THE QUANTUM FLOW OF ELECTRONIC TRANSPORT I: THE FINITE VOLUME CASE

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Abstract. This article provides a model for the dissipative dynamics and electronic transport in Anderson insulators. This model is based upon quantum stochastic flows which satisfy a given stochastic differential equation. The Lindblad master equation follows from a projection of the quantum flow. For fixed parameters of the model, the Gibbs state is the unique stationary state of the quantum dynamical semigroup associated to the Lindblad generator. The current produced by an applied constant electric field is computed within the linear response approach. This yields a novel expression for the DC conductivity.

Contents

1. Introduction

This work is aimed at describing a family of quantum kinetic models for dissipative transport of electrons in a solid with finite volume. An important consequence is the rigorous proof of the validity of the linear response theory leading to a formula for the electrical conductivity of a Green-Kubo type. This is a preliminary step towards a generalization of our study to the case of an infinite volume aperiodic solid.

The construction of our model follows similar lines than those currently used in Quantum Optics [1, 2, 3, 4, 5, 6, 7]. We start from an *ab initio* theory involving all degrees of freedom from both, the atom and the quantized electromagnetic field. Tracing out the degrees of freedom of the field in the corresponding Liouville-von Neumann equation, an integro-differential equation is obtained for the density matrix of the atom (Nakajima-Zwanzig equation) [7]. By using a Markov approximation and second order perturbation theory, a master equation follows [1, 2, 3, 7]. This differential equation is generally of the Lindblad type [8]. It describes the single dynamics of the atom. It has been shown that this kind of master equation appears in some specific models involving the atom alone, submitted to random time-dependent external forces (noises) [9, 10, 11, 12, 13, 14, 15]. These models involve classical stochastic noises and give rise to effective non linear stochastic Schrödinger equations. Indeed, these equations are non linear due to a re-normalization procedure introduced to keep the norm of the atomic wave packet conserved at all time. In a non-equilibrium statistical approach, one may also use equivalent linear stochastic Schrödinger equations, for which the square norm of the wave packet is conserved only after averaging over the noise [16, 17, 14, 18]. The use of stochastic Schrödinger equations is quite efficient as far as numerical computations are concerned. Indeed, let N denotes the number of relevant atomic eigenstates. Then, while the master equation is a system of N^2 coupled linear differential equations for the density matrix, within the stochastic approach instead, one is reduced to solve N equations for each realization of the noises, saving dramatically for large N both memory and computing time.

Electrons in a solid are also submitted to dissipative mechanisms, such as electron-phonon or electron-electron collisions. Similarly, a master equation may be derived too, whenever the coupling between electrons and the other degrees of freedom are small enough for perturbation theory to hold. There is, however, a major difference compared to atoms: while atoms are usually represented by a system with a finite number of levels, electrons in a solid may eventually explore an infinite lattice, requiring the use of a Hamiltonian in an infinite dimensional Hilbert space. For perfect crystals, however, a translation symmetry argument allows to reduce the problem to a finite number of bands, leading to a situation analogous to that of Quantum Optics. For aperiodic solids, no translation symmetry survives in general, so that the infinite volume limit becomes more involved.

In a series of previous works [19, 20, 16, 17, 21], kinetic models were proposed, along the lines of the Drude [22] and Lorentz models [23], in which the dissipation mechanism was represented through a classical external time-dependent noise. The Relaxation Time Approximation (RTA) was first investigated in [19] giving rise to a Kubo formula that was used to analyze the width of plateaux in the Integer Quantum Hall Effect, and in [20] to analyze the effect of anomalous transport arising in quasicrystals [24]. In [16], the kinetic model was fully developed for the impurity band electrons in a semiconductor. It was proved that the instantaneous random evolution operators exist and are almost surely unbounded at the infinite volume limit, even though the evolution is square-norm preserving after averaging over the noise.

In the present work, the classical noises are replaced by their quantum counterpart, following the ideas developed in Noncommutative Stochastic Calculus [25, 26]. For indeed, the master equation of Lindblad type may be obtained from a Schrödinger equation with a quantum noise as will be shown here. This fact has been put forward in Quantum Optics by Gardiner and Collet [27] (see [3]). This leads to the characterization of the so-called *Quantum Flow*, from which the *Quantum Dynamical Semigroup* is obtained by taking the average. The Quantum Dynamical Semigroup has a generator of the Lindblad type [8], which is the adjoint of the generator appearing in the master equation. The main advantages of this approach are two. First, the instantaneous evolution is unitary at all time, making the mathematical analysis much easier. This is because the degrees of freedom that are the source of dissipation in the real problem, are represented here by a Bose gas of virtual particles driven by the same master equation. Secondly, since Poisson and Wiener processes can be all obtained from quantum noises defined over a suitable Fock space [25, 26], all previous stochastic Schrödinger equations involving classical noises are contained in the quantum stochastic differential equation (see also [28]). As long as quantum computing is not available, this quantum stochastic differential equation approach will however not be efficient in numerical calculations!

We focus ourselves on a specific family of models which are physically relevant for transport in disordered solids in the strong localization regime (Anderson insulators) [29]. It is known that the electronic spectrum in such solids is pure point near the Fermi energy and the corresponding eigenfunctions are exponentially localized, even in the infinite volume limit [30, 31]. The electrons are coupled to low energy acoustic phonons. If an electric field is applied, this coupling induces electronic hopping from one localized state into another (hopping transport). The corresponding Lindblad equation is similar to the Quantum Optical Master Equation [21], although it is more conveniently written in the second quantization framework.

This paper is organized as follows. We start by motivating our model by some heuristic considerations on open quantum systems in section 2. These are well known results, connected with the derivation of master equations, which throw light on the underlying physical approximations. Section 3 provides the mathematical framework of our analysis and introduce our model. The specific quantum flow and its average, the quantum dynamical semigroup, are obtained in the foregoing section. The generator of the semigroup yields the master equation in Lindblad form. The analysis of the equilibrium and stationary states is the subject of the fifth section. The final section is devoted to the computation of the conductivity in our model.

2. Heuristics

This section is devoted to a brief review of the basic ideas and different approximations involved from *ab initio* in the derivation of master equations for open quantum systems coupled to infinite reservoirs. Excellent books on the subject are available where the reader can find more details (see e.g. [7, 1, 3, 32]). Even though, for the sake of clarity we feel necessary to state here our basic approximations and assumptions on times scales, to precise for which physical systems the kinetic models of the next section could be relevant.

2.1. **Starting from Quantum Statistical Mechanics.** Within the framework of Algebraic Field Theory in Quantum Statistical Mechanics [33, 34], a quantum system S is described by its C^*-algebra $\mathcal{A}$ of observables, which will be unital. One of the basic facts of Statistical Mechanics is that there are conserved quantities beside the total energy, such as the number of particles of a given species, the volume, or the total momentum. In the algebraic framework, these conserved quantities are the infinitesimal generators of a locally compact Lie group G, called the *gauge group* acting on $\mathcal{A}$ via automorphisms, $g \in G \mapsto \theta_g \in \mathrm{Aut}(\mathcal{A})$. The conservation of these physical quantities is then expressed by demanding that G be a symmetry of the evolution, namely $\alpha_t^{(S)} \circ \theta_g = \theta_g \circ \alpha_t^{(S)}$ for all $t \in \mathbb{R}$, $g \in G$, where $\alpha_t^{(S)}$ is the 1-parameter group of automorphisms of $\mathcal{A}$ associated to the time evolution. It is convenient to consider the time itself as one component of G, so that $\theta_{(t,0)} = \alpha_t^{(S)}$. The corresponding conserved quantity is the total energy. In most applications, G can be taken as an Abelian group of the form $G = \mathbb{R}^l \times \mathbb{T}^m$, where the first l component correspond to first integrals which are continuous whereas the m others correspond to the discrete ones. In such case, it is meaningful to consider holomorphic continuation of θ in the complexification of G. Then $\mathcal{A}^{(0)}$ will denote a dense subalgebra made of elements $A \in \mathcal{A}$ such that the map $g \in G \mapsto \theta_g(A) \in \mathcal{A}^{(0)}$ can be continued as an entire holomorphic function on $\mathbb{C}_{l,m} = \mathbb{C}^l \times (\mathbb{T} + i\mathbb{R})^m$. The equilibrium state of S is described by a KMS state. Namely, it is a G-invariant state ω on $\mathcal{A}$ for which there exists $\beta \in \mathbb{R}_+^{l+m}$ and, for any A, $B \in \mathcal{A}^{(0)}$, a function $F_{A,B}(z)$ holomorphic and bounded in the strip $\{z \in \mathbb{C}_{l,m}; 0 < \Im(z_i) < \beta_i, i = 1, \dots, l+m\}$, such that

$$F_{A,B}(g) = \omega(A\theta_g(B)), \qquad F_{A,B}(g + i\beta) = \omega(\theta_g(B)A), \qquad g \in G\,.$$

The parameters $\beta = (\beta_1, \cdots, \beta_{l+m})$ are the Lagrange multipliers associated to the conserved quantities, such as the inverse temperature $1/k_B T$ (k_B is the Boltzmann constant), the chemical potential μ, the pressure, etc...)

In the particular situation investigated in this work, the system S is an open system that is, it interacts with thermal baths generically denoted B. An evolution towards a non equilibrium steady state is created by turning on, at initial time, some external forces, which may depend on time and space, and/or by creating a gradient in the family of Lagrange multipliers β defining the equilibrium of the system. In practice, such a gradient is usually created by coupling the system to two or more thermal bath with different values of β. The C^*-algebra of observables for the total system $S \cup B$ is the tensor product $\mathcal{A} \otimes \bigotimes_r \mathcal{B}_r$ of the observable algebras $\mathcal{A}$ of the system and $\mathcal{B}_r$ of each bath. The quantum evolution of the system and the family of baths is described through a 1-parameter group of automorphisms $t \in \mathbb{R} \mapsto \alpha_t \in \mathrm{Aut}(\mathcal{A} \otimes \mathcal{B})$. The automorphisms could include external forces, denoted $\mathcal{E}$, in some cases. If the external forces depend on time, the new evolution is no longer a group, but it is a 2-parameters family of automorphisms $\alpha_{t,s}$ such that:

1. $\alpha_{t,s} \in \mathrm{Aut}(\mathcal{A} \otimes \mathcal{B})$ for all $t, s \in \mathbb{R}$.
2. $\alpha_{s,s} = id$ for all $s \in \mathbb{R}$.
3. $\alpha_{t,s} = \alpha_{t,u} \circ \alpha_{u,s}$ for all $t, u, s \in \mathbb{R}$.

The equilibrium state of the bath is the tensor product $\omega^{(B)} = \bigotimes_r \omega_{\beta^{(r)}}^{(B_r)}$ of the KMS state of each bath with Lagrange multipliers $\beta^{(r)}$. These Lagrange multipliers may also depend on time. Starting at time t_0, the state $\omega_0^{(S\cup B)} = \omega_\beta^{(S)} \otimes \omega_\beta^{(B)}$, is transformed into $\omega_0^{(S\cup B)} \circ \alpha_{t,t_0}$ at time t.

2.2. **The Markov approximation.** The next step consists in restricting the evolution to the system S only. In the Heisenberg picture, this can be done by defining the unity-preserving linear maps Φ_{t,t_0} from $\mathcal{A}$ into itself such that, for any $A \in \mathcal{A}$,

$$\omega_\beta^{(S)} \circ \Phi_{t,t_0}(A) = \omega_0^{(S\cup B)} \circ \alpha_{t,t_0}(A \otimes \mathbf{1})\,. \tag{2.1}$$

The evolution of the observables is given by $A(t) = \Phi_{t,t_0}(A(t_0))$. As shown by Kraus [35], Φ_{t,t_0} is a *completely positive map* for any $t \geq t_0$. Namely, for any matrix $\hat{A} = (A_{i,j})_{i,j=1}^n$, the matrix $(\Phi_{t,t_0}((\hat{A}^*\hat{A})_{i,j}))_{i,j=1}^n$ is positive in $\mathcal{A} \otimes M_n(\mathbb{C})$. In general, Φ_{t,t_0} is not an automorphism of $\mathcal{A}$ and do not satisfy the property (3) above.

To go forward, it is necessary to discuss more precisely the physical situation. For indeed, different time scales can be well distinguished in practice. The shortest one is the *correlation time τ_c of the bath*, also called the memory time. This time is of the order of, or is greater than $\hbar/(k_B T)$. It depends only on the bath and on its interaction Hamiltonian with S (see [1]). For times $t - t_0$ much bigger than τ_c, one can neglect memory effects [7] and approximate the evolution Φ_{t,t_0} by some linear maps $\Phi_{t,t_0}^{(M)} : \mathcal{A} \to \mathcal{A}$ satisfying the properties (2) and (3) above for any $t \geq u \geq s$. This approximation is called the *Markov approximation*. Clearly, $\Phi_{t,t_0}^{(M)}$ must be completely positive for times $t - t_0 \gg \tau_c$, but its positivity could fail for times $t - t_0 \simeq \tau_c$ for which the Markov approximation is not valid [36]. The evolution of observables for times $t - t_0 \gg \tau_c$ is described via a linear master equation :

$$\frac{dA}{dt}(t) = \mathcal{L}_t(A(t))\,, \tag{2.2}$$

where $\mathcal{L}_t$ is the generator of the Markov evolution. In concrete cases, $\mathcal{L}_t$ is often computed to lowest order in the system-bath coupling constant λ, starting from the Nakajima-Zwanzig equations and using a "Markov-Born" approximation (see [7] and references therein). This approximation is valid provided $\lambda\tau_c \ll \hbar$. If time-dependent forces are applied, one must assume that the $x_i \in \Lambda$ and $x_j \in \Lambda$ typical variation time $\Delta t_{\mathcal{E}}$ of these forces is much bigger than τ_c. Then the generator $\mathcal{L}_t$ depends on time t. Let $\alpha_{t,t_0}^{(S)}$ be the two-parameter group of automorphisms of $\mathcal{A}$ describing the evolution of the system S uncoupled to the baths and $H(t)$ be the associated Hamiltonian (the time argument indicates that time-dependent external forces must be included). One can always write $\mathcal{L}_t$ as the sum of the generator $\mathcal{L}_{H(t)}$ of $\alpha_{t,t_0}^{(S)}$ and of a *dissipative generator* $\mathcal{D}_t$ describing the effect of the baths on the dynamics of S,

$$\mathcal{L}_t(A) = \mathcal{L}_{H(t)} + \mathcal{D}_t(A)\ , \qquad \mathcal{L}_{H(t)}(A) = i[H(t), A]\,.$$

By the time-dependent version of Lindblad's theorem [8, 37], if $\mathcal{A}$ is the von Neumann algebra of all bounded operators on a given Hilbert space, the unity preserving maps $\Phi_{t,t_0}^{(M)}$ are completely positive and ultraweakly continuous (normal) for any $t \geq t_0$ and $(t, t_0) \mapsto \Phi_{t,t_0}^{(M)}(A)$ is ultraweakly continuous for any $A \in \mathcal{A}$, and $\mathcal{D}_t$ can be written in the canonical Lindblad form, namely there exist some operators $L_\ell(t)$ acting on the Hilbert space such that:

$$\mathcal{D}_t(A) = \sum_\ell \Big(L_\ell^*(t) A L_\ell(t) - \frac{1}{2} L_\ell^*(t) L_\ell(t) A - \frac{1}{2} A\, L_\ell^*(t) L_\ell(t) \Big)\,. \tag{2.3}$$

In general, the bath is also responsible for some renormalization of the energies of S (e.g. the Lamb shift in Quantum Optics), even though, this effect can always be included in $H(t)$.

