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Geometry of quantum active subspaces and of effective Hamiltonians

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We propose a geometric formulation of the theory of effective Hamiltonians associated with active spaces. We analyze particularly the case of the time-dependent wave operator theory. This formulation is related to the geometry of the manifold of the active spaces, particularly to its Kählerian structure. We introduce the concept of quantum distance between active spaces. We show that the time-dependent wave operator theory is, in fact, a gauge theory, and we analyze its relationship with the geometric phase concept. © *2007 American Institute of Physics.*
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I. INTRODUCTION

The numerical study of the interaction of a molecule with a strong laser field leads to a need for long computational times and large computer memory capacity when use is made of a wave packet approach, which involves a direct integration of the time-dependent Schrödinger equation. This computational problem is even greater for the study of control processes, since the repetition of many propagations is needed to find the optimum values of several adjustable parameters which describe the nonlinear effects due to ultrashort laser pulses.

Fortunately, it turns out that a reasonable description of the matter-field interaction can often be made by using an active space of small dimension, provided that the basis sets used consist of instantaneous Floquet eigenvectors[1] or generalized Floquet eigenvectors.[2] This feature makes an effective Hamiltonian approach attractive, and Guérin and Jauslin[3] have proposed such an approach, based on the quantum analog of the Kolmogorov-Arnold-Moser (KAM) transformation,[4] with resonant effects being treated by a rotating wave approximation. The superadiabatic Floquet approach,[5] which uses a sequence of unitary transformations to produce bases which follow the nonadiabatic evolution, is also very similar to an effective Hamiltonian approach. Finally, the constrained adiabatic trajectory method[6] is a method consisting to define an effective Hamiltonian by adding a time-dependent complex potential. The time-dependent wave operator theory is another example of effective Hamiltonian theory for time-dependent systems. It has long been used to describe photoreactive processes[7,8] and has several features which make it useful in the search for an efficient description of nonadiabatic effects. The theory of time-dependent wave operators, and their stationary equivalents, the Bloch wave operators, has been the subject of several works.[9–11]

We consider a separable Hilbert space $\mathcal{H}$ which is used to describe the states of a quantum system. The dynamical system is described by a time-dependent Hamiltonian $H(t)$, and its associated time-dependent Schrödinger equation and has the time evolution operator $U(t,0)$ $(\forall t \in [0,T])$. The idea of the wave operator theory is to consider a *fixed active subspace* S_0 of $\mathcal{H}$, such that the dynamics projected into this subspace can be integrated by using an effective Hamiltonian. S_0 should be chosen to describe the strong and fast part of the dynamics issuing from the initial state; this choice has been made previously by using artificial intelligence

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approaches[12,13] and a wave operator sorting algorithm.[8,14] After the solution of the Schrödinger equation in the active space S_0, the wave operator Ω which generates H^{eff} is used to transform the solution in S_0 into the true solution in the Hilbert space $\mathcal{H}$. The above description can be summarized as follows:

$$\forall t, \quad \Omega(t): \begin{array}{c} S(t) \to \mathcal{H} \\ \psi_0(t) \mapsto \psi(t), \end{array} \tag{1}$$

where $\psi(t)$ is a solution of the Schrödinger equation

$$\imath\hbar \partial_t \psi(t) = H(t)\psi(t) \tag{2}$$

and where $\psi_0(t)$, defined as the projection of ψ into S_0, is a solution of the equation

$$\imath\hbar \partial_t \psi_0(t) = H^{\text{eff}}(t)\psi_0(t). \tag{3}$$

The effective Hamiltonian (which describes the approximate dynamics in S_0) is defined by $H^{\text{eff}}(t)=P_0H(t)\Omega(t)$, and the target space is $S(t)=P_0U(t,0)S_0 \subset S_0$, with P_0 being the projector on S_0. The time-dependent wave operator can be written as

$$\Omega(t) = U(t)(P_0U(t,0)P_0)^{-1}, \tag{4}$$

where $(P_0U(t,0)P_0)^{-1}=P_0(P_0U(t,0)P_0)^{-1}P_0$ is the inverse of $U(t)$ within S_0 $[\text{dom}(P_0U(t,0)P_0)^{-1}=S_0]$.

Finally, the wave function can be written as follows:

$$\psi(t) = \Omega(t)U^{\text{eff}}(t,0)\psi_0, \tag{5}$$

where $\imath\hbar\partial_t U^{\text{eff}}(t,0)=H^{\text{eff}}(t)U^{\text{eff}}(t,0)$.

It is possible to define a stationary analog to the time-dependent wave operator. We will now consider (in the same separable Hilbert space $\mathcal{H}$) the operator H and the eigenvalue equation

$$H\psi = \lambda\psi. \tag{6}$$

We consider two subspaces S_0 and S of $\mathcal{H}$. We call them the active and target subspaces, and we denote the projectors of these subspaces by P_0 and P. We are interested in eigenvectors included in S such that $P\psi=\psi$. As for the previous time-dependent problem, we reduce this problem to one within the active subspace. We then introduce the Bloch wave operator:

$$\Omega: \begin{array}{c} S_0 \to S \\ \psi_0 \mapsto \psi \end{array}, \tag{7}$$

where ψ is a solution of the eigenvalue equation [Eq. (6)] and ψ_0 is a solution of

$$H^{\text{eff}}\psi_0 = \lambda\psi_0. \tag{8}$$

The effective operator is defined by $H^{\text{eff}}=P_0H\Omega$. The Bloch wave operator is formally given by the expression

$$\Omega = P(P_0PP_0)^{-1}, \tag{9}$$

where $(P_0PP_0)^{-1}$ is the inverse of P within S_0.

The time-dependent wave operator is a generalization of the Møller wave operators $\Omega^{\pm} = \lim_{t\to\mp\infty} e^{-\imath\hbar^{-1}Ht}e^{\imath\hbar^{-1}H_0t}$, which compare the dynamics induced by a time-independent Hamiltonian H with the dynamics induced by a simplest Hamiltonian H_0. The time-dependent wave operator has the same function; it compares the true dynamics with the effective dynamics condensed in a fixed active space. The time-dependent wave operator techniques consist then to separate the subdynamics governed by $H^{\text{eff}}(t)$ from the dynamics outside S_0 which is induced by

$\Omega(t)$. The aim of this paper is to show that this method has a geometric formulation very close to usual geometric theories of dynamical systems. We show that the separation in two parts of the dynamics is associated with a fiber bundle formalism; the effective dynamics is associated with the base manifold of the bundle, whereas the true dynamics is associated with the total space of the bundle. The wave operator action, consisting to built the true wave function from the effective one, is, in fact, a horizontal lift of the effective dynamics in the bundle with respect to a particular connection explicated in this paper. The effective dynamics, which is condensed in the base manifold, can be geometrically formulated by a complexification of the Poincaré form formulation of classical dynamics. With this geometric formulation of the dynamics in the base manifold, we have a consistent geometric point of view of the time-dependent wave operator method. Section III is dedicated to this analysis.

Since the time-dependent wave operator geometric formulation is associated with a principal bundle, it is very close to the non-Abelian geometric phase theory. We show in this paper that the time-dependent wave operator can be assimilated with an operator which multiplies the effective wave function by a non-Abelian geometric phase.

In 1984, Berry[15] proved, in the context of the standard adiabatic approximation, that the wave function of a quantum dynamical system takes the form

$$\psi(t) = e^{-\imath\hbar^{-1}\int_0^t E_a(\mathbf{R}(t'))dt' - \int_0^t \langle a,\mathbf{R}(t')|\partial_{t'}|a,\mathbf{R}(t')\rangle dt'}|a,\mathbf{R}(t)\rangle, \tag{10}$$

where E_a is a nondegenerate instantaneous eigenvalue isolated from the rest of the Hamiltonian spectrum and having instantaneous eigenvector $|a,\mathbf{R}(t)\rangle$. $\mathbf{R}$ is a set of classical control parameters used to model the time-dependent environment of the system. The set of all configurations of $\mathbf{R}$ is supposed to form a $\mathcal{C}^\infty$-manifold $\mathcal{M}$. The important result is the presence of the extra phase term, called the Berry phase $e^{-\int_0^t \langle a,\mathbf{R}(t')|\partial_{t'}|a,\mathbf{R}(t')\rangle dt'}$. Simon[16] found the mathematical structure which models the Berry phase phenomenon, namely, a principal bundle with base space $\mathcal{M}$ and with structure group $U(1)$. If we eliminate the dynamical phase by a gauge transformation which involves redefining the eigenvector at each time, then expression (10) is the horizontal lift of the curve $\mathcal{C}$ described by $t\mapsto\mathbf{R}(t)$ with the gauge potential $A=\langle a,\mathbf{R}|d_{\mathcal{M}}|a,\mathbf{R}\rangle$. If $\mathcal{C}$ is closed, then the Berry phase $e^{-\oint_{\mathcal{C}}A}\in U(1)$ is the holonomy of the horizontal lift.

In 1987, Aharonov and Anandan[17] proved that the appearance of geometric phases such as the Berry phase is not restricted to the use of adiabatic approximation but arises in a more general context. Let $t\mapsto\psi(t)$ be a wave function such that $\psi(T)=e^{\imath\phi}\psi(0)$ and $H(t)$ be the Hamiltonian of the system. Suppose that the Hilbert space is n dimensional (the case $n=+\infty$ is not excluded); then the wave function defines a closed curve $\mathcal{C}$ in the complex projective space $\mathbb{C}P^{n-1}$. If one redefines the wave function such that $\tilde{\psi}(T)=\tilde{\psi}(0)$, then

$$\psi(t) = e^{-\imath\hbar^{-1}\int_0^t\langle\tilde{\psi}(t')|H(t')|\tilde{\psi}(t')\rangle dt' - \int_0^t\langle\tilde{\psi}(t')|\partial_{t'}|\tilde{\psi}(t')\rangle dt'}\tilde{\psi}(t). \tag{11}$$

The extra phase in addition to the dynamical phase is called the Aharonov-Anandan phase (or nonadiabatic Berry phase). We can eliminate the dynamical phase by a gauge transformation; the Aharonov-Anandan phase then appears as the horizontal lift of $\mathcal{C}$ in the principal bundle with base space $\mathbb{C}P^{n-1}$, the structure group $U(1)$, and with the $(2n-1)$-dimensional sphere S^{2n-1} as total space. The Berry-Simon model and the Aharonov-Anandan model are related by the universal classifying theorem of principal bundles;[18,19] more precisely, the Aharonov-Anandan principal bundle is a universal bundle for the Berry-Simon principal bundle. The base space $\mathbb{C}P^{n-1}$ is endowed with a natural metric called the Fubini-Study metric. Anandan and Aharonov[20] have proved that this metric measures the quantum distance between the quantum states. The connection bewteen geometric phases and universal classifying spaces is explained in Refs. 21–23

A non-Abelian geometric phase (based on the gauge group $U(M)$) was introduced by Wilczek and Zee in 1984 Ref. 24 and its universal structure was studied by Bohm and Mostafazadeh in 1994.[22] In a previous article,[25] we have proposed a geometric structure based on the concept of principal composite bundle to describe in the context of the adiabatic approximation, the non-Abelian geometric phase when it does not commute with the dynamical phase (see also the works of Sardanashvily[26,27]).

The wave operator formalism is associated with a fixed active space. In the present work, we are also interested by the possibility to use an evolutive active space, i.e., a time-dependent active space which adapts to the time evolution rather than the use of a time-dependent wave operator to lift an effective dynamics within a fixed subspace. Although these two concepts seems to have radically different philosophies, we show that they have very close geometric formulations and that they differ only from the choice of the connection in the principal bundle of the active spaces. Section II is devoted to the geometric formalism of the evolutive active space theory. The methods of effective Hamiltonians [Eqs. (1)–(6)] based on a Floquet eigenbasis can be viewed as methods using an evolutive active space, the space spanned by the Floquet eigenvectors depending on the time through the Floquet variable.

The results of this paper could permit to clarify the connections between some techniques used in quantum dynamics (effective Hamiltonians, geometric phases, and time-dependent basis representation) by showing that the geometric formulation unifies them.

The theory of active subspaces could be a fruitful framework for the study of problems of quantum computing in the context of realistic dynamical systems (atoms or molecules interacting with a field). Indeed, an elementary quantum computation unit, a *qubit*, is a two-dimensional space which can be identified with a two-dimensional active space of a quantum dynamical system. More generally, a system of n qubits can be assimilated to a 2^n-dimensional active space. Moreover, the logical operations are represented by unitary operators. In a geometric method of quantum computing called holonomic quantum computation (see Refs. 28–34), the logical operations are described by a gauge theory in the bundle of the active spaces. The present work, analyzing the geometric representation of dynamical systems in the context of evolutive active spaces, could be a first step to the application of the efficient methods of the quantum dynamics (wave operator theory, adiabatic assumption, evolutive active space method, effective Hamiltonian methods, etc.) to quantum computation.

