The Quantum Jumps Approach for Infinitely Many States

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Abstract. A new class of models describing the dissipative dynamics of an open quantum system by means of random time evolutions of its wavefunction is considered. The random evolutions are linear and defined by Poisson processes. At the random Poissonian times, the wavefunction experiences discontinuous changes (quantum jumps). These changes are implemented by some non unitary operators satisfying a locality condition. The stochastic dynamics gives the Lindblad master equation back after averaging over the random times. If the Hilbert space of the system is infinite dimensional, the models involve an infinite number of independent Poisson processes and the total frequency of jumps is infinite. We show that the random evolutions are then given by some almost-surely defined unbounded random evolution operators obtained by a limit procedure. The relevance of the models in the field of electronic transport in Anderson insulators is briefly discussed.

1 Introduction

The dissipative dynamics of an open quantum system S can be described in two different ways. The first and most popular approach consists in coupling S with a reservoir R. The density matrix ρ_{tot} of the total system $S + R$ is assumed to follow a Liouville–von Neumann equation, i.e., one assumes that $S+R$ is a closed system. A state of S is specified by the reduced density matrix ρ, defined as the partial trace of ρ_{tot} over the reservoir's Hilbert space. ρ does not describe a single system but a statistical ensemble. By tracing out the degrees of freedom of R in the Liouville–von Neumann equation, one obtains an integro–differential equation for ρ (Nakajima–Zwanzig equation). Using a suitable Markov approximation to eliminate memory effects, this equation is then transformed into a simpler first-order linear differential equation, called the *master equation* [1]. The reduced dynamics does not conserve pure states. It has been shown by Lindblad [2] that the Markovian master equation is of the form:

$$\frac{\mathrm{d}\rho}{\mathrm{d}t} = \mathcal{L}\rho = -\mathrm{i}[H_S,\rho] + \frac{1}{2}\sum_{\ell}\Big([L_\ell\,\rho, L_\ell^\dagger] + [L_\ell, \rho L_\ell^\dagger]\Big)\ . \tag{1}$$

H_S is the Hamiltonian of S (including the energy shifts due to the coupling with the reservoir), and L_ℓ are some operators acting on the Hilbert space $\mathcal{H}_S$ of S, called the Lindblad operators in the sequel. An alternative approach for the same problem is based on stochastic evolutions of pure states. The state of S is specified by a random wavefunction (RW) in $\mathcal{H}_S$, evolving according to a linear or nonlinear *stochastic Schrödinger equation*. Different stochastic evolutions have been proposed in the last two decades in various fields of physics and mathematics, especially Quantum Optics [3,4], Quantum Measurement Theory [5–14] and Electronic Transport in Solids [15–17]. Consistency with the master equation approach requires that the pure state evolution gives the density matrix evolution back after averaging over the dynamical noise. Apart from being intuitively appealing, the RW models provide quite efficient tools for solving master equations numerically. Actually, one is led to integrate N coupled differential equations for the wavefunction, where N is the dimension of $\mathcal{H}_S$, for a large enough number of realizations of the dynamical noise. For large N, this is generally much more efficient than integrating the $N \times N$ coupled master equations for the density matrix. However, the RW models are more than simple mathematical or numerical tools: they describe the real evolution of the system S under continuous monitoring by means of measurements (photons counting, homodyne or heterodyne detections) [18]. The randomness of their dynamics is a consequence of our ignorance of the result of a measurement in quantum mechanics. At the end of the eighties, experiments on the fluorescence of single ions in magnetic traps have shown records of 'quantum jumps' between an excited atomic state and a lower state, occurring at random times [18]. These sudden jumps – which were already assumed to exist by Einstein in his paper on the A and B atomic coefficients [19] – correspond to the absorption or emission of a photon by the ion at the corresponding transition. Such direct observations have motivated the study of the RW models in Quantum Optics.

The aim of this paper is to study a particular quantum jumps model in the limit where infinitely many levels of the system are coupled by the dissipative dynamics. The model is built in such a way as to give the classical kinetic theory back, such as Boltzmann's equation, when quantum effects can be neglected. Unlike in the models studied in [3,4,6], the stochastic evolution for the wavefunction is linear, which makes the mathematical analysis easier. The price we pay for this convenience is the non conservation of the norm of the random wavefunction.

Many systems with non-degenerate spectra are correctly described by the master equation (1) with $\ell = (i,j)$, $i \neq j$, and:

$$\hat{L}_{i\to j} = \sqrt{\Gamma_{i\to j}}\, a_j^\dagger a_i \ . \tag{2}$$

$a_i^\dagger, a_i$ are the creation and annihilation operators in the one–particle energy eigenstate $|i\rangle$. $\Gamma_{i\to j}$ is the one–particle transition rate from $|i\rangle$ to $|j\rangle$. It can be calculated perturbatively by means of Fermi golden rule [20]. Examples of systems correctly described by this master equation are: (1) an atom coupled to the quantized electromagnetic field radiating in the vacuum [20]; (2) independent electrons in strongly disordered solids coupled to phonons at very low temperatures [21]. The inverse life-time of eigenstate $|i\rangle$ is $\Gamma_i = \sum_{j \neq i} \Gamma_{i \to j}$. If we ignore level shifts, the dynamics of S is completely characterized by its Hamiltonian H_S and by the set of the transition rates $\Gamma_{i \to j}$ for all pairs (i, j) of one–particle eigenstates. In the RW model studied in this paper, the rates $\Gamma_{i \to j}$ give the probability per unit time of occurrence of quantum jumps. For an infinite dimensional Hilbert space $\mathcal{H}_S$, it usually happens that the double sum $\sum_{i,j} \Gamma_{i \to j}$ is infinite, i.e., that an infinite number of jumps occur in any finite time interval. Our main result shows that, provided the discontinuous changes of the wavefunction at the jumps are sufficiently 'local', the stochastic dynamics in $\mathcal{H}_S$ is also well–defined in this case, and is given by an almost surely unbounded random evolution operator obtained by a limit procedure.

The physical situation which motivates our work is electronic transport in strongly disordered solids [22]. The electronic eigenfunctions are exponentially localized in such solids (Anderson localization [23]). The electrical conductivity thus vanishes at zero temperature. At non zero temperature $T > 0$, transport occurs via phonon–assisted hopping of electrons from one localized eigenstate into another. At small T, a phenomenological argument due to Mott [24] shows that the hopping conductivity σ is given by $\sigma = \sigma_0 \exp(-(T_0/T)^\gamma)$, where the exponent $\gamma = 1/(d+1)$ depends on the dimension d ($d = 1, 2, 3$) only and T_0 is a constant which depends on the localization length and the density of states at the Fermi energy. Efros and Shklovskii have shown that the presence of a wide Coulomb gap in the density of state modifies γ, which then equals $1/2$ for all dimensions [22]. Hopping transport occurs for instance in lightly doped compensated semiconductors at low temperature, in amorphous solids, in two–dimensional electron gases in zero or strong magnetic field, and in the quasicrystal i–AlPdRe [22,25]. The electrons in the disordered potential created by the ions, impurities or defects are coupled to low energy acoustic phonons. Since phonons do not carry current, the study of transport requires the knowledge of the electron dynamics only. The system S of all electrons is thus an open quantum system. If we ignore electron–electron interactions, it can be shown that, at low enough temperature, its dissipative dynamics is correctly described by the master equation (1) with the Lindblad operators (2) [21]. The transition rate $\Gamma_{i \to j}$ between two localized one–electron eigenstates $|i\rangle$ and $|j\rangle$ decreases exponentially with the distance $|i - j|$ between their localization centers, and depends strongly at low temperature on their energies E_i and E_j. The widely used relaxation time approximation, which amounts to replace all the $\Gamma_{i \to j}$'s by a single damping constant, is thus completely unjustified in hopping transport.

A fundamental question addressed by mathematical physicists in the theory of solids concerns the study of the spectrum and of the time evolution of the relevant electronic observables at the thermodynamic limit. Letting the volume of a strongly disordered solid tend to infinity an infinite number of localized eigenstates $|i\rangle$ with energies close to the Fermi energy E_F comes into play. Thus, a well–defined RW dynamics in an infinite dimensional Hilbert space $\mathcal{H}_S$ must be specified. The quantum jump model studied in this paper is a candidate for such a RW dynamics in solids, giving the time evolution of the electrons under electron–phonon or another coupling.

