ARNOLD, ANTON

The Relaxation-Time von Neumann-Poisson Equation

This paper is concerned with the relaxation-time von Neumann-Poisson (or quantum Liouville-Poisson) equation in three spatial dimensions which describes the self-consistent time evolution of an open quantum mechanical system that include some relaxation mechanism. This model and the equivalent relaxation-time Wigner-Poisson system play an important role in the simulation of quantum semiconductor devices.

We prove that the evolution is a positivity preserving map, satisfying the Lindblad condition. The nonlinear evolution problem is formulated as an abstract Cauchy problem in the space of Hermitian trace class operators. For initial density matrices with finite kinetic energy we prove the global-in-time existence and uniqueness of mild solutions. A key ingredient for our analysis is a new generalization of the Lieb-Thirring inequality for density matrix operators. We also present a local convergence result towards the steady state of the system.

1. Introduction

In this paper we shall discuss the relaxation-time von Neumann-Poisson ($RT-vNP$) equation, which is the simplest physically relevant quantum mechanical model to account for electron–phonon scattering. Together with the equivalent RT-Wigner-Poisson equation, it is an important model for the numerical simulation of ultra-integrated semiconductor devices, like resonant tunneling diodes ([11], [6], [7]). Here, we will mainly focus on existence and uniqueness results for this problem in three spatial dimensions, and on the large-time behavior of its solution. For results on the (technically much simpler) RT-Wigner-Poisson system in one dimension with space-periodic boundary conditions we refer to [1].

With a constant RT $\tau > 0$ the $RT-vNP$ system is the following time evolution equation for the density matrix operator $\widehat{\rho}$, which describes the quantum mechanical state of the considered electron ensemble at each time t:

$$\begin{aligned} &i\widehat{\rho}_t = H(t)\widehat{\rho} - \widehat{\rho}H(t) - \tfrac{i}{\tau}(\widehat{\rho} - \widehat{\rho}_0), \qquad H(t) = -\tfrac{1}{2}\Delta + V(x,t), \quad t > 0, \\ &\widehat{\rho}(t=0) = \widehat{\rho}^I, \end{aligned} \tag{1}$$

with the self–consistent electrostatic potential

$$V(x,t) = \frac{1}{4\pi} \int_{\mathbb{R}^3} \frac{n(y,t)}{|x-y|} dy, \quad x \in \mathbb{R}^3. \tag{2}$$

When considering $\widehat{\rho}$ as an integral operator on $L^2(\mathbb{R}^3)$, the (non–negative) particle density $n[\widehat{\rho}]$ is (formally) obtained from the integral kernel as $n(x,t) = \rho(x,x,t)$. $\widehat{\rho}_0$ is usually chosen as a steady state of the vNP (or, equivalently, the Schrödinger–Poisson) system, and it models the state of phonons in thermodynamic equilibrium (see, e.g., [12]). The presented framework also allows to include more realistic self–consistent interaction potentials, which are important in several applications to semiconductor devices. In the simplest case, exchange-correlation potentials are of the form $V_{ex}(x,t) = -\alpha n(x,t)^{\frac{1}{3}}$, $\alpha > 0$ ([8]), and this extension of the model (1-2) will be analyzed in a subsequent paper.

The usual framework for (1) in quantum statistical mechanics is to consider $\widehat{\rho}$ as a positive, Hermitian trace class operator. For physical applications of model (1-2) one always assume $\widehat{\rho}^I \geq 0$, $\widehat{\rho}_0 \geq 0$, and $\operatorname{Tr}\widehat{\rho}^I = \operatorname{Tr}\widehat{\rho}_0 = 1$. This implies $\widehat{\rho}(t) \geq 0$, $\operatorname{Tr}\widehat{\rho}(t) = 1$ (see §2), and it allows us to verify that the open quantum system (1) is in Lindblad form [5,9]. In the sequel $(\mu_k, \varphi_k)_{k\in\mathbb{N}}$ denotes the eigenpairs of $\widehat{\rho}_0$. Since $\{\varphi_k\}_{k\in\mathbb{N}}$ is a complete o.n.s. of $L^2(\mathbb{R}^3)$, it is easy to verify that the RT-term of (1) can be represented as