At this point we give a brief summary of our notation. We denote a principal bundle with base space M, total space P, projection π, and structure group G by (P,M,G,π). The set of the sections of a bundle is denoted by $\Gamma(M,P)$. The set of differential n forms of M is denoted by $\Omega^n M$. The tangent space of a manifold M at the point $p \in M$ is denoted by T_pM. The set of complex matrices with n rows and p columns is denoted by $\mathcal{M}_{n\times p}(\mathbb{C})$. The $\bar{Z}$ denotes the complex conjugation, whereas Z^* or $Z^\#$ denote other involutions specified by the context.

II. GEOMETRY OF EVOLUTIVE QUANTUM ACTIVE SPACES

We consider a quantum dynamical system described by the Hamiltonian $t \mapsto H(t)$ in the Hilbert space $\mathcal{H}$. Let $U(t,0)$ be the evolution operator of the dynamical system, i.e., the unitary operator which is the solution of the Schrödinger equation

$$\imath\hbar \partial_t U(t,0) = H(t)U(t,0), \quad U(0,0) = 1. \tag{12}$$

We denote by $\{|i\rangle\}$ a reference orthonormal basis of $\mathcal{H}$. In practice, if the quantum system is a molecule interacting with a field, then $\{|i\rangle\}_i$ is the eigenbasis of the unperturbed molecule. We want to describe the quantum dynamical system by using evolutive active subspaces. This section presents the mathematical theory of this concept. We first need to define the evolutive active subspaces.

Definition 1: *An M dimensional evolutive active subspace of a quantum dynamical system $(H(t),\mathcal{H})$ is defined by specifying two kinds of data*:

- *a map $t \mapsto S(t)$ from the time line to the M-dimensional subspaces of $\mathcal{H}$ such that $\forall \psi_0 \in S(0)$, $U(t,0)\psi_0 \in S(t) \forall t > 0$ and*
- *a map $t \mapsto \{|\alpha(t)\rangle\}_\alpha$ from the time line to a basis of $S(t)$.*

We note that if $S(t)$ is an evolutive active subspace associated with a self-adjoint Hamiltonian, then the orthogonal projector associated with $S(t)$, $P(t)$, satisfies the Schrödinger–von Neumann equation

$$\imath\hbar\frac{\mathrm{d}P(t)}{\mathrm{d}t}=[H(t),P(t)]. \tag{13}$$

(The equation for a non-self-adjoint Hamiltonian is studied in Sec. II C). The concept of an evolutive active space is particularly interesting if it is possible to find a basis $\{|\alpha(t)\rangle\}_\alpha$ without integrating the Schrödinger equation, as, for example, happens in the adiabatic theory where $\{|\alpha(t)\rangle\}_\alpha$ is a set of instantaneous eigenvectors.

Regarding Eq. (13), the time-dependent projection operator can be identified with a specific example of a dynamical invariant (Ref. 35). Indeed, the definition of an active subspace $\psi_0 \in S_0 \Rightarrow U(t,0)\psi_0 \in S(t)$ is similar to the definition of an invariant subspace $\mathfrak{S}$ under the action of the semigroup $t\mapsto U(t,0)$, i.e., $\psi_0\in\mathfrak{S}\Rightarrow U(t,0)\psi\in\mathfrak{S}$. The evolutive active space is an example of "dynamical invariant subspaces" which are generally spanned by eigenvectors of a Lewis invariant. The relation between periodic or cyclic dynamical invariants and non-Abelian geometric phases is discussed in Refs. 36–38. The present work focuses on the connection between geometric phases with nonperiodic and noncyclic dynamical invariants which satisfy the projection prescription $P(t)^2=P(t)$. Since we want to relate this analysis to the wave operator theory, we prefer to refer to the range of $P(t)$ (the active space) rather than to the dynamical invariant theory.

Sections II A and II B explore the connection between the geometric phase concept and the evolutive active space theory. They show that the complete dynamics of the wave function can be computed by a horizontal lift from the dynamics of the evolutive active space governed by the Schrödinger–von Neumann equation. This dynamics appears then as a subdynamics condensed in the base space of the bundle where the horizontal lift takes place. Section II C shows that this subdynamics, analytically defined by the Eq. (13), can be geometrically formulated. We have then a consistent geometric formulation of the quantum dynamics in the active space formalism.

A. Generalized geometric phases

The following proposition proves that the geometric phase phenomenon is associated with the evolutive active space description.

Proposition 1: *Let $(H(t),\mathcal{H})$ be a quantum dynamical system and $(S(t),\{|\alpha(t)\rangle\}_{\alpha=1,\ldots,M})$ be an evolutive active space. Let $\{|\alpha(t)\#\rangle\}_{\alpha=1,\ldots,M}$ be a set biorthogonal to $\{|\alpha(t)\rangle\}_{\alpha=1,\ldots,M}$, i.e.,*

$$\forall t,\ \forall\ \alpha,\beta=1,\ldots,M,\quad \langle\alpha(t)\sharp|\beta(t)\rangle=\delta_{\alpha\beta}. \tag{14}$$

(We do not suppose that $\{|\alpha(t)\rangle\}$ is orthonormal). Let $\psi_\alpha(t)$ be the solution of the Schrödinger equation

$$\imath\hbar\partial_t\psi_\alpha(t)=H(t)\psi_\alpha(t),\quad \psi_\alpha(0)=|\alpha(0)\rangle. \tag{15}$$

By the definition of the evolutive active space, we have $\psi_\alpha(t)\in S(t)$. Then, the representation of ψ_α on the active space is

$$\psi_\alpha(t)=\sum_{\beta=1}^{M}[\mathbb{T}e^{-\imath\hbar^{-1}\int_0^t E(t')\mathrm{d}t'-\int_0^t A(t')\mathrm{d}t'}]_{\beta\alpha}|\beta(t)\rangle, \tag{16}$$

where the matrices E and A of $\mathcal{M}_{M\times M}(\mathbb{C})$ are defined by

$$E(t)_{\alpha\beta}=\langle\alpha(t)\sharp|H(t)|\beta(t)\rangle,\quad A(t)_{\alpha\beta}=\langle\alpha(t)\sharp|\partial_t|\beta(t)\rangle. \tag{17}$$

$\mathbb{T}e$ *is the time-ordering exponential (the Dyson series), i.e., $D(t)=\mathbb{T}e^{\int_0^t X(t)}$ is a solution of $\partial_t D(t)=X(t)D(t)$ for all $X\in\mathcal{M}_{M\times M}(\mathbb{C})$. The matrices E and A generate, respectively, the non-Abelian dynamical and geometric phases.*

Proof: We know that $\psi_\alpha(t) \in S(t) \forall t$, since $\{|\alpha(t)\rangle\}$ is a basis of $S(t)$, $\forall \alpha$ and $\forall t$, $\exists \{U_{\beta\alpha}(t) \in \mathbb{C}\}_{\beta=1,\ldots,M}$ such that

$$\psi_\alpha(t) = \sum_{\beta=1}^{M} U_{\beta\alpha}(t)|\beta(t)\rangle. \tag{18}$$

We group the numbers $\{U_{\beta\alpha}\}_{\alpha\beta}$ into a matrix $U \in \mathcal{M}_{M\times M}(\mathbb{C})$. ψ_α is a solution of the Schrödinger equation. By using expression (18), we find the equation

$$\imath\hbar\sum_\beta \dot{U}_{\beta\alpha}(t)|\beta(t)\rangle + \imath\hbar\sum_\beta U_{\beta\alpha}(t)\partial_t|\beta(t)\rangle = \sum_\beta U_{\beta\alpha}(t)H(t)|\beta(t)\rangle. \tag{19}$$

We project this equation on $\langle\gamma(t)\#|$ to give

$$\dot{U}_{\gamma\alpha} = -\imath\hbar^{-1}\sum_\beta U_{\beta\alpha}\langle\gamma(t)\sharp|H(t)|\beta(t)\rangle - \sum_\beta U_{\beta\alpha}\langle\gamma(t)\sharp|\partial_t|\alpha(t)\rangle. \tag{20}$$

This equation can be written in a matrix form,

$$\partial_t U = (-\imath\hbar^{-1}E(t) - A(t))U. \tag{21}$$

This last equation has for its solution the Dyson series

$$U(t) = \mathbb{T}e^{-\imath\hbar^{-1}\int_0^t E(t')dt' - \int_0^t A(t')dt'}. \tag{22}$$

■

By virtue of the intermediate representation theorem (Ref. 40), we can write

$$U(t) = \mathbb{T}e^{-\int_0^t A(t')dt'}\mathbb{T}e^{-\imath\hbar^{-1}\int_0^t \mathbb{T}e^{\int_0^{t'}A(t'')dt''}E(t')\mathbb{T}e^{-\int_0^{t'}A(t'')dt''}dt'}. \tag{23}$$

We can then isolate for study the pure geometric term $\mathbb{T}e^{-\int_0^t A(t')dt'}$. The precise relation between the pure non-Abelian geometric phase and the non-Abelian geometric and dynamical phase is explained in Refs. 25–27. This proposition defines a more general context in which a geometric phase appears in quantum dynamics. If $S(t)$ is an instantaneous spectral subspace, with $\{|\alpha(t)\rangle\}$ being an orthonormalized set of instantaneous eigenvectors of a self-adjoint Hamiltonian $H(t)$, then the proposition reproduces the non-Abelian Berry phase of the adiabatic approximation; if $\{|\alpha(t)\rangle\}$ is an orthonormalized cyclic basis, then the proposition reproduces the non-Abelian Aharonov-Anandan phase (in these cases, $|\alpha\sharp\rangle = |\alpha\rangle$). If $H(t)$ is a non-self-adjoint Hamiltonian, with $\{|\alpha(t)\rangle\}$ a set of generalized eigenvectors of $H(t)$ and $\{|\alpha(t)\sharp\rangle\}$ the associated generalized eigenvectors of $H(t)^\dagger$, then the proposition gives rise to the Berry phase of a non-self-adjoint Hamiltonian in the adiabatic approximation.

If $\mathcal{H}$ is finite dimensional with $\dim\mathcal{H} = N$, then one can then introduce the matrices $Z \in \mathcal{M}_{N\times M}(\mathbb{C})$ and $Z^\sharp \in \mathcal{M}_{N\times M}(\mathbb{C})$ defined by

$$Z(t) = \begin{pmatrix} \langle 1|1(t)\rangle & \ldots & \langle 1|M(t)\rangle \\ \vdots & & \vdots \\ \langle N|1(t)\rangle & \ldots & \langle N|M(t)\rangle \end{pmatrix}, \quad Z^\sharp(t) = \begin{pmatrix} \langle 1|1(t)\sharp\rangle & \ldots & \langle 1|M(t)\sharp\rangle \\ \vdots & & \vdots \\ \langle N|1(t)\sharp\rangle & \ldots & \langle N|M(t)\sharp\rangle \end{pmatrix}, \tag{24}$$

where $\{|i\rangle\}$ is a reference Hermitian basis on which the Hamiltonian has a finite $N\times N$ matrix representation,

$$E(t) = Z^\sharp(t)^\dagger H(t)Z(t), \quad A(t) = Z^\sharp(t)^\dagger\frac{d}{dt}Z(t). \tag{25}$$

We now introduce an important property.