2 The Model

2.1 The Stochastic Scheme

Let us consider a quantum system composed of identical non-interacting particles coupled to their environment. We denote by H the one–particle Hamiltonian, acting on the one–particle Hilbert space $\mathcal{H}$, and $\hat{H}$ the second quantized of H, acting on the Fock space $\mathcal{F} = \oplus_{n=0}^{\infty} P_{\pm} \mathcal{H}^{\otimes n}$. $P_{(\pm)}$ is the particle (anti) symmetrizer. We shall assume that $H = V + T$ is the sum of a (possibly unbounded) self–adjoint operator V with dense domain $\mathcal{D}(H)$ and pure point spectrum, and of a bounded self–adjoint operator T. Let $\{|i\rangle; i \in \Lambda\}$ be the orthonormal basis of $\mathcal{H}$ formed by the eigenfunctions of V, where Λ is an infinite subset of $\mathbb{Z}^d$. If the system is a doped semiconductor, we can think of Λ as the impurity sites in the host crystal $\mathbb{Z}^3$; then H acts on the Hilbert space $\mathcal{H} = \ell^2(\Lambda)$ and $\{|i\rangle; i \in \Lambda\}$ is the canonical basis (see below). The annihilation and creation operators of a particle in state $|i\rangle$, $i \in \Lambda$, are denoted by a_i and $a_i^\dagger$, respectively. For each pair $(i,j) \in \Lambda^2$, $|i-j|$ is the Euclidean distance between $i \in \mathbb{Z}^d$ and $j \in \mathbb{Z}^d$. *Instantaneous jumps* take place at some random times

$$0 \leq t_{i\to j}^1 \leq \ldots \leq t_{i\to j}^m \leq \ldots \quad , \quad i,j \in \Lambda \; .$$

These jumps are labelled by pairs $(i,j) \in \Lambda^2$ of indices and by an integer m, which counts the number of jumps (i,j) that occurred since the initial time $t = 0$. The time delays between two consecutive jumps (i,j), $s_{i\to j}^m = t_{i\to j}^m - t_{i\to j}^{m-1}$, $m = 2, 3, \ldots$, and the first jump times $s_{i\to j}^0 = t_{i\to j}^1$, for all $i,j \in \Lambda$, are assumed to be mutually independent random variables distributed according to the exponential law $p(ds) = \Gamma_{i\to j} e^{-s\,\Gamma_{i\to j}} ds$, where $\Gamma_{i\to j} \geq 0$ depends on (i,j) but not on m. In other words, for any fixed (i,j), the jump times $t_{i\to j}^m$, $m \in \mathbb{N}^\star$ are given by a Poisson process with parameter $\Gamma_{i\to j}$. The *transition rates* $\Gamma_{i\to j}$ are considered here as phenomenological parameters. In concrete situations, they can be computed by using the Fermi golden rule. They contain all the quantitative physical information on the interaction of the system's particles with the environment (e.g., the coupling constant). If the environment is a thermal bath, they depend on its temperature.

Each jump modifies in a discontinuous way the wavefunction of the system in the Fock space $\mathcal{F}$. These discontinuous changes are implemented by some bounded operators $\hat{W}_{i\to j}$ (called *jump operators* in the sequel). More precisely, if the system's wavefunction is $|\psi\rangle \in \mathcal{F}$ just before a jump (i,j), it becomes $\hat{W}_{i\to j}|\psi\rangle$ just after it:

$$\text{jump } (i,j): \qquad |\psi\rangle \to \hat{W}_{i\to j}|\psi\rangle \; . \tag{3}$$

The jump operators describe the qualitative effect of the interaction between S and its environment (e.g., the effect on S of the absorption or the emission of external particles such as photons, phonons, ...). They do not depend on the damping rates or on the temperature of the bath.

Between two consecutive jumps, the system evolves according to the Schrödinger equation with Hamiltonian $\hat{H}+\hat{K}$, where $\hat{K}$ is a bounded operator describing both some damping effects and some energy renormalizations due to the coupling with the environment. We will restrict ourself in this work to systems with a norm–preserving average dynamics, namely, such that $\mathbb{E}\|\psi(t)\|^2 = 1$, where $\mathbb{E}$ is the average over all times $t^m_{i\to j}$. As we shall see below, in order that $\|\psi(t)\|^2$ be conserved in average, the damping operator $\hat{K}$ must be given, *up to a self–adjoint operator*, by:

$$\hat{K} = \hat{K}_1 \equiv \frac{1}{2\mathrm{i}} \sum_{i,j\in\Lambda} \Gamma_{i\to j} \big(\hat{W}^\dagger_{i\to j} + 1\big)\big(\hat{W}_{i\to j} - 1\big) \; . \tag{4}$$

This means that $\hat{K}$ is *not* self–adjoint.

The wavefunction at time t, $t_p \le t < t_{p+1}$, is thus formally given by:

$$\begin{aligned} |\psi(t)\rangle = e^{-\mathrm{i}(t-t_p)(\hat{H}+\hat{K})}\hat{W}_{i_p\to j_p} e^{-\mathrm{i}(t_p-t_{p-1})(\hat{H}+\hat{K})} \dots \\ \dots \hat{W}_{i_1\to j_1} e^{-\mathrm{i}t_1(\hat{H}+\hat{K})}|\psi\rangle \; , \end{aligned} \tag{5}$$

where $|\psi\rangle \in \mathcal{F}$ is the wavefunction at time $t=0$, $0 \le t_1 \le \ldots \le t_p \le \ldots$ are the times of occurrence of *any* jump, and (i_p, j_p) is the random pair of indices corresponding to the jump that takes place at time t_p. As it will be clear below, the formula (5) is only meaningful if:

$$\Gamma \equiv \sum_{i,j\in\Lambda} \Gamma_{i\to j} < \infty \; . \tag{6}$$

A way to define the random wavefunction when $\Gamma = \infty$ will be given in the next section.

From a mathematical point of view, it is convenient to represent each sequence of random times $(t^m_{i\to j})_{m\in\mathbb{N}^*}$ by a counting process $(N_{i\to j}(t))_{t\ge 0}$ [26]. Here $t^m_{i\to j}$ are the left discontinuities of the counting function $N_{i\to j}(t)$. For any compact interval $I \subset \mathbb{R}_+$, $N_{i\to j}(I)$ is the (random) number of jumps (i,j) occurring at times $t \in I$, namely:

$$N_{i\to j}(I) = \sum_{m=1}^{\infty} \chi(t^m_{i\to j} \in I) \; , \tag{7}$$

where χ is the characteristic function ($\chi(\mathcal{P}) = 1$ if the property $\mathcal{P}$ is true, 0 otherwise). We set $N_{i\to j}(t) = N_{i\to j}([0,t])$. The stochastic scheme described above is thus specified by the infinite set of independent Poisson processes $(N_{i\to j}(t))_{t\geq 0}$ with parameters $\Gamma_{i\to j}$, for all $i,j \in \Lambda$. If (6) holds, the staircase function:

$$N(t) = \sum_{i,j\in\Lambda} N_{i\to j}(t) \ , \tag{8}$$

which counts the total number of jumps between 0 and t, define a Poisson process of parameter Γ. The left discontinuities of this function are the jump times t_p above. As follows from the independence of the Poisson processes $(N_{i\to j}(t))_{t\geq 0}$, the probability that the p–th jump is a jump (i,j) is:

$$\mathbb{P}\big((i_p,j_p) = (i,j)\big) = \frac{\Gamma_{i\to j}}{\Gamma} \ . \tag{9}$$

2.2 Examples

In order to be more concrete, let us give two examples corresponding to physical systems for which the above approach applies.

'Classical' Model Consider a system made of fermions initially in an eigenstate of the Hamiltonian $\hat{H}$, $H = V$. The eigenstates of $\hat{H}$ are of the form $|\underline{n}\rangle = \prod_i (a_i^\dagger)^{n_i}|0\rangle$, where $|0\rangle$ is the vacuum and $\underline{n} = (n_i)_{i\in\Lambda} \in \{0,1\}^\Lambda$. Let $\hat{n}_i = a_i^\dagger a_i$ be the number operator in state $|i\rangle$. Let $\Gamma_{i\to i} = 0$ and:

$$\hat{W}_{i\to j} = 1 - \hat{n}_i + \hat{n}_i\hat{n}_j + a_j^\dagger a_i \ , \ i \neq j \tag{10a}$$

$$\hat{K} = 0 \ . \tag{10b}$$

The jump operator $\hat{W}_{i\to j}$ transforms an eigenstate $|\underline{n}\rangle$ into $a_j^\dagger a_i|\underline{n}\rangle$ if $n_i = 1$ and $n_j = 0$, and leaves $|\underline{n}\rangle$ unchanged otherwise. Let the system evolve from $t = 0$ until time t according to the quantum jump scheme described above. If we restrict ourself to initial wavefunctions $|\psi(0)\rangle = |\underline{n}\rangle$, with $\underline{n} \in \{0,1\}^\Lambda$, the wavefunction $|\psi(t)\rangle$ at time $t \geq 0$ is in an eigenstate $|\underline{n}(t)\rangle$ at all time and its norm is conserved. Actually, $|\psi(t)\rangle$ remains unchanged up to a phase, as long as there is no jump. When a jump occurs, it may (or may not) jump from an eigenstate $|\underline{n}\rangle$ into another eigenstate $|\underline{n}'\rangle$. The RW at time t is thus completely specified by the sequence of random numbers $\underline{n}(t) \in \{0,1\}^\Lambda$. Define the average population $\rho_i(t)$ in the one–particle state $|i\rangle$ as the average of $n_i(t)$, $\rho_i(t) = \mathbb{E}n_i(t)$. In order to determine the equation satisfied by the ρ_i's, let us compute the amount of change $\mathrm{d}\rho_i = \mathrm{d}\rho_i^+ - \mathrm{d}\rho_i^-$ of $\rho_i(t)$ between times t and $t + \mathrm{d}t$. The gain $\mathrm{d}\rho_i^+$ is equal to the sum over $j \in \Lambda$ of the probability $\Gamma_{j\to i}\,\mathrm{d}t$ that a jump (j,i) occurs between t and $t + \mathrm{d}t$, multiplied by the probability $\rho_j(t)(1 - \rho_i(t))$ that this jump modifies the wavefunction. Similarly, the loss $\mathrm{d}\rho_i^-$ is equal to the sum over $j \in \Lambda$ of the probability $\Gamma_{i\to j}\,\mathrm{d}t$ that a jump (i,j) occurs between t and $t+\mathrm{d}t$, multiplied by $\rho_i(t)(1-\rho_j(t))$. Hence, $\rho_i(t)$ satisfies the Boltzmann equation:

$$\frac{\mathrm{d}\rho_i}{\mathrm{d}t} = \sum_{j\in\Lambda, j\neq i} \Big(\Gamma_{j\to i}\,\rho_j(t)\big(1-\rho_i(t)\big) - \Gamma_{i\to j}\,\rho_i(t)\big(1-\rho_j(t)\big)\Big) \ . \qquad (11)$$

