

Motion of the Reduced Density Operator

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Spring 2009

Introduction. Quantum mechanical decoherence, dissipation and measurements all involve the interaction of the system of interest with an environmental system (reservoir, measurement device) that is typically assumed to possess a great many degrees of freedom (while the system of interest is typically assumed to possess relatively few degrees of freedom). The state of the composite system is described by a density operator ρ which in the absence of system-bath interaction we would denote $\rho_s \otimes \rho_e$, though in the cases of primary interest that notation becomes unavailable, since in those cases the states of the system and its environment are entangled. The observable properties of the system are latent then in the **reduced density operator**

$$\rho_s = \text{tr}_e \rho \tag{1}$$

which is produced by “tracing out” the environmental component of ρ .

Concerning the specific meaning of (1). Let $\{|n\rangle\}$ be an orthonormal basis in the state space \mathcal{H}_s of the (open) system, and $\{|N\rangle\}$ be an orthonormal basis in the state space \mathcal{H}_e of the (also open) environment. Then $\{|n\rangle \otimes |N\rangle\}$ comprise an orthonormal basis in the state space $\mathcal{H} = \mathcal{H}_s \otimes \mathcal{H}_e$ of the (closed) composite system. We are in position now to write

$$\begin{aligned} \text{tr}_e \rho &\equiv \sum \{ \mathbf{1}_s \otimes \langle N| \} \rho \{ \mathbf{1}_s \otimes |N\rangle \} \\ &\downarrow \\ &= \rho_s \cdot \text{tr} \rho_e \quad \text{in separable cases} \end{aligned}$$

The dynamics of the composite system is generated by Hamiltonian of the form

$$\mathbf{H} = \mathbf{H}_s + \mathbf{H}_e + \mathbf{H}_i$$

where

$$\begin{aligned}
\mathbf{H}_s &= \mathbf{h}_s \otimes \mathbf{I}_e \\
&= \sum_{m,n} \sum_N \langle m | \mathbf{h}_s | n \rangle \left\{ (|m\rangle \otimes |N\rangle) \cdot (\langle n| \otimes \langle N|) \right\} \\
\mathbf{H}_e &= \mathbf{I}_s \otimes \mathbf{h}_e \\
&= \sum_n \sum_{M,N} \left\{ (|n\rangle \otimes |M\rangle) \cdot (\langle n| \otimes \langle N|) \right\} \langle M | \mathbf{h}_e | N \rangle \\
\mathbf{H}_i &= \sum_{m,n} \sum_{M,N} (|m\rangle \otimes |M\rangle) \left\{ (\langle m| \otimes \langle M|) \mathbf{H}_i (|n\rangle \otimes |N\rangle) \right\} (\langle n| \otimes \langle N|)
\end{aligned}$$

—all components of which we will assume to be time-independent.

Interaction picture. In the Schrödinger picture one has (on the assumption that the Hamiltonian is time-independent)

$$i \hbar \partial_t |\psi\rangle_t = \mathbf{H} |\psi\rangle_t \implies |\psi\rangle_t = \mathbf{U}(t) |\psi\rangle_0 \quad \text{with} \quad \mathbf{U}(t) = e^{-(i/\hbar) \mathbf{H} t}$$

Looking to the quantum motion of the expectation value of a time-independent observable \mathbf{A} , we in the Schrödinger picture have

$$\langle \mathbf{A} \rangle_t = {}_t \langle \psi | \mathbf{A} | \psi \rangle_t = {}_0 \langle \psi | \mathbf{U}^\dagger(t) \mathbf{A} \mathbf{U}(t) | \psi \rangle_0$$

which in the Heisenberg picture becomes

$$= {}_0 \langle \psi | \mathbf{A}_t | \psi \rangle_0 \quad \text{with} \quad \mathbf{A}_t \equiv \mathbf{U}^\dagger(t) \mathbf{A}_0 \mathbf{U}(t)$$

giving

$$i \hbar \partial_t \mathbf{A} = [\mathbf{A}, \mathbf{H}]$$

Compare this with the equation that in the Schrödinger picture is satisfied by the density matrix $\rho \equiv |\psi\rangle\langle\psi|$:

$$i \hbar \partial_t \rho = [\mathbf{H}, \rho]$$

which entails $\rho_t = \mathbf{U}(t) \rho_0 \mathbf{U}^\dagger(t)$. We have

$$\langle \mathbf{A} \rangle_t = \begin{cases} \text{tr} \{ \rho_t \mathbf{A}_0 \} & \text{in the Schrödinger picture} \\ \text{tr} \{ \rho_0 \mathbf{A}_t \} & \text{in the Heisenberg picture} \end{cases}$$

which shows very clearly the distinction between and equivalence of the two pictures.

Suppose now that the Hamiltonian can be resolved into the sum

$$\mathbf{H} = \mathbf{H}_0 + \mathbf{H}_1$$

of an “easy/uninteresting part” \mathbf{H}_0 and a relatively “difficult/interesting part” \mathbf{H}_1 . In the absence of \mathbf{H}_1 we would have $|\psi\rangle_0 \longrightarrow |\psi\rangle_t = \exp[-\frac{i}{\hbar}\mathbf{H}_0 t]|\psi\rangle_0$ so the time-dependent unitary transformation

$$|\psi\rangle_t \longrightarrow |\Psi\rangle_t = \exp\left[+\frac{i}{\hbar}\mathbf{H}_0 t\right]|\psi\rangle_t$$

produces a state vector that in the absence of \mathbf{H}_1 would not move at all. In the presence of \mathbf{H}_1 we have