Property 1: *Let $\{t \mapsto \psi_\alpha(t)\}_\alpha$ be a set of wave functions within the evolutive active $S(t)$ such that $\psi_\alpha(0) = |\alpha(0)\rangle$. $\{\psi_\alpha\}$ are the wave functions of the evolutive active space without dynamical phase, i.e.,*

$$\psi_\alpha(t) = \sum_{\beta=1}^{M} [\mathbb{T}e^{-\int_0^t A(t')dt'}]_{\beta\alpha}|\beta(t)\rangle, \tag{26}$$

if and only if

$$\forall \alpha,\beta, \quad \langle C^\sharp(t)\psi_\alpha(t)|\partial_t|\psi_\beta(t)\rangle = 0, \tag{27}$$

where $C^\sharp(t)$ is an operator of $S(t)$ defined by

$$\forall \alpha, \quad C^\sharp(t)|\alpha(t)\rangle = |\alpha(t)\sharp\rangle. \tag{28}$$

Proof: First, we suppose that ψ_α is the evolutive active space wave function, i.e., $\psi_\alpha(t) = \Sigma_\beta U_{\beta\alpha}|\beta(t)\rangle$, with $U(t) = \mathbb{T}e^{-\int_0^t A(t')dt'}$. We then have

$$\partial_t \psi_\alpha = -\sum_{\beta,\gamma} A_{\beta\gamma}U_{\gamma\alpha}|\beta(t)\rangle + \sum_\beta U_{\beta\alpha}\partial_t|\beta(t)\rangle. \tag{29}$$

By projecting this equation on to $\langle C^\sharp \psi_\epsilon| = \Sigma_\delta \bar{U}_{\epsilon\delta}\langle\delta(t)\sharp|$, we obtain

$$\langle C^\sharp \psi_\epsilon|\partial_t|\psi_\alpha\rangle = -[U^\dagger A U]_{\epsilon\alpha} + [U^\dagger A U]_{\epsilon\alpha} = 0. \tag{30}$$

Second, we suppose that $\langle C^\sharp \psi_\gamma|\partial_t|\psi_\alpha\rangle = 0$. $\psi_a(t) \in S(t)$ and $\{|\alpha(t)\rangle\}$ is a basis of $S(t)$, then $\exists U_{\beta\alpha}(t) \in \mathbb{C}$ such that $\psi_\alpha(t) = \Sigma_\beta U_{\beta\alpha}(t)|\beta(t)\rangle$. Then

$$\langle C^\sharp \psi_\gamma|\partial_t|\psi_\alpha\rangle = 0 \Rightarrow \sum_{\delta,\beta} \bar{U}_{\delta\gamma}\dot{U}_{\beta\alpha}\langle\delta(t)\sharp|\beta(t)\rangle + \sum_{\beta,\delta} \bar{U}_{\delta\gamma}U_{\beta\alpha}\langle\delta(t)\sharp|\partial_t|\beta(t)\rangle \tag{31}$$

$$\Rightarrow [U^\dagger \dot{U}]_{\gamma\alpha} = -[U^\dagger A U]_{\gamma\alpha}, \tag{32}$$

and finally $\dot{U} = -AU$. ■

B. The principal bundle of the active spaces

To simplify the discussion, we suppose that H is self-adjoint and that we can choose an orthonormal basis of the active space (i.e., $Z^\sharp = Z$). In this section we explore the geometric structure describing the evolutive active space of the dynamical system. Initially, we suppose that the Hilbert space is finite dimensional, $\mathcal{H} = \mathbb{C}^N$, and we select evolutive active spaces with dimension equal to M. By using a matrix representation associated with a basis of $\mathbb{C}^N$, we can consider the evolution operator $U(t,0)$ associated with the dynamical system as an application from the time line to $U(N)$ (the Lie group of unitary matrices of order N). We do not choose the fixed basis $\{|i\rangle\}$, but the following time-dependent basis $\mathcal{B}(t) = (|1(t)\rangle, \ldots, |M(t)\rangle, |1(t)\perp\rangle, \ldots, |N-M(t)\perp\rangle)$, where $\mathcal{B}_0(t) = (|1(t)\rangle, \ldots, |M(t)\rangle)$ is the orthonormal basis of $S(t)$, the evolutive active space, and where $\mathcal{B}_\perp(t) = (|1(t)\perp\rangle, \ldots, |N-M(t)\perp\rangle)$ is a basis of $S^\perp(t)$, the orthogonal supplement of $S(t)$. The time-dependent representation $D_{\mathcal{B}(t)}(U(t,0))$ of $U(t,0)$ in the basis $\mathcal{B}(t)$ is a unitary matrix. Since $S(t)$ is an evolutive active space, and since we choose the initial conditions of the dynamics inside $S(0)$, then a transformation which only affects the region outside the active space has no influence on the wave function. In the Lie group $U(N)$, we have then the equivalence relation defined by $\forall U, V \in U(N)$, $U \sim V \Leftrightarrow U = VG$, with $G \in U(N-M)$. It is then clear that the space of evolution operators associated with the inner dynamics of the active space is $U(N)/U(N-M)$. This manifold is known in the literature[18] as the complex Stiefel manifold $V_M(\mathbb{C}^N) = U(N)/U(N-M)$. As we have seen in previous paragraph, the evolution inside the active space gives rise to a non-

Abelian phase $\mathbb{T}e^{-\imath\hbar^{-1}\int_0^t E(t')dt' - \int_0^t A(t')dt'}$. The manifold describing the evolution without this non-Abelian phase is $G_M(\mathbb{C}^N)=U(N)/(U(N-M)\times U(M))$ called the complex Grassmannian manifold (Ref. 18). We can show Ref. 18 that

$$V_M(\mathbb{C}^N) = \{Z \in \mathcal{M}_{N\times M}(\mathbb{C}) | Z^\dagger Z = I_M\}. \tag{33}$$

A matrix $Z\in V_M(\mathbb{C}^N)$ can be interpreted as the matrix of the basis vectors of an active space, as expressed in the fixed basis of $\mathbb{C}^N$, $\{|i\rangle\}$. The Stiefel manifold $V_M(\mathbb{C}^N)$ is then the space of all M-dimensional active spaces of $\mathbb{C}^N$ endowed with an orthonormal basis. The Grassmannian manifold $G_M(\mathbb{C}^N)=V_M(\mathbb{C}^N)/U(M)$ is the space of all M-dimensional active spaces without a particular basis. Moreover, we can show that

$$G_M(\mathbb{C}^N) = \{P \in \mathcal{M}_{N\times N}(\mathbb{C}) | P^2 = P, P^\dagger = P, \mathrm{tr}\, P = M\}. \tag{34}$$

$P\in G_M(\mathbb{C}^N)$ can be identified with the orthogonal projector of the active space. To summarize, we now have produced the structure of the principal bundle on the right $\mathcal{U}=(V_M(\mathbb{C}^N),G_M(\mathbb{C}^N),U(M),\pi_U)$ with $\forall Z\in V_M(\mathbb{C}^N)$, $\pi_U(Z)=ZZ^\dagger$. Let $\mathcal{E}=(E,G_M(\mathbb{C}^N),\mathbb{C}^M,\pi_E)$ be the associated vector bundle of $\mathcal{U}$. The active space (with a vector space structure), defined on $P\in G_M(\mathbb{C}^N)$, is $\pi_E^{-1}(P)$. In other words, if $P(t)\in G_M(\mathbb{C}^N)$ is the solution of a Schrödinger–von Neumann equation, then the evolutive active space is $S(t)=\pi_E^{-1}(P(t))$ and it is endowed with a basis chosen in $\Gamma(G_M(\mathbb{C}^n),V_M(\mathbb{C}^n))$ (the set of the sections of $\mathcal{U}$).

By virtue of the Narasimhan-Ramaman theorem,[41] we can endow $\mathcal{U}$ with a natural connection, called universal, defined by the gauge potential

$$A(ZZ^\dagger) = Z^\dagger dZ \in \Omega^1(G_M(\mathbb{C}^N),\mathfrak{u}(M)), \tag{35}$$

where $\mathfrak{u}(M)$ is the Lie algebra of $U(M)$ (the set of anti-self-adjoint matrices of order M). Let $t\mapsto(|1(t)\rangle,\dots,|M(t)\rangle)=Z(t)$ be a section of $\mathcal{U}$ over the path $\pi_U(Z(t))=P(t)\in G_M(\mathbb{C}^N)$ [$P(t)$ being a solution of the Schrödinger–von Neumann equation]. The horizontal lift of this path which passes by $|\alpha(0)\rangle\in E$ is

$$\psi_\alpha(t) = \sum_{\beta=1}^{M} [\mathbb{T}e^{-\int_0^t Z^\dagger(t')\partial_{t'}Z(t')dt'}]_{\beta\alpha}|\beta(t)\rangle. \tag{36}$$

This is precisely the non-Abelian geometric phase. It is possible to explain the connection in more detail. $\forall X\in\mathfrak{u}(M)$, its associated fundamental vector field is $\hat{X}$ defined by

$$\forall F \in V_M(\mathbb{C}^N), \quad \hat{X}(F) = \left[\frac{d}{dt}R(e^{-tX})F\right]_{t=0} = \left[\frac{d}{dt}Fe^{tX}\right]_{t=0} = FX, \tag{37}$$

where R is the canonical right action of $U(M)$ on $V_M(\mathbb{C}^N)$. The tangent space $T_F V_M(\mathbb{C}^N)$ can be identified with M vectors of $\mathbb{C}^N$ and so to a matrix of $\mathcal{M}_{N\times M}(\mathbb{C})$. Let $\omega\in\Omega^1 V_M(\mathbb{C}^N)$ be the 1-form defined by

$$\forall F \in V_M(\mathbb{C}^N), \quad \forall\,\Phi \in T_F V_M(\mathbb{C}^N), \quad \omega(\Phi) = F^\dagger\Phi. \tag{38}$$

It is clear that $\omega(FX)=X\in\mathfrak{u}(M)$, and the equivariance of ω follows immediately from its definition; ω is then a connection 1-form. Let $[-1,1]\ni t\mapsto F(t)\in V_M(\mathbb{C}^N)$, $\omega([dF/dt]_{t=0}) =[F^\dagger(d/dt)F]_{t=0}\in\mathfrak{u}(M)$. Let $Z(t)\in V_M(\mathbb{C}^N)$ be such that $\pi_U(Z(t))$ is a solution of the Schrödinger–von Neumann equation. Letting $\Psi(t)$ be a matrix of M wave functions such that $\pi_U(\Psi(t)) =\pi_U(Z(t))$, then

$$\Psi(t) = Z(t)\mathbb{T}e^{-\imath\hbar^{-1}\int_0^t Z^\dagger(t')\partial_{t'}Z(t')dt'} \Leftrightarrow \Psi^\dagger\partial_t\Psi = 0 \Leftrightarrow \omega(\partial_t\Psi) = 0. \tag{39}$$

We see that the relation $\Psi^\dagger\partial_t\Psi=0$ proved in the previous section is, in fact, the horizontality condition.

If $\mathcal{H}$ is infinite dimensional, then we can define the manifolds of the active spaces by an inductive limit,

$$G_M(\mathbb{C}^\infty) = \{P \in \mathcal{B}(\mathcal{H}) | P^2 = P, P^\dagger = P, \mathrm{tr}\, P = M\}, \tag{40}$$

$$V_M(\mathbb{C}^\infty) = \{(\psi_1, \ldots, \psi_M) \in \mathcal{H}^M | \forall\, i,j \langle \psi_i | \psi_j \rangle = \delta_{ij}\}, \tag{41}$$

with $\mathcal{B}(\mathcal{H})$ being the Banach space of bounded operators of $\mathcal{H}$. If $H(t)$ is not self-adjoint, then the structure is the same with the replacement of $U(M)$ by $GL(M,\mathbb{C})$, of $V_M(\mathbb{C}^N)$ by the noncompact Stiefel manifold (see Ref. 18) $V_M^{\mathrm{u}}(\mathbb{C}^N) = GL(N,\mathbb{C})/GL(N-M,\mathbb{C})$, and of $Z^\dagger$ by $Z^{*\dagger}$, where Z^* is the matrix of the eigenvectors of $H^\dagger$. Note that

$$V_M^{\mathrm{u}}(\mathbb{C}^N) = V_M(\mathbb{C}^N) \times T(M,\mathbb{C}), \tag{42}$$

with $T(M,\mathbb{C})$ being the manifold of upper triangular matrices of order M with positive diagonal elements. To simplify the analysis, in the sequel we will suppose that H is self-adjoint.