This example shows that the RW model of sect.2.1 can be seen as a quantum generalization of a classical kinetic model. In the quantum case, the classical 'random collisions' between particles of the system and of the bath are replaced by 'random quantum jumps'. If we would have worked with single particle systems, the same Boltzmann equation (11) without the Pauli exclusion factors $(1-\rho_i(t))$ would have been obtained.

The Anderson Model Let us consider a crystal the atoms of which are located at the vertices of a Bravais lattice in dimension d. Using labelling of the lattice sites by integers, we can identify it with $\mathbb{Z}^d$. Some random sites are actually occupied by impurities instead of atoms of the original species. These sites form an infinite (random) set $L \subset \mathbb{Z}^d$. At low enough temperature, conducting electrons are almost all in the impurity band, i.e., they are in linear combinations of impurity orbitals. Neglecting the other electrons and assuming only one orbital par impurity, the one–electron Hilbert space $\mathcal{H}$ is identified with $\ell^2(L)$. The one–electron Hamiltonian can be chosen as the Anderson Hamiltonian:

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

$|x\rangle$, $x \in L$, are the canonical basis vectors, describing an electronic state in the impurity orbital at site x. ϵ_x are independent identically distributed random variables and t_{xy} are hopping terms. The randomness of the site energies ϵ_x, describing disorder in the solid, must be distinguished from the dynamical randomness above, which describes dissipation. As is well-known, for strong enough disorder, i.e., if $\langle \Delta\epsilon_x\rangle$ is large enough compared with t_{xy}, the eigenfunctions of H with energies close to the Fermi energy are exponentially localized (Anderson localization [23]). A first choice for the basis vectors $|i\rangle$ is $|i\rangle = |x\rangle$, for any $i \in \Lambda = L$. Then H is non-diagonal, i.e. $T \neq 0$. However, because the Lindblad operators (2) describing the electron-phonon interaction processes at very low temperature are expressed in terms of the eigenfunctions of H, another interesting choice is to take $|i\rangle$ equal to these eigenfunctions. Then $T = 0$ and $|i\rangle$ is an exponentially localized wavefunction differing from the canonical basis vectors $|x\rangle$. The set Λ can be considered as the set of the localization centers of $|i\rangle$, i.e., as the lattice points $i \in L$ where the amplitude of $|i\rangle$ is maximum.

We now describe how the electrons are kicked by phonons. We choose $\Gamma_{i\to i}=0$ and

$$\hat{W}_{i\to j}=1+a_j^\dagger a_i \quad , \quad i\neq j \ . \tag{12}$$

The damping operator $\hat{K}$ is taken according to (4), i.e.

$$\hat{K}=-\frac{\mathrm{i}}{2}\sum_{i,j\in\Lambda}\Gamma_{i\to j}\,\hat{n}_i(1-\hat{n}_j)-\mathrm{i}\sum_{i\neq j\in\Lambda}\Gamma_{i\to j}\,a_j^\dagger a_i \tag{13}$$

(we have set $\hbar=1$). $\hat{K}$ adds an imaginary part to the eigenenergies of $\hat{H}$ and introduce some new hopping terms $\Gamma_{i\to j}\,a_j^\dagger a_i$.

3 Case of Infinitely Many States

Suppose that the one–particle Hilbert space $\mathcal{H}$ is infinite dimensional, i.e., that the set Λ is infinite. As said in the introduction, if the double sum Γ in (6) diverges, the total number $N(I)$ of jumps in any finite interval $I\subset\mathbb{R}_+$ is infinite with probability one. One can even shows [27] that, if there exists $\beta>0$ such that $\sum_j\Gamma_{i\to j}\geq\beta$ for infinitely many indices $i\in\Lambda$, then the sup over i of $\sum_j N_{i\to j}(I)$ is infinite with probability one. The random times t_p and the random indices (i_p,j_p) in (5) are therefore not well–defined. The idea for computing the random evolution in $\mathcal{F}$ when $\Gamma=\infty$ runs as follows: (1) restrict Λ to a finite 'box' $B\subset\Lambda$ and determine the wavefunction at time t using (5); (2) let the size of the box increase to reach the limit $B\uparrow\Lambda$.

The theorem stated in this section shows that the limit exists provided suitable conditions on the $\Gamma_{i\to j}$ and $\hat{W}_{i\to j}$ are made. We restrict our analysis to jump operators $\hat{W}_{i\to j}$ which are the second quantized of some one–particle operators $W_{i\to j}$:

Assumption 1
For any $i,j\in\Lambda$, $\hat{W}_{i\to j}$ is a single particle operator, i.e.,

$$\hat{W}_{i\to j}=\sum_{k,l\in\Lambda}\langle k|W_{i\to j}|l\rangle\,a_k^\dagger a_l \ .$$

Let $\{|\underline{n}\rangle,\underline{n}\in S\}$ be the occupation number basis of $\mathcal{F}$:

$$|\underline{n}\rangle=\prod_{i\in\Lambda}\frac{1}{\sqrt{n_i!}}\big(a_i^\dagger\big)^{n_i}|0\rangle \quad , \quad \underline{n}=(n_i)_{i\in\Lambda}\in S \ , \tag{14}$$

where $|0\rangle$ is the vacuum, $S=S_+=\mathbb{N}^\Lambda$ if the the system's particles are bosons and $S=S_-=\{0,1\}^\Lambda$ if they are fermions. Assumption 1 implies that $\langle \underline{n}|\hat{W}_{i\to j}|\underline{n}'\rangle = 0$ if $|\underline{n}'\rangle$ is different from $c^{(\pm)}_{kl}(\underline{n})\, a^\dagger_l a_k |\underline{n}\rangle$ for some $k,l \in \Lambda$, where $c^{(\pm)}_{kl}(\underline{n})$ is a normalization constant:

$$c^{(+)}_{kl}(\underline{n}) = \big(n_k(1+n_l-\delta_{kl})\big)^{-1/2} \quad , \quad n_k \neq 0 \tag{15a}$$

$$c^{(-)}_{kl}(\underline{n}) = 1 \quad , \quad n_k(1-n_l) \neq 0 \; . \tag{15b}$$

The sign $+$ refers to bosons and $-$ to fermions. δ_{kl} is the Kronecker delta ($\delta_{kl} = 1$ if $k = l$ and 0 otherwise). Similarly, let $c_{ijkl}(\underline{n}) = \| a^\dagger_j a^\dagger_l a_i a_k |\underline{n}\rangle \|^{-1}$. For any $n \in \mathbb{N}^\star$, we denote by $S^{(n)}$ the subset $\{\underline{n} \in S; \sum_{i\in\Lambda} n_i = n\}$ of S. The jump rates $\Gamma_{i\to j}$, the jump operators $\hat{W}_{i\to j}$, the damping operator $\hat{K}$ and the off–diagonal Hamiltonian $\hat{T}$ are assumed to fulfill the following requirements:

Assumption 2

There is $r_1 > 0$ such that:

$$\sup_{i\in\Lambda} \sum_{j\in\Lambda} \Gamma_{i\to j}\, e^{r_1|i-j|} < \infty \quad , \quad \sup_{i\in\Lambda} \sum_{j\in\Lambda} \Gamma_{j\to i}\, e^{r_1|i-j|} < \infty \; .$$