2.3. **The adiabatic approximation.** Other relevant time scales are given by the *Heisenberg time* $\tau_{H(t)} = \hbar/\Delta E(t)$, where $\Delta E(t)$ is the typical energy interval between nearest eigenvalues of $H(t)$, and by the typical *relaxation time* τ_{rel} of the system. That time is the typical rate of variation of a state of the system under the dissipative generator $(\mathcal{D}_t)_*$. In the perturbative regime $\lambda\tau_c \ll \hbar$, τ_{rel} is of order $\hbar^2\lambda^{-2}\tau_c^{-1}$ and is much bigger than τ_c [1]. If the Hamiltonian $H(t)$ have a discrete spectrum, λ is small enough and the force variation time $\Delta t_{\mathcal{E}}$ big enough for the inequalities

$$\tau_{H(t)} \ll \tau_{rel}\ , \qquad \tau_{H(t)} \ll \Delta t_{\mathcal{E}}$$

to hold for any $t \geq 0$, one can further simplify (2.2) by means of an adiabatic approximation. This approximation is performed by making a local averaging in time as follows. Let δt be a time interval satisfying:

$$\sup_{t\geq 0} \tau_{H(t)} \ll \delta t \ll \tau_{rel}\ , \qquad \delta t \ll \Delta t_{\mathcal{E}}\,. \tag{2.4}$$

One writes equation (2.2) in the interaction picture by defining :

$$\tilde{A}_t(s) = e^{-(t-s)\mathcal{L}_{H(s)}} A(s)\,.$$

Then the variation $\delta\tilde{A}_t$ of $\tilde{A}(s)$ between t and $t+\delta t$ is given by :

$$\frac{\delta\tilde{A}_t}{\delta t} = \int_t^{t+\delta t} \frac{ds}{\delta t}\Big(e^{-(s-t)\mathcal{L}_{H(s)}}\mathcal{D}_s\, e^{(s-t)\mathcal{L}_{H(s)}}\tilde{A}_t(s) - (s-t)\frac{d\mathcal{L}_{H(s)}}{ds}\tilde{A}_t(s)\Big)\,.$$

Since $\tilde{A}_t(s)$ and $H(s)$ vary in time respectively on scales τ_{rel} and $\Delta t_{\mathcal{E}}$ much bigger than δt one can replace, up to a small error, $\tilde{A}(s)$ and $H(s)$ in the integrand by their values at $s=t$. The last term inside the parenthesis is of order $\delta t/\Delta t_{\mathcal{E}}$ and can be neglected with respect to the first. Thus:

$$\frac{\delta\tilde{A}_t}{\delta t} \simeq \int_0^{\delta t} \frac{ds}{\delta t}\, e^{-s\mathcal{L}_{H(t)}}\mathcal{D}_t\, e^{s\mathcal{L}_{H(t)}} A(t)\,. \tag{2.5}$$

If one is only interested in the evolution of the observable A on the time scale δt, one can approximate the left hand side by the exact derivation $d\tilde{A}/ds|_t = -\mathcal{L}_{H(t)}A(t) + dA/dt$ (coarse graining in time). The last step consists in letting δt (or, more precisely, $\delta t/\tau_{H(t)}$) tend to infinity in the right hand side of (2.5). The error in doing so is small, because the matrix elements of the integrand in the basis of eigenvectors of $H(t)$ are constant or oscillating functions of s with period $\tau_{H(t)} \gg \delta t$ or more. Therefore, the separation of time scales (2.4) allows to approximate the master equation(2.2) by the often simpler expression:

$$\frac{dA}{dt} = \mathcal{L}_t^{(ad)} A(t)\ , \qquad \mathcal{L}_t^{(ad)} = \mathcal{L}_{H(t)} + \widetilde{\mathcal{D}}_t\,, \tag{2.6}$$

where

$$\widetilde{\mathcal{D}}_t = \lim_{\delta t\to\infty}\int_0^{\delta t}\frac{ds}{\delta t}\, e^{-s\mathcal{L}_{H(t)}}\mathcal{D}_s\, e^{s\mathcal{L}_{H(t)}}\ ,\ \mathcal{L} \in \mathcal{B}(\mathcal{A})\,. \tag{2.7}$$

We do not enter here into the mathematical details about the topology involved in this definition (a more precise analysis is postponed for a separate publication).

The adiabatic approximation is thus equivalent to replace the generator $\mathcal{L}_t = \mathcal{L}_{H(t)} + \mathcal{D}_t$ by $\widetilde{\mathcal{L}}_t = \mathcal{L}_{H(t)} + \widetilde{\mathcal{D}}_t$. The dissipative part $\widetilde{\mathcal{D}}_t$ is of Lindblad form (2.3) even if $\mathcal{D}_t$ is not (i.e., if $\Phi^{(M)}_{t,t_0}$ violate positivity for $t - t_0 \simeq \tau_c$). It is clear from (2.7) that $\mathcal{L}_{H(t)}$ and $\widetilde{\mathcal{L}}_t$ commute.

Definition 2.1. A generator $\mathcal{L}$ of a quantum dynamical semigroup is said to be adiabatic with respect to $\mathcal{L}_H = i[H, \cdot]$ if $\mathcal{L} \circ \mathcal{L}_H = \mathcal{L}_H \circ \mathcal{L}$.

Thus, the system S coupled to the baths B_r can be described by an adiabatic generator if the time scales of the problem are such that :

$$\tau_c \ll \delta t \ll \Delta t_{\mathcal{E}} \ , \qquad \sup_{t \geq 0} \tau_{H(t)} \ll \delta t \ll \tau_{rel} \ , \tag{2.8}$$

and if the derivative dA/dt in eq. (2.6) is understood as a coarse-grained rate of variation $\delta A/\delta t$ on the time scale δt.

The second inequality in (2.8) can never be satisfied in any macroscopic solid, since $\tau_{H(t)}$ tends to zero in the thermodynamic limits. However, the adiabatic approximation still holds if any pair of eigenfunctions of $H(t)$, associated with eigenvalues whose difference is of the order of, or less than $\hbar/\delta t$, are nearly uncoupled by the dissipative generator $(\mathcal{D}_t)_*$. This situation is realized at very low temperature in disordered solids in the Anderson localization regime. Indeed, the spectrum of H is pure point at the infinite volume limit and its eigenfunctions are exponentially localized in this regime [31]. Lack of symmetry makes degeneracies highly improbable, so that one can ignore the effect of weak external forces on the spectrum, at least at finite volume. The probability of bath-driven transition from an eigenfunction into another is exponentially small with the distance between the two localization centers [29]. As a consequence of the finite density of states at the Fermi level, eigenfunctions associated to close eigenvalues around the Fermi energy are localized far apart. Thus, matrix elements of the right hand side of (2.5) between two eigenfunctions with eigenvalues very close to each other can be neglected. A more quantitative analysis in the variable range hopping regime shows that the adiabatic approximation is indeed valid at low enough temperatures [21]. On the other hand, for disordered or perfect metals and perfect quasicrystals, the eigenfunctions are not exponentially localized and the adiabatic approximation leading to (2.6) is expected to fail.

2.4. **The current and the conductivity.** The aim of linear transport theory is the study of the average value of observables $\omega^{(S)}_\beta(A(t))$ or of their derivative (currents) in the limit of weak external forces and/or gradients. To be specific, let S be a finite system composed of charge carriers, of charge q, coupled to two baths of chemical potentials $\mu_\diamond$, $\mu_\star$, respectively. At $t = 0$, these two chemical potentials coincide and S is at equilibrium. For $t > 0$ they evolve towards different values. Let us study the response of S to an external time-dependent electric field $\mathcal{E}(t)$ applied at $t = 0$. The time-dependent Hamiltonian is $\hat{H}(t) = \hat{H}(0) - q\,\mathcal{E}(t)\,\hat{X}$, where $\hat{H}(0)$ and $\hat{X}$ are respectively the Hamiltonian of S in absence of field and the position operator of the charge carriers in second quantization. The evolution is given by an adiabatic quantum dynamical semigroup whose generator is $\mathcal{L}$. Charge transport can only occur in a finite sample if there are exchanges of carriers with the baths. Therefore it makes sense to separate $\mathcal{L}$ into two parts:

$$\mathcal{L}_t = \mathcal{L}^{(int)}_t + \mathcal{L}^{(ext)}_t = \mathcal{L}_{\hat{H}(t)} + \mathcal{D}^{(int)}_t + \mathcal{D}^{(ext)}_t \ ,$$

where $\mathcal{D}_t^{(int)}$ corresponds to the dissipative evolution which keeps the number of particles in S unchanged, while $\mathcal{D}_t^{(ext)}$ instead, involves a variation in the number of particles in S. In other words, $\mathcal{D}_t^{(int)}$ is a generator characterized by operators L_ℓ which commute with the number operator $\hat{N}$, and $\mathcal{D}_t^{(ext)}$ is the remaining part; $\mathcal{L}_t = \mathcal{L}_{\hat{H}(t)} + \mathcal{D}_t^{(int)}$.

The adiabatic current operator is:

$$\hat{J}^{ad}(t) = q \left. \frac{\delta \hat{X}(t)}{\delta t} \right|_{int} = q\, \Phi_{t,0} \circ \mathcal{L}_t^{(int)}(\hat{X}) . \tag{2.9}$$

If one uses the adiabatic master equation (2.6) for the evolution of observables, the coarse grained velocity $\delta \hat{X}/\delta t = \mathcal{L}_t^{(int)}(\hat{X})$ must be used to compute the current, instead of the usual "instantaneous" velocity $d\hat{X}/dt = i[\hat{H}(t), \hat{X}] = \mathcal{L}_{\hat{H}}(\hat{X})$. $\hat{J}^{ad}(t)$ is only defined for systems with finite volume V. In the thermodynamic limit, the limit of $\hat{J}^{ad}(t)/V$ as $V \uparrow \mathbb{R}^d$ should be studied. The current density at time t is [21]:

$$j(t) = \omega_\beta^{(S)}(\hat{J}^{ad}(t)) = \omega_\beta^{(S)} \circ \Phi_{t,0}\big(\mathcal{L}_t^{(int)}(\hat{X})\big) . \tag{2.10}$$

In section 6, we will be interested in the DC current, i.e, to the case of an applied electric field $\mathcal{E}(t)$ growing rapidly after $t = 0$ and attaining a constant value $\mathcal{E}$ for $t \geq \Delta t_{\mathcal{E}} > 0$, where $\Delta t_{\mathcal{E}}$ satisfies (2.8). Similarly, the difference $\mu_\star - \mu_\diamond$ between the chemical potentials of the two baths is assumed to be constant after a fixed time which is supposed to be $>> \delta t$. More precisely, one assumes that $f(t)$ is a uniformly increasing function equal to 1 for $t > \Delta t_{\mathcal{E}}$. The steady-state current density is:

$$j = \lim_{T\to\infty} \frac{1}{T} \int_0^T \omega_\beta^{(S)} \circ \big(\Phi_{\mathcal{E},\mu_\diamond,\mu_\star}\big)_t \big(\mathcal{L}_{\mathcal{E}}^{(int)}(\hat{X}) dt\big) . \tag{2.11}$$

Here $\Phi^{\mathcal{E},\mu_\diamond,\mu_\star}$ is the quantum dynamical semigroup of generator $\mathcal{L}_{\mathcal{E},\mu_\diamond,\mu_\star} = \mathcal{L}_{\mathcal{E}}^{(int)} + \mathcal{L}_{\mathcal{E},\mu_\diamond,\mu_\star}^{(ext)}$ describing the adiabatic Markovian evolution of the system submitted to the (time-independent) electric field $\mathcal{E}$ and coupled to the two bath of chemical potential $\mu_\diamond$, $\mu_\star$.

3. Introducing the model

3.1. **Preliminary notations.** Consider a fixed finite lattice $\Lambda \subset \mathbb{Z}^d$ and let denote $\mathfrak{h}^1 = \mathbb{C}^\Lambda$ the complex finite-dimensional Hilbert space used to represent a single electron on this lattice, in the tight binding representation. Throughout this paper, the customary notation $\mathcal{B}(\mathfrak{h}^1)$ will be used for the algebra of all bounded linear operators on the given Hilbert space $\mathfrak{h}^1$. We now go through the second quantization procedure on the Fermi-Fock space $\Gamma_f(\mathfrak{h}^1)$ [33]. We denote $|0\rangle$ the vacuum vector in $\Gamma_f(\mathfrak{h}^1)$. Given $\psi \in \mathfrak{h}^1$, the associated *creation* (respectively *annihilation*) operator on $\Gamma_f(\mathfrak{h}^1)$ is denoted $c^\dagger(\psi)$ (resp. $c(\psi)$). To simplify notations we simply write $c_i^\dagger = c^\dagger(\psi_i)$, $c_i = c(\psi_i)$, for all $i \in I$. The second quantization of a given self-adjoint operator $B \in \mathcal{B}(\mathfrak{h}^1)$ is self-adjoint and denoted $\hat{B}$:

$$\hat{B} = \sum_{i,j} \langle \psi_j, B\psi_i \rangle c_j^\dagger c_i \ \in \mathcal{B}(\Gamma_f(\mathfrak{h}^1)).$$

The space $\Gamma_f(\mathfrak{h}^1)$ will be referred from now on as the *initial space* for the dynamics.