$$\begin{aligned} i\hbar\partial_t|\Psi\rangle_t &= \exp\left[+\frac{i}{\hbar}\mathbf{H}_0 t\right]\left\{-\mathbf{H}_0|\psi\rangle_t + i\hbar\partial_t|\psi\rangle_t\right\} \\ &= \exp\left[+\frac{i}{\hbar}\mathbf{H}_0 t\right]\left\{-\mathbf{H}_0|\psi\rangle_t + (\mathbf{H}_0 + \mathbf{H}_1)|\psi\rangle_t\right\} \\ &= \mathbf{U}_0^{-1}(t)\mathbf{H}_1\mathbf{U}_0(t)|\Psi\rangle_t \quad \text{with} \quad \mathbf{U}_0(t) \equiv \exp\left[-\frac{i}{\hbar}\mathbf{H}_0 t\right] \\ &\equiv \mathbf{G}(t)|\Psi\rangle_t \end{aligned} \quad (2)$$

where the hermiticity of the time-dependent operator $\mathbf{G}(t)$ is manifest, as is the fact that $\mathbf{G}(t) \rightarrow \mathbf{I}$ in cases where $\mathbf{H}_1 \rightarrow \mathbf{0}$. We now have

$$\langle \mathbf{A} \rangle_t = {}_t\langle \psi | \mathbf{A} | \psi \rangle_t = {}_t\langle \Psi | \mathbf{B}(t) | \Psi \rangle_t$$

where

$$\mathbf{B}(t) \equiv \mathbf{U}_0^{-1}(t)\mathbf{A}\mathbf{U}_0(t)$$

executes simple \mathbf{H}_1 -independent Heisenberg motion:

$$i\hbar\partial_t\mathbf{B}(t) = [\mathbf{B}(t), \mathbf{H}_0]$$

The solution of (2) is famously difficult to construct (involves chronological ordering), but has necessarily the form

$$\begin{aligned} |\Psi\rangle_t &= \mathbf{V}(t)|\Psi\rangle_0 \quad : \quad \mathbf{V}(t) \text{ is unitary} \\ &\downarrow \\ &= |\Psi\rangle_0 \quad \text{for all } t \text{ in cases where } \mathbf{H}_1 \text{ vanishes} \end{aligned}$$

From $|\psi\rangle_t = \mathbf{U}_0(t)|\Psi\rangle_t = \mathbf{U}_0(t)\mathbf{V}(t)|\Psi\rangle_0 = \mathbf{U}_0(t)\mathbf{V}(t)|\psi\rangle_0 = \mathbf{U}(t)|\psi\rangle_0$ we see that we have in effect factored $\mathbf{U}(t) = \exp\left[-\frac{i}{\hbar}(\mathbf{H}_0 + \mathbf{H}_1)t\right]$, and have thus placed ourselves in position to write

$$\begin{aligned} \langle \mathbf{A} \rangle_t &= \text{tr}\{\rho_t \mathbf{A}_0\} = \text{tr}\{\mathbf{U}_0(t)\mathbf{V}(t)\rho_0\mathbf{V}^{-1}(t)\mathbf{U}_0^{-1}(t)\mathbf{A}_0\} \\ &= \text{tr}\{\mathbf{V}(t)\rho_0\mathbf{V}^{-1}(t) \cdot \mathbf{U}_0^{-1}(t)\mathbf{A}_0\mathbf{U}_0(t)\} \end{aligned}$$

in which ρ is propelled (prograde) by

$$\mathbf{V}(t) = e^{+(i/\hbar)\mathbf{H}_0 t} \cdot e^{-(i/\hbar)(\mathbf{H}_0 + \mathbf{H}_1)t} \quad (3)$$

while \mathbf{A} is propelled (retrograde) by $\mathbf{U}_0(t) = e^{-(i/\hbar)\mathbf{H}_0 t}$.

The expression on the right hand side of (3) is easy to write down but in typical cases is difficult to evaluate explicitly. In favorable cases one can appeal to Campbell-Baker-Hausdorff theory, but more commonly one works from

$$i\hbar\partial_t\mathbf{V}(t) = \mathbf{G}(t)\mathbf{V}(t) \quad : \quad \mathbf{G}(t) \equiv \mathbf{U}_0^{-1}(t)\mathbf{H}_1\mathbf{U}_0(t)$$

which is a version of (2), follows directly from (3), and can be formulated

$$\mathbf{V}(t) = \mathbf{V}(0) + \frac{1}{i\hbar} \int_0^t \mathbf{G}(s) \mathbf{V}(s) ds$$

and by iteration gives

$$\mathbf{V}(t) = \overleftarrow{\wp} \exp \left\{ -\frac{i}{\hbar} \int_0^t \mathbf{G}(s) ds \right\} \cdot \mathbf{V}(0) \quad (4)$$

where $\overleftarrow{\wp}$ is the chronological ordering operator. Typically (as in QED) \mathbf{H}_1 is time-dependent (abruptly/slowly switched on then off): in such cases one cannot write $\mathbf{U}(t) = \exp \left\{ -\frac{i}{\hbar} (\mathbf{H}_0 + \mathbf{H}_1) t \right\}$ so (3) fails and one has no alternative but to work from (4).

From (2)—which describes the motion of $|\Psi\rangle_t$ in the interaction picture—we get

$$i\hbar \partial_t \rho(t) = [\mathbf{G}(t), \rho(t)] \quad (5.1)$$

where $\rho(t) = |\Psi\rangle_t \langle \Psi| = \mathbf{U}_0^{-1}(t) \rho_t \mathbf{U}_0(t)$ is the interaction picture version of the density operator. Equivalently,

$$\rho(t) = \rho(0) + \frac{1}{i\hbar} \int_0^t [\mathbf{G}(s), \rho(s)] ds \quad (5.2)$$

Returning with these ideas to the quantum theory of open systems, it becomes natural to

- identify $\mathbf{H}_s + \mathbf{H}_e$ with \mathbf{H}_0 ;
- identify \mathbf{H}_i with \mathbf{H}_1 .