Assumption 3

For any $i,j,k,l \in \Lambda$, one has:

$$\big|\langle \underline{n}|(\hat{W}_{i\to j} - 1)\, a^\dagger_l a_k |\underline{n}\rangle\big| \leq \frac{1}{c^{(\pm)}_{kl}(\underline{n})} (f_{il} + f_{jl})(f_{ik} + f_{jk})$$

for all $\underline{n} \in S_\pm$, $n_k(1 \pm n_l) \neq 0$, where $f_{ij} = f_{ji} > 0$ is such that there is $r_2 > 0$,

$$\sup_{i\in\Lambda} \sum_{j\in\Lambda} f_{ij}\, e^{r_2|i-j|} < \infty \; .$$

Assumption 4

There is $r_3 > 0$ such that, for all $n \in \mathbb{N}^\star$,

$$\sup_{\underline{n}\in S^{(n)}} \Bigg\{ \sum_{k,l\in\Lambda} c_{kl}(\underline{n}) \, \big|\langle \underline{n}|\,(\hat{T}+\hat{K})\, a^\dagger_l a_k |\underline{n}\rangle\big| \, e^{r_3|k-l|} + \sum_{i,j,k,l\in\Lambda} c_{ijkl}(\underline{n}) \, \big|\langle \underline{n}|\hat{K}| a^\dagger_j a^\dagger_l a_i a_k |\underline{n}\rangle\big| \, e^{r_3 \min\{|i-j|+|k-l|,|i-l|+|k-j|\}} \Bigg\} < \infty \; .$$

Assumption 2 basically means that the rates $\Gamma_{i\to j}$ decrease exponentially with the distance $|i-j|$. Clearly, this does *not* imply that $\Gamma < \infty$ (for instance, $\sum_{ij} \exp(-r|i-j|) = \infty$). Assumption 3 means that a jump (i,j), up to small corrections, can remove a particle in state $|l\rangle$ and create one in a far state $|k\rangle$ only if l is 'exponentially close' to i and k is 'exponentially close' to j, or vice versa. For instance, the jump operators (12) satisfies this assumption with $f_{ij} = \delta_{ij}$. It will be shown below that assumptions 1 to 3 imply that the damping operator $\hat{K}_1$ in (4) satisfies assumption 4 with $r_3 = \min\{r_1/2, r_2\}$.

If $\hat{H}$ is an unbounded operator, with dense domain $\mathcal{D}(\hat{H})$, some care about domains must be taken. Let $\mathcal{B}(\mathcal{F})$ be the C^*–algebra of bounded operators on $\mathcal{F}$. Consider the subspace of $\mathcal{B}(\mathcal{F})$:

$$\left\{ \hat{A} \in \mathcal{B}(\mathcal{F}); \hat{A}\,\mathcal{D}(\hat{H}) \subset \mathcal{D}(\hat{H}) \text{ and } [\hat{H}, \hat{A}] : \mathcal{D}(\hat{H}) \to \mathcal{F} \text{ is bounded } \right\} .$$

This subspace is denoted by $D(\mathcal{L}_{\hat{H}})$, as it is the ultraweakly dense domain of the Liouvillian $\mathcal{L}_{\hat{H}} : \hat{A} \in D(\mathcal{L}_{\hat{H}}) \mapsto \mathrm{i}\big[\hat{H}, \hat{A}\big] \in \mathcal{B}(\mathcal{F})$ [28].

Assumption 5
$\hat{W}_{i\to j}$, $\hat{T}$ and $\hat{K}$ belong to $D(\mathcal{L}_{\hat{H}})$ for any $i, j \in \Lambda$.

Let us denote $\mathcal{F}_n = P_{\pm}\mathcal{H}^{\otimes n}$ the n–particles subspace of $\mathcal{F}$. We say that a sequence $(|\psi_\nu\rangle)_{\nu\in\mathbb{N}}$ of random vectors in $\mathcal{F}_n$ converges *almost surely* to $|\psi\rangle$ if the set of outcomes of all the Poisson processes $(N_{i\to j}(t))_{t\geq 0}$ for which $|\psi_\nu\rangle \to |\psi\rangle$ has a probability one. Note that the limit $|\psi\rangle$ is also a random vector (it takes different values for different outcomes). Our main mathematical result is summarized in the theorem below.

Theorem: *Let $|\psi\rangle \in \mathcal{F}_n$, $n \in \mathbb{N}^*$, and $B \subset \Lambda$ be a finite box of Λ. Consider the random variables:*

- $0 \leq t_1^B \leq \ldots \leq t_p^B \leq \ldots$, *the times of occurrence of* any *jump $(i,j) \in B^2$, i.e., the left discontinuities of the counting function*
$$N_B(t) = \sum_{i,j\in B} N_{i\to j}(t) \ ;$$
- (i_p^B, j_p^B)*, the random pair of indices corresponding to the actual jump $(i,j) \in B^2$ that takes place at time t_p^B:*
$$t_p^B = t^{\,m}_{i_p^B \to j_p^B} \quad \textit{for some } m \in \mathbb{N}.$$

Let $\hat{U}_B(t)$ be the random evolution operator defined by (5)*:*

$$\begin{aligned} \hat{U}_B(t) = {} & e^{-\mathrm{i}(t-t_p^B)(\hat{H}+\hat{K})}\, \hat{W}_{i_p^B \to j_p^B}\, e^{-\mathrm{i}(t_p^B - t_{p-1}^B)(\hat{H}+\hat{K})} \ldots \\ & \ldots \hat{W}_{i_1^B \to j_1^B}\, e^{-\mathrm{i}t_1^B(\hat{H}+\hat{K})} \quad \textit{for } 0 \leq t_p^B \leq t < t_{p+1}^B \ . \end{aligned} \tag{16}$$

Then, under assumptions 1 to 5, $\hat{U}_B(t)|\psi\rangle$ converges almost surely to a random vector $|\psi(t)\rangle = \hat{U}(t)|\psi\rangle \in \mathcal{F}_n$ as $B \uparrow \Lambda$. The convergence for a fixed outcome is uniform with respect to t on finite intervals of $\mathbb{R}_+$ (on a set of outcomes of probability one). Moreover, for any $t \geq 0$ and any bounded operator $\hat{A}$ on $\mathcal{F}_n$, the limit $B \uparrow \Lambda$ and the mean $\mathbb{E}$ over the times $t^m_{i\to j}$ can be inverted when calculating expectation values:

$$\mathbb{E}\,\langle\psi|\,\hat{U}(t)^\dagger \hat{A}\,\hat{U}(t)\,|\psi\rangle = \lim_{B\uparrow\Lambda} \mathbb{E}\,\langle\psi|\,\hat{U}_B(t)^\dagger \hat{A}\,\hat{U}_B(t)\,|\psi\rangle \ . \tag{17}$$

Sketch of the proof. The theorem has been proved elsewhere [27] in the one-particle case, i.e., for RW dynamics in the one-particle Hilbert space $\mathcal{H}$. The proof in the n-particles case considered here is identical excepted that: (1) the basis vectors $|i\rangle \in \mathcal{H}$, $i \in \Lambda$, must be replaced by the basis vectors $|\underline{n}\rangle \in \mathcal{F}_n$, $\underline{n} \in S^{(n)}$; (2) the norms:

$$\|A\|_r = \max\Big\{ \sup_{i\in\Lambda} \sum_{j\in\Lambda} |\langle i|A|j\rangle| e^{r|i-j|} \, , \, (A \leftrightarrow A^\dagger) \Big\} \quad , \quad r \geq 0 \, , \tag{18}$$

on sub-algebras of $\mathcal{B}(\mathcal{H})$ must be replaced by some appropriate norms $\|.\|_r^{(n)}$ on sub-algebras of $\mathcal{B}(\mathcal{F}_n)$. These norms may be constructed as follows. For any $\underline{n}, \underline{n}' \in S^{(n)}$, one can find $i_1, i_1, \ldots, i_n, i_n' \in \Lambda$ such that $|\underline{n}\rangle$ and $|\underline{n}'\rangle$ are respectively equal to $a_{i_1}^\dagger \ldots a_{i_n}^\dagger |0\rangle$ and $a_{i_1'}^\dagger \ldots a_{i_n'}^\dagger |0\rangle$ up to normalization constants. It is easy to see that:

$$d(\underline{n}, \underline{n}') = \min_{\sigma : \{i_1, \ldots, i_n\} \to \{i_1', \ldots, i_n'\} \text{ bijection}} \sum_{\nu=1}^{n} |i_\nu - \sigma(i_\nu)| \, ,$$

defines a distance on $S^{(n)}$. Clearly, $d(\underline{n}, \underline{n}') = |i-j|$ if $|\underline{n}'\rangle = c_{ij}(\underline{n}) \, a_j^\dagger a_i |\underline{n}\rangle$. One sets for any $r \geq 0$ and $\hat{A} \in \mathcal{B}(\mathcal{F}_n)$:

$$\big\|\hat{A}\big\|_r^{(n)} = \max\Big\{ \sup_{\underline{n}\in S^{(n)}} \sum_{\underline{n}'\in S^{(n)}} |\langle \underline{n}|\hat{A}|\underline{n}'\rangle| e^{r d(\underline{n},\underline{n}')} \, , \, (\hat{A} \leftrightarrow \hat{A}^\dagger) \Big\} \, . \tag{19}$$

