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Berry's transport and minimization of averaged distances

M Maamache†, J-P Provost‡ and G Vallée§

† Département de Physique, Université de Sétif, Sétif 19000, Algeria

‡ Institut Non Linéaire de Nice, UMR CNRS 129, 1361 Route des Lucioles, Sophia Antipolis 06560 Valbonne, France

§ Laboratoire J A Dieudonné, URA CNRS 168, Université de Nice Sophia Antipolis, Parc Valrose, 06108 Nice Cedex 2, France

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Abstract. In this paper we consider the metric approach to the Berry's transport (geometrical part of the adiabatic evolution) of any pure or mixed state, for possibly degenerate Hamiltonians. We emphasize that explicit formulae for the transport of such states need the introduction of an averaging procedure; in analogy with the classical case this quantum averaging involves multiplying each energy eigenstate by a different phase and then integrating over these phases. We show in particular how the transport of non-stationary pure states, rays and density matrices arise from the minimization of Hilbert, Fubini–Study and Bures averaged distances respectively.

1. Introduction

In this introduction we briefly recall the different approaches to Berry's phase focusing on the metric derivation which we develop in this paper. In section 2 we argue that these approaches have been essentially formulated for stationary states and need to be generalized for non-stationary pure states and mixed states; by introducing an averaging technique we provide explicit new expressions for the transport of arbitrary pure states. The main result, obtained in section 3, concerns the application of this technique to a metric derivation of the adiabatic Berry's transport of density operators, using the Bures distance.

Historically, the Berry's phase and more generally the Berry's transport, are geometrical concepts which have emerged from recent reconsiderations of the quantum adiabatic theorem. As is well known, this theorem describes the evolution of the stationary states of systems with Hamiltonians, $H(\boldsymbol{X})$, depending on a set of slowly time-varying parameters $(\boldsymbol{X}(t) \equiv X_1(t), X_2(t), \ldots, X_r(t))$. In its original form [1], it asserts that an initial stationary state remains an eigenstate of the instantaneous Hamiltonian, i.e. it belongs at each time to the eigensubspace $\mathcal{H}_{E(\boldsymbol{X}(t))}$ (hereafter simply denoted $\mathcal{H}_E(t)$) of the Hilbert space, $\mathcal{H}$, associated with the energy level $E(\boldsymbol{X}(t))$. An important physical consequence is that the adiabatic evolution does not induce transitions between stationary states of different energies. The complement given by Berry [2] for a non-degenerate level, and generalized in [3] for the degenerate case, deals with the evolution inside the subspaces $\mathcal{H}_E(t)$. It states that an initial state, $\Psi_E(0)$, in $\mathcal{H}_E(0)$ evolves into the state $\underline{\Psi}_E(t) = \Psi_E(t) \exp -\frac{\mathrm{i}}{\hbar} \int_0^t E(\boldsymbol{X}(s))\, \mathrm{d}s$ of $\mathcal{H}_E(t)$ which contains, besides the expected dynamical phase factor, a slowly time-varying contribution, $\Psi_E(t)$, determined by the condition

$$\boldsymbol{P}_E\, \mathrm{d}\Psi_E = 0 \tag{1}$$

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with $\boldsymbol{P}_E$ (a shorter notation for $\boldsymbol{P}_{E(\boldsymbol{X}(t))}$) being the projector onto $\mathcal{H}_E(t)$. This condition amounts to the requirement that the evolved state, $\underline{\Psi}_E(t)$, satisfies the Schrödinger equation projected onto the eigensubspace associated with $E(\boldsymbol{X}(t))$ (which, for $\Psi_E(t)$, implies the relation $\boldsymbol{P}_E \mathrm{i}\hbar\partial_t \Psi_E(t) = 0$ which is equivalent to (1)).

First noticed by Simon in the non-degenerate case (where (1) reduces to $\langle \Psi_E, \mathrm{d}\Psi_E\rangle = 0$) [4], relation (1) defines a unitary geometrical transport, the Berry's transport, on the fibre bundle with basis the parameters space and fibre over $\boldsymbol{X}$ the space $\mathcal{H}_{E(\boldsymbol{X})}$. If an orthonormal basis of reference states $\Psi^{(0)}_{E,r}(\boldsymbol{X}(t))$ is introduced in $\mathcal{H}_E(t)$, i.e. if $\Psi_E(t)$ is written as

$$\Psi_E(t) = \sum_r C_{E,r}(t)\Psi^{(0)}_{E,r}(\boldsymbol{X}(t)) \tag{2}$$

the transport is explicitly given from (1) by the equations

$$\begin{aligned} \mathrm{d}C_{E,r} &= -\sum_s C_{E,s}\langle \Psi^{(0)}_{E,r}(\boldsymbol{X}), \partial_{\boldsymbol{X}}\Psi^{(0)}_{E,s}(\boldsymbol{X})\rangle \,\mathrm{d}\boldsymbol{X} \\ &= \mathrm{i}\sum_s C_{E,s}\boldsymbol{A}^E_{r,s}(\boldsymbol{X})\,\mathrm{d}\boldsymbol{X}. \end{aligned} \tag{3}$$