$$-\frac{1}{\tau}(\widehat{\rho}\operatorname{Tr}\widehat{\rho}_0 - \widehat{\rho}_0\operatorname{Tr}\widehat{\rho}) = \sum_{j,k\in\mathbb{N}} L_{jk}^* L_{jk}\widehat{\rho} + \widehat{\rho}L_{jk}^* L_{jk} - 2L_{jk}\widehat{\rho}L_{jk}^*, \tag{3}$$

with the Lindblad operators $L_{jk} = \sqrt{\mu_k/\tau}\,|\varphi_k><\varphi_j|$. Hence, the time evolution of (1) can be physically realized through the interaction of the considered electron ensemble with some "environment". The evolution of this larger, closed quantum system (i.e., electrons + environment) is then unitary [9].

In the next Section we will sketch the existence and uniqueness analysis of the $RT - vNP$ system, and give a local convergence result towards the steady state $\widehat{\rho}_0$. For the details of the proofs we refer to [2].

2. Analysis

In this Section we will establish the existence and uniqueness of mild, global-in-time solutions to the $RT - vNP$ problem (1-2) for initial data $\widehat{\rho}^I$ having finite mass and finite kinetic energy. We remark that this equation cannot be written as a system of Schrödinger equations that are weakly coupled in terms of the potential V. In contrast to the situation in the Wigner-Poisson equation [3], the relaxation term introduces here a mixing of the 'pure quantum states', i.e., eigenvectors of $\widehat{\rho}^I$.

We first introduce the notation $\mathfrak{J}_1$ for the space of trace class operators acting on $L^2(\mathbb{R}^3)$, endowed with the norm $\|\widehat{\rho}\|_1 = \operatorname{Tr}|\widehat{\rho}|$. For a Hermitian trace class operators $\widehat{\rho}$ let $\{\lambda_j\}_{j\in\mathbb{N}}$ denote its eigenvalues, and $\{\psi_j\}_{j\in\mathbb{N}}$ its eigenfunctions, which form a complete o.n.s. in $L^2(\mathbb{R}^3)$.

We now define the particle density n and the kinetic energy E_{kin} associated with the (not necessarily positive) Hermitian operator $\widehat{\rho}$. They coincide with the usual physical notions only for 'physical quantum states', i.e., for positive operators $\widehat{\rho}$.

$$n(x) := \sum_{j\in\mathbb{N}} \lambda_j |\psi_j(x)|^2, \tag{4}$$

$$E_{\text{kin}}(\widehat{\rho}) := \frac{1}{2}\sum_{j\in\mathbb{N}} \lambda_j \|\nabla\psi_j\|_2^2 = \operatorname{Tr}\big(\,\overline{H_0^{\frac{1}{2}}\widehat{\rho} H_0^{\frac{1}{2}}}\,\big), \tag{5}$$

where $H_0 = -\frac{1}{2}\Delta$ is the free Hamiltonian. The bar in (5) denotes the extension of the operator from its original domain $H^1(\mathbb{R}^3)$ to $L^2(\mathbb{R}^3)$ (if $\widehat{\rho}$ is regular enough).

The Cauchy problem (1-2, 4) will now be considered in the (real) Banach space

$$Z := \{\widehat{\rho} \in \mathfrak{J}_1 \mid \widehat{\rho} \text{ Hermitian}, \overline{H_0^{\frac{1}{2}}\widehat{\rho} H_0^{\frac{1}{2}}} \in \mathfrak{J}_1\},$$

equipped with the norm $\|\widehat{\rho}\|_Z = \|\widehat{\rho}\|_1 + \|H_0^{\frac{1}{2}}\widehat{\rho} H_0^{\frac{1}{2}}\|_1$. The local-in-time analysis is based on considering the nonlinearity of (1),

$$F(\widehat{\rho}) = -i(V\widehat{\rho} - \widehat{\rho}V) - 1/\tau(\widehat{\rho} - \widehat{\rho}_0)$$

