0^\infty k^2\,dk \int_{S^2} \cdot\, d\mathbf{u} = \int_0^\infty D(\varepsilon)\,d\varepsilon \int_{S^2} \cdot\, d\mathbf{u}$$

where $\mathbf{k} = k\mathbf{u}$, $|\mathbf{u}| = 1$ and $D(\varepsilon) = (2\alpha)^{3/2}(1+2a\varepsilon)\sqrt{\varepsilon + a\varepsilon^2}$.

Rewriting the operators in terms of ε, a straight calculation gives:

$$\int_{B_n} (-\nu(\mathbf{k})f(\mathbf{k}) + (Kf)(\mathbf{k}))\,d\mathbf{k} =$$

$$= -(n_q+1)\int_{\hbar\omega}^{n\hbar\omega} D(\varepsilon-\hbar\omega)\int_{S^2\times S^2} \mathcal{G}(\varepsilon,\varepsilon-\hbar\omega,\mathbf{u},\mathbf{u}')D(\varepsilon)f(\varepsilon,\mathbf{u})\,d\mathbf{u}\,d\mathbf{u}'\,d\varepsilon$$

$$- n_q\int_0^{n\hbar\omega} D(\varepsilon+\hbar\omega)\int_{S^2\times S^2} \mathcal{G}(\varepsilon,\varepsilon+\hbar\omega,\mathbf{u},\mathbf{u}')D(\varepsilon)f(\varepsilon,\mathbf{u})\,d\mathbf{u}\,d\mathbf{u}'\,d\varepsilon$$

$$- \int_0^{n\hbar\omega} D^2(\varepsilon)\int_{S^2\times S^2} \mathcal{G}_0(\varepsilon,\varepsilon,\mathbf{u},\mathbf{u}')f(\varepsilon,\mathbf{u})\,d\mathbf{u}\,d\mathbf{u}'\,d\varepsilon \tag{3.9}$$

$$+ (n_q+1)\int_0^{n\hbar\omega} D(\varepsilon)\int_{S^2\times S^2} \mathcal{G}(\varepsilon,\varepsilon+\hbar\omega,\mathbf{u},\mathbf{u}')D(\varepsilon+\hbar\omega)f(\varepsilon+\hbar\omega,\mathbf{u}')\,d\mathbf{u}\,d\mathbf{u}'\,d\varepsilon$$

$$+ n_q\int_{\hbar\omega}^{n\hbar\omega} D(\varepsilon)\int_{S^2\times S^2} \mathcal{G}(\varepsilon,\varepsilon-\hbar\omega,\mathbf{u},\mathbf{u}')D(\varepsilon-\hbar\omega)f(\varepsilon-\hbar\omega,\mathbf{u}')\,d\mathbf{u}\,d\mathbf{u}'\,d\varepsilon$$

$$+ \int_0^{n\hbar\omega} D^2(\varepsilon)\int_{S^2\times S^2} \mathcal{G}_0(\varepsilon,\varepsilon,\mathbf{u},\mathbf{u}')f(\varepsilon,\mathbf{u}')\,d\mathbf{u}\,d\mathbf{u}'\,d\varepsilon\,. \tag{3.10}$$

We get immediately that (3.9) + (3.10) = 0, and, shifting ε variable in the other terms in a way to have $f(\varepsilon,\mathbf{u}')$ inside the integrals and using the symmetry of the kernel $\mathcal{G}$, we obtain the r.h.s. of (3.8). Hence the lemma is completely proved. ■

Now we are able to characterize the generator T in the following way.

Theorem 3.2 *Assume that there exists $n_0 \in \mathbb{N}$ such that $\mathcal{G}$, as a function of ϵ, is a strictly positive function for $\epsilon > n_0$ and that there exists $q < 1$ such that for all $n \geq n_0$*

$$\sup_{B_{n+1}\setminus B_n} \mathcal{G}(\varepsilon,\varepsilon-\hbar\omega,\mathbf{u},\mathbf{u}') \leq q\frac{n_q+1}{n_q} \inf_{B_n\setminus B_{n-1}} \mathcal{G}(\varepsilon,\varepsilon-\hbar\omega,\mathbf{u}',\mathbf{u}), \tag{3.11}$$

then $T = \overline{-\nu I + K}$.

Proof. Following Lemma 3.1 we denote by b_n the right-hand side of (3.8). The proof of the characterization of the generator T relies on proving (3.7) of Theorem 3.1, that is, that the limit of the sequence b_n, that exists by the assumption $-\nu f + Kf \in X$, is non-negative. So, suppose on the contrary that $\lim_{n\to\infty} b_n < 0$. Then there exist n_0 and $b > 0$ such that $b_n < -b$ and the assumption (3.11) holds for all $n > n_0$. Let

$$G_n = \sup_{B_{n+1}\setminus B_n} \mathcal{G}(\varepsilon, \varepsilon - \hbar\omega, \mathbf{u}, \mathbf{u}'), \quad c_{n+1} = 4\pi \int_{S^2} \int_{n\hbar\omega}^{(n+1)\hbar\omega} D(\varepsilon) f(\varepsilon, \mathbf{u}')\, d\varepsilon d\mathbf{u}',$$

$$g_n = \inf_{B_{n+1}\setminus B_n} \mathcal{G}(\varepsilon, \varepsilon - \hbar\omega, \mathbf{u}', \mathbf{u}), \quad c_n = 4\pi \int_{S^2} \int_{n\hbar\omega}^{(n+1)\hbar\omega} D(\varepsilon - \hbar\omega) f(\varepsilon - \hbar\omega, \mathbf{u}')\, d\varepsilon d\mathbf{u}'.$$