3.2. **Describing the dynamics.** The electrons on the lattice Λ are coupled with two baths denoted $\star$ and $\diamond$, which have the same inverse temperature β but may have different chemical potentials $\mu_\star$ and $\mu_\diamond$. To describe the dynamics of the electrons, we will consider three main dynamical phenomena. Firstly, the Hamiltonian dynamics. Secondly, the dissipative effects due to the coupling of electrons with phonons. Thirdly, the exchanges of electrons between the system and the baths.

The non dissipative dynamics of the single particle is described by a *bare* Hamiltonian H acting on $\mathfrak{h}^1$, which has a set of eigenvectors $(\psi_i)_{i\in I}$ where I is a finite set of indexes, with corresponding eigenvalues $(E_i)_{i\in I}$. The second quantized $\hat{H}$ of H,

$$\hat{H} = \sum_{i\in I} E_i c_i^\dagger c_i, \tag{3.1}$$

describes the Hamiltonian dynamics of the whole system of electrons. The self-adjoint bounded operator $\hat{H}$ has an orthonormal basis of eigenvectors in $\Gamma_f(\mathfrak{h}^1)$, which we construct as follows. Call $\mathcal{C} = \{0,1\}^I$ the set of *configurations* (also known as the set of *occupation numbers*). Given any $\eta = (\eta_i)_{i\in I} \in \mathcal{C}$, the vector

$$|\eta\rangle = \prod_{i\in I} c_i^{\dagger\eta_i}|0\rangle, \tag{3.2}$$

is an eigenvector of $\hat{H}$. It is convenient to add two indices $\star \notin I$ and $\diamondsuit \notin I$ referring to the two baths, to the set I labelling the eigenstates of H. Call $L = (I \cup \{\star,\diamondsuit\}) \times (I \cup \{\star,\diamondsuit\})$. Each couple $\ell = (i,j) \in L$ will be interpreted as an oriented segment, labeling a transition from i to j.

The description of the dissipative effects and the exchanges of electrons with the baths are obtained by means of the collection of *jump operators* $C_{i,j}$, and the corresponding *jump rates* $\gamma_{i,j} \geq 0$. The jump operators are defined on the space $\Gamma_f(\mathfrak{h}^1)$ as follows:

$$C_{i,j} = \begin{cases} c_j^\dagger c_i & \text{if } i,j \in I,\ i \neq j \\ c_j^\dagger & \text{if } i \in \{\diamond,\star\},\ j \in I \\ c_i & \text{if } i \in I,\ j \in \{\diamond,\star\} \\ 0 & \text{otherwise.} \end{cases} \tag{3.3}$$

The jump rates $\gamma_{i,j}$ will be supposed to satisfy the following detailed balance hypothesis:

$$\gamma_{i,j} = e^{\beta(E_i - E_j)}\gamma_{j,i} \tag{3.4}$$

$$\gamma_{\star,j} = e^{-\beta(E_j - \mu_\star)}\gamma_{j,\star} \tag{3.5}$$

$$\gamma_{\diamond,j} = e^{-\beta(E_j - \mu_\diamond)}\gamma_{j,\diamond} \tag{3.6}$$

for $i,j \in I,\ i \neq j$.

The quantum evolution is given via a *quantum cocycle* $(U(t))_{t\geq\mathbb{R}_+}$, defined on $\mathcal{B}(\mathfrak{H})$, that we will characterize in differential form according to the following steps.

- Firstly, the jump operators $C_{i,j}$ will be used to model the action of both the coupling with phonons and the loss or gain of electrons in the baths. If $i,j \in I$, $C_{i,j}$ implement a quantum jump of one electron from an eigenfunction ψ_i into another ψ_j. If i or $j \in \{\star,\diamond\}$, $C_{i,j}$ implement a loss or a gain of an electron in the baths. The probability per unit of time that a jump $\ell = (i,j)$ occurs is given by the jump rates $\gamma_{i,j}$.

- Secondly, the evolution includes stochastic terms which will be expressed through *quantum noises*, namely, by bosonic creation and annihilation operator, $A_\ell^\dagger(t)$ and $A_\ell(t)$ respectively, depending on the time t and on $\ell = (i,j)$. These stochastic terms represent a Bose gas of virtual particles which mimics the effects of both the phonons and the baths on the electrons.
- Thirdly, $\hat{H}$, $C_{i,j}$ and $\gamma_{i,j}$ determine a unique quantum cocycle $(U(t))_{t\geq 0}$, which is the solution of the *quantum stochastic differential equation* (QSDE):

$$dU(t) = \left[\left(-i\hat{H} + \hat{K}\right) dt + \sum_\ell \left(L_\ell^*\, dA_\ell(t) - L_\ell\, dA_\ell^\dagger(t)\right)\right] U(t), \tag{3.7}$$

  with:

$$L_\ell = \sqrt{\gamma_\ell}\, C_\ell,\ \ (\ell \in L) \tag{3.8}$$

  and

$$\hat{K} = -\frac{1}{2}\sum_\ell L_\ell^* L_\ell = -\frac{1}{2}\sum_\ell \gamma_\ell\, C_\ell^* C_\ell. \tag{3.9}$$

  The evolution operators $U(t)$ are bounded on the bigger space:

$$\mathfrak{H} = \Gamma_f(\mathfrak{h}^1) \otimes \Gamma_b(L^2(\mathbb{R}_+, \mathbb{C}^L)),$$

  where the symbol $\Gamma_b(\cdot)$ is used for the Boson-Fock space.
- The cocycle determines a *quantum flow* $B \mapsto k_t(B)$ from $\mathcal{B}(\Gamma_f(\mathfrak{h}^1))$ into $\mathcal{B}(\mathfrak{H})$. The projection of this flow on the algebra $\mathcal{B}(\Gamma_f(\mathfrak{h}^1))$ gives the *quantum dynamical (or Markov) semigroup* used to describe the averaged dynamics. This semigroup has an infinitesimal generator expressed in Lindblad form (see [8]).

3.3. **Physical discussion.** In this paper we are concerned with a disordered solid of finite volume in the strong localization regime (Anderson insulator). The one-electron Hamiltonian H is e.g. given by the Anderson Hamiltonian:

$$H = \sum_{x\in\Lambda} \epsilon_x |x\rangle\langle x| + \sum_{x,y\in\Lambda, x,y \text{ n.n.}} t_{xy} |x\rangle\langle y|,$$

where $|x\rangle$, $(x \in \Lambda)$ are the canonical basis vectors, t_{xy} are hopping terms between nearest neighbors $x, y \in \Lambda$, and ϵ_x, $(x \in \Lambda)$ are independent identically distributed random energies. The randomness of ϵ_x is due to disorder in the solid and must be distinguished from the randomness introduced above, which describes dissipative effects. It is well-known [30, 31] that, if the disorder is strong enough (i.e., if $\langle \Delta\epsilon_x^2\rangle / t_{xy}$ is large enough), the eigenfunctions ψ_i of H with energies close to the Fermi energy μ are exponentially localized. As a result, the jump rates $\gamma_{i,j}$ decrease exponentially with the distance $|x_i - x_j|$ between their localization centers $x_i \in \Lambda$ and $x_j \in \Lambda$. The two baths are considered to be connected to the solid through two electric wires. This induces the existence of two privileged wavefunctions $\psi_{i(\star)}$ and $\psi_{i(\diamond)}$, whose localization centers $x_{i(\star)}$ and $x_{i(\diamond)}$ are closer to the wires than those of the other wavefunctions. The rates $\gamma_{i,\star}$ and $\gamma_{i,\diamond}$, $i \in I$, decrease exponentially with the distance between x_i and the wires. Hence the rates $\gamma_{i(\star),\star}$ and $\gamma_{i(\diamond),\diamond}$ are much bigger than the other rates $\gamma_{i,\star}$ and $\gamma_{i,\diamond}$, respectively.

3.4. **The basic spaces.** Consider the Boson-Fock space $\Gamma_b(L^2(\mathbb{R}_+,\mathbb{C}^L))$. We denote coherent vectors there by the symbol $e(f)$, where $f \in L^2(\mathbb{R}_+,\mathbb{C}^L)$, that is

$$e(f) = \sum_{n\geq 0} \frac{1}{\sqrt{n!}} f^{\otimes n}.$$

Moreover, we denote $(\delta_\ell;\ \ell \in L)$ an orthonormal basis of $\mathbb{C}^L$.

As we mentioned before, the total Hilbert space for the evolution is $\mathfrak{H} = \Gamma_f(\mathfrak{h}^1)\otimes\Gamma_b(L^2(\mathbb{R}_+,\mathbb{C}^L))$. The space $\mathfrak{H}$ is generated by vectors of the form $\Psi\otimes e(f)$, $(\Psi \in \Gamma_f(\mathfrak{h}^1),\ f \in L^2(\mathbb{R}_+,\mathbb{C}^L))$. Furthermore, given a set A, the notation 1_A is used for the characteristic function of the set A. Given any $\Psi \in \Gamma_f(\mathfrak{h}^1)$ and $f \in L^2(\mathbb{R}_+,\mathbb{C}^L)$, the elements of the form $\Psi \otimes e(f1_{[0,t]})$ generate the space:

$$\mathfrak{H}_{t]} = \Gamma_f(\mathfrak{h}^1) \otimes \Gamma_b(L^2([0,t],\mathbb{C}^L)),\ (t \geq 0).$$

$\mathfrak{H}$ has the *continuous tensor product property*, i.e.

$$\mathfrak{H} = \mathfrak{H}_{t]} \otimes \mathfrak{H}_{[t},$$

where $\mathfrak{H}_{[t} = \Gamma_b(L^2([t,\infty[,\mathbb{C}^L))$. For any $t \geq 0$, the algebra of all linear bounded operators on $\mathfrak{H}_{t]}$ is denoted $\mathcal{B}_t = \mathcal{B}(\mathfrak{H}_{t]})$. Any element $x_t \in \mathfrak{H}_{t]}$ will be identified with $x_t \otimes e(0_{[t}) \in \mathfrak{H}$, where $e(0_{[t})$ is the vacuum in $\mathfrak{H}_{[t}$. Similarly, any operator $B_t \in \mathcal{B}_t$ will be identified with $B_t \otimes \mathbf{1}_{[t}$, where $\mathbf{1}_{[t}$ is the identity operator acting on $\mathfrak{H}_{[t}$. In particular, $\Gamma_f(\mathfrak{h}^1)$ is embedded in $\mathfrak{H}$ through the identification of $\Psi \in \Gamma_f(\mathfrak{h}^1)$ with $\Psi \otimes e(0) \in \mathfrak{H}$ and, for any operator $B \in \mathcal{B}_0 = \mathcal{B}(\Gamma_f(\mathfrak{h}^1))$, $B(\Psi \otimes e(f))$ means $(B\Psi)\otimes e(f)$. With these identifications, $(\mathcal{B}_t)_{\geq 0}$ is an increasing family of sub-algebras of $\mathcal{B}$. Given a family $V = (V(t))_{t\geq 0}$ of operators, such that $V(t) \in \mathcal{B}_t$ for any $t \geq 0$, then $B \mapsto k_t(B) = V(t)BV(t)^*$ maps $\mathcal{B}_0$ into the algebra $\mathcal{B}_t$.

For any $t \geq 0$, we define projections E_t from $\mathfrak{H}$ onto $\mathfrak{H}_{t]}$ by:

$$E_t\Psi \otimes e(f) = \Psi \otimes e(f1_{[0,t]}) \otimes e(0_{[t}).$$

In addition, a projection $\mathbb{E}_{t]}$ between the algebras of operators $\mathcal{B}$ and $\mathcal{B}_t$ is associated to each E_t as follows:

$$\mathbb{E}_{t]}(Z) = E_t Z E_t, (Z \in \mathcal{B}).$$

In particular, E_0 and $\mathbb{E}_{0]}$ will be written simply as E and $\mathbb{E}$.

3.5. **Quantum Noises.** With these notations, creation, annihilation and number (or conservation) processes are respectively characterized as follows:

$$A^\dagger_\ell(t)\Psi \otimes e(f) = \frac{d}{d\epsilon}\Psi \otimes e(f + \epsilon 1_{[0,t]}\delta_\ell)\ |_{\epsilon=0}, \tag{3.10}$$

$$A_\ell(t)\Psi \otimes e(f) = \langle \delta_\ell 1_{[0,t]}, f\rangle \Psi \otimes e(f), \tag{3.11}$$

$$N_{\ell,m}(t) = A^\dagger_\ell(t)A_m(t), \tag{3.12}$$

for all $t \geq 0$, $u \in \Gamma_f(\mathfrak{h}^1)$, $f \in L^2(\mathbb{R}_+,\mathbb{C}^L)$, $\ell, m \in \mathbb{L}$ where the scalar product $\langle\cdot,\cdot\rangle$ is that of $L^2(\mathbb{R}_+,\mathbb{C}^L)$.

Notice that for any fixed $t \geq 0$, the ranges of $A^\dagger_\ell(t)$, $A_\ell(t)$, $N_{\ell m}(t)$ are included in $\mathfrak{H}_{t]}$. These quantum noises satisfy two important families of relations:

- *The canonical commutation relations (CCR):*

$$[A_\ell(s), A_m^\dagger(t)] = \langle 1_{[0,s]}\delta_\ell, 1_{[0,t]}e_m\rangle \mathbf{1} = \delta_{\ell m}\min(s,t)\mathbf{1},\ (s,t\geq 0). \tag{3.13}$$

$$[A_\ell(s), A_m(t)] = [A_\ell^\dagger(s), A_m^\dagger(t)] = 0. \tag{3.14}$$

From this two fundamental relations, it follows that

$$\begin{aligned} [A_k(s), N_{\ell m}(t)] &= \delta_{\ell k}\min(s,t)A_m(t) \\ [A_k^\dagger(s), N_{\ell m}(t)] &= -\delta_{\ell k}\min(s,t)A_\ell^\dagger(t). \end{aligned}$$

- *The Itô table for differentials:* An integration theory for these quantum noises has been developed by Hudson and Parthasarathy (see e.g. [25], which allows to give an interpretation to $dA_\ell(s)$, $dA_\ell^\dagger(t)$ in terms of stochastic integrals). This leads to the following table which synthesizes the fundamental formulae of this non commutative extension of Itô calculus.