as a locally Lipschitz perturbation of the free evolution operator $h_0(\widehat{\rho}) = -i(\,\overline{H_0\widehat{\rho} - \widehat{\rho}H_0}\,)$ in the space Z. From the analysis in [4], Chap. XVII B, §5 it easily follows that h_0 is the infinitesimal generator of an isometric C_0 group $G_0(t)$ on Z, which has the explicit representation

$$G_0(t)\widehat{\rho} = e^{-iH_0t}\widehat{\rho}\, e^{iH_0t}.$$

The key point of the analysis is the proof that, for $\widehat{\rho}_0 \in Z$, F maps Z into itself. This is based on a new generalization of the Lieb-Thirring inequality ([2], [10]), which reads in $\mathbb{R}^3$:

$$\|n\|_q \le C_q \|\widehat{\rho}\|_1^\theta [\operatorname{Tr}(H_0^{\frac{1}{2}}|\widehat{\rho}|H_0^{\frac{1}{2}})]^{1-\theta}, \qquad 1 \le q \le 3, \qquad \theta = \frac{3-q}{2q}. \tag{6}$$

From (2) one then easily obtains the following estimate for $V = V[\widehat{\rho}]$:

$$\|V\|_\infty + \|\nabla V\|_3 + \|\Delta V\|_2 \le C\|\widehat{\rho}\|_Z, \tag{7}$$

which suffices to prove $F : Z \to Z$. By standard arguments of semigroup theory this proves existence and uniqueness of a local solution $\widehat{\rho} \in C([0, t_{\max}); Z)$.

To show that this solution exists globally in time it remains to derive *a-priori* estimates for $\|\widehat{\rho}\|_Z$.

L e m m a 1. *Let $\widehat{\rho}^I$, $\widehat{\rho}_0 \in Z$, and $\widehat{\rho}^I \ge 0$, $\widehat{\rho}_0 \ge 0$. Then, $\widehat{\rho}(t) \ge 0$ for $t \in [0, t_{\max})$, and*

$$Tr\,\widehat{\rho}(t) = e^{-\frac{t}{\tau}}\, Tr\,\widehat{\rho}^I + (1 - e^{-\frac{t}{\tau}})\, Tr\,\widehat{\rho}_0. \tag{8}$$

Proof. Using the unitary propagator $U(t,s)$ associated with the Hamiltonian $H_0 + V(t)$, we can represent the solution of (1) as

$$\widehat{\rho}(t) = e^{-\frac{t}{\tau}} U(t,0)\widehat{\rho}^I U(0,t) + \frac{1}{\tau}\int_0^t e^{-\frac{t-s}{\tau}} U(t,s)\widehat{\rho}_0 U(s,t) ds, \tag{9}$$

and the assertion follows immediately.

For the energy estimate we first introduce the potential energy of the state $\widehat{\rho}$:

$$E_{\rm pot}(\widehat{\rho}) = \frac{1}{2}\,\mathrm{Tr}\,(V[\widehat{\rho}]\widehat{\rho}) = \frac{1}{2}\|\nabla V[\widehat{\rho}]\|_2^2. \tag{10}$$

The total energy of the system is then given by $E_{\rm tot}(\widehat{\rho}) = E_{\rm kin}(\widehat{\rho}) + E_{\rm pot}(\widehat{\rho})$, and both of these terms are non-negative. If $\widehat{\rho}^I \geq 0$ and $\widehat{\rho}_0 \geq 0$ one then derives the estimate (see [2])

$$E_{\rm tot}(\widehat{\rho}(t)) \leq e^{-\frac{t}{\tau}} E_{\rm tot}(\widehat{\rho}^I) + (1 - e^{-\frac{t}{\tau}}) E_{\rm tot}(\widehat{\rho}_0). \tag{11}$$

Relations (8) and (11) show that $\|\widehat{\rho}\|_Z$ stays uniformly bounded, and we can thus formulate the main result of this Section in

Theorem 2. *Let $\widehat{\rho}^I$, $\widehat{\rho}_0 \in Z$, and $\widehat{\rho}^I \geq 0$, $\widehat{\rho}_0 \geq 0$. Then the $RT-vNP$ system (1-2) has a unique mild, global solution $\widehat{\rho} \in C_B([0,\infty); Z)$.*