Let $n = n_0 + k$. Then, for any $k \geq 0$, using the fact that D is an increasing function

$$b_n \geq -n_q D((n_0 + k + 1)\hbar\omega) G_{n_0+k} c_{n_0+k} + (n_q + 1) D((n_0 + k - 1)\hbar\omega) g_{n_0+k} c_{n_0+k+1}.$$

To shorten the notation we introduce $\beta_k = n_q D((n_0 + k + 1)\hbar\omega) G_{n_0+k}$, and $\alpha_k = (n_q + 1) D((n_0 + k - 2)\hbar\omega) g_{n_0+k-1}$, then, in the new notation, we have

$$0 > -b \geq b_n \geq -\beta_k c_{n_0+k} + \alpha_{k+1} c_{n_0+k+1}, \qquad \forall k \geq 0,$$

and we obtain the recurrence for c_{n_0+k+1}:

$$c_{n_0+k+1} \leq -\frac{b}{\alpha_{k+1}} + \frac{\beta_k}{\alpha_{k+1}} c_{n_0+k} \qquad \forall k \geq 0.$$

By induction, it is easy to show that

$$c_{n_0+k} \leq -bA_k + c_{n_0} B_k = B_k \left(-b \frac{A_k}{B_k} + c_{n_0} \right) \tag{3.12}$$

where

$$A_k = \frac{1}{\alpha_k} \sum_{l=1}^{k} \prod_{i=1}^{k-l} \frac{\beta_{k-i}}{\alpha_{k-i}}, \qquad B_k = \prod_{i=0}^{k-1} \frac{\beta_i}{\alpha_{i+1}}$$

and we put $\prod_{i=1}^{0} = 1$. Now it is easy to show that the sequence A_k/B_k is not divergent. In fact, if we assume $\lim_{k\to\infty} A_k/B_k = \infty$, it follows that $-b\frac{A_k}{B_k} + c_{n_0} \to -\infty$. Thus $c_{n_0+k} < 0$ for k sufficiently large; but this is impossible as by definition $c_{n_0+k} > 0$. After a simple manipulation we have

$$\frac{A_k}{B_k} = \sum_{l=0}^{k} \prod_{i=1}^{l} \frac{\alpha_i}{\beta_i},$$

hence the previous conclusion means that the series $\sum_{l=0}^{\infty} C_l = \sum_{l=0}^{\infty} \prod_{i=1}^{l} \frac{\alpha_i}{\beta_i}$ converges. The generic term of this series has the form

$$C_l = \frac{(n_q + 1) D((n_0 + l - 2)\hbar\omega) g_{n_0+l-1}}{n_q D((n_0 + l + 1)\hbar\omega) G_{n_0+l}} \cdot \ \ldots \ \cdot \frac{(n_q + 1) D((n_0 - 1)\hbar\omega) g_{n_0}}{n_q D((n_0 + 1)\hbar\omega) G_{n_0+1}}.$$

From the hypothesis there exists a $q < 1$ such that $G_{n_0+l} \leq q\frac{(n_q+1)}{n_q} g_{n_0+l-1}$ for l sufficiently large. Since $\lim_{l\to\infty} \frac{D((n_0+l-2)\hbar\omega)}{D((n_0+l+1)\hbar\omega)} = 1$, we can find $q' < 1$ such that for l sufficiently large,

$$\frac{(n_q+1)D((n_0+l-2)\hbar\omega)g_{n_0+l-1}}{n_q D((n_0+l+1)\hbar\omega)G_{n_0+l}} \geq q' > 1$$

which shows that the sum does not converge. Hence inequality (3.7) is proved and Theorem 3.1 gives the result. ■

In this paper we have studied the initial value problem (1.1) obtaining existence and uniqueness of the evolution substochastic semigroup by standard semigroup theory. In Theorem 3.1 we have proved a condition on the growth of the collision kernel $\mathcal{G}$, as function of the energy, sufficient to characterize the generator T by the closure of the physical operator $-\nu I + K$. Condition (3.11) implies that the collision kernel, as function of ϵ, belongs to the L^1 space with the weighted measure $p^\epsilon d\epsilon$, with $p < \frac{n_q}{q(n_q+1)}$. Conversely, we can observe that if the collision kernel is of a polynomial growth or behaves as p^ϵ with $p \leq \sqrt{\frac{n_q+1}{n_q}}$ for large ϵ, then condition (3.11) is satisfied.

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References

1. L. Arlotti, *Acta Applicandae Mathematicae* **23**, 129 (1991).
2. J. Banasiak, *Math. Mod. Meth. Appl. Sci.* **10**(2), 163 (2000).
3. J. Banasiak, *Math. Meth. in the Appl. Sci.* **23**, 1237 (2000).
4. J. Banasiak, *Taiwanese J. of Mathematics* **5**(1), 169 (2001).
5. J. Banasiak, *Transport Theory Stat. Phys.* (2001) (submitted).
6. T. Kato, *J. Math. Soc. Japan* **6**, 1 (1954).
7. A. Majorana and C. Milazzo, *J. Math. Anal. Appl.* **259**(2), 609 (2001).
8. A. Majorana, *Transport Theory Statist. Phys.* **20**, 261 (1991).