Let $[0,T] \ni t \mapsto Z(t)Z^\dagger(t) \in G_M(\mathbb{C}^N)$ be a map which satisfies the Schrödinger–von Neumann equation, and let $\mathcal{C}$ be the path in $G_M(\mathbb{C}^N)$ associated with this map. The non-Abelian geometric phase associated with this map is then the horizontal lift of $\mathcal{C}$, i.e.,

$$\mathbb{T}e^{-\int_0^T Z^\dagger(t)\partial_t Z(t)\mathrm{d}t} = \mathbb{P}e^{-\int_{\mathcal{C}} A}, \tag{43}$$

where $\mathbb{P}$e is the exponential order with respect to the path (see Ref. 42). In general, the non-Abelian geometric phase does not commute with the dynamical phase. It is then necessary to have a structure describing simultaneously the two phases. This structure is a principal composite bundle as explained in Refs. 25–27. Following Ref. 25, let $\mathcal{U}$ be the principal bundle describing the geometric phase endowed with the connection with gauge potential $A = Z^\dagger dZ$, and let $\mathcal{Q} = (Q, \mathbb{R}, U(N), \pi_Q)$ be the principal bundle with the time line as base space, endowed with the connection describing the evolution operators. Consider the space $G_M(\mathbb{C}^N) \times \mathbb{R}$ as the trivial bundle $\mathcal{S}$ with base space the time line $\mathbb{R}$ and with the typical fiber $G_M(\mathbb{C}^N)$. If we consider $\mathcal{U}$ as a structure bundle, $\mathcal{Q}$ as a transversal bundle, and $\mathcal{S}$ as a base bundle (see Ref. 25 for the definitions of these notions), we construct a composite principal bundle (this construction is based on the local trivializations of the different bundles, see Ref. 25). The connections of $\mathcal{U}$ and of $\mathcal{Q}$ define a natural connection in the composite principal bundle (see Ref. 25) associated with the gauge potential,

$$A_{+,H}(ZZ^\dagger, t) = \imath\hbar^{-1} Z^\dagger H(t) Z \mathrm{d}t + Z^\dagger \mathrm{d}Z \in \Omega^1(G_M(\mathbb{C}^N) \times \mathbb{R}). \tag{44}$$

Let $t \mapsto Z(t)Z^\dagger(t)$ be the solution of $\imath\hbar\partial_t(Z(t)Z^\dagger(t)) = [H(t), Z(t)Z^\dagger(t)]$, $[0,T] \ni t \mapsto (Z(t)Z^\dagger(t), t)$ that appears as a path in $G_M(\mathbb{C}^N) \times \mathbb{R}$, and its horizontal lift in the principal composite bundle is

$$U(T) = \mathbb{T}e^{-\imath\hbar^{-1}\int_0^T E(t)\mathrm{d}t - \int_0^T Z(t)^\dagger \partial_t Z(t)\mathrm{d}t}. \tag{45}$$

The dynamics is then described as follows. Let $\imath\hbar^{-1}H(t)\mathrm{d}t$ be a connection in $\mathcal{Q}$; then the horizontal lift of $[0,T]$ in $\mathcal{Q}$ induces a path in $G_M(\mathbb{C}^N)$ parametrized by $Z(t)Z^\dagger(t)$ satisfying the Schödinger–von Neumann equation. $t \mapsto (Z(t)Z^\dagger(t), t)$ is a path in $G_M(\mathbb{C}^N) \times \mathbb{R}$ for which the horizontal lift in the composite bundle, associated with the connection $A_{+,H}$, describes the non-Abelian total phase. The integration of the dynamics is then decomposed in two steps. The first one consists to find the path $t \mapsto Z(t)Z(t)^\dagger \in G_M(\mathbb{C}^N)$ and the second one consists to lift the result of this first step. Section II C presents the geometric formulation of the subdynamics in $G_M(\mathbb{C}^N)$ constituting the first step.

C. Geometric formulation of the subdynamics of the evolutive active space in the base manifold

This section shows that the subdynamics of the evolutive active space can be geometrically formulated.

1. The self-adjoint case

Definition 2: *Let $C \in \mathcal{L}(\mathcal{H})$ be a self-adjoint operator of the Hilbert $\mathcal{H}=\mathbb{C}^N$ (with possibly $N=+\infty$) considered as an observable of the quantum system. Let f: $G_M(\mathbb{C}^N) \to \mathbb{C}$ be the function defined by*

$$f(Z,Z^\dagger) = C^i_j \bar{Z}^j_\alpha Z^\alpha_i = \mathrm{tr}(Z^\dagger C Z). \tag{46}$$

We call f the weak version of the observable C.

Let f and g be the weak versions of two observables C and B, and the Poisson bracket of f and g is the weak version of the commutator of C and B; indeed,

$$\{f,g\} = \frac{\partial f}{\partial Z^\alpha_i}\frac{\partial g}{\partial \bar{Z}^i_\alpha} - \frac{\partial f}{\partial \bar{Z}^i_\alpha}\frac{\partial g}{\partial Z^\alpha_i} \tag{47}$$

$$= \bar{Z}^j_\alpha (C^i_j B^k_i - B^i_j C^k_i) Z^\alpha_k \tag{48}$$

$$= \mathrm{tr}(Z^\dagger [C,B] Z). \tag{49}$$

Proposition 2: *Let H be the self-adjoint Hamiltonian of the quantum system supposed to be time independent. Let $\mathcal{H}(Z,Z^\dagger)=H^i_j\bar{Z}^j_\alpha Z^\alpha_i$ be its weak version. Let $\mathcal{F}=\mathrm{tr}\,F=\mathrm{d}\bar{Z}^i_\alpha \wedge \mathrm{d}Z^\alpha_i$ be the Kähler form of $G_M(\mathbb{C}^N)$ (see the Appendix). A curve $t \mapsto \Psi(t)\Psi^\dagger(t) \in G_M(\mathbb{C}^N)$ satisfies the Schrödinger–von Neumann equation if and only if*

$$i_X \mathcal{F} = \imath\hbar^{-1}\mathrm{d}\mathcal{H}, \tag{50}$$

where $X=(\mathrm{d}\Psi^\alpha_i/\mathrm{d}t)(\partial/\partial Z^\alpha_i)+(\mathrm{d}\bar{\Psi}^i_\alpha/\mathrm{d}t)(\partial/\partial \bar{Z}^i_\alpha)$ is the tangent vector field to the curve and where i is the inner product of $G_M(\mathbb{C}^N)$.

Proof:

$$i_X\mathcal{F} = \frac{\mathrm{d}\bar{\Psi}^i_\alpha}{\mathrm{d}t}\mathrm{d}Z^\alpha_i - \frac{\mathrm{d}\Psi^\alpha_i}{\mathrm{d}t}\mathrm{d}\bar{Z}^i_\alpha. \tag{51}$$

Moreover,

$$\mathrm{d}\mathcal{H} = H^i_j Z^\alpha_i \mathrm{d}\bar{Z}^j_\alpha + H^i_j \bar{Z}^j_\alpha \mathrm{d}Z^\alpha_i. \tag{52}$$

Then,

$$i_X\mathcal{F} = \imath\hbar^{-1}\mathrm{d}\mathcal{H}(\Psi,\Psi^\dagger) \tag{53}$$

$$\Leftrightarrow \imath\hbar\frac{\mathrm{d}\bar{\Psi}^i_\alpha}{\mathrm{d}t}\mathrm{d}Z^\alpha_i - \imath\hbar\frac{\mathrm{d}\Psi^\alpha_i}{\mathrm{d}t}\mathrm{d}\bar{Z}^i_\alpha = -H^i_j\Psi^\alpha_i\mathrm{d}\bar{Z}^j_\alpha - H^i_j\bar{\Psi}^j_\alpha\mathrm{d}Z^\alpha_i, \tag{54}$$

and then,

$$\left(\imath\hbar\frac{\mathrm{d}\bar{\Psi}^{i}_{\alpha}}{\mathrm{d}t}+H^i_j\bar{\Psi}^j_\alpha\right)\mathrm{d}Z^\alpha_i+\left(-\imath\hbar\frac{\mathrm{d}\Psi^\alpha_j}{\mathrm{d}t}+H^i_j\Psi^\alpha_i\right)\mathrm{d}\bar{Z}^j_\alpha=0. \tag{55}$$

Since $(Z^\alpha_i,\bar{Z}^i_\alpha)$ are degenerate coordinates for $G_M(\mathbb{C}^N)$, these variables are not independent. We have the relation

$$Z^\dagger Z=I_M \tag{56}$$

$$\Rightarrow \mathrm{d}Z^\dagger Z+Z^\dagger \mathrm{d}Z=0 \tag{57}$$

$$\Leftrightarrow \forall\ \alpha,\beta,\quad Z^\alpha_i\mathrm{d}\bar{Z}^i_\beta+\bar{Z}^i_\beta\mathrm{d}Z^\alpha_i=0. \tag{58}$$

For all functions $\{\Lambda^\beta_\alpha(t)\}$, we have $\Lambda^\beta_\alpha(Z^\alpha_i\mathrm{d}\bar{Z}^i_\beta+\bar{Z}^i_\beta\mathrm{d}Z^\alpha_i)=0$. $\{\Lambda^\beta_\alpha(t)\}$ are Lagrange factors associated with the constraint on the variables. Equation (55) is then equivalent to the two following equations:

$$\imath\hbar\frac{\mathrm{d}\Psi^\alpha_i}{\mathrm{d}t}+\Lambda^\alpha_\beta\Psi^\beta_i=H^i_j\Psi^\alpha_i\Leftrightarrow\imath\hbar\frac{\mathrm{d}}{\mathrm{d}t}(\Psi\mathbb{T}e^{-\imath\hbar^{-1}\int_0^t\Lambda(t')\mathrm{d}t'})=H\Psi\mathbb{T}e^{-\imath\hbar^{-1}\int_0^t\Lambda(t')\mathrm{d}t'}, \tag{59}$$

$$-\imath\hbar\frac{\mathrm{d}\bar{\Psi}^i_\alpha}{\mathrm{d}t}+\Lambda^\beta_\alpha\bar{\Psi}^i_\beta=H^i_j\bar{\Psi}^j_\alpha\Leftrightarrow\left(\imath\hbar\frac{\mathrm{d}}{\mathrm{d}t}(\Psi\mathbb{T}e^{-\imath\hbar^{-1}\int_0^t\Lambda(t')\mathrm{d}t'})\right)^\dagger=(H\Psi\mathbb{T}e^{-\imath\hbar^{-1}\int_0^t\Lambda(t')\mathrm{d}t'})^\dagger. \tag{60}$$

Finally, we have

$$\imath\hbar\frac{\partial\Psi\Psi^\dagger}{\partial t}=\imath\hbar\frac{\partial\Psi\Upsilon\Upsilon^\dagger\Psi^\dagger}{\partial t} \tag{61}$$

$$=\imath\hbar\frac{\partial\Psi\Upsilon}{\partial t}\Upsilon^\dagger\Psi^\dagger+\imath\hbar\Psi\Upsilon\frac{\partial(\Psi\Upsilon)^\dagger}{\partial t} \tag{62}$$

$$=H\Psi\Upsilon\Upsilon^\dagger\Psi^\dagger+\Upsilon\Upsilon^\dagger\Psi^\dagger H \tag{63}$$

$$=[H,\Psi\Psi^\dagger], \tag{64}$$

where $\Upsilon=\mathbb{T}e^{-\imath\hbar^{-1}}\int_0^t\Lambda(t')\mathrm{d}t'$ with $\Upsilon^\dagger\Upsilon=\Upsilon\Upsilon^\dagger=1$. ■

We remark that we recover the invariance of the Schrödinger equation with respect to the local gauge choice $\mathbb{T}e^{-\imath\hbar^{-1}}\int_0^t\Lambda(t')\mathrm{d}t'$.

We suppose now that the system Hamiltonian is time dependent. Let $A_{+,H}=\imath\hbar^{-1}Z^\dagger H(t)Z\mathrm{d}t+Z^\dagger\mathrm{d}Z$ be the connection of the composite bundle. Let $F_{+,H}=dA_{+,H}+A_{+,H}\wedge A_{+,H}$ be the curvature of the composite bundle. Moreover, we consider the following forms:

$$\mathcal{A}_+=\mathrm{tr}(A_{+,H})=\bar{Z}^i_\alpha\mathrm{d}Z^\alpha_i+\imath\hbar^{-1}\mathcal{H}\mathrm{d}t \tag{65}$$

and

$$\mathcal{F}_+=\mathrm{tr}(F_{+,H})=\mathrm{d}\bar{Z}^i_\alpha\wedge\mathrm{d}Z^\alpha_i+\imath\hbar^{-1}\mathrm{d}\mathcal{H}\wedge\mathrm{d}t, \tag{66}$$

where $\mathcal{H}(Z,Z^\dagger,t)=H^i_j(t)\bar{Z}^j_\alpha Z^\alpha_i$.

Proposition 3: *Let $\mathcal{H}(Z,Z^\dagger,t)$ be the weak version of the time-dependent self-adjoint Hamiltonian of the quantum system. A curve $t\mapsto(\Psi(t),\Psi^\dagger(t))$ satisfies the Schrödinger equation if and only if*

TABLE I. Comparison between classical dynamics and quantum dynamics with active spaces.