Working first in the Schrödinger picture, we have

$$\rho_t = \mathbf{U}(t) \rho_0 \mathbf{U}^{-1}(t) \iff i\hbar \partial_t \rho_t = [\mathbf{H}, \rho_t]$$

where ρ_t and \mathbf{H} both refer to the total (composite) system. Tracing out the environmental terms, we get¹

$$\rho_{st} = \text{tr}_e \{ \mathbf{U}(t) \rho_0 \mathbf{U}^{-1}(t) \} \iff i\hbar \partial_{st} \rho_t = \text{tr}_e \{ [\mathbf{H}, \rho_t] \}$$

I know from low-dimensional numerical experiments that the spectrum of ρ_{st} is time-dependent, so the transformation $\rho_{s0} \longrightarrow \rho_{st}$ cannot be unitary (even though the experiments indicate that it is trace-preserving). Breuer & Petruccione (their page 114) draw

$$\begin{array}{ccc} \rho_{t_1} & \longleftarrow & \rho_{t_2} \equiv \mathbf{U}(t_2, t_1) \rho_{t_1} \mathbf{U}^{-1}(t_2, t_1) \\ \downarrow & & \downarrow \\ \rho_{st_1} \equiv \text{tr}_e \rho_{t_1} & \longrightarrow & \rho_{st_2} \equiv \text{tr}_e \rho_{t_2} \end{array}$$

¹ Compare Heinz-Peter Breuer & Francesco Petruccione, *The Theory of Open Quantum Systems* (2006), page 112.

to emphasize that, while the transformations $\mathcal{T}(t_2, t_1) : \rho_{t_1} \longrightarrow \rho_{t_2}$ are clearly elements of a group with an obvious composition law $\mathcal{T}(t_3, t_2)\mathcal{T}(t_2, t_1) = \mathcal{T}(t_3, t_1)$, obvious identity $\mathcal{T}(t, t)$ and obvious inversion law $\mathcal{T}^{-1}(t_2, t_1) = \mathcal{T}(t_1, t_2)$, the induced transformations $\mathcal{T}_s(t_2, t_1) : \rho_{st_1} \longrightarrow \rho_{st_2}$ are *not* elements of a group: they satisfy the same composition law, but are *non-invertible*. To invert $\mathcal{T}_s(t_2, t_1)$ one would, as STEP #1 (see the diagram), have to invert $\rho_{t_2} \longrightarrow \rho_{st_2}$ which—since the step entails loss of information (is essentially projective)—is impossible. The transformations $\mathcal{T}_s(t_2, t_1)$ are elements not of a group but of a *semigroup*.

In realistic situations we do not know nearly enough about the quantum mechanics of the environment—the quantum mechanics generated by $\mathbf{H}_e + \mathbf{H}_i$ to permit us to proceed by direct application of the process diagrammed above to useful information about the process of interest: $\mathcal{T}_s(t_2, t_1) : \rho_{st_1} \longrightarrow \rho_{st_2}$. What we need is an approximation scheme that permits us to describe the evolution of ρ_s in terms of operators that act on \mathcal{H}_s , and into which the physics generated by \mathbf{H}_e and \mathbf{H}_i enters only in a simplified way, as an “influence.” Equations that accomplish that objective are called “master equations,” and come in several flavors. My own discussion of this subject borrows from the following sources: Maximillian Schlosshauer, *Decoherence & the Quantum-to-Classical Transition* (2007), especially Chapter 4 (“Master-equation formulations of decoherence”); H.-P. Breuer & F. Petruccione, *The Theory of Open Quantum Systems* (2006), especially §3.2.1–4; U. Weiss, *Quantum Dissipative Systems* (3rd edition 2008), §2.3.

Quantum dynamical map. We work from

$$\rho_{st} = \text{tr}_e \{ \mathbf{U}(t) \rho_0 \mathbf{U}^{-1}(t) \} \quad (6)$$

and from the assumption that initially ρ_0 factors

$$\rho_0 = \rho_{s0} \otimes \rho_{e0}$$

We assume moreover—quite unrealistically (!), but in service of our formal objective—that we possess the spectral resolution of ρ_{e0} :

$$\rho_{e0} = \sum_{\alpha} \lambda_{\alpha} |\phi_{\alpha}\rangle \langle \phi_{\alpha}|$$

where the λ_{α} are positive real numbers that sum to unity. Let $\{|\psi_{\beta}\rangle\}$ comprise an orthonormal basis in \mathcal{H}_e , and with its aid construct

$$\begin{aligned} \rho_{st} &= \text{tr}_e \{ \mathbf{U}(t) \rho_0 \mathbf{U}^{-1}(t) \} \\ &= \sum_{\beta} [\mathbf{I}_s \otimes \langle \psi_{\beta}|] \mathbf{U}(t) [\rho_{s0} \otimes \sum_{\alpha} \lambda_{\alpha} |\phi_{\alpha}\rangle \langle \phi_{\alpha}|] \mathbf{U}^{-1}(t) [\mathbf{I}_s \otimes |\psi_{\beta}\rangle] \end{aligned}$$