In the non-degenerate case, (3) leads simply to the expression $C_E(t) = C_E(0)\exp \mathrm{i}\gamma_E(t)$ where $\gamma_E(t)$, the Berry's phase, is the integral of the connection one-form:

$$\mathrm{d}\gamma_E = \mathrm{i}\langle \Psi^{(0)}_E(\boldsymbol{X}), \partial_{\boldsymbol{X}}\Psi^{(0)}_E(\boldsymbol{X})\rangle \,\mathrm{d}\boldsymbol{X} = \mathrm{i}\langle \Psi^{(0)}_E(\boldsymbol{X}), \mathrm{d}_X\Psi^{(0)}_E(\boldsymbol{X})\rangle. \tag{4}$$

Besides these approaches of the Berry's transport, a less known metric one also exists which we consider now. In the non-degenerate case this approach is connected with the Fubini–Study distance defined in the projective Hilbert space of rays

$$d^2_{FS}(\tilde{\Psi}_1, \tilde{\Psi}_2) = \mathrm{Inf}_{\phi_1,\phi_2}\, \|\Psi_1 \mathrm{e}^{\mathrm{i}\phi_1} - \Psi_2 \mathrm{e}^{\mathrm{i}\phi_2}\|^2 \tag{5}$$

or more precisely with the associated metric

$$\begin{aligned} d^2_{FS}(\tilde{\Psi}, \widetilde{\Psi + \mathrm{d}\Psi}) &\equiv \mathrm{Inf}_{\mathrm{d}\phi}\, \|\Psi - (\Psi + \mathrm{d}\Psi)\mathrm{e}^{\mathrm{i}\,\mathrm{d}\phi}\|^2 \\ &= \langle \mathrm{d}\Psi, \mathrm{d}\Psi\rangle - |\langle \Psi, \mathrm{d}\Psi\rangle|^2. \end{aligned} \tag{6}$$

Indeed, identifying Ψ with the state $\Psi_E(t)$ and $(\Psi + \mathrm{d}\Psi)$ with $\Psi_E(t + \mathrm{d}t)$, the gauge invariance [5] of the metric implies that the transport condition $\langle \Psi_E, \mathrm{d}\Psi_E\rangle = 0$ also reads

$$\langle \mathrm{d}\Psi_E, \mathrm{d}\Psi_E\rangle \qquad \text{minimum} \tag{7}$$

(the rays $\tilde{\Psi}_E$ and $\widetilde{(\Psi_E + \mathrm{d}\Psi_E)}$ being fixed). In other words, the transport simply associates to any vector state of the ray $\tilde{\Psi}_E(t)$ and the state of the ray $\tilde{\Psi}_E(t + \mathrm{d}t)$ which is the closest to it.

A more general formalism, to which we refer below, has recently been developed by Uhlmann [6] and Hubner [7]. Let $\mathcal{B}^2(\mathcal{H})$ be the space of (Hilbert–Schmidt) linear operators, W, from $\mathcal{H}$ to $\mathcal{H}$ such that:

$$WW^\dagger = \rho \qquad \mathrm{Tr}\,\rho < \infty. \tag{8}$$

Then, the space $\mathcal{B}^1(\mathcal{H})^+$ of positive trace class operators, ρ, can be considered as the basis of a fibre bundle, with fibre over ρ the set of operators $\rho^{\frac{1}{2}}U$ (since W in (8) is defined modulo the right action of a unitary operator U). From the distance on $\mathcal{B}^2(\mathcal{H})$

$$d^2_{HS}(W_1, W_2) = \mathrm{Tr}((W_1 - W_2)(W_1 - W_2)^\dagger) \tag{9}$$

which is analogous to the distance $\mathrm{d}^2(\Psi_1, \Psi_2) = \|\Psi_1 - \Psi_2\|^2$ between vector states, one can define a distance in $\mathcal{B}^1(\mathcal{H})^+$

$$d^2_B(\rho_1, \rho_2) = \mathrm{Inf}_{U_1,U_2}\,\mathrm{Tr}((\rho_1^{\frac{1}{2}}U_1 - \rho_2^{\frac{1}{2}}U_2)(\rho_1^{\frac{1}{2}}U_1 - \rho_2^{\frac{1}{2}}U_2)^\dagger) \tag{10}$$

which generalizes the Fubini–Study distance (5). This distance is nothing but the Bures distance initially introduced in the more general framework of normal states of Von Neumann algebras [8]. Its associated metric

$$d_B^2(\rho, \rho + \mathrm{d}\rho) = \mathrm{Inf}_{\mathrm{d}U}\, \mathrm{Tr}(\mathrm{d}W\, \mathrm{d}W^\dagger) \qquad \text{with } \mathrm{d}W = \mathrm{d}(\rho^{\frac{1}{2}}) + \rho^{\frac{1}{2}}\, \mathrm{d}U \tag{11}$$

which generalizes (6), can be considered as the most natural one between density matrices. Then, in analogy with (7) which characterizes the Berry transport $\Psi \to \Psi + \mathrm{d}\Psi$ of vector states, one can define a transport $W \to W + \mathrm{d}W$, named by Uhlman 'parallel transport along density operators', by the condition:

$$d_{HS}^2(W, W + \mathrm{d}W) = \mathrm{Tr}(\mathrm{d}W\, \mathrm{d}W^\dagger) \qquad \text{minimum.} \tag{12}$$