If $\hat{A} = \sum_{k,l} \langle k|A|l\rangle a_k^\dagger a_l$ is a single–particle operator, then $\|\hat{A}\|_r^{(n)} \leq n^2 \|A\|_r$. Let F and G be the operators on $\mathcal{H}$ given by [27]:

$$F = \sum_{i,j\in\Lambda} f_{ij} |i\rangle\langle j| \quad , \quad G = \sum_{i,j\in\Lambda} \Gamma_{i\to j} (|i\rangle + |j\rangle)(\langle i| + \langle j|) \, .$$

Then assumption 2, the hypothesis on the f_{ij}'s in assumption 3 and assumption 4 can be rewritten as $\|G\|_{r_1} < \infty$, $\|F\|_{r_2} < \infty$ and $\|\hat{K} + \hat{T}\|_{r_3}^{(n)} < \infty$, respectively. □

The following estimates are obtained by using assumptions 1 to 3:

$$\begin{aligned} \Big\| \sum_{i,j\in\Lambda} \Gamma_{i\to j} (\hat{W}_{i\to j}^\dagger - 1)(\hat{W}_{i\to j} - 1) \Big\|_r^{(n)} &\leq 8n^2 \|F\|_r^4 \|G\|_{2r} \\ \Big\| \sum_{i,j\in\Lambda} \Gamma_{i\to j} (\hat{W}_{i\to j} - 1) \Big\|_r^{(n)} &\leq 2n \|F\|_r^2 \|G\|_r \, . \end{aligned}$$

They show that assumptions 1 to 3 imply that $\|\hat{K}_1\|_{r_3}^{(n)} < \infty$ if $r_3 \leq r_1/2$ and $r_3 \leq r_2$, i.e, that the damping operator $\hat{K}_1$ in (4) satisfies assumption 4.

Let us come back to the Anderson model of sect.2.2. Since the one–electron eigenfunctions $|i\rangle$ are exponentially localized, the jump rates $\Gamma_{i\to j}$ decrease exponentially with the distance $|i-j|$ between their localization center [22]. Moreover, $\hat{W}_{i\to j}$ and $\hat{K}$ in (12) and (13) satisfy assumptions 3 and 4. Therefore, the theorem above shows that the stochastic dynamics in $\mathcal{F}$ is well–defined at the infinite volume limit $B \uparrow \Lambda$.

Remark: The theorem does not solve completely the question of convergence at thermodynamic limit, since it is only valid for a finite number n of particles. The study of the limit $B \uparrow \Lambda$, $n \to \infty$, $n/|B| = const.$ is a difficult open problem.

4 Equivalence with the Master Equation

Let us show that the stochastic dynamics in $\mathcal{F}$ of sect.2 gives the Lindblad master equation (1) after averaging over the random times $t^m_{i\to j}$. Ignoring energy shifts, this master equation reads:

$$\frac{\mathrm{d}\rho}{\mathrm{d}t} = \mathcal{L}\rho = -\mathrm{i}[\hat{H},\rho] + \frac{1}{2}\sum_{i,j\in\Lambda}\Big([\hat{L}_{i\to j}\,\rho,\hat{L}^\dagger_{i\to j}] + [L_{i\to j},\rho\hat{L}^\dagger_{i\to j}]\Big)\ . \tag{20}$$

We shall see that, for arbitrary Lindblad operators $\hat{L}_{i\to j}$, its solution $\rho(t) = e^{t\mathcal{L}}\rho$ for $\rho = |\psi\rangle\langle\psi|$ can be written as the mean value $\mathbb{E}\,|\psi(t)\rangle\langle\psi(t)|$, where $|\psi(t)\rangle$ is the random wavefunction (5).

4.1 Decomposition of the Generator $\mathcal{L}$ into a Jump and a Damping Parts

We assume in this section that $\Gamma < \infty$. We set:

$$\hat{L}_{i\to j} = \sqrt{\Gamma_{i\to j}}(\hat{W}_{i\to j} - \alpha_{i\to j})\ , \tag{21}$$

where $\alpha_{i\to j}$, $i,j \in \Lambda$, are some complex numbers such that:

$$\lambda_\alpha = \sum_{i,j\in\Lambda}\Gamma_{i\to j}\big(1+\alpha^*_{i\to j}\big)\big(1-\alpha_{i\to j}\big) < \infty\ .$$

The arbitrariness of the parameters $\alpha_{i\to j}$ is linked to the fact that, for fixed Lindblad operators $\hat{L}_{i\to j}$, different choices for the jump operators $\hat{W}_{i\to j}$ are possible; it will be shown below that all these choices lead to the same Lindblad equation. Equation (20) yields:

$$\mathcal{L}\,\rho = -\mathrm{i}[\hat{H},\rho] + \sum_{i,j\in\Lambda}\Gamma_{i\to j}\Big(\hat{W}_{i\to j}\,\rho\,\hat{W}^\dagger_{i\to j} - \alpha_{i\to j}\,\rho\,\hat{W}^\dagger_{i\to j}$$
$$-\alpha^*_{i\to j}\hat{W}_{i\to j}\,\rho + |\alpha_{i\to j}|^2\rho - \frac{1}{2}\Big\{(\hat{W}^\dagger_{i\to j} - \alpha^*_{i\to j})(\hat{W}_{i\to j} - \alpha_{i\to j}),\rho\Big\}\Big)\ ,$$

with $\{A, B\} = AB + BA$. Let us set:

$$\hat{K}_\alpha = \frac{1}{2\mathrm{i}} \sum_{i,j\in\Lambda} \Gamma_{i\to j} \big(\hat{W}^\dagger_{i\to j} + \alpha^*_{i\to j}\big)\big(\hat{W}_{i\to j} - \alpha_{i\to j}\big) - \frac{\lambda_\alpha}{2\mathrm{i}} \tag{22}$$

and define the operators:

$$\mathcal{W}_{i\to j}\, \rho = \hat{W}_{i\to j}\, \rho\, \hat{W}^\dagger_{i\to j} \tag{23a}$$

$$\mathcal{L}_\alpha\, \rho = -\mathrm{i}[\hat{H}, \rho] - \mathrm{i}\hat{K}_\alpha \rho + \mathrm{i}\rho \hat{K}^\dagger_\alpha \tag{23b}$$

acting on density matrices. $\mathcal{W}_{i\to j}$ gives the discontinuous transformation of the density matrix during a jump (i, j) (compare with (3)). One can easily check by time differentiation that:

$$e^{t\mathcal{L}_\alpha} \rho = e^{-\mathrm{i}(\hat{H}+\hat{K}_\alpha)}\, \rho\, e^{\mathrm{i}(\hat{H}+\hat{K}^\dagger_\alpha)} \; . \tag{24}$$

$\hat{K}_\alpha$ coincides with $\hat{K}_1$ in (4) for $\alpha_{i\to j} = 1$. In the general case, $\hat{K}_\alpha$ and $\hat{K}_1$ differ by a self–adjoint operator. A simple computation gives:

$$\mathcal{L}\, \rho = \mathcal{L}_\alpha\, \rho + \sum_{i,j\in\Lambda} \Gamma_{i\to j} (\mathcal{W}_{i\to j} - 1)\, \rho \; . \tag{25}$$

It is assumed here that the $\hat{W}_{i\to j}$ are uniformly bounded in i, j, so that the sum converges in norm.

4.2 Average over Quantum Trajectories

Following Carmichael [4], the solution of (20) is expanded as an infinite Dyson series:

$$\begin{aligned}\rho(t) = e^{t\mathcal{L}} \rho = e^{t\mathcal{L}_\alpha} \rho + \sum_{p=1}^{\infty} \sum_{i_1, j_1, \ldots, i_p, j_p \in \Lambda} \Gamma_{i_1\to j_1} \ldots \Gamma_{i_p\to j_p} \int_0^t \mathrm{d}t_p \ldots \int_0^{t_2} \mathrm{d}t_1 \\ e^{(t-t_p)\mathcal{L}_\alpha} (\mathcal{W}_{i_p\to j_p} - 1) \ldots e^{(t_2-t_1)\mathcal{L}_\alpha} (\mathcal{W}_{i_1\to j_1} - 1)\, e^{t_1\mathcal{L}_\alpha} \rho \; ,\end{aligned} \tag{26}$$

with $\rho = \rho(t = 0)$. The expression inside the sum over p is equal to:

$$\rho_p(t) = \sum_{q=0}^{p} \frac{(-\Gamma t)^q}{q!}\, \mathcal{J}_{p-q}(t)\, \rho \; , \tag{27}$$

with $\mathcal{J}_0(t) = e^{t\mathcal{L}_\alpha}$ and, for any $p \geq 1$,

$$\begin{aligned}\mathcal{J}_p(t) = \sum_{i_1, j_1, \ldots, i_p, j_p \in \Lambda} \Gamma_{i_1\to j_1} \ldots \Gamma_{i_p\to j_p} \int_0^t \mathrm{d}t_p \ldots \int_0^{t_2} \mathrm{d}t_1 \\ e^{(t-t_p)\mathcal{L}_\alpha} \mathcal{W}_{i_p\to j_p} \ldots e^{(t_2-t_1)\mathcal{L}_\alpha} \mathcal{W}_{i_1\to j_1} e^{t_1\mathcal{L}_\alpha} \; .\end{aligned} \tag{28}$$