Use

$$[\rho_{s0} \otimes \sum_{\alpha} \lambda_{\alpha} |\phi_{\alpha}\rangle \langle \phi_{\alpha}|] = \sum_{\alpha} [\mathbf{I}_s \otimes \sqrt{\lambda_{\alpha}} |\phi_{\alpha}\rangle] \rho_{s0} \otimes \mathbf{1} [\mathbf{I}_s \otimes \sqrt{\lambda_{\alpha}} \langle \phi_{\alpha}|]$$

to obtain (since $[\boldsymbol{\rho}_{s0} \otimes 1] = \boldsymbol{\rho}_{s0}$)

$$\boldsymbol{\rho}_{st} = \sum_{\alpha,\beta} \mathbf{W}_{\alpha\beta}(t) \boldsymbol{\rho}_{s0} \mathbf{W}_{\alpha\beta}^+(t) \quad (7.1)$$

with

$$\begin{aligned} \sqrt{\lambda_\alpha} [\mathbf{I}_s \otimes \langle \psi_\beta |] \mathbf{U}(t) [\mathbf{I}_s \otimes |\phi_\alpha \rangle] &\equiv \mathbf{W}_{\alpha\beta}(t) \\ \sqrt{\lambda_\alpha} [\mathbf{I}_s \otimes \langle \phi_\alpha |] \mathbf{U}^+(t) [\mathbf{I}_s \otimes |\psi_\beta \rangle] &= \mathbf{W}_{\alpha\beta}^+(t) \end{aligned} \quad (7.2)$$

The dimensions of the matrices that enter into the preceding definitions conform to the following pattern



where the short sides have length s , the long sides have length $s + e$. It now follows from $\sum_\beta |\psi_\beta \rangle \langle \psi_\beta| = \mathbf{I}_e$, normality $\langle \phi_\alpha | \phi_\alpha \rangle = 1$ and $\sum_\alpha \lambda_\alpha = 1$ that

$$\begin{aligned} &\sum_{\alpha,\beta} \mathbf{W}_{\alpha\beta}^+(t) \mathbf{W}_{\alpha\beta}(t) \\ &= \sum_\alpha \lambda_\alpha [\mathbf{I}_s \otimes \langle \phi_\alpha |] \mathbf{U}^+(t) [\mathbf{I}_s \otimes \sum_\beta |\psi_\beta \rangle \langle \psi_\beta|] \mathbf{U}(t) [\mathbf{I}_s \otimes |\phi_\alpha \rangle] \\ &= \sum_\alpha \lambda_\alpha [\mathbf{I}_s \otimes \langle \phi_\alpha |] \mathbf{U}^+(t) [\mathbf{I}_s \otimes \mathbf{I}_e] \mathbf{U}(t) [\mathbf{I}_s \otimes |\phi_\alpha \rangle] \\ &= \sum_\alpha \lambda_\alpha [\mathbf{I}_s \otimes \langle \phi_\alpha |] \mathbf{I}_{s+e} [\mathbf{I}_s \otimes |\phi_\alpha \rangle] \\ &= \sum_\alpha \lambda_\alpha [\mathbf{I}_s \otimes \langle \phi_\alpha |] [\mathbf{I}_s \otimes |\phi_\alpha \rangle] \quad \text{by } \mathbf{I}_s \cdot \mathbf{I}_s = \mathbf{I}_s \text{ and } \mathbf{I}_e |\phi_\alpha \rangle = |\phi_\alpha \rangle \\ &= \sum_\alpha \lambda_\alpha [\mathbf{I}_s \otimes 1] \\ &= \mathbf{I}_s \end{aligned} \quad (8)$$

Returning with this information to (7.1), we have

$$\text{tr}\{\boldsymbol{\rho}_{st}\} = \text{tr}\{\boldsymbol{\rho}_{s0} \cdot \sum_{\alpha,\beta} \mathbf{W}_{\alpha\beta}^+(t) \mathbf{W}_{\alpha\beta}(t)\} = \text{tr}\{\boldsymbol{\rho}_{s0}\} = 1$$

Note that we *could but need not* identify $\{|\psi_\alpha \rangle\}$ with $\{|\phi_\alpha \rangle\}$, as Breuer & Petruccione elected to do.

Equations (7) do provide a description of $\boldsymbol{\rho}_{s0} \mapsto \boldsymbol{\rho}_{st}$, but presume that we possess information—the spectral representation of $\boldsymbol{\rho}_{e0}$, an evaluation of $\mathbf{U}(t) = \exp\{- (i/\hbar)(\mathbf{h}_s \otimes \mathbf{h}_e + \mathbf{H}_i) t\}$ —that in realistic cases we cannot expect to have. It is, in this respect, gratifying to observe that in the absence of system-environmental interaction we have $\mathbf{U}(t) = \mathbf{U}_s(t) \otimes \mathbf{U}_e(t)$ and (7) reads

$$\begin{aligned}
 \rho_{st} &= [\mathbf{U}_s(t) \rho_{s0} \mathbf{U}_s^\dagger(t)] \otimes \sum_{\alpha,\beta} \langle \psi_\beta | \mathbf{U}_e(t) | \phi_\alpha \rangle \lambda_\alpha \langle \phi_\alpha | \mathbf{U}_e^\dagger(t) | \psi_\beta \rangle \\
 &= [\mathbf{U}_s(t) \rho_{s0} \mathbf{U}_s^\dagger(t)] \otimes \text{tr} \{ \mathbf{U}_e(t) \rho_{e0} \mathbf{U}_e^\dagger(t) \} \\
 &= \mathbf{U}_s(t) \rho_{s0} \mathbf{U}_s^\dagger(t)
 \end{aligned}$$

The motion of ρ_{st} has in the absence of interaction become unitary. It is the presence of the $\sum_{\alpha,\beta}$ that destroys the unitarity of (7).