(ρ and $\rho + \mathrm{d}\rho$ being fixed, this condition specifies now $\mathrm{d}U$ in the expression $\mathrm{d}W = \rho^{\frac{1}{2}}\, \mathrm{d}U$.) Writing condition (12) under the equivalent form

$$W^\dagger\, \mathrm{d}W \qquad \text{Hermitian} \tag{13}$$

Uhlman was able to recover the Berry's transport (3) ($\boldsymbol{P}_E\, \mathrm{d}\Psi_{E,r} = 0$) of an orthonormal basis $\{\Psi_{E,r}\}$, in the degenerate case, by choosing $W = \sum_r |\Psi_{E,r}\rangle\langle r|$ where $\{|r\rangle\}$ is an arbitrary fixed orthonormal basis in $\mathcal{H}$ [6]. One of the results of section 2 will be to provide a more natural metric derivation of this transport. To end this introduction, we stress the fact that condition (12) does not define a transport of density matrices, transport is the main purpose of this paper.

2. Berry's transport and averaging generalized

The Berry's phase for individual stationary states, besides its mathematical interest, has also proved itself to be fruitful from an experimental point of view [9]. However, this interest is not limited to considerations about stationary states as illustrated by the two following examples. The first one, of a theoretical nature, deals with the semiclassical relationship $\frac{\partial \gamma_n}{\partial I} = -\frac{1}{\hbar}\theta_I$ between the Berry's phase γ_n (the principal quantum number, n, labels the energy level) and its classical counterpart, for an integrable Hamiltonian, the Hannay's angle θ_I (the action $I = n\hbar$ labels the trajectory in phase space) [10]. A simple quantum way to derive this relationship consists of transport 'action-angle' coherent states (or better rays), which have been shown to be the adapted tools to describe points in the classical phase space with action angle coordinates [11]. Let these states $|I, \theta, \boldsymbol{X}\rangle$ be defined, in the classical limit, by

$$|I, \theta, \boldsymbol{X}\rangle = \sum_{n \simeq I/\hbar} |C_n| \mathrm{e}^{\mathrm{i}n\theta} |\Psi_n^{(0)}(\boldsymbol{X})\rangle \tag{14}$$

the sum over n being 'peaked' ($\Delta n \simeq (I\hbar^{-1})^{\frac{1}{2}}$) around the value given by the correspondence principle. Then it is easy to verify that, up to a global phase factor, the change $\Psi_n^{(0)}(\boldsymbol{X}(0)) \to \mathrm{e}^{\mathrm{i}\gamma_n(t)}\Psi_n^{(0)}(\boldsymbol{X}(t))$ of the stationary states induces the change $|I, \theta, \boldsymbol{X}(0)\rangle \to |I, \theta + \theta_I(t), \boldsymbol{X}(t)\rangle$ of the coherent states. However, this change (Hannay's transport) of the coherent states, which is induced by the Berry's transport of stationary states, does not correspond to conditions such as $\langle \Psi, \mathrm{d}\Psi\rangle = 0$ or $\langle \mathrm{d}\Psi, \mathrm{d}\Psi\rangle$ minimum: these conditions need to be modified for non-stationary states. The second example, of a practical nature, deals with experiments such as those performed by Bitter and Dubbers [12] where one measures the change in the polarization of slow neutrons propagating in an inhomogeneous static magnetic field. In such experiments one studies the adiabatic evolution of density (polarization) matrices. Although it is clearly understood that this

evolution is the one induced by the evolution of the individual stationary states there is also, in this case, the need for a direct definition of the Berry's transport. As we shall see this definition requires a notion of averaging. We now define this notion and apply it to the transport of pure states (formulae (17)–(19)), postponing the case of density matrices to section 3.

Averaging is a concept which lies at the basis of the demonstration of the classical adiabatic theorem [13] but which is, surprisingly, rarely evocated in the quantum case. Quantum averaging concerns the phase of the stationary states in the same way as the classical one concerns the angle variable on trajectories of fixed action in phase space [14]. Technically, the adiabatic average, $\overline{\mathcal{F}}$, of any functional, $\mathcal{F}$, of the reference stationary states $\Psi^{(0)}_{E,r}(\boldsymbol{X}(t))$ is defined by:

$$\overline{\mathcal{F}} = \int_0^{2\pi}\int_0^{2\pi}\dots\int_0^{2\pi} \mathcal{F}(\{\mathrm{e}^{\mathrm{i}\alpha_E}\Psi^{(0)}_{E,r}(\boldsymbol{X}(t))\})\Pi_E \frac{\mathrm{d}\alpha_E}{2\pi}. \tag{15}$$