Classical dynamical systems	Quantum dynamical systems
Phase space: $\mathbb{R}^{2M}$	Grassmannian: $G_M(\mathbb{C}^N)$
Variables: q^i	Variables: Z_i^α
Conjugate variables: p_i	Conjugate variables: $\bar{Z}_\alpha^i$
Symplectic metric: $d\ell^2 = dp_i dq^i$	Kählerian metric: $d\ell^2 = d\bar{Z}_\alpha^i dZ_i^\alpha - d\bar{Z}_\alpha^i Z_i^\beta \bar{Z}_\beta^j dZ_j^\alpha$
Observables algebra: $(\mathcal{C}^\infty(\mathbb{R}^{2M},\mathbb{C}),+,\{.,.\})$	Weak observables algebra: $(\{C_j^i \bar{Z}_\alpha^j Z_i^\alpha\},+,\{.,.\})$
Poincaré 1-form: $\lambda = p_i dq^i$	Trace of the gauge potential: $\mathcal{A} = \bar{Z}_\alpha^i dZ_i^\alpha$
$\Lambda = p_i dq^i - \mathcal{H} dt$	$\mathcal{A}_+ = \bar{Z}_\alpha^i dZ_i^\alpha + \imath\hbar^{-1}\mathcal{H} dt$
Poincaré 2-form: $\omega = dp_i \wedge dq^i$	Kähler form: $\mathcal{F} = d\bar{Z}_\alpha^i \wedge dZ_i^\alpha$
$\Omega = dp_i \wedge dq^i - d\mathcal{H}\wedge dt$	$\mathcal{F}_+ = d\bar{Z}_\alpha^i \wedge dZ_i^\alpha + \imath\hbar^{-1} d\mathcal{H}\wedge dt$
Fundamental equation: $i_X\omega = -d\mathcal{H}$	Fundamental equation: $\imath\hbar i_X \mathcal{F} = -d\mathcal{H}$
$i_X\Omega = 0$	$\imath\hbar i_X \mathcal{F}_+ = 0$

$$i_X \mathcal{F}_+ = 0, \tag{67}$$

where $X = (d\Psi_i^\alpha/dt)(\partial/\partial Z_i^\alpha) + (d\bar{\Psi}_\alpha^i/dt)(\partial/\partial \bar{Z}_\alpha^i) - \partial/\partial t$ *is the tangent vector field to the curve and where* i *is the inner product of* $G_M(\mathbb{C}^N)\times\mathbb{R}$.

Proof:

$$i_X \mathcal{F}_+(Z,Z^\dagger,t) = 0 \tag{68}$$

$$\Leftrightarrow \frac{d\bar{\Psi}_\alpha^i}{dt} dZ_i^\alpha - \frac{d\Psi_i^\alpha}{dt} d\bar{Z}_\alpha^i + \imath\hbar^{-1} H_j^i(t)\Psi_i^\alpha \frac{d\bar{\Psi}_\alpha^j}{dt} dt - \imath\hbar^{-1} H_j^i(t)\bar{\Psi}_\alpha^j \frac{d\Psi_i^\alpha}{dt} dt = 0 \tag{69}$$

$$\Leftrightarrow \imath\hbar \frac{d\bar{\Psi}_\alpha^i}{dt} dZ_i^\alpha - \imath\hbar \frac{d\Psi_i^\alpha}{dt} d\bar{Z}_\alpha^i = H_j^i(t)\Psi_i^\alpha d\bar{Z}_\alpha^j - H_j^i(t)\bar{\Psi}_\alpha^j dZ_i^\alpha . \tag{70}$$

The demonstration is then totally equivalent to the previous one. ■

We see that the quantum dynamics with active spaces has a geometric formalism very close to that of classical dynamics, with $\mathcal{A}$ or $\mathcal{A}_+$ playing the role of the Poincaré 1-form and $\mathcal{F}$ or $\mathcal{F}_+$ playing the role of the Poincaré 2-form. A comparison between classical and quantum systems is given Table I.

To summarize, we obtain the active space dynamics as being a curve on $G_M(\mathbb{C}^N)$ satisfying $i_X\mathcal{F}_+=0$, with the state dynamics being obtained by the horizontal lift of this curve with respect to the composite connection of gauge potential $A_{+,H}$.

2. The non-self-adjoint case

If $H(t)$ is not self-adjoint, the dynamics is quite different. Let $\{|\alpha(t)\rangle\}_\alpha$ be the generalized eigenvectors of $H(t)$, i.e., the states satisfying for some $n\in\mathbb{N}$ the equation $(H(t)-E_i(t))^n|\alpha(t)\rangle = 0$, where $E_i(t)$ is an eigenvalue of $H(t)$. The number of generalized eigenvectors satisfying this equation for a particular E_i is equal to the algebraic multiplicity of E_i (see Ref. 39, Remark 6.5). $\{|\alpha(t)\rangle\}_\alpha$ are not orthonormalized but are biorthogonal to the generalized eigenvectors of $H(t)^\dagger:\{|\alpha*(t)\rangle\}_\alpha$. The operator C such that $C|\alpha(t)\rangle = |\alpha*(t)\rangle$ is antilinear with $CH=H^\dagger C$ (see Refs. 44 and 45). The general case can be difficult since, in general, C is time dependent. However, if we suppose that H is symmetric (i.e., $H^{\mathfrak{t}}=H$, where the symbol $\mathfrak{t}$ denotes the transposition), it is easy to show that C is then the complex conjugation (without the transposition), and then $|\alpha*(t)\rangle = \overline{|\alpha(t)\rangle}$. In the sequel, we assume that H is symmetric or more generally that the antilinear operator C associated with the transformation of the eigenvectors of $H(t)$ to the eigenvectors of $H^{\dagger}(t)$ is independent of time and so defines an operation extensible to any vectors of $\mathcal{H}$ independent of t.

Let $t \mapsto \Psi^{\alpha}(t)$ be the solution of the Schödinger equation with $\Psi^{\alpha}(0)=|\alpha(0)\rangle$ (now $\{|\alpha(t)\rangle\}_{\alpha}$ is the basis of the active space and it is not necessarily generated by eigenvectors). The equation of the dual solution $\Psi^{*\alpha}=C\Psi^{\alpha}$ is obtained by setting

$$C\left(\imath\hbar\frac{\mathrm{d}\Psi^{\alpha}}{\mathrm{d}t}\right)=C(H\Psi^{\alpha}), \tag{71}$$

$$-\imath\hbar\frac{\mathrm{d}C\Psi^{\alpha}}{\mathrm{d}t}=H^{\dagger}C\Psi^{\alpha}, \tag{72}$$

$$-\imath\hbar\frac{\mathrm{d}\Psi^{*\alpha}}{\mathrm{d}t}=H^{\dagger}\Psi^{*\alpha}. \tag{73}$$

The operator $P(t)=\Psi(t)\Psi(t)^{*\dagger}$ does not satisfy the Schrödinger–von Neumann equation but obeys the equation $\imath\hbar\dot{P}=HP+PH=[H,P]_{+}$. We refer to this equation as being the anti–Schrödinger–von Neumann equation.

Let $Z,Z^{*}\in\mathcal{M}_{N\times M}(\mathbb{C})$ be such that $Z^{*\dagger}Z=I_M$, where Z^{*} is the conjugate matrix by C of Z. Z now represents a point of the noncompact Stiefel manifold $V_M^{\mho}(\mathbb{C}^N)$. Z_i^{α} and $\bar{Z}_{\alpha}^{*i}$ can be considered as another degenerate coordinate system for $G_M(\mathbb{C}^N)$. Let J be the almost complex structure of $G_M(\mathbb{C}^N)$ (see Refs. 42 and 43) defined by $\forall\alpha,i$:

$$J\frac{\partial}{\partial Z_i^{\alpha}}=\imath\frac{\partial}{\partial Z_i^{\alpha}}, \tag{74}$$

$$J\frac{\partial}{\partial \bar{Z}_{\alpha}^{*i}}=-\imath\frac{\partial}{\partial \bar{Z}_{\alpha}^{*i}}, \tag{75}$$

where $J^2=-1$. Moreover, let $J^{\ddagger}$ be the adjoint of J for the duality bracket of the tangent space, i.e., $\forall X\in T_{ZZ^{*\dagger}}G_M(\mathbb{C}^N)$ and $\phi\in\Omega^1G_M(\mathbb{C}^N)$, $\langle\phi,JX\rangle=\langle J^{\ddagger}\phi,X\rangle$. It is easy to show that

$$J^{\ddagger}\mathrm{d}Z_i^{\alpha}=-\imath\mathrm{d}Z_i^{\alpha}, \tag{76}$$

$$J^{\ddagger}\mathrm{d}\bar{Z}_{\alpha}^{*i}=\imath\mathrm{d}\bar{Z}_{\alpha}^{*i}. \tag{77}$$

Proposition 4: *Let H be the non-self-adjoint Hamiltonian of the quantum system supposed to be time independent. Let $\mathcal{H}(Z,Z^{*\dagger})=H_j^i\bar{Z}_{\alpha}^{j*}Z_i^{\alpha}=\mathrm{tr}(Z^{*\dagger}HZ)$ be its weak version. Let $\mathcal{F}=\mathrm{d}\bar{Z}_{\alpha}^{*i}\wedge\mathrm{d}Z_i^{\alpha}$ be the pseudo-Kähler form. A curve $t\mapsto\Psi(t)\Psi^{*}(t)\in G_M(\mathbb{C}^N)$ satisfies the anti-Schrödinger–von Neumann equation if and only if*

$$J^{\ddagger}\hbar i_X\mathcal{F}=-\mathrm{d}\mathcal{H} \tag{78}$$

$$\Leftrightarrow\hbar i_{JX}\mathcal{F}=-\mathrm{d}\mathcal{H}, \tag{79}$$

where $X=(\mathrm{d}\Psi_i^{\alpha}/\mathrm{d}t)(\partial/\partial Z_i^{\alpha})+(\mathrm{d}\bar{\Psi}_{\alpha}^{*i}/\mathrm{d}t)(\partial/\partial\bar{Z}_{\alpha}^{*i})$ is the tangent vector field to the curve and where i is the inner product of $G_M(\mathbb{C}^N)$.

Proof:

$$i_X\mathcal{F} = \frac{d\bar{\Psi}^{*i}_{\alpha}}{dt} dZ^{\alpha}_i - \frac{d\Psi^{\alpha}_i}{dt} d\bar{Z}^{*i}_{\alpha}, \tag{80}$$

$$J^{\ddagger}\hbar i_X\mathcal{F} = -\imath\hbar\frac{d\bar{\Psi}^{*i}_{\alpha}}{dt} dZ^{\alpha}_i - \imath\hbar\frac{d\Psi^{\alpha}_i}{dt} d\bar{Z}^{*i}_{\alpha}. \tag{81}$$

By a demonstration similar of the previous one, we have

$$J^{\ddagger}\hbar i_X\mathcal{F} = -d\mathcal{H} \tag{82}$$

$$\Leftrightarrow\left(-\imath\hbar\frac{d\bar{\Psi}^{*i}_{\alpha}}{dt} + H^i_j\bar{\Psi}^{*j}_{\alpha}\right)dZ^{\alpha}_i + \left(-\imath\hbar\frac{d\Psi^{\alpha}_j}{dt} + H^i_j\Psi^{\alpha}_i\right)d\bar{Z}^{*j}_{\alpha} = 0 \tag{83}$$

$$\Leftrightarrow\begin{cases}\imath\hbar\dfrac{d}{dt}(\Psi\mathbb{T}e^{-\imath\hbar^{-1}\int_0^t\Lambda(t')dt'}) = H\Psi\mathbb{T}e^{-\imath\hbar^{-1}\int_0^t\Lambda(t')dt'}\\ \left(-\imath\hbar\dfrac{d}{dt}(\Psi^*\mathbb{T}e^{\imath\hbar^{-1}\int_0^t\Lambda(t')dt'})\right)^{\dagger} = (H^{\dagger}\Psi^*\mathbb{T}e^{\imath\hbar^{-1}\int_0^t\Lambda(t')dt'})^{\dagger}.\end{cases} \tag{84}$$

. ■

By comparison of the equation $J^{\ddagger}\hbar i_X\mathcal{F}=-d\mathcal{H}$ with the equation of the self-adjoint case $\imath\hbar i_X\mathcal{F}=-d\mathcal{H}$, we see that the non-self-adjoint case arises mainly by substituting $\imath$ by the almost complex structure $J^{\ddagger}$.

In the same way, if H is a time-dependent non-self-adjoint Hamiltonian, the dynamical equation is

$$J^{\ddagger}\hbar i_X\mathcal{F}_+ = 0, \tag{85}$$

where

$$\mathcal{F}_+ = d\bar{Z}^{*i}_{\alpha}\wedge dZ^{\alpha}_i + \imath\hbar^{-1}d\mathcal{H}\wedge dt \tag{86}$$

(and with, by convention, $J^{\ddagger}dt=\imath dt$).

III. GEOMETRIC FORMULATION OF THE TIME-DEPENDENT WAVE OPERATORS

The previous section has analyzed the geometry of a dynamics in the evolutive active space formalism. Now we consider the status of the time-dependent wave operator in the bundle of the active spaces. We assume in this section that the Hamiltonian is self-adjoint, and the non-self-adjoint case can be easily obtained by substitutions as $Z^{\dagger}$ by $Z^{*\dagger}$ for example. We use in this section the distances in $G_M(\mathbb{C}^N)$ defined in the Appendix.