Breuer & Petruccione write

$$\rho_{st} = \sum_{\alpha,\beta} \mathbf{W}_{\alpha\beta}(t) \rho_{s0} \mathbf{W}_{\alpha\beta}^\dagger(t) \equiv \mathcal{V}(t) \rho_{s0} \quad (9)$$

where $\mathcal{V}(t)$ is an operator (what Breuer & Petruccione call a “super-operator”) that achieves a certain linear reorganization of the elements of ρ_{s0} . Suppose, for example, that \mathcal{H}_s is 2-dimensional, and that ρ_{s0} can be represented

$$\rho_{s0} = \begin{pmatrix} \rho_{0,11} & \rho_{0,12} \\ \rho_{0,21} & \rho_{0,22} \end{pmatrix}$$

Then the upshot of (9) can be described

$$\begin{pmatrix} \rho_{t,11} \\ \rho_{t,12} \\ \rho_{t,21} \\ \rho_{t,22} \end{pmatrix} = \begin{pmatrix} V_{11,11}(t) & V_{11,12}(t) & V_{11,21}(t) & V_{11,22}(t) \\ V_{12,11}(t) & V_{12,12}(t) & V_{12,21}(t) & V_{12,22}(t) \\ V_{21,11}(t) & V_{21,12}(t) & V_{21,21}(t) & V_{21,22}(t) \\ V_{22,11}(t) & V_{22,12}(t) & V_{22,21}(t) & V_{22,22}(t) \end{pmatrix} \begin{pmatrix} \rho_{0,11} \\ \rho_{0,12} \\ \rho_{0,21} \\ \rho_{0,22} \end{pmatrix}$$

and abbreviated

$$\vec{\rho}_{st} = \mathbb{V}(t) \vec{\rho}_{s0}$$

Proceeding on the assumption that it is possible to write $\mathbb{V}(t) = \exp \{ \mathbb{L} t \}$ we are led to a differential equation of “Markovian” form

$$\frac{d}{dt} \vec{\rho}_{st} = \mathbb{L} \vec{\rho}_{st}$$

This equation illustrates the explicit meaning of the equation that Breuer & Petruccione write

$$\frac{d}{dt} \rho_{st} = \mathcal{L} \rho_{st} \quad (10)$$

and call the “Markovian quantum master equation.” We undertake now to develop the explicit meaning of the $\mathcal{L} \rho_{st}$.

Suppose \mathcal{H}_s to be n -dimensional. Let operators $\mathbf{F}_i, i = 1, 2, \dots, n^2$ span the space of linear operators on \mathcal{H}_s . Assume without loss of generality that the \mathbf{F}_i are orthonormal in the tracewise sense

$$(\mathbf{F}_i, \mathbf{F}_j) \equiv \frac{1}{n} \text{tr} \{ \mathbf{F}_i^\dagger \mathbf{F}_j \} = \delta_{ij}$$

Assume more particularly that $\mathbf{F}_1 = \mathbf{I}$. The remaining basis operators are then necessarily traceless: $(\mathbf{F}_1, \mathbf{F}_{i \neq 1}) = 0 \sim \text{tr}\{\mathbf{F}_{i \neq 1}\}$. For any linear operator \mathbf{A} on \mathcal{H}_s we have

$$\mathbf{A} = \sum_{i=1}^{n^2} \mathbf{F}_i (\mathbf{F}_i, \mathbf{A})$$

In particular, we have

$$\mathbf{W}_{\alpha\beta} = \sum_{i=1}^{n^2} \mathbf{F}_i (\mathbf{F}_i, \mathbf{W}_{\alpha\beta})$$

which by (9) gives

$$\begin{aligned} \mathcal{V}(t)\rho_{s0} &= \sum_{i,j=1}^{n^2} \sum_{\alpha,\beta} \mathbf{W}_{\alpha\beta}(t) \rho_{s0} \mathbf{W}_{\alpha\beta}^+(t) \\ &= \sum_{i,j=1}^{n^2} \underbrace{\sum_{\alpha,\beta} (\mathbf{F}_i, \mathbf{W}_{\alpha\beta})(\mathbf{F}_j, \mathbf{W}_{\alpha\beta})^*}_{c_{ij}(t)} \mathbf{F}_i \rho_{s0} \mathbf{F}_j^+ \end{aligned}$$

Taking now into account the unique simplicity of $\mathbf{F}_1 = \mathbf{I}$, we have

$$\mathcal{L}\rho_{st} = \dot{c}_{11}\rho_{s0} + \sum_{i=2}^{n^2} \left(\dot{c}_{i1}\mathbf{F}_i \rho_{s0} + \dot{c}_{1i}\rho_{s0} \mathbf{F}_i^+ \right) + \sum_{i,j=2}^{n^2} \dot{c}_{ij}\mathbf{F}_i \rho_{s0} \mathbf{F}_j^+$$

All the computational difficulty resides now in the functions $\dot{c}_{ij}(t)$. At $t = 0$ those become constants $a_{ij} \equiv \dot{c}_{ij}(0)$ and the preceding equation reads

$$\begin{aligned} \mathcal{L}\rho_{s0} &= a_{11}\rho_{s0} + \sum_{i=2}^{n^2} \left(a_{i1}\mathbf{F}_i \rho_{s0} + a_{1i}\rho_{s0} \mathbf{F}_i^+ \right) + \sum_{i,j=2}^{n^2} a_{ij}\mathbf{F}_i \rho_{s0} \mathbf{F}_j^+ \\ &= a_{11}\rho_{s0} + (\mathbf{F}\rho_{s0} + \rho_{s0}\mathbf{F}^+) + \sum_{i,j=2}^{n^2} a_{ij}\mathbf{F}_i \rho_{s0} \mathbf{F}_j^+ \end{aligned} \quad (11)$$

which serves to define the action of the ‘‘super-generator’’ \mathcal{L} . Here

$$\mathbf{F} \equiv \sum_{i=2}^{n^2} a_{i1}\mathbf{F}_i \implies \mathbf{F}^+ = \sum_{i=2}^{n^2} a_{1i}\mathbf{F}_i^+ \quad \text{by the hermiticity of } \|c_{ij}(t)\|$$