It is obtained by multiplying each reference state by a phase factor associated with the corresponding energy level (possibly degenerated) and by integrating over these phases $\{\alpha_E\}$ (the same for all r). If $\mathcal{F}$ depends on an arbitrary state Ψ it is understood in (15) that one decomposes Ψ as

$$\Psi(t) = \sum_E \Psi_E(t) \qquad \text{with } \Psi_E(t) = \sum_r C_{E,r}(t)\Psi^{(0)}_{E,r}(\boldsymbol{X}(t)) \tag{16}$$

before taking the average. As a consequence the coefficients $C_{E,r} = \langle\Psi^{(0)}_{E,r}, \Psi\rangle$ must be considered as unaffected by the change of phases. In contrast, a variation $\mathrm{d}\Psi$ ('d of Ψ') is affected by this change.

As a first application of the averaging procedure it is easy to verify the equality $\overline{\langle\Phi, \mathrm{d}\Psi\rangle} = \sum_E \langle\Phi_E, \mathrm{d}\Psi_E\rangle$ for any two vectors, Φ and Ψ, in the Hilbert space $\mathcal{H}$. This allows us to specify the Berry's transport, $\boldsymbol{P}_E\,\mathrm{d}\Psi_E = 0$ for all E, of an arbitrary pure state, Ψ, by the unique condition (generalization of (1)):

$$\overline{\langle\Phi, \mathrm{d}\Psi\rangle} = 0 \qquad \forall\Phi \in \mathcal{H}. \tag{17}$$

This condition infers that, on average, $\mathrm{d}\Psi$ is orthogonal to any vector in $\mathcal{H}$.

A second application of the averaging procedure is the derivation of the Berry's transport from the extremum principle:

$$\delta\left[\int \overline{\langle\Psi, \mathrm{d}\Psi\rangle}\right] = 0 \qquad \left(\mathrm{d}\Psi = \frac{\partial\Psi}{\partial t}\,\mathrm{d}t\right). \tag{18}$$

Indeed, using decomposition (16) and differentiating $\overline{\langle\Psi, \mathrm{d}\Psi\rangle}$ with respect to the complex conjugate coefficients, $C^*_{E,r}$, it is easy to recover (17) from (18). This result is a direct consequence of the fact that, in the quantum case as in the classical one, the adiabatic hypothesis consists of changing the Lagrangian $\mathcal{L}$ ($\mathcal{L} = \langle\Psi, (\mathrm{i}\hbar\partial_t - H)\Psi\rangle$ for the Schrödinger equation) by its average $\overline{\mathcal{L}}$ [14].

Finally, we combine the averaging procedure with the metric approach and show that the condition

$$\overline{\langle\mathrm{d}\Psi, \mathrm{d}\Psi\rangle} \qquad \text{minimum} \tag{19}$$

is a simple metric way to define the Berry's transport for arbitrary pure vector states. For this demonstration, as for those which lead, in section 3, to the transport of rays and density matrices, it is useful to separate, into the total variation, $\mathrm{d}\Psi$, of a state, the contribution $\mathrm{d}_X\Psi = \sum_{E,r} C_{E,r}\,\mathrm{d}_X\Psi^{(0)}_{E,r}(\boldsymbol{X})$ associated with a given variation, $\mathrm{d}\boldsymbol{X}$, of the parameters from the contribution $\mathrm{d}_C\Psi = \sum_{E,r}\mathrm{d}C_{E,r}\,\Psi^{(0)}_{E,r}(\boldsymbol{X})$ associated with the variations $\{\mathrm{d}C_{E,r}\}$

of the components of Ψ onto the moving basis (the transport being specified, in the metric approach, by the variation $\mathrm{d}_C\Psi$ which, for a given $\mathrm{d}_X\Psi$, satisfies condition (19)). One has:

$$\mathrm{d}\Psi = \mathrm{d}_X\Psi + \mathrm{d}_C\Psi \qquad \text{with } (\boldsymbol{I} - \boldsymbol{P}_E)\,\mathrm{d}_C\Psi_E = 0. \tag{20}$$

Then, from the equality

$$\begin{aligned}\overline{\langle \mathrm{d}\Psi, \mathrm{d}\Psi\rangle} &= \sum_E \langle \mathrm{d}\Psi_E, \mathrm{d}\Psi_E\rangle \\ &= \sum_E \|\boldsymbol{P}_E\,\mathrm{d}\Psi_E\|^2 + \|(\boldsymbol{I} - \boldsymbol{P}_E)\,\mathrm{d}_X\Psi_E\|^2\end{aligned} \tag{21}$$

and the remark that the last term on the r.h.s. of (21) is independent of the variations $\{\mathrm{d}C_{E,r}\}$, one verfies that the minimum of (21) is obtained when the transport conditions (1), $\boldsymbol{P}_E\,\mathrm{d}\Psi_E = 0$ for all E, are satisfied.