A. Bloch wave operators and time-dependent wave operators

Let $P_0, P\in G_M(\mathbb{C}^N)$, $Z\in\pi_U^{-1}(P)$, and $Z_0\in\pi_U^{-1}(P_0)$. If $\mathrm{dist}_{FS}(Z,Z_0)<\pi/2$ then $(P_0PP_0)^{-1}$ exists and we can define a type of Bloch wave operator $P(P_0PP_0)^{-1}$. Let $\{|\alpha_0\rangle\}$ and $\{|\alpha\rangle\}$ be the bases defined by Z_0 and Z. We have

$$P_0PP_0 = \sum_{\alpha\beta\gamma}|\alpha_0\rangle\langle\alpha_0|\beta\rangle\langle\beta|\gamma_0\rangle\langle\gamma_0| \tag{87}$$

$$=\sum_{\alpha\gamma}[Z_0^\dagger ZZ^\dagger Z_0]_{\alpha\gamma}|\alpha_0\rangle\langle\gamma_0| \tag{88}$$

and then

$$(P_0PP_0)^{-1}=\sum_{\alpha\gamma}[(Z^\dagger Z_0)^{-1}(Z_0^\dagger Z)^{-1}]_{\alpha\gamma}|\alpha_0\rangle\langle\gamma_0|, \tag{89}$$

from which we find

$$P(P_0PP_0)^{-1}=\sum_{\alpha\beta\gamma}[(Z^\dagger Z_0)^{-1}(Z_0^\dagger Z)^{-1}]_{\alpha\gamma}|\beta\rangle\langle\beta|\alpha_0\rangle\langle\gamma_0| \tag{90}$$

$$=\sum_{\beta\gamma}[Z^\dagger Z_0(Z^\dagger Z_0)^{-1}(Z_0^\dagger Z)^{-1}]_{\beta\gamma}|\beta\rangle\langle\gamma_0| \tag{91}$$

$$=\sum_{\beta\gamma}[(Z_0^\dagger Z)^{-1}]_{\beta\gamma}|\beta\rangle\langle\gamma_0|. \tag{92}$$

The Bloch wave operator $P(P_0PP_0)^{-1}$ is then a linear map from $\pi_E^{-1}(P_0)$ to $\pi_E^{-1}(P)$ represented by the matrix $(Z_0^\dagger Z)^{-1}$.

Now we focus on the time-dependent wave operator $\Omega(t)=U(t,0)(P(0)U(t,0)P(0))^{-1}$. Let $V(t)=\mathbb{T}e^{-\imath\hbar^{-1}\int_0^t E(t')\mathrm{d}t'-\int_0^t A(t')\mathrm{d}t}$, where $E(t)=Z^\dagger(t)H(t)Z(t)$, $A(t)=Z^\dagger(t)\partial_t Z(t)$, and $\pi_U(Z(t))=P(t)$ is a solution of the Schrödinger–von Neumann equation. We have

$$\psi_\alpha(t)=U(t,0)|\alpha(0)\rangle=\sum_\beta V(t)_{\beta\alpha}|\beta(t)\rangle, \tag{93}$$

and then $\langle\beta(t)|U(t,0)|\alpha(0)\rangle=V(t)_{\beta\alpha}$ and

$$U(t,0)=\sum_{\alpha\beta}V(t)_{\beta\alpha}|\beta(t)\rangle\langle\alpha(0)|. \tag{94}$$

We can then write

$$P(0)U(t,0)P(0)=\sum_{\alpha\beta\gamma\delta}V(t)_{\beta\alpha}|\gamma(0)\rangle\langle\gamma(0)|\beta(t)\rangle\langle\alpha(0)|\delta(0)\rangle\langle\delta(0)| \tag{95}$$

$$=\sum_{\gamma\alpha}[Z^\dagger(0)Z(t)V(t)]_{\gamma\alpha}|\gamma(0)\rangle\langle\alpha(0)|, \tag{96}$$

giving

$$(P(0)U(t,0)P(0))^{-1}=\sum_{\gamma\alpha}[V(t)^{-1}(Z^\dagger(0)Z(t))^{-1}]_{\gamma\alpha}|\gamma(0)\rangle\langle\alpha(0)| \tag{97}$$

and thus

$$U(t,0)(P(0)U(t,0)P(0))^{-1}=\sum_{\alpha\beta\gamma\delta}V(t)_{\beta\delta}[V(t)^{-1}(Z^\dagger(0)Z(t))^{-1}]_{\gamma\alpha}|\beta(t)\rangle\langle\delta(0)|\gamma(0)\rangle\langle\alpha(0)| \tag{98}$$

$$=\sum_{\beta\alpha}[V(t)V(t)^{-1}(Z^\dagger(0)Z(t))^{-1}]_{\beta\alpha}|\beta(t)\rangle\langle\alpha(0)| \tag{99}$$

$$= \sum_{\beta\alpha} [(Z^\dagger(0)Z(t))^{-1}]_{\beta\alpha} |\beta(t)\rangle\langle\alpha(0)|. \tag{100}$$

We see that the time-dependent wave operator is, in fact, a type of Bloch wave operator $\Omega(t)=P(t)(P(0)P(t)P(0))^{-1}$, where $P(t)$ is solution of the Schrödinger–von Neumann equation.

B. The time-dependent wave operator as a horizontal lift of the bundle of active spaces

Let $Z\in V_M(\mathbb{C}^N)$, $\forall W\in V_M(\mathbb{C}^N)$, such that $\mathrm{dist}_{\mathrm{FS}}(W,Z)<\pi/2$, and $Z_W=W(Z^\dagger W)^{-1}$ is such that $Z_W^\dagger Z=I_M$; indeed, $Z_W^\dagger Z=(W^\dagger Z)^{-1}W^\dagger Z=I_M$. The set of vectors defined by Z_W is biorthogonal to the basis defined by Z. Now consider $Z(t)$ such that $\pi_U(Z(t))=P(t)$ is a solution of the Schrödinger–von Neumann equation and such that $\forall t$, $\mathrm{dist}_{\mathrm{FS}}(Z(t),Z(0))<\pi/2$. We know by Proposition 1 that the wave function Ψ, a solution of the Schrödinger equation, is

$$\Psi(t) = Z(t)\mathbb{T}e^{-\imath\hbar^{-1}\int_0^t E_0^\sharp(t')\mathrm{d}t' - \int_0^t A_0^\sharp(t')\mathrm{d}t'}, \tag{101}$$

where

$$A_0^\sharp(t) = (Z^\dagger(0)Z(t))^{-1}Z^\dagger(0)\partial_t Z(t), \quad E_0^\sharp(t) = (Z^\dagger(0)Z(t))^{-1}Z^\dagger(0)H(t)Z(t). \tag{102}$$

In other words, $A_0^\sharp = Z_{Z(0)}^\dagger(t)\partial_t Z$ and $E_0^\sharp = Z_{Z(0)}^\dagger(t)H(t)Z(t)$. Letting $\tilde{\Omega}(t)=(Z^\dagger(0)Z(t))^{-1}$, then

$$\frac{\mathrm{d}}{\mathrm{d}t}(Z^\dagger(0)Z(t))^{-1} = -(Z^\dagger(0)Z(t))^{-1}Z^\dagger(0)\frac{\mathrm{d}Z(t)}{\mathrm{d}t}(Z^\dagger(0)Z(t))^{-1}. \tag{103}$$

In other words,

$$\frac{\mathrm{d}}{\mathrm{d}t}\tilde{\Omega}(t) = -A_0^\sharp(t)\tilde{\Omega}(t). \tag{104}$$

We conclude that

$$\Omega(t) = \sum_{\alpha\beta} [\mathbb{T}e^{-\int_0^t A_0^\sharp(t')\mathrm{d}t'}]_{\beta\alpha} |\beta(t)\rangle\langle\alpha(0)|. \tag{105}$$

The time-dependent wave operator is a horizontal lift for the connection defined by the gauge potential $A_{Z(0)}^\sharp(ZZ_{Z(0)}^\dagger)=(Z(0)^\dagger Z)^{-1}Z^\dagger(0)\mathrm{d}Z\in\Omega^1(K_{Z(0)},\mathfrak{gl}(M,\mathbb{C}))$, where $K_W=\{ZZ_W^\dagger | Z \in V_M(\mathbb{C}^N), \mathrm{dist}_{\mathrm{FS}}(Z,W)<\pi/2\}$ [K_W can be injected in its universal classifying space $G_M(\mathbb{C}^N)$]. In fact, the time-dependent wave operator theory is associated with a family of connections defined by

$$V_M(\mathbb{C}^N) \to \Omega^1(K_W,\mathfrak{gl}(M,\mathbb{C})),$$

$$W \mapsto A_W^\sharp(ZZ_W^\dagger) = (W^\dagger Z)^{-1}W^\dagger\mathrm{d}Z = Z_W^\dagger\mathrm{d}Z. \tag{106}$$

This family of connections is also defined by a family of connection 1-form ω_W:

$$\forall F \in V_M^\upsilon(\mathbb{C}^N),\ \forall\,\Phi \in T_F V_M^\upsilon(\mathbb{C}^N), \quad \omega_W(\Phi) = (W^\dagger F)^{-1}W^\dagger\Phi, \tag{107}$$

for which the horizontality conditions are

$$(W^\dagger\Psi(t))^{-1}W^\dagger\partial_t\Psi(t) = 0. \tag{108}$$

We thus recover the general structure of generalized geometric phases. In the usual time-dependent wave operator theory, we choose the connection associated with the initial condition $Z(0)$.

Note that to define the wave operator connection, we have considered the group extension $(V_M(\mathbb{C}^N), K_W, U(M), \pi_K) \hookrightarrow (V_M^{\mho}(\mathbb{C}^N), K_W, GL(M,\mathbb{C}), \pi_K)$, because the wave operator theory does not preserve the self-adjointness of the Hamiltonian representation.

In the expression for ψ_α, we wish to separate the geometric phase from the dynamical phase. By virtue of the intermediate representation theorem [Eq. (40)], we have

$$\psi_\alpha(t) = \sum_\beta [\mathbb{T}e^{-\imath\hbar^{-1}\int_0^t E_0^\sharp(t')dt' - \int_0^t A_0^\sharp(t')dt'}]_{\beta\alpha}|\beta(t)\rangle \tag{109}$$

$$= \sum_{\beta\gamma} \underbrace{[\mathbb{T}e^{-\int_0^t A_0^\sharp(t')dt}]_{\beta\gamma}}_{\tilde{\Omega}(t)_{\beta\gamma}} [\mathbb{T}e^{-\imath\hbar^{-1}\int_0^t \tilde{\Omega}^{-1}(t')E_0^\sharp(t')\tilde{\Omega}(t')dt'}]_{\gamma\alpha}|\beta(t)\rangle. \tag{110}$$

However, we also have

$$\tilde{\Omega}^{-1}(t)E_0^\sharp(t)\tilde{\Omega}(t) = Z^\dagger(0)Z(t)(Z^\dagger(0)Z(t))^{-1}Z^\dagger(0)H(t)Z(t)(Z^\dagger(0)Z(t))^{-1} \tag{111}$$

$$= Z^\dagger(0)H(t)Z(t)(Z^\dagger(0)Z(t))^{-1}, \tag{112}$$

and thus

$$[\tilde{\Omega}^{-1}(t)E_0^\sharp(t)\tilde{\Omega}(t)]_{\alpha\beta} = \sum_\gamma \langle\alpha(0)|H|\gamma(t)\rangle\langle\gamma(t)|\Omega(t)|\beta(0)\rangle. \tag{113}$$

Finally, we obtain

$$\sum_{\alpha\beta} [\tilde{\Omega}^{-1}(t)E_0^\sharp(t)\tilde{\Omega}(t)]_{\alpha\beta}|\alpha(0)\rangle\langle\beta(0)| = P_0 H(t)\Omega(t) = H^{\text{eff}}(t), \tag{114}$$

and thus

$$\psi_\alpha(t) = \Omega(t)\mathbb{T}e^{-\imath\hbar^{-1}\int_0^t H^{\text{eff}}(t')dt'}|\alpha(0)\rangle. \tag{115}$$

We see that the time-dependent wave operator theory is just a geometric phase phenomenon where we have separated the geometric and the dynamical phases. The effective Hamiltonian of the wave operator theory emerges spontaneously as being the generator of the dynamical phase conjugated by the geometric phase (the wave operator).