In fact, (27) is clearly true for $p = 1$; let us assume that it holds for p and show that then it also holds for $p+1$. One has:

$$\rho_{p+1}(t) = \sum_{i,j\in\Lambda} \Gamma_{i\to j} \int_0^t \mathrm{d}t\, e^{(t-\tau)\mathcal{L}_\alpha}(\mathcal{W}_{i\to j} - 1)\rho_p(\tau)\ .$$

Moreover,

$$\frac{\mathrm{d}}{\mathrm{d}\tau}\Big(e^{-\tau\mathcal{L}_\alpha}\mathcal{J}_{p-q+1}(\tau)\Big) = \sum_{i,j\in\Lambda} \Gamma_{i\to j}\, e^{-\tau\mathcal{L}_\alpha}\mathcal{W}_{i\to j}\mathcal{J}_{p-q}(\tau)\ .$$

This identity and (27) yields:

$$\begin{aligned}\rho_{p+1}(t) = \sum_{q=0}^{p}\ e^{t\mathcal{L}_\alpha}\int_0^t \mathrm{d}\tau\, \frac{(-\Gamma\tau)^q}{q!}\Big\{\frac{\mathrm{d}}{\mathrm{d}\tau}\Big(e^{-\tau\mathcal{L}_\alpha}\mathcal{J}_{p-q+1}(\tau)\Big)\rho \\ -\Gamma e^{-\tau\mathcal{L}_\alpha}\mathcal{J}_{p-q}(\tau)\,\rho\Big\} = \sum_{q=0}^{p+1}\frac{(-\Gamma t)^q}{q!}\,\mathcal{J}_{p-q+1}(t)\,\rho\ .\end{aligned}$$

The last equality follows from an integration by parts. Hence (27) holds for $p+1$ and thus for all $p \in \mathbb{N}^\star$.

As a result,

$$\begin{aligned}\rho(t) &= \sum_{p=0}^{\infty}\sum_{q=0}^{p}\frac{(-\Gamma t)^q}{q!}\,\mathcal{J}_{p-q}(t)\,\rho = \sum_{q=0}^{\infty}\sum_{p=q}^{\infty}\frac{(-\Gamma t)^q}{q!}\mathcal{J}_{p-q}(t)\,\rho \\ &= e^{-\Gamma t}\sum_{r=0}^{\infty}\mathcal{J}_r(t)\,\rho\ . \end{aligned} \tag{29}$$

We may therefore rewrite the Dyson series (26) as follows:

$$\begin{aligned}\rho(t) = e^{t\mathcal{L}_\alpha}\rho + \sum_{p=1}^{\infty}\sum_{i_1,j_1,\dots,i_p,j_p\in\Lambda}\frac{\Gamma_{i_1\to j_1}}{\Gamma}\cdots\frac{\Gamma_{i_p\to j_p}}{\Gamma}\int_{0\le t_1\le\dots\le t_p\le t} \\ \mathrm{d}P_p(t_1,\dots,t_p)\, e^{(t-t_p)\mathcal{L}_\alpha}\mathcal{W}_{i_p\to j_p}\dots e^{(t_2-t_1)\mathcal{L}_\alpha}\mathcal{W}_{i_1\to j_1}e^{t_1\mathcal{L}_\alpha}\rho\ ,\end{aligned} \tag{30}$$

with $\mathrm{d}P_p(t_1,\dots,t_p) = \Gamma^p\, e^{-\Gamma t}dt_1\dots dt_p$. We now come back to the Poisson process (8) of parameter Γ. Actually, $dP_p(t_1,\dots,t_p)$ is precisely the joint probability that p first jump times immediately following $t=0$ occur respectively in the time intervals $[t_1, t_1+\mathrm{d}t_1]$, …, $[t_p, t_p+\mathrm{d}t_p]$, and that no other jump occurs between 0 and t. Moreover, by (9), the quantity before the integrals in (30) is the probability that these p jumps are jumps (i_1, j_1), …, (i_p, j_p). We may therefore interpret (30) as an average over all the independent Poisson processes $(N_{i\to j}(t))_{t\ge0}$:

$$\rho(t) = \mathbb{E}\, e^{(t-t_p)\mathcal{L}_\alpha}\mathcal{W}_{i_p\to j_p}\dots e^{(t_2-t_1)\mathcal{L}_\alpha}\mathcal{W}_{i_1\to j_1}e^{t_1\mathcal{L}_\alpha}\rho\ . \tag{31}$$

The remarkable fact in this formula is that the random operator acting on the density matrix inside the mean conserve pure states. More precisely, it follows from (23a) and (24) that, if $\rho = |\psi\rangle\langle\psi|$, then:

$$\rho(t) = \mathbb{E}\,|\psi(t)\rangle\langle\psi(t)|\ , \tag{32}$$

with $|\psi(t)\rangle$ given by (5).

4.3 Comments

The calculation above shows that the average of the random pure state $|\psi(t)\rangle\langle\psi(t)|$ given by (5) defines a density matrix $\rho(t)$ satisfying the Lindblad equation (20). Using the terminology of [4], the map $t \mapsto |\psi(t)\rangle$ for a fixed outcome of the Poisson processes is called a *quantum trajectory*. The average over all quantum trajectories thus gives the density matrix evolution back. The formula (21) connects the Lindblad operators $\hat{L}_{i\to j}$ with the jump rates and operators. For given $\hat{L}_{i\to j}$, one has many different random evolutions, all giving the same master equation, which correspond to different choices for $\hat{W}_{i\to j}$ and $\alpha_{i\to j}$, in accordance with (21). These different random evolutions are characterized by different damping operators $\hat{K} = \hat{K}_\alpha$, defined by (22). However, there exists only one choice for the complex numbers $\alpha_{i\to j}$ such that assumption 3 holds. Actually, changing $\alpha_{i\to j}$ is the same as adding a constant to $\hat{W}_{i\to j}$; but if assumption 3 is true for $\hat{W}_{i\to j}$, then it is not true for $\hat{W}_{i\to j} + c$ if the constant c differs from zero. As a result, $\hat{K}_\alpha$ and the random evolution may not be defined when $\Gamma = \infty$ except for particular values of the $\alpha_{i\to j}$'s.

For instance, if $\hat{L}_{i\to j}$ is given by (2), one must take $\alpha_{i\to j} = 1$ for all but a finite number of pairs (i,j). Taking $\alpha_{i\to j} = 1$ for any $i,j \in \Lambda$, one ends up with the model discussed at the end of sect.2.2. The corresponding Lindblad equation describes the electronic dynamics at very low temperature due to phonon absorption/emission processes; it does not take into account the elastic electron–phonon scattering. It should be noted that the equation for the diagonal and for the off-diagonal elements of $\rho(t)$ in the eigenbasis $\{|i\rangle\}$ are decoupled. This is a special property of this Lindblad generator, related to an adiabatic approximation [21]. The diagonal elements $\rho_{ii}(t)$ satisfy the Boltzmann equation (11).

5 Stochastic Hamiltonians

Let us assume that the jump operators can be expressed as exponentials, i.e. that there exists some bounded operators $\hat{V}_{i\to j} \in D(\mathcal{L}_{\hat{H}})$ such that:

$$\hat{W}_{i\to j} = e^{-\mathrm{i}\hat{V}_{i\to j}}\ ,\ i,j \in \Lambda\ . \tag{33}$$

This is the case for instance in the model for electrons in strongly disordered solids of sect.2.2. Actually, $(a_i)^2 = 0$ for fermions, hence the operators (12) satisfy (33) with $\hat{V}_{i\to j} = \mathrm{i}\, a_j^\dagger a_i$. It is shown in this section that the random dynamics of the preceding sections can be found by solving formally the stochastic Schrödinger equation:

$$\mathrm{i}\,\frac{\mathrm{d}|\psi\rangle}{\mathrm{d}t} = \Big(\hat{H} + \hat{K} + \sum_{i,j\in\Lambda} \hat{V}_{i\to j} \sum_{m=1}^{\infty} \delta\big(t - t_{i\to j}^{m}\big)\Big)\,|\psi(t)\rangle \ . \tag{34}$$

The last term in the time–dependent stochastic Hamiltonian is a random kicked Hamiltonian (noise term). The second term, which is time independent and non random, can be interpreted as a 'damping term', by analogy with the Langevin equation for Brownian motion.

Let us restrict as before Λ to a finite box $B \subset \Lambda$ and compute the solution of the corresponding stochastic Schrödinger equation,

$$\mathrm{i}\,\frac{\mathrm{d}|\psi_B\rangle}{\mathrm{d}t} = \Big(\hat{H} + \hat{K}_B + \sum_{p=1}^{\infty} \hat{V}_{i_p^B\to j_p^B}\,\delta\big(t - t_p^B\big)\Big)\,|\psi(t)\rangle \ . \tag{35}$$

As usual (see e.g. [30]), this solution is found in two steps: (1) replace the Dirac distribution δ by a smooth function δ_ε of compact support $\operatorname{supp}\delta_\varepsilon \subset [-\varepsilon,\varepsilon]$ and integral unity:

$$\int_{\mathbb{R}} \mathrm{d}t\,\delta_\varepsilon(t) = 1 \ \ , \ \ \varepsilon > 0 \ ;$$

(2) find the limit as $\varepsilon \to 0+$ of the corresponding solution $|\psi_{B,\varepsilon}(t)\rangle$.