Resolving \mathbf{F} into its hermitian and anti-hermitin parts

$$\mathbf{F} = \frac{1}{2}(\mathbf{F} + \mathbf{F}^+) + \frac{1}{2}(\mathbf{F} - \mathbf{F}^+) \equiv \mathbf{g} - i\mathbf{H}$$

we have

$$(\mathbf{F}\rho_{s0} + \rho_{s0}\mathbf{F}^+) = -i(\mathbf{H}\rho_{s0} - \rho_{s0}\mathbf{H}) + (\mathbf{g}\rho_{s0} + \rho_{s0}\mathbf{g})$$

and find that (11) can be written

$$\mathcal{L}\rho_{s0} = -i[\mathbf{H}, \rho_{s0}] + \{\mathbf{G}, \rho_{s0}\} + \sum_{i,j=2}^{n^2} a_{ij} \mathbf{F}_i \rho_{s0} \mathbf{F}_j^\dagger \quad (12)$$

with

$$\mathbf{G} = \frac{1}{2}a_{11}\mathbf{I} + \mathbf{g}$$

From

$$\rho_{st} = e^{\mathcal{L}t}\rho_{s0} = \rho_{s0} + t \cdot \mathcal{L}\rho_{s0} + \dots$$

and the previously established fact that $\text{tr}\{\rho_{st}\} = \text{tr}\{\rho_{s0}\}$ we conclude from (12) that

$$0 = \text{tr}\left\{\left(2\mathbf{G} + \sum_{i,j=2}^{n^2} a_{ij} \mathbf{F}_j^\dagger \mathbf{F}_i\right)\rho_{s0}\right\} \quad : \quad \text{all } \rho_{s0}$$

whence

$$\mathbf{G} = -\frac{1}{2} \sum_{i,j=2}^{n^2} a_{ij} \mathbf{F}_j^\dagger \mathbf{F}_i$$

Equation (12) now presents what Breuer & Petruccione call the “first standard form”

$$\mathcal{L}\rho_s = -i[\mathbf{H}, \rho_s] + \sum_{i,j=2}^{n^2} a_{ij} \left(\mathbf{F}_i \rho_s \mathbf{F}_j^\dagger - \frac{1}{2}\{\mathbf{F}_j^\dagger \mathbf{F}_i, \rho_s\} \right) \quad (13)$$

of the description of the action achieved by the super-generator \mathcal{L} .

Further progress requires that we sharpen what we know about the coefficients

$$c_{ij}(t) \equiv \sum_{\alpha,\beta} (\mathbf{F}_i, \mathbf{W}_{\alpha\beta})(\mathbf{F}_j, \mathbf{W}_{\alpha\beta})^*$$

It is, as previously remarked, immediate that $\|c_{ij}(t)\|$ is hermitian. Moreover

$$\sum_{i,j} v_i^* c_{ij} v_j = \sum_{\alpha,\beta} \left| \left(\sum_k (v_k \mathbf{F}_k, \mathbf{W}_{\alpha\beta}) \right) \right|^2 \geq 0 \quad : \quad \text{all complex vectors } v$$

so the eigenvalues of $\|c_{ij}(t)\|$ must all be non-negative. The same can, of course, be said of $\|a_{ij}\|$. And of the sub-matrix that results from restricting the range of i and j , as is done in (13).

Let u_{ip} be elements of the unitary matrix that diagonalizes $\|a_{ij}\|$:

$$a_{ij} = \sum_{p,q} u_{ip} \Lambda_{pq} \bar{u}_{jq} \quad \text{with} \quad \|\Lambda_{pq}\| = \begin{pmatrix} \lambda_2 & 0 & \dots & 0 \\ 0 & \lambda_3 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \lambda_{n^2} \end{pmatrix}$$

Equation (13) becomes

$$\begin{aligned}
\mathcal{L}\rho_s &= -i[\mathbf{H}, \rho_s] + \sum_{i,j,p,q=2}^{n^2} u_{ip}\Lambda_{pq}\bar{u}_{jq} \left(\mathbf{F}_i \rho_s \mathbf{F}_j^\dagger - \frac{1}{2}\{\mathbf{F}_j^\dagger \mathbf{F}_i, \rho_s\} \right) \\
&= -i[\mathbf{H}, \rho_s] + \sum_{i,j,p,q=2}^{n^2} \lambda_p \delta_{pq} \left(u_{ip} \mathbf{F}_i \rho_s \bar{u}_{jq} \mathbf{F}_j^\dagger - \frac{1}{2}\{\bar{u}_{jq} \mathbf{F}_j^\dagger u_{ip} \mathbf{F}_i, \rho_s\} \right) \\
&= -i[\mathbf{H}, \rho_s] + \sum_{p=2}^{n^2} \lambda_p \left(\mathbf{A}_p \rho_s \mathbf{A}_p^\dagger - \frac{1}{2} \mathbf{A}_p^\dagger \mathbf{A}_p \rho_s - \frac{1}{2} \rho_s \mathbf{A}_p^\dagger \mathbf{A}_p \right) \quad (14)
\end{aligned}$$

with

$$\mathbf{A}_p = \sum_{i=2}^{n^2} u_{ip} \mathbf{F}_i$$

The operators $\mathbf{A}_p, p = 2, 3, \dots, n^2$ are called ‘‘Lindblad’’ operators, and