We wish to add an important comment. In contrast with the universal connection, the wave operator connections are not defined for all the manifold $V_M^{\mho}(\mathbb{C}^N)$. Letting $W \in V_M(\mathbb{C}^N)$, the wave operator gauge potential $A_W^\sharp = (W^\dagger Z)^{-1}W^\dagger dZ$ is only defined for $\pi_U(Z)$ in the open ball of center $\pi_U(W)$ and of radius $\pi/2$ (in the Fubini-Study distance); in other words, the domain of the connection 1-form is

$$\text{dom}\,\omega_W^\sharp = \left\{ Z \in V_M^{\mho}(\mathbb{C}^N) \middle| \text{dist}_{\text{FS}}(W,Z) < \frac{\pi}{2} \right\}. \tag{116}$$

The wave operator connection is flat; indeed, if we compute the wave operator curvature, we find

$$F_W^\sharp = dA_W^\sharp + A_W^\sharp \wedge A_W^\sharp = -(W^\dagger Z)^{-1}W^\dagger dZ(W^\dagger Z)^{-1} \wedge W^\dagger dZ + (W^\dagger Z)^{-1}W^\dagger dZ \wedge (W^\dagger Z)^{-1}W^\dagger dZ = 0. \tag{117}$$

Let $\Psi \in \mathcal{M}_{N\times M}(\mathbb{C})$ be a solution of the Schrödinger equation $\imath\hbar\partial_t\Psi(t) = H(t)\Psi(t)$ and let $\Psi_W(t) = W(\Psi(t)^\dagger W)^{-1}$,

$$\imath\hbar\frac{d\Psi_W}{dt} = -W\imath\hbar(\Psi^\dagger W)^{-1}\frac{d\Psi^\dagger}{dt}W(\Psi^\dagger W)^{-1} \tag{118}$$

$$=W(\Psi^\dagger W)^{-1}\Psi^\dagger H^\dagger W(\Psi^\dagger W)^{-1} \tag{119}$$

$$=W(\Psi^\dagger W)^{-1}((W^\dagger\Psi)^{-1}W^\dagger H\Psi)^\dagger \tag{120}$$

$$=\Psi_W(\Psi_W^\dagger H\Psi)^\dagger \tag{121}$$

$$=\Psi_W E_W^{\sharp,\dagger}. \tag{122}$$

This last equation, $\imath\hbar\partial_t\Psi_W=\Psi_W E_W^{\sharp,\dagger} \Leftrightarrow -\imath\hbar\partial_t\Psi_W^\dagger=E_W^\sharp\Psi_W^\dagger$, is the dual equation of the Schrödinger equation with the new local conjugate variables $\bar{Z}^i_{W\alpha}$. In a geometric framework, the wave operator theory consists then to the lift with respect to the connection $A_W^\sharp+\imath\hbar^{-1}E_W^\sharp\mathrm{d}t$ of the curve $\Psi(t)\Psi(t)_W^\dagger$ obtained as a solution of the equation $\imath\hbar(\mathrm{d}\Psi\Psi_W^\dagger/\mathrm{d}t)=H\Psi\Psi_W^\dagger-\Psi\Psi_W^\dagger H\Psi\Psi_W^\dagger$.

IV. CONCLUSION

We have seen that the theory of active spaces, effective Hamiltonians, and wave operators is, in fact, a gauge theory. The active space theory is defined by the principal bundle $\mathcal{U}=(V_M(\mathbb{C}^N),G_M(\mathbb{C}^N),U(M),\pi_U)$, where the Grassmannian manifold models the space of the active space projectors, and where the Stiefel manifold models the space of the active space basis. The fibers $\pi_E^{-1}(P)$ of the associated vector bundle $\mathcal{E}=(E,G_M(\mathbb{C}^N),\mathbb{C}^M,\pi_E)$ model the active spaces with the vector space structure. The Grassmannian manifold is endowed with a metric associated with its Kählerian structure. This metric measures the quantum distance between the active spaces, i.e., the probabilistic compatibility between the active spaces (see Appendix).

$\mathcal{U}$ is endowed with the connection $A=Z^\dagger dZ$, which is universal in the sense of the Narasimhan-Ramaman theorem (see Ref. 41). The universal connection is, in fact, the single connection compatible with the Kählerian metric of the Grassmannian, like the Levi-Civita connection in the Riemannian case. The horizontal lifts in this connection define the non-Abelian Aharonov-Anandan geometric phases. Moreover, $\mathcal{U}^{\mho}$ is also endowed with a family of connections $A_W=(W^\dagger Z)^{-1}W^\dagger dZ$ for which the horizontal lifts define the time-dependent wave operators. The wave operator appears then as a geometric phase, and the effective Hamiltonian of the wave operator theory emerges spontaneously in the geometric framework as being the generator of the dynamical phase conjugated by the geometric phase.

In a more general framework, if $Z\in\mathcal{M}_{N\times M}(\mathbb{C})$ represents a basis of an evolutive active space with $Z^\sharp\in\mathcal{M}_{N\times M}(\mathbb{C})$, a biorthogonal basis $(Z^{\sharp\dagger}Z=I_M)$ such that the passage from Z to $Z^\sharp$ is a time-independent procedure. The evolution path of the active space on the Grassmannian is then a solution of

$$\imath\hbar i_X\mathcal{F}_+=0 \quad \text{if } H \text{ is self-adjoint},$$

$$J^\ddagger\hbar i_X\mathcal{F}_+=0 \quad \text{if } H \text{ is non-self-adjoint}, \tag{123}$$

where X is the tangent vector field of the curve, and with

$$\mathcal{F}_+=\mathrm{d}\bar{Z}^{\sharp i}_\alpha\wedge\mathrm{d}Z^\alpha_i+\imath\hbar^{-1}\mathrm{d}\,\mathrm{tr}(Z^{\sharp\dagger}HZ)\wedge\mathrm{d}t, \tag{124}$$

with $J^\ddagger$ being the dual of the almost complex structure

$$J\frac{\partial}{\partial Z^\alpha_i}=\imath\frac{\partial}{\partial Z^\alpha_i},\quad J\frac{\partial}{\partial\bar{Z}^{*i}_\alpha}=-\imath\frac{\partial}{\partial\bar{Z}^{*i}_\alpha}. \tag{125}$$

The wave functions are obtained by the horizontal lift of this curve with respect to the composite connection $A_+=Z^{\sharp\dagger}\mathrm{d}Z+\imath\hbar^{-1}Z^{\sharp\dagger}HZ\mathrm{d}t$. $Z^{\sharp\dagger}HZ$ (or its conjugate by the geometric phase) is the effective Hamiltonian associated with the evolutive active space.

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APPENDIX: GEOMETRY OF THE BASE MANIFOLD

$G_M(\mathbb{C}^N)$ is the base manifold of the bundle of active spaces. In this present appendix, we explore some geometric properties of $G_M(\mathbb{C}^N)$ where the subdynamics of the evolutive active space or where the effective dynamics of the wave operator theory takes place.

Let A be the gauge potential of $\mathcal{U}$, so that

$$A = Z^\dagger \mathrm{d}Z, \tag{A1}$$

where $Z \in \mathcal{M}_{N\times M}(\mathbb{C})$ such that $Z^\dagger Z = I_M$. Z represents a point in the Stiefel manifold $V_M(\mathbb{C}^N)$, and the equivalence class of Z for the relation $Z \sim ZU$ with $U \in U(M)$ represents a point in the Grassmann manifold $G_M(\mathbb{C}^N)$ $(\pi_U(Z))$.

The curvature associated with the connection is obtained by the Cartan structure equation

$$F = \mathrm{d}A + A \wedge A = \mathrm{d}Z^\dagger \wedge \mathrm{d}Z + (Z^\dagger \mathrm{d}Z) \wedge (Z^\dagger \mathrm{d}Z), \tag{A2}$$

and it satisfies the Bianchi identity

$$\mathrm{d}F + [A,F] = 0. \tag{A3}$$

We note, moreover, that

$$Z^\dagger Z = 1 \Rightarrow \mathrm{d}Z^\dagger Z = -Z^\dagger \mathrm{d}Z \Leftrightarrow A^\dagger = -A. \tag{A4}$$

We know that the complex Grassmannian $G_M(\mathbb{C}^N)$ is endowed with the structure of a Kählerian manifold,[42,43] with its Kähler potential being

$$K = \frac{1}{2} \ln \det(W^\dagger Z), \tag{A5}$$

with ln being the principal value of the complex natural logarithm. The Kähler form $\mathcal{F}$ can be deduced from K by the relation

$$\mathcal{F} = (2\imath \bar{\partial}\partial K)_{|W=Z}, \tag{A6}$$

where ∂ and $\bar{\partial}$ are the Dolbeault differentials.[42,43] Introducing $Z_i^\alpha = \langle i|\alpha\rangle$ and $\bar{Z}_\alpha^i = \langle \alpha | i\rangle$ with $\alpha = 1,\ldots,M$ and $i=1,\ldots,N$, as a degenerate coordinate system, we find that

$$\mathcal{F} = \mathrm{tr}\, F = \mathrm{d}\bar{Z}_\beta^j \wedge \mathrm{d}Z_j^\beta - (Z_k^\gamma \mathrm{d}\bar{Z}_\beta^k) \wedge (\bar{Z}_\gamma^j \mathrm{d}Z_j^\beta). \tag{A7}$$

Proof: In this section, we adopt the Einstein convention for the Latin indices but not for the Greek indices. We denote by S_M the group of permutations of $(1,\ldots,M)$ and by $(-1)^\sigma$ the signature of the permutation σ. The detailed derivative associated with Eq. (A7) is as follows.

$$\det W^\dagger Z = \sum_{\sigma\in S_M} (-1)^\sigma \prod_{\alpha=1}^{M} \bar{W}_{\sigma(\alpha)}^i Z_i^\alpha, \tag{A8}$$

$$\partial \ln \det W^\dagger Z = \frac{1}{\det W^\dagger Z} \sum_{\sigma\in S_M} (-1)^\sigma \sum_{\beta=1}^{M} \prod_{\alpha\neq\beta} \bar{W}_{\sigma(\alpha)}^i Z_i^\alpha \bar{W}_{\sigma(\beta)}^j \mathrm{d}Z_j^\beta, \tag{A9}$$

$$\bar\partial\partial \ln \det W^\dagger Z = \frac{1}{\det W^\dagger Z}\sum_{\sigma\in S_M}(-1)^\sigma \sum_{\beta=1}^{M}\sum_{\gamma\neq\beta}\prod_{\alpha\neq\beta,\gamma}\bar W^i_{\sigma(\alpha)}Z^\alpha_i \bar W^j_{\sigma(\beta)}Z^\gamma_k \mathrm{d}\bar W^k_{\sigma(\gamma)}\wedge \mathrm{d}Z^\beta_j + \frac{1}{\det W^\dagger Z}\sum_{\sigma\in S_M}(-1)^\sigma\sum_{\beta=1}^{M}\prod_{\alpha\neq\beta}\bar W^i_{\sigma(\alpha)}Z^\alpha_i \mathrm{d}\bar W^j_{\sigma(\beta)}\wedge \mathrm{d}Z^\beta_j - \frac{1}{(\det W^\dagger Z)^2}\left(\sum_{\sigma\in S_M}(-1)^\sigma\sum_{\beta=1}^{M}\prod_{\alpha\neq\beta}\bar W^i_{\sigma(\alpha)}Z^\alpha_i Z^\beta_j \mathrm{d}\bar W^j_{\sigma(\beta)}\right)\wedge\left(\sum_{\sigma\in S_M}(-1)^\sigma\sum_{\beta=1}^{M}\prod_{\alpha\neq\beta}\bar W^i_{\sigma(\alpha)}Z^\alpha_i \bar W^j_{\sigma(\beta)}\mathrm{d}Z^\beta_j\right), \quad \text{(A10)}$$

$$(\bar\partial\partial \ln \det W^\dagger Z)_{|W=Z} = \sum_{\sigma\in S_M}(-1)^\sigma\sum_{\beta=1}^{M}\sum_{\gamma\neq\beta}\prod_{\alpha\neq\beta,\gamma}(Z^\dagger Z)^\alpha_{\sigma(\alpha)}\bar Z^j_{\sigma(\beta)}Z^\gamma_k \mathrm{d}\bar Z^k_{\sigma(\gamma)}\wedge \mathrm{d}Z^\beta_j + \sum_{\sigma\in S_M}(-1)^\sigma\sum_{\beta=1}^{M}\prod_{\alpha\neq\beta}(Z^\dagger Z)^\alpha_{\sigma(\alpha)}\mathrm{d}\bar Z^j_{\sigma(\beta)}\wedge \mathrm{d}Z^\beta_j - \left(\sum_{\sigma\in S_M}(-1)^\sigma\sum_{\beta=1}^{M}\prod_{\alpha\neq\beta}(Z^\dagger Z)^\alpha_{\sigma(\alpha)}Z^\beta_j \mathrm{d}\bar Z^j_{\sigma(\beta)}\right)\wedge\left(\sum_{\sigma\in S_M}(-1)^\sigma\sum_{\beta=1}^{M}\prod_{\alpha\neq\beta}(Z^\dagger Z)^\alpha_{\sigma(\alpha)}\bar Z^j_{\sigma(\beta)}\mathrm{d}Z^\beta_j\right) \quad \text{(A11)}$$