3. Berry's transport of rays and density matrices

As the Fubini–Study metric (6) is the extension to rays of the Hilbert metric $\langle \mathrm{d}\Psi, \mathrm{d}\Psi\rangle$ for vector states, let us average it and examine the condition

$$\overline{\langle \mathrm{d}\Psi, \mathrm{d}\Psi\rangle - |\langle \Psi, \mathrm{d}\Psi\rangle|^2} \qquad \text{minimum.} \tag{22}$$

We now show that it leads to the transport of rays and therefore generalizes (19). (We keep the possibility that some eigenspaces, $\mathcal{H}_E$, are degenerate.) An important remark is that, because each variation $\mathrm{d}_C\Psi_E$ belongs to the corresponding eigensubspace $\mathcal{H}_E$, the quantity $\langle \Psi, \mathrm{d}_C\Psi\rangle$ is equal to its average $\overline{\langle \Psi, \mathrm{d}_C\Psi\rangle}$. So one can write:

$$\langle \Psi, \mathrm{d}\Psi\rangle - \overline{\langle \Psi, \mathrm{d}\Psi\rangle} = \langle \Psi, \mathrm{d}_X\Psi\rangle - \overline{\langle \Psi, \mathrm{d}_X\Psi\rangle}. \tag{23}$$

Then, considering each side of (23) as random variables (functions of the random phases $\{\alpha_E\}$ entering into the averaging procedure) one gets the equality of their variances:

$$\overline{|\langle \Psi, \mathrm{d}\Psi\rangle|^2} - |\overline{\langle \Psi, \mathrm{d}\Psi\rangle}|^2 = \overline{|\langle \Psi, \mathrm{d}_X\Psi\rangle|^2} - |\overline{\langle \Psi, \mathrm{d}_X\Psi\rangle}|^2. \tag{24}$$

Since the r.h.s. of (24) is independent of the variations $\{\mathrm{d}C_{E,r}\}$ it follows that $\overline{|\langle \Psi, \mathrm{d}\Psi\rangle|^2}$ can be replaced by $|\overline{\langle \Psi, \mathrm{d}\Psi\rangle}|^2$ in (22). The quantity to minimize thus reads $\sum_E \|\boldsymbol{P}_E\,\mathrm{d}\Psi_E\|^2 - |\sum_E \langle \Psi_E, \mathrm{d}\Psi_E\rangle|^2$. According to the Schwartz inequality, the minimum is obtained when $\boldsymbol{P}_E\,\mathrm{d}\Psi_E = \mathrm{d}\lambda\Psi_E$ (for all E). One can verify that the normalization of Ψ implies that $\mathrm{d}\lambda$ is purely imaginary. Therefore condition (22) leads to:

$$\boldsymbol{P}_E\,\mathrm{d}\Psi_E = \mathrm{i}\,\mathrm{d}\varphi\Psi_E. \tag{25}$$

One obtains the Berry's transport of vector states up to a global (the same for all E and r) phase factor, i.e. (22) actually defines the Berry's transport of rays. (When the states Ψ are the action-angle states (14) relation (22) provides a metric transport of the classical trajectories in phase space [15].)

The generalization of this transport to statistical mixtures of quantum states requires a notion of distance between density operators. As explained in the introduction, the natural one is the Bures distance (10) (although the distance $\mathrm{Tr}(\rho_2 - \rho_1)^2$ has also been considered in this context [16]). An explicit expression for the associated metric (11) was first obtained by Hubner [7] by means of the calculation of $d_B(\rho, \rho + t\,\mathrm{d}\rho)$ up to second order in t and then by Braunstein and Caves [17] using arguments of a statistical nature. This expression,

also obtained in the appendix from a direct determination of the infimum by means of Lagrange multipliers, reads

$$d_B^2(\rho, \rho + \mathrm{d}\rho) = \frac{1}{2} \sum_{\lambda_\alpha + \lambda_\beta \neq 0} \frac{|\langle \Phi_\alpha | \mathrm{d}\rho | \Phi_\beta \rangle|^2}{\lambda_\alpha + \lambda_\beta} \tag{26}$$

where $\{\Phi_\alpha\}$ is a basis of eigenvectors of ρ and $\{\lambda_\alpha\}$ is the associated spectrum. In the particular case of a projector $\rho = \boldsymbol{P}_\Psi = |\Psi\rangle\langle\Psi|$, identifying the pure state, Ψ, with the eigenstate Φ_0, (26) reads $\sum_{\alpha \neq 0} |\langle \Phi_\alpha, \mathrm{d}\Psi \rangle|^2 = \langle \mathrm{d}\Psi, (\boldsymbol{I} - \boldsymbol{P}_\Psi)\, \mathrm{d}\Psi \rangle = \langle \mathrm{d}\Psi, \mathrm{d}\Psi \rangle - |\langle \Psi, \mathrm{d}\Psi \rangle|^2$ and the Bures metric reduces to the Fubini–Study one (6) (as expected since $\rho = \boldsymbol{P}_\Psi$ is another way to specify the quantum ray $\tilde{\Psi}$). Let us now consider the transport of density operators defined by the condition