$$\frac{d}{dt} \rho_{st} = -i[\mathbf{H}, \rho_{st}] + \underbrace{\sum_{p=2}^{n^2} \lambda_p \left(\mathbf{A}_p \rho_{st} \mathbf{A}_p^\dagger - \frac{1}{2} \mathbf{A}_p^\dagger \mathbf{A}_p \rho_{st} - \frac{1}{2} \rho_{st} \mathbf{A}_p^\dagger \mathbf{A}_p \right)}_{\mathcal{D}(\rho_{st})} \quad (15)$$

is called the ‘‘Lindblad equation.’’² The \mathbf{H} term generates a unitary motion which is distinct from that which in the absence of system-environmental interaction would have been generated by \mathbf{H}_s ; the interaction term \mathbf{H}_i was seen above to enter into the construction of $\mathbf{H} = i\frac{1}{2}(\mathbf{F} - \mathbf{F}^\dagger)$. It is the ‘‘dissipator’’ $\mathcal{D}(\rho_{st})$ that accounts for the non-unitarity of $\rho_{s0} \mapsto \rho_{st}$.

Much freedom attended our selection of an orthonormal basis

$$\{\mathbf{I}, \mathbf{F}_2, \mathbf{F}_3, \dots, \mathbf{F}_{n^2}\}$$

in the ‘‘Liouville space’’ of linear operators on \mathcal{H}_s , so the expression on the right side of (15) is highly non-unique. If, for example, we write

$$\sqrt{\lambda_p} \mathbf{A}_p = \sum_q u_{pq} \sqrt{\mu_q} \mathbf{B}_q$$

we obtain

$$\begin{aligned}
\mathcal{D}(\rho_{st}) &= \sum_{p=2}^{n^2} \lambda_p \left(\mathbf{A}_p \rho_{st} \mathbf{A}_p^\dagger - \frac{1}{2} \mathbf{A}_p^\dagger \mathbf{A}_p \rho_{st} - \frac{1}{2} \rho_{st} \mathbf{A}_p^\dagger \mathbf{A}_p \right) \quad (16) \\
&= \sum_{p,q,r=2}^{n^2} \left(u_{pq} \sqrt{\mu_q} \mathbf{B}_q \rho_{st} \bar{u}_{pr} \sqrt{\mu_r} \mathbf{B}_r^\dagger \right. \\
&\quad \left. - \frac{1}{2} \bar{u}_{pr} \sqrt{\mu_r} \mathbf{B}_r^\dagger u_{pq} \sqrt{\mu_q} \mathbf{B}_q \rho_{st} - \frac{1}{2} \rho_{st} \bar{u}_{pr} \sqrt{\mu_r} \mathbf{B}_r^\dagger u_{pq} \sqrt{\mu_q} \mathbf{B}_q \right)
\end{aligned}$$

² Breuer & Petruccione cite G. Lindblad, ‘‘On the generator of quantum mechanical semigroups,’’ *Commun. Math. Physics* **48**, 119–130 (1976).

which, if we impose the unitarity assumption $\sum_p u_{pq} \bar{u}_{pr} = \delta_{qr}$, becomes

$$\mathcal{D}(\rho_{st}) = \sum_{q=2}^{n^2} \mu_q \left(\mathbf{B}_q \rho_{st} \mathbf{B}_q^+ - \frac{1}{2} \mathbf{B}_q^+ \mathbf{B}_q \rho_{st} - \frac{1}{2} \rho_{st} \mathbf{B}_q^+ \mathbf{B}_q \right)$$

which is structurally identical to (16). Or consider

$$\mathbf{A}_p \longmapsto \mathbf{A}_p + a_p \mathbf{I}$$

which (working again from (16)) sends

$$\begin{aligned} \mathcal{D}(\rho_{st}) &\longmapsto \mathcal{D}(\rho_{st}) + \sum_{p=2}^{n^2} \lambda_p \left\{ \left(a_p \rho_{st} \mathbf{A}_p^+ - \frac{1}{2} \mathbf{A}_p^+ a_p \rho_{st} - \frac{1}{2} \rho_{st} \mathbf{A}_p^+ a_p \right) \right. \\ &\quad \left. + \left(\mathbf{A}_p \rho_{st} \bar{a}_p - \frac{1}{2} \bar{a}_p \mathbf{A}_p \rho_{st} - \frac{1}{2} \rho_{st} \bar{a}_p \mathbf{A}_p \right) \right\} + \mathbf{0} \\ &\downarrow \\ \mathcal{D}(\rho_{st}) &+ \frac{1}{2} \sum_{p=2}^{n^2} \lambda_p \left\{ a_p [\rho_{st}, \mathbf{A}_p^+] - \bar{a}_p [\rho_{st}, \mathbf{A}_p] \right\} \\ &\downarrow \\ \mathcal{D}(\rho_{st}) &+ \left[\rho_{st}, \frac{1}{2} \sum_{p=2}^{n^2} \lambda_p \left(a_p \mathbf{A}_p^+ - \bar{a}_p \mathbf{A}_p \right) \right] \end{aligned}$$

The additive term can be absorbed into a redefinition of the effective Hamiltonian:

$$\mathbf{H} \longmapsto \mathbf{H} + i \frac{1}{2} \sum_{p=2}^{n^2} \lambda_p \left(a_p \mathbf{A}_p^+ - \bar{a}_p \mathbf{A}_p \right) \quad (17)$$

Note the manifest hermiticity of the added term.