$\nearrow$	$dA_\ell(t)$	$dN_{\ell m}(t)$	$dA_\ell^\dagger(t)$	$dt\mathbf{1}$
$dA_\ell(t)$	0	$dA_\ell(t)$	$dt\mathbf{1}$	0
$dN_{\ell m}(t)$	0	$dN_{\ell m}(t)$	$dA_\ell^\dagger(t)$	0
$dA_\ell^\dagger(t)$	0	0	0	0
$dt\mathbf{1}$	0	0	0	

3.6. **Cocycles.** The evolution of our system will be characterized by a quantum cocycle which will lead to a quantum dynamical semigroup and a flow. The reader who is less aware of this kind of description may first think to the simplest case of a hamiltonian dynamics, described by a unitary group $(U(t))_{t\geq 0}$ defined by $U(t) = e^{-it\hat{H}}$. The evolution operators $U(t)$ satisfy the group property $U(t+s) = U(t)U(s)$, which is a particular case of cocycle. They are the solutions of the differential equation $dU(t) = -i\hat{H}\,dt\,U(t)$, with $U(0) = \mathbf{1}$ (see e.g. [38]). In our case, due to dissipative effects, the process $U(t)$ will not correspond to a group, but to a less simpler cocycle, and the above differential equation will be replaced by:

$$dU(t) = dY(t)\,U(t)\ ,\quad U(0) = \mathbf{1}, \tag{3.15}$$

where $Y(t)$ is a process involving bosonic quantum noises. Since bosonic quantum noises are unbounded operators, it is not clear whether this equation is well-posed, as $U(t)$ may not preserve their domains. Thus, the rigorous treatment of (3.15) is easier to achieve through solving the adjoint equation:

$$dV(t) = V(t)\,dZ(t)\ ,\quad V(0) = \mathbf{1}$$

with $Z(t) = Y(t)^*$. Indeed, it will be shown below that its integral form:

$$V(t) = \mathbf{1} + \int_0^t V(s)\,dZ(s), \tag{3.16}$$

is well-posed in the strong topology and has a unique solution $V(t) \in \mathcal{B}(\mathfrak{H})$, where all the stochastic integrals are computed following the theory of Hudson and Parthasarathy (see [25, 26]). Although this implies that (3.15) is well-defined in the weak sense (its solution being $U(t) = V(t)^*$), it is not necessarily well-posed in the strong sense as (3.16) is. This is why, whereas (3.15) is more according to the physical tradition, mathematicians do prefer to work with (3.16) instead (see e.g. [25, 26]).

To express the cocycle property rigorously, one needs to introduce first the usual time shift in $L^2(\mathbb{R}_+, \mathbb{C}^L)$:

$$\sigma_t f(s) = \begin{cases} f(s-t) & \text{if } s > t \\ 0 & \text{otherwise} \end{cases}.$$

Take then the second quantization $\Gamma(\sigma_t)$ of this shift which yields to a map $Z \mapsto \Gamma(\sigma_t) Z \Gamma(\sigma_t)^*$. This map can be canonically extended to a map θ_t, called *covariant quantum shift* over the algebra $\mathcal{B}$. A straightforward computation shows that the projections $\mathbb{E}_{t]}$ satisfy the following *covariant property*:

$$\mathbb{E} = \mathbb{E}_{t]} \circ \theta_t, \quad (t \geq 0). \tag{3.17}$$

Definition 3.1. A family $(V(t))_{t\geq 0}$ (respectively $(U(t))_{t\geq 0}$) of linear bounded operators in $\mathfrak{H}$ is a **left cocycle** (resp. **right-cocycle**) if for every $s, t \geq 0$ it holds:

$$V(t+s) = V(s)\,\theta_s(V(t)), \text{ (resp. } U(t+s) = \theta_s\,(U(t))U(s)).$$

Notice that if V is a left-cocycle, its adjoint $U(t) = V(t)^*$ is a right-cocycle. Cocycles are related to solutions of some classes of stochastic differential equations, as it has been shown in the seminal articles of Hudson and Parthasarathy (see e.g. [25, 26]), further extended by Fagnola to the case of equations with unbounded coefficients (see [39, 40]).

In our model, according to (3.7), the stochastic differential equation is given by (3.16) with:

$$dZ(t) = (i\hat{H} + \hat{K})dt + \sum_\ell \left(L_\ell dA_\ell^\dagger(t) - L_\ell^* dA_\ell(t) \right) \tag{3.18}$$

and L_ℓ and $\hat{K}$ are defined in (3.8) and (3.9), respectively. It is worth noticing here that, like $\hat{H}$, all the L_ℓ's and $\hat{K}$ are bounded operators in $\Gamma_f(\mathfrak{h}^1)$. We now precise the conditions under which the equation (3.16) makes sense and has a solution which is a unitary cocycle.

Theorem 3.2. *Given Z defined by* (3.18)*, the equation* (3.16) *is well posed and has a unique solution $V(t)$, which is a unitary cocycle.*

Proof. This theorem is a corollary of Propositions 26.1, 26.2 and Theorem 26.3 of [25], from which it also follows that

$$\sup_{0\leq t\leq T} \sup_{\Psi\in\Gamma_f(\mathfrak{h}^1):\, \|\Psi\|\leq 1} \|V(t)\Psi \otimes e(f)\| < \infty,$$

for every $f \in L^2(\mathbb{R}_+, \mathbb{C}^L)$, $T > 0$.

Although the unitary property is a consequence of Theorem 26.3 of [25], it is instructive to check this for $V(t)$ in our case. Indeed, since $V(0) = \mathbf{1}$, it suffices to prove that $d(V^*(t)V(t)) = 0 = d(V(t)V^*(t))$. We first apply the integration by parts formula:

$$\begin{aligned} d(V(t)V^*(t)) &= (dV(t))V^*(t) + V(t)dV^*(t) + dV(t)dV^*(t) \\ &= V(t)\left[dZ(t) + dZ^*(t) + dZ(t)dZ^*(t)\right]V^*(t) \\ &= V(t)\left[2\hat{K} + \sum_\ell L_\ell^* L_\ell\right]V^*(t) \\ &= 0. \end{aligned}$$

¿From this it follows that

$$V(t)V^*(t) = \mathbf{1}, \text{ for all } t \geq 0.$$

Thus, each $V(t)$ is a coisometry.

To verify that $V(t)$ is unitary, it remains to show that it is an isometry. For this we need to introduce the so called *dual cocycle*. We start by taking the customary *time reversal* operator in $L^2(\mathbb{R}_+, \mathbb{C}^L)$:

$$(\mathbf{r}_t f) = \begin{cases} f(t-s) & \text{if } t \geq s \\ f(s) & \text{otherwise,} \end{cases} \tag{3.19}$$

for any $f \in L^2(\mathbb{R}_+, \mathbb{C}^L)$. Now, take the second quantization $\Gamma(\mathbf{r}_t)$ of the above operator:

$$\Gamma(\mathbf{r}_t)e(f) = e(\mathbf{r}_t f), \tag{3.20}$$

and finally define the *time reversal map* in $\mathcal{B}(\mathcal{H})$ as

$$\mathcal{R}_t(X) = \Gamma(\mathbf{r}_t)X\Gamma(\mathbf{r}_t)^*, \tag{3.21}$$

for any $X \in \mathcal{B}(\mathcal{H})$. The *dual cocycle* of V is defined as

$$\tilde{V}(t) = \mathcal{R}_t(V(t)^*), \ (t \geq 0). \tag{3.22}$$

It is shown in e.g. [40] that $\tilde{V}$ is indeed a cocycle that satisfies the stochastic differential equation:

$$d\tilde{V}(t) = \tilde{V}\, dZ(t)^*. \tag{3.23}$$

Moreover, (3.22) yields $\tilde{V}(t)\tilde{V}(t)^* = \mathcal{R}_t(V(t)^*V(t))$.This allows to prove that $V(t)$ is an isometry if and only if $\tilde{V}(t)$ is a coisometry. For that we use (3.23) and the formula of integration by parts again:

$$d(\tilde{V}(t)\tilde{V}(t)^*) = \tilde{V}(t)\left[dZ(t)^* + dZ(t) + dZ(t)^* dZ(t)\right]\tilde{V}(t)^* = 0. \tag{3.24}$$

Therefore $d(\tilde{V}(t)\tilde{V}(t)^*) = 0$ and V is an isometry. Since V is also a coisometry, it is unitary. □

4. The quantum dynamical semigroup

4.1. **The quantum Markov flow and the associated semigroup.** The cocycle property of $V(t)$ and $U(t) = V(t)^*$ and the structure of projections on the given Fock space are related to an extension of the concept of Markov process to a non commutative framework. Indeed, let us introduce the *Quantum Flow* $(k_t)_{t\geq 0}$ associated to the cocycle U as follows: for any $t \geq 0$, $k_t(\cdot)$ is the map $\mathcal{B}_0 \to \mathcal{B}_t$ defined by:

$$k_t(B) = U(t)^* B U(t) \tag{4.1}$$

for all $B \in \mathcal{B}_0$. It is clear that $k_t(\cdot) \circ \mathbb{E}_{t]} = \mathbb{E}_{t]} \circ k_t(\cdot)$. The cocycle property implies that:

$$\Phi_t(B) = \mathbb{E}(k_t(B)), \ \ (B \in \mathcal{B}_0, \ t \geq 0). \tag{4.2}$$

defines a semigroup Φ. It can be shown [25, 26] (see also [40]) that Φ is a *Quantum Dynamical Semigroup*, i.e., it is a w^*-continuous semigroup of completely positive normal maps (the complete positivity is a consequence of Stinespring's theorem [41]).

The stochastic differential equation satisfied by $k_t(B)$ can be readily derived from the stochastic differential equation (3.15) for $U(t)$. Notice first that $k_0(B) = B$ and $k_t(\mathbf{1}) = \mathbf{1}$, since U is unitary. Moreover, each $k_t(\cdot)$ is a *-homomorphism of algebras. By means of the integration by parts formula, one obtains formally:

$$\begin{aligned} dk_t(B) &= dU(t)^* BU(t) + U(t)^* B\, dU(t) + dU(t)^* B\, dU(t) \\ &= U(t)^* \big(dY(t)^* B + B\, dY(t) + dY(t)^* B\, dY(t) \big) U(t). \end{aligned}$$

In our model,

$$dY(t) = \hat{G}\, dt + \sum_{\ell \in L} \Big({L_\ell}^*\, dA_\ell(t) - L_\ell\, dA_\ell^\dagger(t) \Big)\,, \tag{4.3}$$

with:

$$\hat{G} = -i\hat{H} + \hat{K} = -i\hat{H} - \frac{1}{2} \sum_{\ell \in L} L_\ell^* L_\ell\,. \tag{4.4}$$

Hence, since $U(t)$ commutes with $dA_\ell(t)$ and $dA_\ell^\dagger(t)$,

$$\begin{aligned} U(t)^* dY(t)^* BU(t) &= k_t(G^* B)\, dt + \sum_\ell \big(k_t(L_\ell B)\, dA_\ell^\dagger(t) - k_t(L_\ell^* B)\, dA_\ell(t) \big). \\ U(t)^* B\, dY(t) U(t) &= k_t(BG)\, dt + \sum_\ell \big(k_t(BL_\ell^*)\, dA_\ell(t) - k_t(BL_\ell)\, dA_\ell^\dagger(t) \big). \end{aligned}$$

Moreover, by using the Itô rules (section 3.5),

$$U(t)^* dY(t)^* B dY(t) U(t) = k_t \left(\sum_\ell L_\ell^* B L_\ell \right) dt\,.$$

We summarize the discussion before as follows.

Theorem 4.1. *The quantum flow $k = (k_t)_{t \geq 0}$ defined by (4.1) solves the structure equation:*

$$dk_t(B) = k_t(\mathcal{L}(B))\, dt + \sum_{\ell \in L} k_t(\alpha_\ell(B))\, dA_\ell^\dagger(t) + \sum_{\ell \in L} k_t(\beta_\ell(B))\, dA_\ell(t), \tag{4.5}$$

where:

$$\mathcal{L}(B) = i[\hat{H}, B] - \frac{1}{2} \sum_\ell \left({L_\ell}^* L_\ell B - 2{L_\ell}^* B L_\ell + B {L_\ell}^* L_\ell \right), \tag{4.6}$$

the operators L_ℓ being defined by (3.8) above, and

$$\alpha_\ell(B) = [L_\ell, B] \tag{4.7}$$

$$\beta_\ell(B) = [B, L_\ell^*]. \tag{4.8}$$

α_ℓ and β_ℓ are known as the structure maps of the flow.

As a result, $\mathcal{L}(\cdot)$ is the infinitesimal generator of the quantum dynamical semigroup Φ defined by (4.2) associated to the flow.

Note that all of the above maps $\mathcal{L}$, α_ℓ, β_ℓ apply the algebra $\mathcal{B}_0$ into itself in the finite volume case. In the infinite volume case their interpretation is rendered delicate by difficulties that arise with the involved domains.

The canonical form of the generator $\mathcal{L}$ of a general uniformly norm continuous quantum dynamical semigroup has been discovered by Lindblad [8]. The generator (4.6) is particular case of the Lindblad form. Its most noticeable property is that it satisfies the adiabatic condition discussed in subsection 2.3.