Let us substitute δ_ε to δ in (35). The solution at time t is expressed in terms of its value at time $\tau < t$ with the help of a Dyson series [29]. For $t_{p-1}^B < \tau \le t_p^B \le t < t_{p+1}^B$ and $\varepsilon \le (t_{p+1}^B - t)/2$, $\varepsilon \le (\tau - t_{p-1}^B)/2$, this yields:

$$\begin{aligned} |\psi_{B,\varepsilon}(t)\rangle = \sum_{q=0}^{\infty} \frac{(-\mathrm{i})^q}{q!}\,\mathcal{T}\int_{[\tau,t]^q} \prod_{r=1}^{q} \big[\mathrm{d}\tau_r\,\delta_\varepsilon(\tau_r - t_p^B)\big]\, e^{-\mathrm{i}(\hat{H}+\hat{K})(t-\tau_q)}\,\hat{V}_{i_p^B\to j_p^B}\ldots \\ \ldots e^{-\mathrm{i}(\hat{H}+\hat{K})(\tau_2-\tau_1)}\,\hat{V}_{i_p^B\to j_p^B}\,e^{-\mathrm{i}(\hat{H}+\hat{K})(\tau_1-\tau)}\,|\psi_{B,\varepsilon}(\tau)\rangle \ , \end{aligned} \tag{36}$$

where $\mathcal{T}$ is the time ordering operator. Letting $\varepsilon \to 0+$, the integrals tend to:

$$e^{-\mathrm{i}(\hat{H}+\hat{K})(t-t_p^B)}\big(\hat{V}_{i_p^B\to j_p^B}\big)^q\,e^{-\mathrm{i}(\hat{H}+\hat{K})(t_p^B-\tau)}|\psi_{B,\varepsilon}(\tau)\rangle \ .$$

It can be easily shown [27] that the series (36) converges strongly uniformly with respect to ε. As a result,

$$\begin{aligned} |\psi_{B,\varepsilon}(t)\rangle &\to \sum_{q=0}^{\infty} \frac{(-\mathrm{i})^q}{q!} e^{-\mathrm{i}(\hat{H}+\hat{K})(t-t_p^B)}\big(\hat{V}_{i_p^B\to j_p^B}\big)^q\,e^{-\mathrm{i}(\hat{H}+\hat{K})(t_p^B-\tau)}|\psi_{B,\varepsilon}(\tau)\rangle \\ &= e^{-\mathrm{i}(\hat{H}+\hat{K})(t-t_p^B)}\hat{W}_{i_p^B\to j_p^B}\,e^{-\mathrm{i}(\hat{H}+\hat{K})(t_p^B-\tau)}|\psi_{B,\varepsilon}(\tau)\rangle \ . \end{aligned} \tag{37}$$

By repeating this operation until $\tau = 0$, we obtain the solution of (35):

$$|\psi_B(t)\rangle \equiv \lim_{\varepsilon\to 0+} |\psi_{B,\varepsilon}(\tau)\rangle = \hat{U}_B(t)|\psi\rangle \ , \tag{38}$$

where $\hat{U}_B(t)$ is the random evolution operator (16). The (formal) solution of the Schrödinger equation (34) is obtained by letting the size of the box B tend to infinity:

$$|\psi(t)\rangle = \lim_{B\uparrow\Lambda} |\psi_B(t)\rangle = \hat{U}(t)|\psi\rangle \ . \tag{39}$$

The limit exists by the theorem above. Note the importance of the order of the limits: we have first taken $\varepsilon \to 0+$ and then $B \uparrow \Lambda$.

Remark: Equation (35) may be rewritten as an Ito stochastic differential equation in the following way:

$$\mathrm{i}\,\mathrm{d}|\psi_B\rangle = \Big((\hat{H} + \hat{K}_B)\mathrm{d}t + \mathrm{i}\sum_{i,j\in B} (\hat{W}_{i\to j} - 1)\,\mathrm{d}N_{i\to j}(t)\Big)|\psi_B(t)\rangle \ . \tag{40}$$

To see that this equation has the same solutions as (35), one can compute the values of the discontinuities of $|\tilde{\psi}_B(t)\rangle = \exp(\mathrm{i}(\hat{H}+\hat{K}_B))\hat{U}_B(t)|\psi\rangle$ at the jump times t_p^B, and use the fact that $|\tilde{\psi}_B(t)\rangle$ is constant between jumps. It should be noticed that, although it might be tempting to replace $\mathrm{d}N_{i\to j}(t)$ by $\sum_m \delta(t - t^m_{i\to j})\mathrm{d}t$, the operator multiplying the stochastic differential in (40) is $\mathrm{i}(\hat{W}_{i\to j} - 1)$, whereas $\hat{V}_{i\to j}$ multiplies the Dirac distributions in (35).

6 Comparison with Other Stochastic Schemes

Other stochastic dynamical schemes with Poisson processes have been introduced by Dalibard, Castin and Mølmer [3], Carmichael [4], Ghirardi, Rimini and Weber [6] and Barchielli and Belavkin [8,9]. Different schemes using Wiener processes have been studied by Gisin and Percival [5], Ghirardi, Pearle and Rimini [7], van Kampen [10] and by other authors [8,11–14]. We outline in this section the main similarities and differences of these models with the model presented above. The reader can find more information and other relevant references in the reviews [4,18,31,32].

6.1 Quantum Jump schemes

To our knowledge, the first quantum jump scheme is due to Ghirardi *et al.* [6], who introduced the following phenomenological model in connection with the problem of the linear superpositions of macroscopically distinguishable states (Schrödinger cat states). The authors consider some jump operators

$$L_{x,\nu} = (\sqrt{\pi}\alpha)^{-1/2} \exp\Big(-\frac{(x - X_\nu)^2}{2\alpha^2}\Big)$$

which implement 'spontaneous collapses' in the position space around some point $x \in \mathbb{R}^3$. X_ν is the position operator of the ν–th particle of a composite system of n particles. The collapse (x,ν) localizes the ν–th particle around x with an accuracy $\alpha > 0$. The operators $L_{x,\nu}$ are self–adjoint and satisfy:

$$\int_{\mathbb{R}^d} dx\, L_{x,\nu}^2 = 1 \quad , \quad \nu = 1, \dots , n \ . \tag{41}$$

In the wavefunction formulation of the model [32], the collapses (jumps) modify discontinuously the wavefunction of the system according to the non-linear transformation:

$$\text{collapse } (x,\nu) : |\psi\rangle \to \left\| L_{x,\nu}|\psi\rangle \right\|^{-1} L_{x,\nu}|\psi\rangle \ .$$

The probability that a collapse (x,ν) (resp. that *any* collapse) occurs between times t and $t + \mathrm{d}t$ is equal to $\mathrm{d}p_\nu(x) = \lambda \| L_{x,\nu}|\psi(t)\rangle\|^2 \mathrm{d}t$ (resp. to $\mathrm{d}p = \sum_\nu \int dx\, \mathrm{d}p_\nu(x) = \lambda n \|\psi(t)\|^2 \mathrm{d}t$), where λ is a characteristic frequency. Between jumps, the composite system evolves according to Schrödinger equation (with no damping operator; this fact is related to assumption (41)). As shown in [6], for macroscopic systems ($n \gg 1$), the stochastic collapses kill very rapidly the coherences between states localized a distance greater than α. Provided one chooses λ small enough, they have little effect on the dynamics of microscopic systems ($n \simeq 1$) at times accessible in a laboratory experiment.