$$\overline{d_B^2(\rho, \rho + \mathrm{d}\rho)} \qquad \text{minimum} \tag{27}$$

which generalizes (19) and (22). In order to make this condition tractable, one expresses $\rho(t)$ in the basis of reference states $\Psi^{(0)}_{E,r}(\boldsymbol{X}(t))$

$$\rho(t) = \sum_{E,r} \sum_{F,s} \rho_{(E,r)(F,s)}(t) |\Psi^{(0)}_{E,r}(\boldsymbol{X}(t))\rangle\langle\Psi^{(0)}_{F,s}(\boldsymbol{X}(t))| \tag{28}$$

and separates as above, in the total variation $\mathrm{d}\rho$ of the density matrix, the contributions associated respectively with the variations $\{\mathrm{d}(\rho_{(E,r)(F,s)})\}$ of the coefficients and with those $\mathrm{d}\boldsymbol{X}$ of the parameters, i.e. one writes

$$\mathrm{d}\rho = \mathrm{d}_C\rho + \mathrm{d}_X\rho \tag{29}$$

with:

$$\begin{aligned} \mathrm{d}_C\rho &= \sum_{E,r} \sum_{F,s} \mathrm{d}(\rho_{(E,r)(F,s)})\, |\Psi^{(0)}_{E,r}(\boldsymbol{X})\rangle\langle\Psi^{(0)}_{F,s}(\boldsymbol{X})| \\ \mathrm{d}_X\rho &= \sum_{E,r} \sum_{F,s} \rho_{(E,r)(F,s)} (|\mathrm{d}_X\Psi^{(0)}_{E,r}(\boldsymbol{X})\rangle\langle\Psi^{(0)}_{F,s}(\boldsymbol{X})| + |\Psi^{(0)}_{E,r}(\boldsymbol{X})\rangle\langle\mathrm{d}_X\Psi^{(0)}_{F,s}(\boldsymbol{X})|). \end{aligned} \tag{30}$$

Then, given a variation, $\mathrm{d}_X\rho$, of ρ, the geometrical transport involves determining the corresponding variation $\mathrm{d}_C\rho$. At this point, it is important to note that, in the same way as the coefficients $C_{E,r}(t) = \langle \Psi^{(0)}_{E,r}(\boldsymbol{X}(t)), \Psi \rangle$ of the decomposition (16) are not affected by the averaging procedure, quantities such as $\langle \Psi^{(0)}_{F,s}(\boldsymbol{X}(t)), \Phi_\beta \rangle$ which appear in the expression of $\langle \Phi_\alpha | \mathrm{d}\rho | \Phi_\beta \rangle$ must not be averaged. Consequently $\langle \Phi_\alpha | \mathrm{d}_C\rho | \Phi_\beta \rangle$ is equal to its average $\overline{\langle \Phi_\alpha | \mathrm{d}_C\rho | \Phi_\beta \rangle}$. Then a derivation similar at all points to the one used to obtain equation (24) leads to the following expression for the variance of the matrix element $\langle \Phi_\alpha | \mathrm{d}\rho | \Phi_\beta \rangle$:

$$\overline{|\langle \Phi_\alpha | \mathrm{d}\rho | \Phi_\beta \rangle|^2} - |\overline{\langle \Phi_\alpha | \mathrm{d}\rho | \Phi_\beta \rangle}|^2 = \overline{|\langle \Phi_\alpha | \mathrm{d}_X\rho | \Phi_\beta \rangle|^2} - |\overline{\langle \Phi_\alpha | \mathrm{d}_X\rho | \Phi_\beta \rangle}|^2. \tag{31}$$

It follows that the terms $\overline{|\langle \Phi_\alpha | \mathrm{d}\rho | \Phi_\beta \rangle|^2}$ can be replaced by $|\overline{\langle \Phi_\alpha | \mathrm{d}\rho | \Phi_\beta \rangle}|^2$ in (27). The condition of minimum is then clearly realized when:

$$\overline{\langle \Phi_\alpha | \mathrm{d}\rho | \Phi_\beta \rangle} = 0 \qquad \forall \alpha, \beta. \tag{32}$$

This relation, which generalizes (17), infers that on average (and in the weak operator topology) the variation $\mathrm{d}\rho$ is equal to zero. It explicitly reads:

$$\begin{aligned} \sum_{E,r} \sum_{F,s} \langle \Phi_\alpha, \Psi^{(0)}_{E,r}(\boldsymbol{X}) \rangle \langle \Psi^{(0)}_{F,s}(\boldsymbol{X}), \Phi_\beta \rangle \Big[& \mathrm{d}(\rho_{(E,r)(F,s)}) \\ & + \sum_u [\langle \Psi^{(0)}_{E,r}(\boldsymbol{X}), \mathrm{d}_X\Psi^{(0)}_{E,u}(\boldsymbol{X}) \rangle \rho_{(E,u)(F,s)} \\ & + \langle \mathrm{d}_X\Psi^{(0)}_{F,u}(\boldsymbol{X}), \Psi^{(0)}_{F,s}(\boldsymbol{X}) \rangle \rho_{(E,r)(F,u)}] \Big] = 0. \end{aligned} \tag{33}$$