Proposition 4.2. *$\mathcal{L}$ is adiabatic with respect to $\mathcal{L}_{\hat{H}}(.) = i[\hat{H}, .]$, i.e., for all $B \in \mathcal{B}_0$ it holds*

$$i[\hat{H}, \mathcal{L}(B)] = \mathcal{L}(i[\hat{H}, B]). \tag{4.9}$$

Proof. Recall that $\mathcal{L}(B) = i[\hat{H}, B] + \mathcal{D}(B)$, where

$$\mathcal{D}(B) = -\frac{1}{2}\sum_\ell \left(L_\ell{}^* L_\ell B - 2L_\ell{}^* B L_\ell + B L_\ell{}^* L_\ell\right).$$

It is enough to show (4.9) for $\mathcal{D}$ instead of $\mathcal{L}$. A straightforward calculation gives:

$$\begin{aligned} &[\hat{H}, \mathcal{D}(B)] - \mathcal{D}\left([\hat{H}, B]\right) \\ &= \frac{1}{2}\sum_\ell \left\{-[\hat{H}, L_\ell^* L_\ell]B + 2[\hat{H}, L_\ell^*]BL_\ell + 2L_\ell^* B[\hat{H}, L_\ell] - B[\hat{H}, L_\ell^* L_\ell]\right\}. \end{aligned} \tag{4.10}$$

To compute the right-hand side of this equation, we have to determine $[\hat{H}, L_{ij}]$ and $[\hat{H}, L_{ij}^* L_{ij}]$, using (3.8) and (3.3).

The canonical anti-commutation relations yields

$$[n_i, c_j^\dagger] = \delta_{ij} c_j^\dagger, \qquad [n_i, c_j] = -\delta_{ij} c_j. \tag{4.11}$$

Thus, it follows easily that $[\hat{H}, c_j^\dagger] = E_j c_j^\dagger$ and $[\hat{H}, c_j] = -E_j c_j$, for all $j \in I$. As a result,

$$[\hat{H}, L_{ij}] = -\big(E_j 1_I(j) + E_i 1_I(i)\big) L_{ij}, \tag{4.12}$$

where 1_A is the customary notation for the characteristic function of the set A (i.e. $1_A(i) = 1$ if $i \in A$, and is zero otherwise). We also obtain:

$$[\hat{H}, L_{ij}^* L_{ij}] = 0\,, \quad (i, j \in L). \tag{4.13}$$

Thus, using (4.12) and (4.13), the right hand side of (4.10) is zero. □

Call $\mathcal{A}_0 = \mathcal{A}_{\hat{H}}$ the Abelian subalgebra of $\mathcal{B}_0$ generated by the bounded self-adjoint operator $\hat{H}$, which is included in its commutant $\mathcal{A}_0'$. The adiabatic property clearly implies that $\Phi_t(\mathcal{A}_0') \subseteq \mathcal{A}_0'$ for all $t \geq 0$.

4.2. **The master equation.** The predual algebra $\mathcal{B}_{0*}$ of $\mathcal{B}_0$ is isomorphic to the space of trace-class operators $\mathfrak{I}_1(\Gamma_f(\mathfrak{h}^1))$ [33]. Thus, any normal state ω will be identified with the unit trace positive operator $\rho \in \mathfrak{I}_1(\Gamma_f(\mathfrak{h}^1))$ such that $\omega(B) = \mathrm{tr}\,(\rho B)$, which we call a *density matrix* on $\Gamma_f(\mathfrak{h}^1)$ in the sequel. The predual semigroup $\Phi_* = (\Phi_{*t})_{t\geq 0}$ defined through

$$\Phi_{*t}(\omega)(B) = \omega(\Phi_t(B)), \;(\omega \in \mathcal{B}_{0*},\; B \in \mathcal{B}_0), \tag{4.14}$$

induces a weakly continuous semigroup of trace-preserving completely positive maps on $\mathfrak{I}_1(\Gamma_f(\mathfrak{h}^1))$. This semigroup is generated by the adjoint map $\mathcal{L}_*(.)$,

$$\mathcal{L}_*(\rho) = -i[\hat{H}, \rho] - \frac{1}{2}\sum_{\ell} \left(L_\ell{}^* L_\ell \rho - 2L_\ell \rho L_\ell^* + \rho L_\ell{}^* L_\ell\right) \ , \ \ (\rho \in \mathfrak{I}_1(\Gamma_f(\mathfrak{h}^1))). \tag{4.15}$$

Thus, the *Master Equation* of the evolution of states is

$$\frac{d\rho_t}{dt} = \mathcal{L}_*(\rho_t), \tag{4.16}$$

where $\rho_t = \Phi_{*t}(\rho)$, $t \geq 0$, with ρ a density matrix.

4.3. **Unravelings of the quantum flow.** The quantum flow obtained in Theorem 4.1 contains several stochastic models for the electronic transport constructed before, using classical stochastic noises. Indeed, it is well known that both, Wiener and Poisson processes can be obtained from quantum noises as follows (see e.g. [26]. Consider first the canonical multidimensional Wiener process (or Brownian motion) $W = (W_\ell)_{\ell \in L}$. Denote $x \cdot y$ the scalar product of two vectors in $\mathbb{C}^L$. The Wiener space $L^2(W)$ is generated by the family of random variables

$$\mathbf{e}_W(f) = \exp\left(\int_0^\infty f(s)\cdot dW(s) - \frac{1}{2}\int_0^\infty \|f(s)\|^2\, ds\right), \ f \in L^2(\mathbb{R}_+, \mathbb{C}^L). \tag{4.17}$$

Moreover, the stochastic process

$$\mathbf{e}_W(f)_t = \mathbf{e}_W(f 1_{[0,t]}), \ (t \in \mathbb{R}_+)$$

satisfies the stochastic differential equation

$$d\mathbf{e}_W(f)_t = \mathbf{e}_W(f)_t f(t)\cdot dW(t), \ (t \geq 0, f \in L^2(\mathbb{R}_+, \mathbb{C}^L)) \tag{4.18}$$

We thus define $T_W : \mathfrak{H} \to L^2(W) \otimes \mathfrak{H}_{0]}$, through the equation

$$T_W \Psi \otimes e(f) = \mathbf{e}_W(f)\Psi, \tag{4.19}$$

for all $f \in L^2(\mathbb{R}_+, \mathbb{C}^L)$.

Now, compute the action of T_W on $A_\ell^\dagger(t)\Psi \otimes e(f)$:

$$\begin{aligned} T_W A_\ell^\dagger(t)\Psi \otimes e(f) &= T_W \Psi \otimes \frac{d}{d\epsilon} e(f + \epsilon 1_{[0,t]}\delta_\ell) \mid_{\epsilon=0} \\ &= \left(W_\ell(t) - \int_0^t f_\ell(s)ds\right)\mathbf{e}_W(f)\Psi. \end{aligned}$$

And,

$$T_W A_\ell(t)\Psi \otimes e(f) = \left(\int_0^t f_\ell(s)ds\right)\mathbf{e}_W(f)\Psi.$$

So that,

$$T_W(A_\ell^\dagger(t) + A_\ell(t))\Psi \otimes e(f) = W_\ell(t) T_W \Psi \otimes e(f).$$

Moreover, consider the process

$$Y_W(t) = Gt - \sum_\ell L_\ell W_\ell(t),$$

which is defined on the same probability space than W and takes values in $\mathcal{B}(\Gamma_f(\mathfrak{h}^1))$. This process coincides with the restriction to $\Gamma_f(\mathfrak{h}^1) = \mathfrak{H}_{0]}$ of the process $T_W Y(t)$, with $Y(t)$ as introduced in (4.3).

A cocycle U_W can be associated to the process Y_W as the unique solution to the classical stochastic differential equation

$$dU_W(t) = dY_W(t)U_W(t), \quad U_W(0) = \mathbf{1}. \tag{4.20}$$

This is a classical stochastic equation, although each $U_W(t) \in L^2(W) \otimes \mathfrak{H}_{0]}$, because we are concerned with classical noises. Call $\mathbb{E}(\cdot)$ the expectation in the underlying probability space (the Wiener space). The flow associated to the cocycle U_W, termed as *classical flow*, is

$$k_t^W(B) = U_W^*(t)BU_W(t), \; (t \geq 0).$$

And the semigroup associated to this flow is the family of completely positive maps

$$B \mapsto \mathbb{E}\left(k_t^W(B)\right).$$

Although the classical and quantum flow are different, they generate the *same* quantum dynamical semigroup.

Proposition 4.3. *The classical flow satisfies the stochastic differential equation*

$$dk_t^W(B) = k_t^W(\mathcal{L}(B))\,dt + \sum_\ell k_t^W(\theta_\ell(B))\,dW_\ell(t), \tag{4.21}$$

where $\mathcal{L}(B)$ is given by (4.6) *and*

$$\theta_\ell(B) = -({L_\ell}^* B + BL_\ell), \tag{4.22}$$

for all $\ell \in L$.

As a result,

$$\Phi_B(t) = \mathbb{E}\left(k_t^W(B)\right), \tag{4.23}$$

for all $t \geq 0$ and $B \in \mathcal{B}_0$.

Proof. Indeed, using the classical Itô's formula, we obtain

$$dk_t^W(B) = dU_W(t)^* BU_W(t) + U_W(t)^* BdU_W(t) + dU_W^*(t)BdU_W(t)$$

$$= U_W^*(t)dY_W^*(t)BU_W(t) + U_W^*(t)BdY_W(t)U_W(t) + U_W^*(t)dY_W(t)^* BdY_W(t)U_W(t).$$

$$\begin{aligned} U_W(t)^* dY_W^*(t)BU_W(t) &= U_W^*(t)G^*BU_W(t)dt \\ &- \sum_\ell U_W^*(t)L_\ell^* BU_W(t)dW_\ell(t) \end{aligned} \tag{4.24}$$

$$\begin{aligned} &= k_t^W(G^*B)dt \\ &- \sum_\ell k_t^W(L_\ell^* B)dW_\ell(t). \end{aligned} \tag{4.25}$$

$$(4.26)\qquad \begin{aligned} U_W^*(t)BdY_W(t)^*U_W(t) &= U_W^*(t)BGU_W(t)dt \\ &- \sum_\ell U_W^*(t)BL_\ell U_W(t)dW_\ell(t) \\ &= k_t^W(BG)dt \\ &- \sum_\ell k_t^W(BL_\ell)dW_\ell(t). \end{aligned}$$

$$(4.27)\qquad \begin{aligned} U_W^*(t)dY_W^*(t)BdY_W(t)U_W(t) &= \sum_\ell U_W^*(t)L_\ell^*BL_\ell U_W(t)dt \\ &= k_t\left(\sum_\ell L_\ell^*BL_\ell\right)dt. \end{aligned}$$

The addition of (4.24), (4.26) and (4.27) yields (4.21).

From (4.21) and taking the expectation of the flow, it follows that its associated semigroup is generated by $\mathcal{L}(\cdot)$. Thus, it coincides with Φ. $\square$

Similar computations are involved in the Poisson unraveling of the quantum flow. Indeed,

following [26], the Boson-Fock space is related with the Poisson space as follows. We denote by $N(t) = (N_\ell(t);\ \ell \in L)$ a canonical multidimensional Poisson process. That is, the N_ℓ's are independent Poisson processes with intensity rate 1, thus each process $M_\ell(t) = N_\ell(t) - t$ is a martingale satisfying the classical Itô table

$$dM_\ell(t)dM_k(t) = \delta_{\ell k}dt.$$

Like in the previous Wiener case, the Poisson space $L^2(N)$ has a total family $(e_N(f);\ f \in L^2(\mathbb{R}_+, \mathbb{C}^L))$ defined by

$$(4.28)\qquad e_N(f) = e^{-\sum_\ell \int_0^\infty f_\ell(s)ds} \prod_{s\geq 0} \left(1 + f(s)\cdot \Delta N(s)\right),$$

where $f(s)\cdot\Delta N(s) = \sum_\ell f_\ell(s)\Delta N_\ell(s)$, and $\Delta N_\ell(s) = N_\ell(s) - N_\ell(s-)$ denotes the jump size (1 or 0) of N_ℓ at time $s \geq 0$.

Define $T_N : \mathfrak{H} \to L^2(N)\otimes \mathfrak{H}_{0]}$ by

$$(4.29)\qquad T_N\psi\otimes e(f) = e_N(f)\otimes\psi,$$

for all $\psi \in \Gamma_f(\mathfrak{h}^1)$, $f \in L^2(\mathbb{R}_+, \mathbb{C}^L)$.

Define

$$(4.30)\qquad Y_N(t) = Gt - \sum_{\ell\in L} L_\ell M_\ell(t),\ (t\geq 0).$$

A straightforward computation, following Meyer [26], p. 73 to 76, shows that the process Y_N coincides with the restriction to $\mathfrak{H}_{0]}$ of the process $T_NY(t)$, with $Y(t)$ as introduced in (4.3).

We can again consider a classical stochastic differential equation, with Poissonian noise, to obtain a classical cocycle U_N and a flow:

$$dU_N = dY_N(t)U_N(t),\ U_N(0) = \mathbf{1}, \tag{4.31}$$

$$k_t^N(B) = U_N(t)^* B U_N(t),\ (t \geq 0,\ B \in \mathcal{B}_0). \tag{4.32}$$

Paraphrasing the computations performed in Proposition 4.33 we obtain

Proposition 4.4. *The classical Poissonian flow satisfies the stochastic differential equation*

$$dk_t^N(B) = k_t^N(\mathcal{L}(B))\,dt + \sum_\ell k_t^N(\vartheta_\ell(B))\,dM_\ell(t), \tag{4.33}$$

where $\mathcal{L}(B)$ is given by (4.6) *and*

$$\vartheta_\ell(B) = -({L_\ell}^* B + BL_\ell), \tag{4.34}$$

for all $\ell \in L$.

As a result,

$$\Phi_B(t) = \mathbb{E}\left(k_t^N(B)\right), \tag{4.35}$$

for all $t \geq 0$ and $B \in \mathcal{B}_0$, where $\mathbb{E}(\cdot)$ denotes the mean taken in the Poisson space.

It is worth noticing that in all cases we recover the same quantum Markov semigroup, moreover, both classical flows have the same structure maps, even though they are defined in different spaces.