Dalibard *et al.* [3] and Carmichael [4] have studied a similar but different model in order to describe photon–atom interactions in Quantum Optics. The original motivation was to reproduce experimental data on the fluorescence of single atoms [18]. Quantum jumps occur as a result of a continuous measurement of photon emission from the atom. The discontinuous change of the wavefunction occurring at a jump (i,j) is given, as in the collapse model above, by a non-linear transformation:

$$\text{jump } (i,j) : |\psi\rangle \to \left\| \hat{L}_{i\to j}|\psi\rangle \right\|^{-1} \hat{L}_{i\to j}|\psi\rangle \ . \tag{42}$$

The Lindblad operators $\hat{L}_{i\to j}$ are arbitrary and do not need to satisfy a relation similar to (41), as in the case considered in this work. A jump (i,j) occurs if a photon of energy equal to the Bohr frequency $\omega_{ij} = \langle i|V|i\rangle - \langle j|V|j\rangle$ is detected. Between jumps, the atom evolves in the following way. Successive measurements on the fluorescence of the atom are performed at short time intervals δt, with the result of no photon detected. These measurements increase our knowledge on the state of the system; it can be shown that the wavefunction evolves between two measurements according to Schrödinger equation but with a non self–adjoint Hamiltonian $\hat{H} + \hat{K}'$. Perturbation theory gives [3]:

$$\hat{K}' = \frac{1}{2\mathrm{i}} \sum_{i,j} \hat{L}_{i\to j}^\dagger \hat{L}_{i\to j} \tag{43}$$

(note the difference with the damping operator $\hat{K}_\alpha$ defined by (22) and (21)). Immediately after a zero–photon measurement, the wavefunction is normalized, $|\psi\rangle \to \|\psi\|^{-1}|\psi\rangle$. If, on the contrary, a photon is detected, the wavefunction is transformed as in (42). The probability of detection of a photon of frequency ω_{ij} is $\delta p_{i\to j} = \|\hat{L}_{i\to j}|\psi(t)\rangle\|^2\,\delta t$. It depends upon the wavefunction $|\psi(t)\rangle$ before the jump, and thus upon t. As a consequence, the time delays $s_{i\to j}$ between consecutive jumps (i,j) are not given by simple exponential laws. The quantum jumps scheme of Dalibard *et al.* and Carmichael is therefore more involved than the one given by a set of independent Poisson processes (this conclusion also holds for the collapse model of ref. [6]). Despite this mathematical complexity, its dynamics is very simple to implement numerically [3]. On time scales greater than δt, the stochastic dynamics is norm–preserving. The same model has been derived by a completely different and more abstract method using quantum stochastic calculus by Barchielli and Belavkin [8].

The main difference between the models of ref. [3,4,6,8] with the model presented in sect.2 is that the stochastic dynamics is linear and not norm–preserving in the latter, and vice versa in the formers. A linear non norm–preserving model based on Poisson processes has also been discussed by Belavkin [9]. This author consider a stochastic differential equation of the form (40) with a damping operator $\hat{K}_B$ given by (22) for $\alpha_{i\to j} = 0$. Correspondingly, the jump operators are related to the Lindblad operators by $\hat{L}_{i\to j} = \sqrt{\Gamma_{i\to j}}\,\hat{W}_{i\to j}$, which means that the discontinuous changes of the wavefunction are given by (42) without normalization. This model thus coincides with the stochastic scheme of sect.2 in the particular case $\alpha_{i\to j} = 0$. For the Lindblad operators (2), this gives the jump operators $\hat{W}_{i\to j} = a_j^\dagger a_i$ which do not satisfy assumption 3 above. Thus, if $\Gamma = \infty$, the limit $B \uparrow \Lambda$ is not defined in this model.

6.2 Quantum Diffusion schemes

As in the schemes of ref. [3,4,6,8], the stochastic scheme investigated by Gisin *et al.* [5], Ghirardi *et al.* [7] and Barchielli *et al.* [8] has a norm–preserving and non-linear stochastic quantum evolution. However, this evolution is given by a stochastic Schrödinger equation with Wiener processes (white noise). Another model based on Wiener processes but with linear stochastic dynamics has been studied in [7,10]. Its wavefunction satisfies the Ito stochastic Schrödinger equation:

$$\mathrm{i}\,\mathrm{d}|\psi\rangle = \Big((\hat{H} + \hat{K}')\,\mathrm{d}t + \mathrm{i}\sum_{i,j} \hat{L}_{i\to j}\,\mathrm{d}\xi_{i\to j}(t)\Big)|\psi(t)\rangle\ , \tag{44}$$

where $\hat{K}'$ is given by (43) and $(\xi_{i\to j}(t))_{t\geq 0}$ are independent complex Wiener processes. The Ito differentials $\mathrm{d}\xi_{i\to j}$ satisfy:

$$\mathrm{d}\xi_{i\to j}\,\mathrm{d}\bar{\xi}_{k\to m} = \delta_{ik}\delta_{jl}\,\mathrm{d}t \quad , \quad \mathrm{d}\xi_{i\to j}\,\mathrm{d}\xi_{k\to m} = 0\ .$$

The link between this linear non norm–preserving model and the norm–preserving non linear one has been emphasized in [7].

As shown in [3–5,7,10], provided that the appropriate damping operator $\hat{K}$ is added to the Hamiltonian $\hat{H}$, all the above models lead to the same trace–preserving average dynamics, given by the Lindblad equation (1). We have seen above that the same holds true for our model. More general stochastic dynamical models, which lead to non-Markovian master equations and use correlated noise, have been introduced recently by several authors [11–14]. In ref. [11,12], two nice derivations of these models by means of a path integral and a coherent states methods have been proposed.

6.3 Comparison with the Model of Sect.2

The main advantage of the stochastic scheme presented in this work compared with the non linear quantum jumps scheme of e.g. Dalibard *et al.* is its simplicity. Because of the use of Poisson processes and of the linearity of the dynamics, the solution of the stochastic Schrödinger equation is known exactly: it is given by formula (5). The mathematical analysis is also more easy, as the operator theory framework can be used to study the stochastic evolution in the Hilbert space. In the most interesting case $\alpha_{i \to j} = 1$, one should probably look for a physical interpretation of the stochastic dynamics in connection with scattering theory (see [17,33]). From the point of view of the average dynamics (i.e., for statistical ensembles of systems), our model is equivalent to the model of Dalibard *et al.* and to the other models discussed in the preceding subsections. Actually, as seen in sect.4, the density matrix $\rho(t) = \mathbb{E}|\psi(t)\rangle\langle\psi(t)|$ follows the same Lindblad equation as in these models.

For general (non unitary) jump operators $\hat{W}_{i \to j}$, the norm of the wave-function for a fixed outcome is not constant (and not continuous) in time (although, as said before, the square norm is conserved *on average*). Indeed, if one insists in describing an open system by a wavefunction, its norm may not be necessarily conserved by the dynamics, since, unlike in a closed system, the dynamics is not unitary. This is related to the fact that the interaction with the environment may provide us with some information on the system.

From the numerical side, the stochastic dynamics in our model could be of interest if the exponentials $e^{-\mathrm{i}s(\hat{H}+\hat{K})}$ were known on a broad interval of times s and if its eigenvalues have a modulus smaller than one. This happens, for example, if $\hat{H} + \hat{K}$ can be diagonalized analytically and has eigenvalues with negative imaginary parts. Then, the computation of the wavefunction at time t requires a multiplication of $2p$ matrices, where p is the number of jumps between $t = 0$ and t (formula (5)), whereas the non linear quantum jumps and the Wiener schemes involve a time integration between 0 and t.

7 Conclusion

We have studied in this work a model describing dissipation in a system of quantum particles by means of a random evolution in time. This model can be seen as a quantum generalization of a classical kinetic model, the classical collisions being replaced by quantum jumps. The input parameters of the models are: (1) a set of transition rates $\Gamma_{i\to j} \geq 0$, for all pairs (i,j) of one–particle states; (2) some operators $\hat{W}_{i\to j}$ acting on the Fock space $\mathcal{F}$ of the system, which describe the discontinuous changes of the wavefunction at a jump. The linear random time evolution $t \mapsto |\psi(t)\rangle \in \mathcal{F}$ is specified by a set of independent Poisson processes, a different Poisson process, with parameter $\Gamma_{i\to j}$, being associated to each pair (i,j). The average density matrix $\rho(t) = \mathbb{E}|\psi(t)\rangle\langle\psi(t)|$ obeys the general Lindblad equation. Our main result is that, if the transition rates decay exponentially with the distance $|i-j|$ and the jump operators satisfy the locality condition 1 and 3 of sect.3, then the stochastic evolution of the system is well–defined as some limit if the double sum $\sum_{i,j} \Gamma_{i\to j}$ diverges. This result is only valid for systems with a finite number of particles. The limit of an infinite number of particles with a finite density (thermodynamic limit) requires a more abstract algebraic approach [28]. For aperiodic solids like strongly disordered solids, one should define a stochastic dynamics on the C^*-algebra of the electronic observables in second quantization, which is the crossed product of a continuous field of C^*-algebras by a groupoid [21].

The use of Poisson processes is natural from a physical point of view, especially if the dissipation mechanism under study is due to absorption and emission of external particles by the system (phonons, photons,...). It is also convenient because of its mathematical simplicity. Unlike in the model defined by Dalibard *et al.* [3] and Carmichael [4], the random time evolution in our model linear, but not norm–preserving. The linearity simplifies greatly the mathematical analysis. The random evolution operators can be computed directly from formula (5). The model thus provides an example of quantum jump scheme for which one can handle rigorously the case where infinitely many levels are coupled together by the environment. It can be applied to study electronic transport in disordered or aperiodic solids. A simple example was given in sect.2.2. However, a theory of linear response similar to that elaborated in [15–17] is still lacking within our stochastic wavefunctions framework. Investigation in this direction will be the object of a separate publication [34].

Acknowledgements: We are grateful to Rolando Rebolledo, Miguel Orszag, Pierre Gaspard, Hermann Schulz–Baldes, Italo Guarneri and Boris Shklovskii for valuable discussions and remarks. D.S. acknowledge support by a Fondecyt postdoctoral grant 3000035.

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