As this equality is true for all α and β one deduces that the $\mathrm{d}(\rho_{(E,r)(F,s)})$'s which minimize $\overline{d_B^2(\rho, \rho + \mathrm{d}\rho)}$ are such that:

$$\mathrm{d}(\rho_{(E,r)(F,s)}) = \mathrm{i} \sum_u [\boldsymbol{A}^E_{ru}(\boldsymbol{X})\rho_{(E,u)(F,s)} - \rho_{(E,r)(F,u)}\boldsymbol{A}^F_{us}(\boldsymbol{X})]\,\mathrm{d}\boldsymbol{X}. \tag{34}$$

This formula for the elements of density matrices generalizes formula (3) for the components of pure states. It infers that the Berry's transport of density matrices is the one induced by the transport of stationary states. Indeed, (34) implies that the matrix elements would be unchanged if they were taken in the basis of the transported stationary states (in place of the basis of the reference stationary states). For example, in the non-degenerate case (34) reduces to

$$\mathrm{d}(\rho_{EF}) = \mathrm{i}\rho_{EF}(\mathrm{d}\gamma_E - \mathrm{d}\gamma_F) \tag{35}$$

and the corresponding transport associates to the density matrix $\rho(0) = \sum_{EF} \rho_{EF}(0)$ $|\Psi^{(0)}_E(\boldsymbol{X}(0))\rangle\langle\Psi^{(0)}_F(\boldsymbol{X}(0))|$ the density matrix:

$$\rho(t) = \sum_{EF} \rho_{EF}(0)\mathrm{e}^{\mathrm{i}(\gamma_E(t) - \gamma_F(t))}|\Psi^{(0)}_E(\boldsymbol{X}(t))\rangle\langle\Psi^{(0)}_F(\boldsymbol{X}(t))|. \tag{36}$$

Appendix

The problem now involves finding the infimum:

$$\mathrm{Inf}_{\mathrm{d}U}\,\mathrm{Tr}(\mathrm{d}W\,\mathrm{d}W^\dagger) = d_B^2(\rho, \rho + \mathrm{d}\rho) \qquad \text{with } \mathrm{d}W = \mathrm{d}(\rho^{\frac{1}{2}}) + \rho^{\frac{1}{2}}\,\mathrm{d}U. \tag{A.1}$$

In the basis of their eigenvectors $\{\Phi_\alpha\}$, ρ and $\rho^{\frac{1}{2}}$ read as

$$\rho = \sum_\alpha \lambda_\alpha |\Phi_\alpha\rangle\langle\Phi_\alpha| \qquad \rho^{\frac{1}{2}} = \sum_\alpha \mu_\alpha |\Phi_\alpha\rangle\langle\Phi_\alpha| \qquad (\lambda_\alpha = \mu_\alpha^2) \tag{A.2}$$

and $\mathrm{d}W$ takes the form

$$\mathrm{d}W = \sum_\alpha \mathrm{d}\mu_\alpha|\Phi_\alpha\rangle\langle\Phi_\alpha| + \mu_\alpha|\mathrm{d}\Phi_\alpha\rangle\langle\Phi_\alpha| + \mu_\alpha|\Phi_\alpha\rangle\langle\mathrm{d}\Phi_\alpha| + \mu_\alpha|\Phi_\alpha\rangle\langle\Phi_\alpha|\,\mathrm{d}U. \tag{A.3}$$

Let us denote $\langle\mathrm{d}\Phi_\alpha| + \langle\Phi_\alpha|\mathrm{d}U \stackrel{\mathrm{def}}{=} \langle\delta\Phi_\alpha|$; the perturbation $\mathrm{d}U$ being a unitary one ($\mathrm{d}U + \mathrm{d}U^\dagger = 0$), the $\{\langle\delta\Phi_\alpha|\}$'s are submitted to the constraints:

$$\langle\delta\Phi_\alpha, \Phi_\beta\rangle + \langle\Phi_\alpha, \delta\Phi_\beta\rangle = 0 \qquad \forall\alpha, \beta. \tag{A.4}$$

The Bures metric then reads:

$$\begin{aligned} d_B^2(\rho, \rho + \mathrm{d}\rho) = \mathrm{Inf}_{\{\langle\delta\Phi_\alpha|\}}\,\mathrm{Tr}\Bigg(\sum_{\alpha\beta}\big((\mathrm{d}\mu_\alpha|\Phi_\alpha\rangle\langle\Phi_\alpha| + \mu_\alpha|\mathrm{d}\Phi_\alpha\rangle\langle\Phi_\alpha| \\ +\mu_\alpha|\Phi_\alpha\rangle\langle\delta\Phi_\alpha|)(\mathrm{d}\mu_\beta|\Phi_\beta\rangle\langle\Phi_\beta| + \mu_\beta|\Phi_\beta\rangle\langle\mathrm{d}\Phi_\beta| + \mu_\beta|\delta\Phi_\beta\rangle\langle\Phi_\beta|) \\ +\mu_\alpha\mu_\beta l_{\alpha\beta}(\langle\delta\Phi_\alpha, \Phi_\beta\rangle + \langle\Phi_\alpha, \delta\Phi_\beta\rangle)\big)\Bigg). \end{aligned} \tag{A.5}$$