5. Analysis of the equilibrium and stationary states

Under the finite volume assumption, there is an infinite number of stationary states for the class of quantum dynamical semigroups Φ associated to the quantum flows considered in the previous section. On the other hand, it is well known (see for instance [33], section 5.3.2) that for finite systems, the KMS condition completely characterizes the Gibbs states $\omega_\beta = \mathrm{tr}\,(\rho_\beta\ \cdot)$, which is given by a density matrix $\rho_\beta \in \mathfrak{I}_1(\Gamma_f(\mathfrak{h}^1))$ of the form:

$$\rho_\beta = \frac{1}{Z(\beta,\mu)} \exp\left(-\beta(\hat{H} - \mu\hat{N})\right). \tag{5.1}$$

$\hat{N} = \sum_{i\in I} n_i$ is the total number operator and $Z(\beta,\mu) = \mathrm{tr}\left(\exp(-\beta(\hat{H} - \mu\,\hat{N}))\right)$ is the grand canonical partition function. It is our purpose to prove that, if the two baths have identical chemical potentials $\mu_\star = \mu_\diamond = \mu$, the detailed balance conditions (3.4), (3.5) and (3.6) imply that the Gibbs state ω_β is the *unique* stationary state of the semigroup Φ. We will actually prove a slightly more general result, showing that the reverse statement is also true provided (3.4), (3.5) and (3.6) are replaced by more general detailed balance conditions in the case where H has degenerate eigenvalues.

Call $\hat{K}_\mu = \hat{H} - \mu\hat{N}$ and Φ_{K_μ} the *-automorphism group on $\mathcal{B}(\Gamma_f(\mathfrak{h}^1))$ defined by the generalized Hamiltonian $\hat{K}_\mu$. In our case, $\exp(-\beta\hat{H})$ is a trace-class operator since $\Gamma_f(\mathfrak{h}^1)$ is finite-dimensional. Then, from [33], Proposition 5.2.23, the Gibbs state ω_β is the unique Φ_{K_μ}-KMS state at the value β. It is clear from (5.1) that ω_β is faithful.

Call $\Phi^{(int)}$ the semigroup generated by $\mathcal{L}^{(int)}(\cdot) = \mathcal{L}(\cdot) - \mathcal{D}^{(ext)}(\cdot)$, where

$$\mathcal{D}^{(ext)}(B) = -\frac{1}{2} \sum_{\ell \in (\{\star,\diamond\}\times I) \cup (I \times \{\star,\diamond\})} \big(L_\ell^* L_\ell B - 2 L_\ell^* B L_\ell + B L_\ell^* L_\ell \big). \tag{5.2}$$

Let say that two indices $i, k \in I \cup \{\star, \diamond\}$ are *connected* if there exists a collection of indices $i_1, \ldots, i_n$ in I such that $\gamma_{i_m, i_{m+1}} > 0$ for all $m = 0, \ldots, n$, with $i_0 = i$ and $i_{n+1} = k$.

The theorem below is the main result of this section.

Theorem 5.1. *Let $\mu_\diamond = \mu_\star = \mu$. Then the Gibbs state ω_β is a stationary state of the quantum dynamical semigroup Φ defined by* (4.2) *if and only if the following detailed balance equations are satisfied:*

$$\gamma_{k,l} = \gamma_{l,k}\, e^{\beta(E_k - E_l)}\ , \quad (l, k \in I, E_k \neq E_l) \tag{5.3}$$

$$(\gamma_{l,\star} + \gamma_{l,\diamond})\, e^{-\beta(E_l - \mu)} - (\gamma_{\star,l} + \gamma_{\diamond,l}) = \frac{1}{e^{\beta(E_l-\mu)} + 1} \sum_{k \in I, E_k = E_i} (\gamma_{k,l} - \gamma_{l,k})\ , \quad (l \in I) \tag{5.4}$$

$$\sum_{k,l \in I, E_k = E_l} \frac{\gamma_{k,l} - \gamma_{l,k}}{e^{\beta(E_k - \mu)} + 1} = 0. \tag{5.5}$$

If these equations hold and every index $i \in I$ is connected to at least one bath $\star, \diamond$, then ω_β is the unique stationary state of Φ. Moreover, if the detailed balance equations hold, then ω_β is also a stationary state of the quantum dynamical semigroup $\Phi^{(int)}$. Furthermore, given any other normal state with density matrix ρ, both $\Phi_{*t}(\rho)$ and $\Phi_{*t}^{(int)}(\rho)$ converge in the w^*-topology towards ρ_β as $t \to \infty$, i.e.

$$\mathrm{tr}\,(\rho\, \Phi_t(B)) = \mathrm{tr}\,(\rho\, \mathbb{E}\,(k_t(B))) \to \mathrm{tr}\,(\rho_\beta\, B) \tag{5.6}$$

as $t \to \infty$ for any $B \in \mathcal{B}_0$ (similarly for $\Phi^{(int)}$).

It is worth noticing that if all the eigenvalues of H are non-degenerate then the above detailed balance equations (5.3), (5.4), (5.5), reduce to the former equations (3.4), (3.5), (3.6).

The proof of the theorem before will be performed in several steps, starting by the following proposition.

Proposition 5.2. *Let $\mu_\diamond = \mu_\star = \mu$. Then a stationary state of the form* (5.1) *exists for the semigroup Φ if and only if* (5.3) *to* (5.5) *hold.*

Proof. We have to prove that (5.3), (5.4) and (5.5) are equivalent to $\mathcal{L}_*(\omega_\beta) = 0$, where $\mathcal{L}_*(.) = -i[\hat{H}, .] + \mathcal{D}_*(.)$ is given by (4.15). A density ρ_β given by (5.1) can be written in the form

$$\rho_\beta = \sum_{\eta \in \mathcal{C}} p(\eta) |\eta\rangle\langle\eta|, \tag{5.7}$$

where the coefficients $p(\eta)$ are positive and satisfy $\sum_{\eta \in \mathcal{C}} p(\eta) = 1$. Clearly, $i[\hat{H}, \rho_\beta] = 0$. By (3.3) and (3.8),

$$L_\ell = \begin{cases} \gamma_{i,j}\, c_j^\dagger c_i & \text{if } \ell = (i,j) \in I^2,\ i \neq j \\ \gamma_{i,j}\, c_j^\dagger & \text{if } \ell = (i,j) \in \{\diamond, \star\} \times I \\ \gamma_{i,j}\, c_i & \text{if } \ell = (i,j) \in I \times \{\diamond, \star\} \end{cases}$$

It then follows from (4.15) that $\mathrm{tr}\left(\rho_\beta\, \mathcal{D}(|\eta\rangle\langle\xi|)\right) = 0$ for any $\eta, \xi \in \mathcal{C}$, $\eta \neq \xi$. Thus $\mathcal{L}_*(\omega_\beta) = 0$ is equivalent to:

$$\mathrm{tr}\left(e^{-\beta \hat{K}_\mu}\mathcal{D}(|\eta\rangle\langle\eta|)\right) = 0\,, \quad (\eta \in \mathcal{C}).$$

We first notice that

$$\kappa(\eta) = \mathrm{tr}\left(e^{-\beta\hat{K}_\mu}|\eta\rangle\langle\eta|\right) = \prod_{i\in I} e^{-\beta\eta_i(E_i-\mu)} = p(\eta) Z(\beta,\mu). \tag{5.8}$$

We easily obtain the following identities:

$$\begin{aligned}
\mathrm{tr}\left(e^{-\beta\hat{K}_\mu} c_i^\dagger |\eta\rangle\langle\eta| c_i\right) &= (1-\eta_i)\kappa(\eta) e^{-\beta(E_i-\mu)}\\
\mathrm{tr}\left(e^{-\beta\hat{K}_\mu} c_j |\eta\rangle\langle\eta| c_j^\dagger\right) &= \eta_j\kappa(\eta) e^{\beta(E_j-\mu)}\\
\mathrm{tr}\left(e^{-\beta\hat{K}_\mu} c_i^\dagger c_j |\eta\rangle\langle\eta| c_j^\dagger c_i\right) &= (1-\eta_i)\eta_j\kappa(\eta) e^{-\beta(E_i-E_j)}\\
\mathrm{tr}\left(e^{-\beta\hat{K}_\mu} n_i(\mathbf{1}-n_j) |\eta\rangle\langle\eta|\right) &= (1-\eta_j)\eta_i\kappa(\eta) = \mathrm{tr}\left(e^{-\beta\hat{K}_\mu}|\eta\rangle\langle\eta| n_i(\mathbf{1}-n_j)\right).
\end{aligned}$$

Therefore, by using (4.15) and the above expression for L_ℓ,

$$\begin{aligned}
\mathrm{tr}\left(e^{-\beta\hat{K}_\mu}\mathcal{D}(|\eta\rangle\langle\eta|)\right) &= \kappa(\eta)\sum_{i,j\in I}\left((1-\eta_i)\eta_j\gamma_{i,j}\, e^{-\beta(E_i-E_j)} - \eta_i(1-\eta_j)\gamma_{i,j}\right)\\
&\quad + \kappa(\eta)\sum_{j\in I}\left(\eta_j(\gamma_{\star,j}+\gamma_{\diamond,j})e^{\beta(E_j-\mu)} - (1-\eta_j)(\gamma_{\star,j}+\gamma_{\diamond,j})\right)\\
&\quad + \kappa(\eta)\sum_{i\in I}\left((1-\eta_i)(\gamma_{i,\star}+\gamma_{i,\diamond})e^{-\beta(E_i-\mu)} - \eta_i(\gamma_{i,\star}+\gamma_{i,\diamond})\right)
\end{aligned}\tag{5.9}$$

To abbreviate, call

$$\theta_{ji} = \gamma_{i,j}\, e^{-\beta(E_i-E_j)} - \gamma_{i,j} \tag{5.10}$$

$$\theta_j = (\gamma_{\star,j}+\gamma_{\diamond,j})e^{\beta(E_j-\mu)} - (\gamma_{j,\star}+\gamma_{j,\diamond}), \tag{5.11}$$

for all $i, j \in I$. Now we exchange the indices j and i in the second term inside the first sum and in the last sum of formula (5.9). This shows that $\mathcal{L}_*(\omega_\beta) = 0$ if and only if

$$\sum_{i,j\in I}(1-\eta_i)\eta_j\theta_{ji} + \sum_{j\in I}\eta_j\theta_j - \sum_{j\in I}(1-\eta_j)\theta_j e^{-\beta(E_j-\mu)} = 0\,, \quad (\eta\in\mathcal{C}). \tag{5.12}$$

Since any $\eta \in \mathcal{C}$ can be written as a characteristic function $\eta = 1_T$ for a given subset T of I, the above equation is equivalent to have

$$\sum_{j\in T}\sum_{i\in I\setminus T}\theta_{ji} + \sum_{j\in T}\theta_j - \sum_{j\in I\setminus T}\theta_j e^{-\beta(E_j-\mu)} = 0. \tag{5.13}$$

From (5.10), (5.11) and (5.13), it is clear that (5.3) and (5.4) are sufficient conditions to have ω_β as a normal stationary state. We prove their necessity. Assume ω_β to be stationary, then (5.13) holds. Take $T = I$ in (5.13), then

$$\sum_{j\in I}\theta_j = 0, \tag{5.14}$$

and the choice $T = \emptyset$ gives

$$\sum_{j\in I} \theta_j e^{-\beta(E_j-\mu)} = 0. \tag{5.15}$$

Using (5.15), (5.13) may be written equivalently as

$$\sum_{j\in T} \sum_{i\in I\setminus T} \theta_{ji} + \sum_{j\in T} \theta_j (1 + e^{-\beta(E_j-\mu)}) = 0. \tag{5.16}$$

On the other hand, as $\theta_{jj} = 0$, replacing $T = \{l\}$ in (5.16), for any fixed $l \in I$, yields

$$\sum_{i\in I} \theta_{li} + \theta_l (1 + e^{-\beta(E_l-\mu)}) = 0. \tag{5.17}$$

Fix, $k, l \in I$ and use (5.13) with $T = \{k, l\}$. Then

$$\sum_{i\notin\{l,k\}} (\theta_{li} + \theta_{li}) + \theta_l(1 + e^{-\beta(E_l-\mu)}) + \theta_k(1 + e^{-\beta(E_k-\mu)}) = 0. \tag{5.18}$$

From equation (5.17) we derive:

$$\sum_{i\notin\{l,k\}} (\theta_{li} + \theta_{ki}) + \theta_{lk} - \theta_{kl} + \left[\theta_l(1 + e^{-\beta(E_l-\mu)}) + \theta_k(1 + e^{-\beta(E_k-\mu)})\right] = 0,$$

so that (5.18) yields

$$\theta_{lk} = -\theta_{kl}.$$

But $\theta_{lk} = -\theta_{kl} e^{-\beta(E_l-E_k)}$, therefore

$$\theta_{lk}(-e^{-\beta(E_l-E_k)} + 1) = 0.$$

It follows that $\theta_{lk} = 0$ if $E_k \neq E_l$, which proves (5.3). Furthermore, (5.17) yields:

$$\theta_l(1 + e^{-\beta(E_l-\mu)}) = \sum_{k, E_k=E_l} \theta_{lk},$$

from which (5.4) follows. Finally, (5.5) is a consequence of (5.14). □

We now show the uniqueness of the stationary state given by (5.1). For this, we strongly use the fact that under the hypotheses of Theorem 5.2 we have the existence of a faithful stationary state, to apply the results of [42]. Indeed, in that case, the set $\mathcal{A}(\Phi)$ of all fixed points of the semigroup Φ is a von Neumann algebra. Let $\mathcal{N}(\Phi)$ be the algebra of all elements $B \in \mathcal{B}_0$ such that $\Phi_t(B^*B) = \Phi_t(B^*)\Phi_t(B)$, for all $t \geq 0$. Then, it is clear that $\mathcal{A}(\Phi) \subseteq \mathcal{N}(\Phi)$. Frigerio (see [42]) was the first to notice that under the above hypothesis, the equality between the two algebras implies the convergence towards the equilibrium for the semigroup.

Lemma 5.3 (Frigerio)**.** *Let Φ be a quantum dynamical semigroup which admits a faithful normal stationary state. Then $\mathcal{A}(\Phi)$ is a von Neumann algebra and there exists a unique Φ-invariant conditional expectation $\mathbb{E}^{\mathcal{A}(\Phi)}(\cdot)$ of $\mathcal{B}_0$ onto $\mathcal{A}_0$ given by*

$$\mathbb{E}^{\mathcal{A}(\Phi)}(B) = w^* - \lim_{T\to\infty} \frac{1}{T} \int_0^T \Phi_t(B) dt, \tag{5.19}$$

for all $B \in \mathcal{B}_0$, where the integral is understood as a weak limit of Riemann sums.*

Moreover, a normal state φ on $\mathcal{B}_0$ is Φ_*-invariant if and only if it is of the form

$$\varphi(\cdot) = \varphi|_{\mathcal{A}(\Phi)} \circ \mathbb{E}^{\mathcal{A}(\Phi)}(\cdot)\,.$$

In particular, if $\mathcal{A} = \mathbb{C}\,\mathbf{1}$, the semigroup Φ has a unique stationary state.