Weiss³ provides this simpler-looking version of the Lindblad equation (15):

$$\frac{d}{dt} \rho_{st} = -i [\mathbf{H}, \rho_{st}] + \underbrace{\frac{1}{2} \sum_{p=2}^{n^2} \lambda_p \left([\mathbf{A}_p \rho_{st}, \mathbf{A}_p^+] + [\mathbf{A}_p, \rho_{st} \mathbf{A}_p^+] \right)}_{\mathcal{D}(\rho_{st})}$$

³ Ulrich Weiss, *Quantum Dissipative Systems* (3rd edition 2008), page 11.

NOTATIONAL REMARK: Breuer & Petruccione’s notation $\mathcal{D}(\rho_s)$ serves well enough to signify a “function of (the matrix elements of) an operator, though $\mathcal{D}(\rho_s)$ would better emphasize that we are talking about an *operator valued* function of an operator. One would expect in that same spirit to write $\mathcal{V}(\rho_s, t)$ and $\mathcal{L}(\rho_s)$ where Breuer & Petruccione elect to write $\mathcal{V}(t)\rho_s$ and $\mathcal{L}\rho_s$, even though the “super-operators” $\mathcal{V}(t)$ and \mathcal{L} are defined always by their functional action, never as stand-alone objects. It’s my guess that they do so to motivate the train of thought that follows from writing $\mathcal{V}(t) = \exp\{\mathcal{V}t\}$. In these respects the matrix notation to which I alluded on page 7 provides a more frankly informative account of the situation.

Alternative derivation of the Lindblad equation. The results obtained in the preceding section are formally exact, but acquire their exactitude from the seldom/never justified assumption that we possess an exact description of

$$\mathbf{U}(t) = \exp\left\{- (i/\hbar)[\mathbf{H}_s + \mathbf{H}_e + \mathbf{H}_i]t\right\}$$

In their §3.3.1 Breuer & Petruccione develop a line of argument that avoids that strong assumption—an argument that owes its success to certain simplifying assumptions (which is why Weiss³ considers the Lindblad equation to be valid “in the Born-Markov approximation). We work in the interaction picture, where operators generally (and \mathbf{H}_i in particular) move as directed by $[\mathbf{H}_s + \mathbf{H}_e]$ and where the density matrix of the composite system moves as directed by the (now time-dependent) interaction Hamiltonian⁴

$$\mathbf{H}_i(t) \equiv \mathbf{U}_0^+(t)\mathbf{H}_i\mathbf{U}_0(t) \quad \text{with} \quad \mathbf{U}_0(t) \equiv \exp[-i[\mathbf{H}_s + \mathbf{H}_e]t]$$

Thus

$$\begin{aligned} \frac{d}{dt}\rho(t) &= -i[\mathbf{H}_i(t), \rho(t)] \\ &\downarrow \\ \rho(t) &= \rho(0) - i\int_0^t [\mathbf{H}_i(s), \rho(s)] ds \end{aligned}$$

Insert the latter into the former (inspired idea!)

$$\frac{d}{dt}\rho(t) = -i[\mathbf{H}_i(t), \rho(0)] - \int_0^t [\mathbf{H}_i(t), [\mathbf{H}_i(s), \rho(s)]] ds$$

trace out the environmental degrees of freedom, assume (on what grounds?) that

$$\text{tr}_e[\mathbf{H}_i(t), \rho(0)] = \mathbf{0}_s$$

⁴ Here I revert to my former assumption that we have adopted units in which $\hbar = 1$.

to obtain

$$\begin{aligned}
 \frac{d}{dt}\rho_s(t) &= - \int_0^t \text{tr}_e[\mathbf{H}_i(t), [\mathbf{H}_i(s), \rho(s)]] ds \\
 &\downarrow \\
 &\approx - \int_0^t \text{tr}_e[\mathbf{H}_i(t), [\mathbf{H}_i(s), \rho_s(s) \otimes \rho_e]] ds \quad \left\{ \begin{array}{l} \text{weak coupling, or} \\ \text{BORN APPROXIMATION} \end{array} \right. \\
 &\downarrow \\
 &\approx - \int_0^t \text{tr}_e[\mathbf{H}_i(t), [\mathbf{H}_i(s), \rho_s(t) \otimes \rho_e]] ds \quad \left\{ \begin{array}{l} \text{time-localized} \\ \text{"Redfield equation"} \end{array} \right.
 \end{aligned}$$

To achieve the MARKOFF APPROXIMATION we must eliminate all reference to history (here: the “start time,” which in the previous discussion was built into the structure of $\mathbf{U}(t, 0)$), To that end, write $s = t - u$

$$\begin{aligned}
 &\downarrow \\
 &= + \int_t^0 \text{tr}_e[\mathbf{H}_i(t), [\mathbf{H}_i(t - u), \rho_s(t) \otimes \rho_e]] du \\
 &= - \int_0^t \text{tr}_e[\mathbf{H}_i(t), [\mathbf{H}_i(t - u), \rho_s(t) \otimes \rho_e]] du
 \end{aligned}$$

and let the upper limit $\uparrow \infty$:

$$= - \int_0^\infty \text{tr}_e[\mathbf{H}_i(t), [\mathbf{H}_i(t - u), \rho_s(t) \otimes \rho_e]] du$$

This **Born-Markoff master equation** approximates the Lindblad equation (15) in a sense (*i.e.*, under physical conditions) that Breuer & Petruccione attempt to summarize on their page 131, but which I am not yet in position to discuss.⁵

⁵ For a helpful discussion of this entire topic, see the class notes of Andrew Fisher at http://www.cmmmp.ucl.ac.uk/ajf~course_notes/node35.html. Fisher cites Breuer & Petruccione’s Chapter 3 (especially §3.2) and also lecture notes by John Preskill (quantum information class at Caltech).