In this relation the Lagrange multipliers, $l_{\alpha\beta}$ $(= l^*_{\beta\alpha})$, ensure that constraints (A.4) are taken into account (their product by $\mu_\alpha\mu_\beta$ being introduced there only for calculational convenience). The infimum of the trace is obtained for variations $\{|\delta\Phi_\alpha\rangle\}$'s such that:

$$\mu_\alpha|\delta\Phi_\alpha\rangle + \mathrm{d}\mu_\alpha|\Phi_\alpha\rangle + \sum_\beta \mu_\beta(\langle\mathrm{d}\Phi_\beta, \Phi_\alpha\rangle + l_{\alpha\beta})|\Phi_\beta\rangle = 0. \tag{A.6}$$

Then, considering linear combinations of the relations deduced from (A.6) by projection onto the basis vectors $\{\Phi_\gamma\}$ and taking into account constraints (A.4) and the Hermitian symmetry of the $\{l_{\alpha\beta}\}$'s, one gets the Lagrange multipliers:

$$l_{\alpha\alpha} = -\frac{1}{2}\frac{\mathrm{d}\lambda_\alpha}{\lambda_\alpha} \qquad l_{\alpha\beta} = \frac{\lambda_\alpha - \lambda_\beta}{\lambda_\alpha + \lambda_\beta}\langle \mathrm{d}\Phi_\beta, \Phi_\alpha\rangle \qquad \alpha \neq \beta. \tag{A.7}$$

Substituting (A.6) and (A.7) into (A.5), the Bures metric reads:

$$d_B^2(\rho, \rho + \mathrm{d}\rho) = \frac{1}{2}\left(\sum_\alpha \frac{(\mathrm{d}\lambda_\alpha)^2}{2\lambda_\alpha} + \sum_{\alpha\neq\beta} |\langle \Phi_\alpha, \mathrm{d}\Phi_\beta\rangle|^2 \frac{(\lambda_\beta - \lambda_\alpha)^2}{\lambda_\beta + \lambda_\alpha}\right) \tag{A.8}$$

or, by using (A.2),

$$d_B^2(\rho, \rho + \mathrm{d}\rho) = \frac{1}{2}\sum_{\alpha\beta} \frac{|\langle \Phi_\alpha|\mathrm{d}\rho|\Phi_\beta\rangle|^2}{\lambda_\beta + \lambda_\alpha} \tag{A.9}$$

which is expression (26) given in section 3.

References

[1] Messiah A 1962 *Quantum Mechanics* vol 2 (Amsterdam: North-Holland) ch XVII
[2] Berry M V 1984 *Proc. R. Soc.* A **392** 45
[3] Wilczek F and Zee A 1984 *Phys. Rev. Lett.* **58** 2111
[4] Simon B 1983 *Phys. Rev. Lett.* **51** 2167
[5] Provost J P and Vallée G 1980 *Commun. Math. Phys.* **76** 289
[6] Uhlmann A 1986 *Rep. Math. Phys.* **24** 229
Uhlmann A 1989 *Ann. Phys., Lpz.* **46** 63
[7] Hubner M 1992 *Phys. Lett.* A **163** 239
Hubner M 1993 *Phys. Lett.* A **179** 226
[8] Bures D 1969 *Trans. Am. Math. Soc.* **135** 199
[9] Shapere A and Wilczek F 1989 *Geometric Phases in Physics (Advanced Series in Mathematical Physics 5)* (Singapore: World Scientific) ch 4
[10] Hannay J H 1985 *J. Phys. A: Math. Gen.* **18** 221
Berry M V 1985 *J. Phys. A: Math. Gen.* **18** 15
[11] Maamache M, Provost J P and Vallée G 1990 *J. Phys. A: Math. Gen.* **23** 5765
[12] Bitter T and Dubbers D 1987 *Phys. Rev. Lett.* **59** 251
[13] Arnold V 1978 *Mathematical Methods of Classical Mechanics (Springer Graduate Texts in Mathematics 60)* (New York: Springer) p 791
[14] Maamache M, Provost J P and Vallée G 1994 *Eur. J. Phys.* **15** 121
[15] Maamache M 1993 *Thèse de Doctorat* Université de Nice Sophia Antipolis, unpublished
[16] Anandan J 1990 A geometric view of quantum mechanics *Quantum Coherence* ed J S Anandan (Singapore: World Scientific)
[17] Braunstein S L and Caves C M 1994 *Phys. Rev. Lett.* **72** 3439