For the proof of this lemma, see [42].

This reduces the study of normal Φ-invariant (stationary) states on $\mathcal{B}_0$ to that of normal states on $\mathcal{A}(\Phi)$. It follows that ω_β is the unique stationary state for Φ as soon as we prove that $\mathcal{A}(\Phi) = \mathbb{C}\mathbf{1}$.

In our case, since $\hat{H}$ is bounded and self-adjoint the following result, borrowed to [43] holds. We use the customary notation $\{B_1, \dots, B_r\}'$ for the algebra of all operators $B \in \mathcal{B}_0$ commuting with all B_i, $i = 1, \dots, r$ (generalized commutant).

Lemma 5.4 (Fagnola-Rebolledo)**.** *Under the hypotheses of Proposition 5.2, the semigroup Φ satisfies*

$$\begin{aligned} \mathcal{A}(\Phi) &= \left\{\hat{H}, L_\ell, L_\ell^*;\ \ell \in L\right\}', \\ \mathcal{N}(\Phi) &= \{L_\ell, L_\ell^*;\ \ell \in L\}'\,. \end{aligned}$$

We refer the reader to [43] for the proof of this fact.

Lemma 5.5. *Assume that all indices $i \in I$ are connected to at least one of the baths $\star, \diamond$. Then*

$$\{L_\ell, L_\ell^*;\ \ell \in L\}' = \mathbb{C}\mathbf{1}. \tag{5.20}$$

As a result, $\mathcal{A}(\Phi) = \mathcal{N}(\Phi) = \mathbb{C}\mathbf{1}$.

Proof. Let first assume that $\gamma_{i,\star} + \gamma_{i,\diamond} > 0$ for any $i \in I$. Then $\{L_\ell, L_\ell^*;\ \ell \in L\}' \subseteq \left\{c_i, c_i^\dagger;\ i \in I\right\}'$. But the set of bounded operators $\left\{c_i, c_i^\dagger;\ i \in I\right\}$ is irreducible on $\Gamma_f(\mathfrak{h}^1)$ (see [33], Proposition 5.2.2), so that $\left\{c_i, c_i^\dagger;\ i \in I\right\}' = \mathbb{C}\mathbf{1}$.

Let $i \in I$ be such that there is $k \in I$, $k \neq i$, for which $\gamma_{i,k} > 0$ and $\gamma_{k,\star} + \gamma_{k,\diamond} > 0$. Then $c_k^\dagger c_i$, c_k and thus $c_i = c_k c_k^\dagger c_i + c_k^\dagger c_i c_k$ are in the algebra generated by the operators L_ℓ and L_ℓ^*. Therefore, $\{L_\ell, L_\ell^*;\ \ell \in L\}' \subset \left\{c_i, c_i^\dagger\right\}'$.

Thus, if every i is connected to $\star$ or $\diamond$, an iteration of the above argument allows to complete the proof. □

Proof. [of Theorem 5.1] This is a consequence of Lemmas 5.3, 5.4 and 5.5 and Proposition 5.2. The final statement is a straightforward application of the main result of [42] (see also [43]). □

6. The hopping conductivity

We derive in this section a formula for the DC conductivity. A field $\mathcal{E}(t)$ is applied to the system at the initial time $t = 0$ and becomes constant in time and equal to $\mathcal{E}$ for $t \geq \Delta t_{\mathcal{E}} > 0$. That is, we assume $\mathcal{E}(t)$ to be a continuous function which grows rapidly to the constant value $\mathcal{E}$. Since we are interested in the stationary regime, we will assume $t \geq \Delta t_{\mathcal{E}}$ or $t = 0$ in any expression depending on the time t below.

We denote by $\hat{H}$ the zero-field Hamiltonian and by $\hat{X}$ the position operator. $\hat{X}$ is the second quantized of the usual position operator X on $\mathfrak{h}^1$, defined by $X\psi(x) = x\,\psi(x)$, $(\psi \in \mathfrak{h}^1,\, x \in \Lambda)$. It is a self-adjoint and bounded operator on $\Gamma_f(\mathfrak{h}^1)$. The matrix elements of X are denoted by:

$$x_{ij} = \langle \psi_i, X\psi_j \rangle, \;\; x_i = x_{ii}, \; (i, j \in I). \tag{6.1}$$

The chemical potentials of the two baths are initially equal to μ, so that the system is in the Gibbs equilibrium state ρ_β at $t = 0$. They are then switched to different values $\mu_\star$ and $\mu_\diamond$, allowing the system to evolve towards the proper steady state. To simplify the discussion, it is assumed that the only eigenfunction ψ_i from which electrons can be lost or gained from the bath $\star$ (resp. from the bath $\diamond$) is $\psi_{i(\star)}$ (resp. $\psi_{i(\diamond)}$). More precisely, the only non-zero rates $\gamma_{i,j}$, (i or $j \in \{\star, \diamond\}$) of jumps from or into the baths are $\gamma_{i(\star),\star}$, $\gamma_{\star,i(\star)}$, $\gamma_{i(\diamond),\diamond}$ and $\gamma_{\diamond,i(\diamond)}$, with $i(\star), i(\diamond) \in I$, $i(\star) \neq i(\diamond)$. This is a simplification of the real situation, in which the rates $\gamma_{i,\star}$ (resp. $\gamma_{i,\diamond}$) are very small compared with $\gamma_{i(\star),\star}$ (resp. $\gamma_{i(\diamond),\diamond}$) due to their exponential decreasing (see subsection 3.3). The variations of chemical potential $\mu_\star - \mu$ and $\mu_\diamond - \mu$ are chosen equal to the electrical potentials $-q\mathcal{E}x_\star$ and $-q\mathcal{E}x_\diamond$ created by the field $\mathcal{E}$ at the localization centers $x_{i(\star)}$ and $x_{i(\diamond)}$, respectively, where q is the charge of the electron. The generalization to the case where several eigenfunctions ψ_i are connected to each bath is straightforward, provided that the two sets $\{x_i; i \in I, \gamma_{i,\star}, \gamma_{\star,i} > 0\}$ and $\{x_i; i \in I, \gamma_{i,\diamond}, \gamma_{\diamond,i} > 0\}$ in $\mathbb{R}^d$ are perpendicular to the field $\mathcal{E}$.

In what follows, all quantities without an explicitly mentioned $\mathcal{E}$-dependence correspond to their values for $\mathcal{E} = 0$ and $\mu_\star = \mu_\diamond = \mu$.

The main result of this section is the following formula for the hopping conductivity.

Theorem 6.1. *Assume that $\hat{H}$ and H have non-degenerated eigenvalues. Let moreover assume that $\gamma_{i,j}(\mathcal{E}) = \gamma_{i,j} + \mathcal{O}(\mathcal{E}^2)$ if i or $j \in \{\star, \diamond\}$. Then $j = \sigma\mathcal{E} + \mathcal{O}(\mathcal{E}^2)$ and the conductivity σ is given by the following formula:*

$$\sigma = \frac{q^2\beta}{V}\mathrm{tr}\left(\rho_\beta\, \hat{P}\big(\mathcal{L}^{-1}\mathcal{L}^{(int)}(\hat{X}_0) - \hat{X}_0\big)\right) = -\frac{q^2\beta}{V}\mathrm{tr}\left(\rho_\beta\, \hat{P}\mathcal{L}^{-1}\mathcal{L}^{(ext)}(\hat{X}_0)\right), \tag{6.2}$$

where $\hat{P}$ is the operator:

$$\hat{P} = \sum_{i,j \in I, i \neq j} \gamma_{j,i}(x_i - x_j)(1 - n_i)n_j \tag{6.3}$$

and $\hat{X}_0$ is the part of the position operator $\hat{X}$ which commutes with $\hat{H}$:

$$\hat{X}_0 = \sum_{i \in I} x_i n_i \in \mathcal{A}_0'. \tag{6.4}$$

This theorem is proved through the remain of this section. Since only the part $\hat{X}_0 \in \mathcal{A}_0'$ contributes to the current, one deals here with a "classical current". As noted in [21], the contribution in j of the off-diagonal part of $\hat{X}$ ("coherent current") vanishes because of the decoherence effects in the adiabatic regime, which suppress for large times the off-diagonal part of observables in the preferential basis formed by the eigenvectors of $\hat{H}$.

The physical interpretation of the operator $\hat{P}$ is the following. The electrical power dissipated during the evolution is given by the electronic observable $-q\mathcal{E}\hat{P}$. Indeed, its matrix elements $-q\mathcal{E}\,\langle \eta|\hat{P}|\eta\rangle$ are the sum, over all $i, j \in I$, of the rates $\gamma_{i,j}$ of an electronic jump from an *occupied*

($\eta_i = 1$) wavefunction $\psi_i \in \mathfrak{h}^1$ into an *unoccupied* ($\eta_j = 0$) wavefunction ψ_j, multiplied by the potential energy $-q\mathcal{E}(x_j - x_i)$ lost during this jump.

6.1. **Discussion.** Let us first discuss how the electric field $\mathcal{E}$ changes the parameters of the model studied in the previous sections.

- The Hamiltonian $\hat{H}$ becomes $\hat{H}_{\mathcal{E}} = \hat{H} - q\mathcal{E}\hat{X}$ in presence of the field. According to standard perturbation theory, the eigenvectors $\psi_i(\mathcal{E})$ and the (non degenerated) eigenvalues $E_i(\mathcal{E})$ of the one-electron Hamiltonian $H_{\mathcal{E}} = H - q\mathcal{E}X$ on $\mathfrak{h}^1$ are given for any $i \in I$ by [44]:

$$\psi_i(\mathcal{E}) = \psi_i - q\mathcal{E} \sum_{j\in I, j\neq i} \frac{x_{ji}}{E_i - E_j}\psi_j + \mathcal{O}(\mathcal{E}^2) \tag{6.5}$$

$$E_i(\mathcal{E}) = E_i - q\mathcal{E}\, x_i + \mathcal{O}(\mathcal{E}^2). \tag{6.6}$$

- The jump rates $\gamma_{i,j}$ are modified by the electric field, in order to satisfy the conditions (3.4), (3.5) and (3.6) with the energies $E_i(\mathcal{E})$. For the choice $\mu_\star = \mu - q\mathcal{E}x_\star$ and $\mu_\diamond = \mu - q\mathcal{E}x_\diamond$ of the two chemical potentials, the rates $\gamma_{i,j}(\mathcal{E})$, ($i$ or $j \in \{\star, \diamond\}$) of jumps from or into the baths differ from their zero-field values only by terms of order $\mathcal{E}^2$. Actually, the change in the chemical potential in (3.5) for $j = i(\star)$ exactly compensates the change in the energy E_j as given by (6.6) (i.e., to first order in $\mathcal{E}$), and the same holds true in (3.6) for $j = i(\diamond)$. Thus the conditions (3.5) and (3.6) still hold for $\mathcal{E} \neq 0$ if $\gamma_{i,j}(\mathcal{E}) = \gamma_{i,j} + \mathcal{O}(\mathcal{E}^2)$, ($i$ or $j \in \{\star, \diamond\}$).
- The jump operators C_ℓ are built from the creation and annihilation operators associated to the eigenvectors $\psi_i(\mathcal{E})$ as explained in section 3. It is easily seen from (3.3) and (6.5) that they are modified by the electric field as follows:

$$C_{i,j}(\mathcal{E}) = C_{i,j} - q\mathcal{E} \sum_{k\in I, k\neq j} \frac{x_{kj}\, 1_I(j)}{E_j - E_k} C_{i,k} - q\mathcal{E} \sum_{k\in I, k\neq i} \frac{x_{ik}\, 1_I(i)}{E_i - E_k} C_{k,j} + \mathcal{O}(\mathcal{E}^2). \tag{6.7}$$

We denote by $\mathcal{L}_{\mathcal{E}}$ the Lindbladian (4.6) corresponding to the values of $C_{i,j}(\mathcal{E})$ and $\gamma_{i,j}(\mathcal{E})$ above. The quantum dynamical semigroup generated by $\mathcal{L}_{\mathcal{E}}$ is denoted by $\Phi^{\mathcal{E}}$.

6.2. **The linear response.** Our starting point is the expression (6.8) below for the current density:

$$j = \frac{q}{V} \lim_{T\to\infty} \int_0^T \frac{dt}{T} \operatorname{tr}\left(\rho_\beta\, \Phi_t^{\mathcal{E}}(\mathcal{L}_{\mathcal{E}}^{(int)}(\hat{X}))\right). \tag{6.8}$$

Proposition 6.2. *The limit in* (6.8) *is well-defined. If the one-electron Hamiltonian H has non-degenerated eigenvalues, then it is equal, to lowest order in $\mathcal{E}$, to:*

$$j = \frac{q}{V} \lim_{T\to\infty} \int_0^T \frac{dt}{T} \operatorname{tr}\left(\rho_\beta\, \Phi_t^{\mathcal{E}}(\mathcal{L}_{\mathcal{E}}^{(int)}(\hat{X}_0))\right) + \mathcal{O}(\mathcal{E}^2). \tag{6.9}$$

where $\hat{X}_0$ is given by (6.4). *Moreover, for any value of the field $\mathcal{E}$, the current j vanishes if $\mu_\star = \mu_\diamond = \mu$.*

Proof. It follows from the existence of a faithful normal stationary state for $\Phi^{\mathcal{E}}$ (Theorem 5.1) and from Frigerio's ergodic theorem (Lemma 5.3) that the $\star$-weak limits:

$$\mathbb{E}^{\mathcal{A}(\Phi^{\mathcal{E}})}(\hat{B}) = w^*\text{-}\lim_{T\to\infty} \int_0^T \frac{dt}{T}\, \Phi_t^{\mathcal{E}}(\hat{B})$$

define a conditional expectation $\mathbb{E}^{\mathcal{A}(\Phi^{\mathcal{E}})} : \mathcal{B}_0 \to \mathcal{A}(\Phi^{\mathcal{E}}) = \ker \mathcal{L}_{\mathcal{E}}$. In particular, the limit (6.8) is well-defined.