We will now turn to the question of convergence $\widehat{\rho}(t) \to \widehat{\rho}_0$ as $t \to \infty$, if $\widehat{\rho}_0$ is a steady state of the vNP equation. For non-trivial steady states to exist, we have to add an external time–independent confinement potential W to the Hamiltonian in (1) (see [12]). We will assume here that it is bounded, satisfying an estimate

$$\|W\|_\infty + \|\nabla W\|_3 + \|\Delta W\|_2 \leq C_1, \tag{12}$$

and such that the self–consistent Hamiltonian $H = H_0 + V[\widehat{\rho}] + V_c$ has a non-vanishing point spectrum. The (non-unique) steady state $\widehat{\rho}_0$ will then be a linear combination of the finite number of corresponding bound states. Including such a confinement potential does not change the above analysis of (1-2). An unbounded potential W, however, would require some technical modifications and is yet an unsolved problem.

We formulate the local convergence result in

Theorem 3. *Let $\widehat{\rho}^I$, $\widehat{\rho}_0 \in Z$, and $\widehat{\rho}^I \geq 0$, $\widehat{\rho}_0 \geq 0$, and assume that $(\widehat{\rho}_0, V_0)$ is a steady state of the $RT-vNP$ equation with a bounded confinement potential W. Then $\widehat{\rho}(t) \overset{t\to\infty}{\to} \widehat{\rho}_0$ in Z for*

$$C\left[\|\widehat{\rho}^I\|_Z + \|\widehat{\rho}_0\|_Z + C_1\right] < \frac{1}{\tau}, \tag{13}$$

with some generic constant C, and C_1 from (12).

Proof. We consider the evolution equation for $\widehat{\sigma}(t) = \widehat{\rho}(t) - \widehat{\rho}_0$:

$$\widehat{\sigma}_t = h_0(\widehat{\sigma}) - i\left[V(t)\widehat{\rho} - \widehat{\rho}\,V(t) - V_0\widehat{\rho}_0 + \widehat{\rho}_0 V_0\right] - i[W\widehat{\sigma} - \widehat{\sigma}W] - \frac{1}{\tau}\widehat{\sigma}. \tag{14}$$

The idea of the proof is that for τ small enough (in comparison with the kinetic energy of the initial and steady states), the RT term compensates the quadratic term in the r.h.s. of (14). Its solution can be represented as

$$\widehat{\sigma}(t) = e^{-\frac{t}{\tau}} G_0(t)\widehat{\sigma}^I - i\int_0^t e^{-\frac{t-s}{\tau}} G_0(t-s)\left[V(s)\widehat{\rho}(s) - \widehat{\rho}(s)V(s) - V_0\widehat{\rho}_0 + \widehat{\rho}_0 V_0 + W\widehat{\sigma}(s) - \widehat{\sigma}(s)W\right] ds. \tag{15}$$

Since $G_0(t)$ is an isometry on Z, we easily estimate using (7) and (12):

$$\|\widehat{\sigma}(t)\|_Z \leq e^{-\frac{t}{\tau}}\|\widehat{\sigma}^I\|_Z + C\int_0^t e^{-\frac{t-s}{\tau}}\left[\|\widehat{\rho}(s)\|_Z + \|\widehat{\rho}_0\|_Z + C_1\right]\|\widehat{\sigma}(s)\|_Z ds.$$

The assertion then follows from $\|\widehat{\rho}(s)\|_Z \leq \|\widehat{\sigma}(s)\|_Z + \|\widehat{\rho}_0\|_Z$ and (13).

We remark that, if $\widehat{\rho}_0$ is a steady state of the vNP system, it trivially is also a steady state of (1-2) with the same confinement potential. However, the uniqueness of steady states of (1-2) is still an open problem. Consequently, the question of global convergence $\widehat{\rho}(t) \to \widehat{\rho}_0$ is yet unsolved.

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3. References

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Addresses: Anton Arnold, Purdue University, Center for Applied Mathematics, West Lafayette, IN 47907, USA.
Fachbereich Mathematik, TU-Berlin, D-10623 Berlin, Germany. *E-mail:* arnold@math.tu-berlin.de