Assume that H has non-degenerated eigenvalues. By standard perturbation theory, the same holds true for $H_{\mathcal{E}}$ if $|\mathcal{E}|$ is sufficiently small. Since $\mathcal{L}_*(\rho_\beta) = \mathcal{L}_*^{(int)}(\rho_\beta) = 0$, one has for any $i, j \in I$:

$$\mathrm{tr}\left(\rho_\beta\, \Phi_t^{\mathcal{E}}(\mathcal{L}_{\mathcal{E}}^{(int)}(c_i^\dagger(\mathcal{E})c_j(\mathcal{E})))\right) = \mathrm{tr}\left(\rho_\beta\, \Phi_t^{\mathcal{E}}(\mathcal{L}_{\mathcal{E}}^{(int)}(c_i^\dagger c_j))\right) + \mathcal{O}(\mathcal{E}^2). \tag{6.10}$$

Let us show that the time-average of the left-hand side vanishes if $i \neq j$. Indeed, by lemma 5.4, $\mathcal{A}(\Phi^{\mathcal{E}})$ is included in the algebra $\mathcal{A}'_{\hat{H}_{\mathcal{E}}}$ of all bounded operators commuting with $\hat{H}_{\mathcal{E}}$. The conditional expectation $\mathbb{E}^{\hat{H}_{\mathcal{E}}} : \mathcal{B}_0 \to \mathcal{A}'_{\hat{H}_{\mathcal{E}}}$ thus satisfies $\mathbb{E}^{\mathcal{A}(\Phi^{\mathcal{E}})}\mathbb{E}^{\hat{H}_{\mathcal{E}}} = \mathbb{E}^{\mathcal{A}(\Phi^{\mathcal{E}})}$. Moreover, by proposition 4.2, $\mathcal{L}_{\mathcal{E}}^{(int)}$ commutes with $\mathbb{E}^{\hat{H}_{\mathcal{E}}}$. Hence:

$$\mathrm{tr}\left(\rho_\beta\, \mathbb{E}^{\mathcal{A}(\Phi^{\mathcal{E}})}\mathcal{L}_{\mathcal{E}}^{(int)}(c_i^\dagger(\mathcal{E})c_j(\mathcal{E}))\right) = \mathrm{tr}\left(\rho_\beta\, \mathbb{E}^{\mathcal{A}(\Phi^{\mathcal{E}})}\mathcal{L}_{\mathcal{E}}^{(int)}\mathbb{E}^{\hat{H}_{\mathcal{E}}}\left(c_i^\dagger(\mathcal{E})c_j(\mathcal{E})\right)\right) = 0$$

for any $i, j \in I$, $i \neq j$. Together with (6.10), this proves (6.9).

Let $\mu_\star = \mu_\diamond = \mu$. It follows from the detailed balance and Theorem 5.1 that:

$$j = \frac{q}{V}\mathrm{tr}\left(\rho_\beta^{(\mathcal{E})}\mathcal{L}_{\mathcal{E}}^{(int)}(\hat{X})\right),$$

where

$$\rho_\beta^{(\mathcal{E})} = \frac{1}{Z(\beta,\mu,\mathcal{E})}\exp\bigl(-\beta(\hat{H}_{\mathcal{E}} - \mu\hat{N})\bigr)$$

is the unique stationary state of the semigroup $\Phi^{\mathcal{E}}$. But this state satisfies ${\mathcal{L}_{\mathcal{E}}}_*^{(int)}(\rho_\beta^{(\mathcal{E})}) = 0$ by theorem 5.1 again. This implies $j = 0$. $\square$

By subtracting to the right-hand side of (6.8) the vanishing current obtained for $\mathcal{E} = 0$ and $\mu_\star = \mu_\diamond = \mu$, one gets to lowest order in $\mathcal{E}$:

$$j = \frac{q}{V}\lim_{T\to\infty}\int_0^T \frac{dt}{T}\,\mathrm{tr}\left(\rho_\beta\,\delta\Phi_t \circ \mathcal{L}^{(int)}(\hat{X}_0) + \rho_\beta\,\Phi_t \circ \delta\mathcal{L}^{(int)}(\hat{X}_0)\right) + \mathcal{O}(\mathcal{E}^2), \tag{6.11}$$

with $\delta\mathcal{L}^{(int)} \equiv \mathcal{L}_{\mathcal{E}}^{(int)} - \mathcal{L}^{(int)}$ and, by Abel's formula,

$$\delta\Phi_t(\cdot) \equiv \Phi_t^{\mathcal{E}}(\cdot) - \Phi_t(\cdot) = \int_0^t \Phi_{t-s}(\,\delta\mathcal{L}\,(\Phi_s(\cdot)))ds + \mathcal{O}(\mathcal{E}^2).$$

A straightforward computation using $\mathcal{L}_*(\rho_\beta) = 0$ yields:

$$\begin{aligned} j \;=\; & \frac{q}{V}\Biggl\{\lim_{T\to\infty}\frac{1}{T}\mathrm{tr}\left(\rho_\beta\,\delta\mathcal{L}\circ(\Phi_T - \mathbf{1})\circ\mathcal{L}^{-2}\circ\mathcal{L}^{(int)}(\hat{X})\right) - \mathrm{tr}\left(\rho_\beta\,\delta\mathcal{L}\circ\mathcal{L}^{-1}\circ\mathcal{L}^{(int)}(\hat{X}_0)\right) \\ & +\mathrm{tr}\left(\rho_\beta\,\delta\mathcal{L}^{(int)}(\hat{X}_0)\right)\Biggr\}. \end{aligned}$$

The limit vanishes by the convergence to equilibrium (see the last statement of theorem 5.1), leading to:

$$j = -\frac{q}{V}\mathrm{tr}\left(\rho_\beta\,\delta\mathcal{L}\circ\mathcal{L}^{-1}\circ\mathcal{L}^{(int)}(\hat{X}_0) - \rho_\beta\,\delta\mathcal{L}^{(int)}(\hat{X}_0)\right). \tag{6.12}$$

6.3. **The computation of the conductivity.** To go further, one needs to compute $\delta\mathcal{L} = \mathcal{L}_{\mathcal{E}} - \mathcal{L}$ to the first order in $\mathcal{E}$. Let $\eta \in \mathcal{C}$. Since ρ_β commutes with $\hat{H}$, $\mathrm{tr}\left(\rho_\beta[\delta\hat{H}, |\eta\rangle\langle\eta|\,]\right) = 0$. By (6.7), the trace:

$$\mathrm{tr}\left(\rho_\beta\big(2\,\delta C_\ell^\star|\eta\rangle\langle\eta|C_\ell + 2C_\ell^\star|\eta\rangle\langle\eta|\,\delta C_\ell - \delta(C_\ell^\star C_\ell)|\eta\rangle\langle\eta| - |\eta\rangle\langle\eta|\,\delta(C_\ell^\star C_\ell)\big)\right)$$

vanishes as well for any $\ell \in L$. Taking into account that $\delta\gamma_{i,j} = \mathcal{O}(\mathcal{E}^2)$ for i or j in $\{\star, \diamond\}$, this proves that, disregarding terms of order $\mathcal{E}^2$,

$$\begin{aligned} \mathrm{tr}\left(\rho_\beta\,\delta\mathcal{L}(|\eta\rangle\langle\eta|)\right) &= \mathrm{tr}\left(\rho_\beta\,\delta\mathcal{L}^{(int)}(|\eta\rangle\langle\eta|)\right) \\ &= \sum_{i,j,i\neq j} \delta\gamma_{i,j}\mathrm{tr}\left(\rho_\beta\,C_{i,j}^\star|\eta\rangle\langle\eta|C_{i,j} - \rho_\beta\,n_i(1-n_j)|\eta\rangle\langle\eta|\right). \end{aligned}$$

The representation of ρ_β in the form (5.7) yields:

$$\begin{aligned} \mathrm{tr}\left(\rho_\beta\,\delta\mathcal{L}(|\eta\rangle\langle\eta|)\right) &= \sum_{i\xrightarrow{\eta}j} \delta\gamma_{i,j}p(\eta + 1_i - 1_j) - \sum_{j\xrightarrow{\eta}i} \delta\gamma_{i,j}p(\eta) + \mathcal{O}(\mathcal{E}^2) \\ &= p(\eta)\sum_{i\xrightarrow{\eta}j}\left(\delta\gamma_{i,j}e^{-\beta(E_i - E_j)} - \delta\gamma_{j,i}\right) + \mathcal{O}(\mathcal{E}^2). \end{aligned} \tag{6.13}$$

Now, as a result of (6.6) and of the detailed balance condition (3.4) for $\mathcal{E} = 0$ and $\mathcal{E} \neq 0$ with the energies $E_i(\mathcal{E})$,

$$\delta\gamma_{i,j}e^{-\beta(E_i-E_j)} - \delta\gamma_{j,i} = \gamma_{j,i}\delta\ln\frac{\gamma_{i,j}}{\gamma_{j,i}} = -q\mathcal{E}\beta\,\gamma_{j,i}(x_i - x_j) + \mathcal{O}(\mathcal{E}^2).$$

Then:

$$\mathrm{tr}\left(\rho_\beta\,\delta\mathcal{L}(\hat{B})\right) = \mathrm{tr}\left(\rho_\beta\,\delta\mathcal{L}^{(int)}(\hat{B})\right) = -q\mathcal{E}\beta\,\mathrm{tr}\left(\rho_\beta\,\hat{P}\hat{B}\right) + \mathcal{O}(\mathcal{E}^2), \tag{6.14}$$

with $\hat{B} = |\eta\rangle\langle\eta|$. Since all eigenvalues of $\hat{H}$ are assumed to be non-degenerated, the projectors $|\eta\rangle\langle\eta|$, $(\eta \in \mathcal{C})$ span $\mathcal{A}_0'$. Thus (6.14) is actually true for any $\hat{B} \in \mathcal{A}_0'$.

But the algebra $\mathcal{A}_0'$ is invariant under the adiabatic generators $\mathcal{L}$ and $\mathcal{L}^{(int)}$ (section 4.1). Moreover, $\hat{X}_0$ belongs to $\mathcal{A}_0'$ by definition. The result (6.1) is obtained from (6.12) and (6.14).

6.4. **Link with the resistor network approach.** According to the work of Miller and Abrahams [45], the hopping current should be equal to the current of a network of electrical resistors connecting all points x_i, $(i \in I)$. It is interesting to check explicitly this affirmation in our model. Consider the normal state $\rho_\infty^{(\mathcal{E})}$ on $\mathcal{B}_0 = \mathcal{B}(\Gamma_f(\mathfrak{h}^1))$ defined as:

$$\mathrm{tr}\left(\rho_\infty^{(\mathcal{E})}\hat{B}\right) = \lim_{T\to\infty}\int_0^T \frac{dt}{T}\,\mathrm{tr}\left(\rho_\beta\,\Phi_t^{\mathcal{E}}(\hat{B})\right), (\hat{B} \in \mathcal{B}_0).$$

It is convenient to *define* some local chemical potentials $\delta\mu_i$ as follows:

$$p_\infty^{(\mathcal{E})}(\eta) \equiv \langle\eta|\rho_\infty^{(\mathcal{E})}|\eta\rangle = \frac{1}{Z(\beta,\mu)}\prod_{i\in I} e^{-\beta(E_i-\mu-\delta\mu_i)\eta_i}, (\eta \in \mathcal{C}).$$

One easily shows that, to lowest order in $\delta\mu_i$, $p_\infty^{(\mathcal{E})}(\eta) = p(\eta)(1+\sum_{i\in I}\delta\mu_i\eta_i)$. A straightforward computation then gives:

$$\mathrm{tr}\left(\left(\rho_\infty^{(\mathcal{E})} - \rho_\beta\right)\mathcal{L}^{(int)}(\hat{B})\right) = \beta \sum_{i,j\in I, i\neq j} \gamma_{j,i}(\delta\mu_i - \delta\mu_j)\,\mathrm{tr}\left(\rho_\beta(1-n_i)n_j\hat{B}\right)$$

for $\hat{B} = |\eta\rangle\langle\eta|$, $\eta \in \mathcal{C}$ and thus for any $\hat{B} \in \mathcal{A}_0'$. It follows from this formula and from (6.11) and (6.14) that:

$$\begin{aligned} j &= \frac{q}{V}\mathrm{tr}\left(\left(\rho_\infty^{(\mathcal{E})} - \rho_\beta\right)\mathcal{L}^{(int)}(\hat{X}_0)\right) + \frac{q}{V}\mathrm{tr}\left(\rho_\beta\,\delta\mathcal{L}^{(int)}(\hat{X}_0)\right) \\ &= \frac{q\beta}{2V}\sum_{i,j,k\in I, i\neq j} x_k\big(\delta\mu_i - q\mathcal{E}x_i - \delta\mu_j + q\mathcal{E}x_j\big)\big\{\gamma_{j,i}\mathrm{tr}\left(\rho_\beta\,(1-n_i)n_jn_k\right) \\ &\quad -\gamma_{i,j}\mathrm{tr}\left(\rho_\beta\,(1-n_j)n_in_k\right)\big\}. \end{aligned}$$

The expression inside the brackets is equal to $(1_k(j) - 1_k(i))R_{ij}^{-1}/(q^2\beta)$, where:

$$R_{ij}^{-1} = q^2\beta\,\gamma_{i,j}f_\mu(E_i)(1-f_\mu(E_j))$$

and $f_\mu(E)$ is the Fermi-Dirac function:

$$f_\mu(E) = \frac{1}{1+e^{\beta(E-\mu)}}.$$

As a result,

$$j = \frac{1}{2qV}\sum_{i,j\in J, i\neq j} R_{ij}^{-1}(x_i - x_j)\big(\delta\mu_j - q\mathcal{E}x_j - \delta\mu_i + q\mathcal{E}x_i\big) \tag{6.15}$$

It is easy to show [21] that the expression one the right-hand side is the average, over all surfaces S perpendicular to $\mathcal{E}$, of the current density through S obtained by Miller and Abrahams ([45], formula III-1). The quantity inside the second parenthesis is the total difference of potential (electrical and chemical) between the localization centers x_i and x_j. Thus, the current is indeed the same as that of a resistor network, each site x_i being connected to all sites x_j, ($j \in I$) by some electric wires of resistances R_{ij}.

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