$$= \sum_{\beta=1}^{M}\sum_{\gamma\neq\beta}\bar Z^j_\beta Z^\gamma_k \mathrm{d}\bar Z^k_\gamma\wedge \mathrm{d}Z^\beta_j - \sum_{\beta=1}^{M}\sum_{\gamma\neq\beta}\bar Z^j_\gamma Z^\gamma_k \mathrm{d}\bar Z^k_\beta\wedge \mathrm{d}Z^\beta_j + \sum_{\beta=1}^{M}\mathrm{d}\bar Z^j_\beta\wedge \mathrm{d}Z^\beta_j - \left(\sum_{\beta=1}^{M}Z^\beta_j \mathrm{d}\bar Z^j_\beta\right)\wedge\left(\sum_{\beta=1}^{M}\bar Z^j_\beta \mathrm{d}Z^\beta_j\right) \quad \text{(A12)}$$

$$= \left(\sum_{\gamma=1}^{M}Z^\gamma_k \mathrm{d}\bar Z^k_\gamma\right)\wedge\left(\sum_{\beta=1}^{M}\bar Z^j_\beta \mathrm{d}Z^\beta_j\right) - \sum_{\beta=1}^{M}Z^\beta_k\bar Z^j_\beta \mathrm{d}\bar Z^k_\beta\wedge \mathrm{d}Z^\beta_j - \sum_{\beta=1}^{M}\sum_{\gamma=1}^{M}(Z^\gamma_k \mathrm{d}\bar Z^k_\beta)\wedge(\bar Z^j_\gamma \mathrm{d}Z^\beta_j) + \sum_{\beta=1}^{M}Z^\beta_k\bar Z^j_\beta \mathrm{d}\bar Z^k_\beta\wedge \mathrm{d}Z^\beta_j + \sum_{\beta=1}^{M}\mathrm{d}\bar Z^j_\beta\wedge \mathrm{d}Z^\beta_j - \left(\sum_{\beta=1}^{M}Z^\beta_j \mathrm{d}\bar Z^j_\beta\right)\wedge\left(\sum_{\beta=1}^{M}\bar Z^j_\beta \mathrm{d}Z^\beta_j\right) \quad \text{(A13)}$$

$$= \sum_{\beta=1}^{M}\mathrm{d}\bar Z^j_\beta\wedge \mathrm{d}Z^\beta_j - \sum_{\beta,\gamma=1}^{M}(Z^\gamma_k \mathrm{d}\bar Z^k_\beta)\wedge(\bar Z^j_\gamma \mathrm{d}Z^\beta_j). \quad \text{(A14)}$$

■

The natural metric of the Grassmannian is then the Kähler form where we "replace" the exterior product $\wedge$ by the tensor product, i.e., $\mathrm{d}l^2 = 2\imath(\partial^2 K/\partial\bar W^j_\beta\partial Z^i_{\alpha|W=Z})\mathrm{d}Z^i_\alpha \mathrm{d}\bar Z^j_\beta$. By the same approach as that given in this appendix, we then have

$$\mathrm{d}l^2 = \mathrm{tr}(\mathrm{d}Z^\dagger \mathrm{d}Z) + \mathrm{tr}((Z^\dagger \mathrm{d}Z)^2) \quad \text{(A15)}$$

$$= \mathrm{tr}(\mathrm{d}Z^\dagger \mathrm{d}Z) - \mathrm{tr}(\mathrm{d}Z^\dagger Z Z^\dagger \mathrm{d}Z) \quad \text{(A16)}$$

$$= \mathrm{d}\bar Z^i_\alpha \mathrm{d}Z^\alpha_i - \mathrm{d}\bar Z^i_\alpha Z^\beta_i \bar Z^j_\beta \mathrm{d}Z^\alpha_j. \quad \text{(A17)}$$

Note that $\mathcal{F} = \mathrm{tr}\, F = \mathrm{d}\bar Z^j_\beta\wedge \mathrm{d}Z^\beta_j$ since $\mathrm{tr}([Z^\dagger \mathrm{d}Z, Z^\dagger \mathrm{d}Z]) = 0$.

The equivalence class $\pi_U(Z)$ of Z represents an M-dimensional active space. The particular choice of a particular element of the equivalence class is associated with a particular choice of basis $(|\alpha\rangle)_\alpha$ for the active space. We wish to find a distance in $G_M(\mathbb{C}^N)$ which characterizes the quantum distance between active spaces. We have two choices. The first is the chordal distance

$$\mathrm{dist}_{\mathrm{ch}}(W,Z) = \sqrt{2}\sqrt{M - \mathrm{tr}(W^\dagger Z Z^\dagger W)} = \sqrt{2}\sqrt{M - \|W^\dagger Z\|_F^2}, \tag{A18}$$

where $\|\cdot\|_F$ is the Frobenius norm of the matrices: $\|A\|_F^2=\mathrm{tr}(A^\dagger A)=\Sigma_{i=1}^N \Sigma_{\beta=1}^M |A_{i\beta}|^2$. The second possible choice is the Fubini-Study distance

$$\mathrm{dist}_{\mathrm{FS}}(W,Z) = \arccos(\det(W^\dagger Z)\det(Z^\dagger W)) = \arccos|\det W^\dagger Z|^2. \tag{A19}$$

Note that these are distances for $G_M(\mathbb{C}^N)$ (the set of equivalence classes), and not for $V_M(\mathbb{C}^N)$. We see that

$$0 \leqslant \mathrm{dist}_{\mathrm{ch}}(W,Z) \leqslant \sqrt{2M}, \tag{A20}$$

$$0 \leqslant \mathrm{dist}_{\mathrm{FS}}(W,Z) \leqslant \frac{\pi}{2}. \tag{A21}$$

The fact that the distances are bounded just reflects the fact that $G_M(\mathbb{C}^N)$ is a compact manifold. The interpretation as quantum distances follows from the fact that if W and Z represent the same active space $W=ZU$, then the distance between W and Z is zero, and also from the following property.

Property 2: *Let E_1 be the active space represented by W and E_2 be the active space represented by Z. Then* $\mathrm{dist}_{\mathrm{ch}}(W,Z)=\sqrt{2M}$ *if and only if $E_1 \perp E_2$ and* $\mathrm{dist}_{\mathrm{FS}}(W,Z)=\pi/2$ *if and only if $E_1^\perp \cap E_2 \neq \{0\}$ or $E_2^\perp \cap E_1 \neq \{0\}$.*

Proof: $W=(|\phi_1\rangle,\ldots,|\phi_M\rangle)$ and $Z=(|\psi_1,\ldots,|\psi_M\rangle)$,

$$\mathrm{tr}(W^\dagger Z Z^\dagger W) = 0 \Leftrightarrow \sum_{i,j} |\langle\psi_i|\phi_j\rangle|^2 = 0 \Leftrightarrow \forall\, i,j, \quad \langle\psi_i|\phi_j\rangle = 0. \tag{A22}$$

If $\det W^\dagger Z=0$, then the column vectors of $Z^\dagger W$ are not linearly independent, and then $\exists \alpha_i$ such that $\Sigma_j \alpha_j \langle\phi_i|\psi_j\rangle=0$, $\forall i$. Letting $|\tilde{\psi}\rangle=\Sigma_j\alpha_j|\psi_j\rangle$, $\forall \phi \in E_1$, we have $\langle\phi|\tilde{\psi}\rangle=0$, and then $\tilde{\psi}\in E_1^\perp$. We conclude that $\det W^\dagger Z=0 \Rightarrow E_1^\perp \cap E_2 \neq \{0\}$. We suppose that $\exists \tilde{\psi} \in E_1^\perp \cap E_2$, $\tilde{\psi}\neq 0$. Since ψ_j is an orthonormal basis of E_2, we have $\tilde{\psi}=\Sigma_j\alpha_j|\psi_j\rangle$ with $\alpha_j=\langle\psi_j|\tilde{\psi}\rangle$. Since $\tilde{\psi}\in E_1^\perp$, we have $\forall i$, $\langle\phi_i|\tilde{\psi}\rangle=0$ and then $\forall i \Sigma_j \alpha_j\langle\phi_i|\psi_j\rangle=0$. The column vectors of $W^\dagger Z$ are not linearly independent and then $\det W^\dagger Z=0$. ■

The two quantum distances are associated with the two notions of quantum incompatibility of active spaces. We say that two active spaces are incompatible in the strong sense if they are orthogonal: the probability of obtaining the same experimental results with a system in a state of E_1 and with a system in a state of E_2 is zero. We say that two active spaces are incompatible in the weak sense if $E_1^\perp \cap E_2=\{0\}$: there exists a state of E_1 for which the probability of obtaining the same measures as that with a system in a state of E_2 is zero.

Property 3: *The two quantum distances induce the Kählerian metric of* $G_M(\mathbb{C}^N)$.

Proof:

$$\mathrm{dist}_{\mathrm{ch}}(Z,Z+\mathrm{d}Z)^2 = 2(M - \mathrm{tr}(Z^\dagger(Z+\mathrm{d}Z)(Z^\dagger+\mathrm{d}Z^\dagger)Z)) \tag{A23}$$

$$=2(M - \mathrm{tr}((1+Z^\dagger\mathrm{d}Z)(1+\mathrm{d}Z^\dagger Z))) \tag{A24}$$

$$=2\,\mathrm{tr}(-Z^\dagger\mathrm{d}Z - \mathrm{d}Z^\dagger\mathrm{d}Z) - \mathrm{tr}(Z^\dagger\mathrm{d}Z\mathrm{d}Z^\dagger Z) \tag{A25}$$

$$=2\ \mathrm{tr}(\mathrm{d}Z^\dagger \mathrm{d}Z) - 2\ \mathrm{tr}(Z^\dagger \mathrm{d}Z\mathrm{d}Z^\dagger Z) \tag{A26}$$

$$=2\mathrm{d}l^2, \tag{A27}$$

where we have used the property $(Z^\dagger + \mathrm{d}Z^\dagger)(Z+\mathrm{d}Z)=1 \Leftrightarrow \mathrm{d}Z^\dagger \mathrm{d}Z + Z^\dagger \mathrm{d}Z + \mathrm{d}Z^\dagger Z = 0$.

We recall that if $\|A\|$ is in a neighborhood of 0 and if A is diagonalizable, then $\det(1+A)=1 + \mathrm{tr}\, A + \frac{1}{2}((\mathrm{tr}\, A)^2 - \mathrm{tr}(A^2)) + \mathcal{O}(\|A\|^3)$. We can further obtain the result

$$\cos \mathrm{dist}_{\mathrm{FS}}(Z,Z+\mathrm{d}Z) = \det(1 + Z^\dagger \mathrm{d}Z)\det(1 + \mathrm{d}Z^\dagger Z) \tag{A28}$$

$$=\left(1 + \mathrm{tr}\, Z^\dagger \mathrm{d}Z + \frac{1}{2}(\mathrm{tr}\, Z^\dagger \mathrm{d}Z)^2 - \frac{1}{2}\mathrm{tr}(Z^\dagger \mathrm{d}Z)^2 + \mathcal{O}(\|\mathrm{d}Z\|^3)\right) \tag{A29}$$

$$\times\left(1 + \mathrm{tr}\, \mathrm{d}Z^\dagger Z + \frac{1}{2}(\mathrm{tr}\, \mathrm{d}Z^\dagger Z)^2 - \frac{1}{2}\mathrm{tr}(\mathrm{d}Z^\dagger Z)^2 + \mathcal{O}(\|\mathrm{d}Z\|^3)\right) \tag{A30}$$

$$=1 + \mathrm{tr}\, Z^\dagger \mathrm{d}Z + \mathrm{tr}\, \mathrm{d}Z^\dagger Z + (\mathrm{tr}\, Z^\dagger \mathrm{d}Z)(\mathrm{tr}\, \mathrm{d}Z^\dagger Z) \tag{A31}$$

$$+ \frac{1}{2}(\mathrm{tr}\, Z^\dagger \mathrm{d}Z)^2 - \frac{1}{2}\mathrm{tr}(Z^\dagger \mathrm{d}Z)^2 + \frac{1}{2}(\mathrm{tr}\, \mathrm{d}Z^\dagger Z)^2 - \frac{1}{2}\mathrm{tr}(\mathrm{d}Z^\dagger Z)^2 + \mathcal{O}(\|\mathrm{d}Z\|^3) \tag{A32}$$

$$=1 - \mathrm{tr}(\mathrm{d}Z^\dagger \mathrm{d}Z) - (\mathrm{tr}\, Z^\dagger \mathrm{d}Z)^2 + (\mathrm{tr}\, Z^\dagger \mathrm{d}Z)^2 - \mathrm{tr}(Z^\dagger \mathrm{d}Z)^2 + \mathcal{O}(\|\mathrm{d}Z\|^3) \tag{A33}$$

$$=1 - \mathrm{tr}(\mathrm{d}Z^\dagger \mathrm{d}Z) - \mathrm{tr}(Z^\dagger \mathrm{d}Z)^2 + \mathcal{O}(\|\mathrm{d}Z\|^3) \tag{A34}$$

$$\simeq 1 - \mathrm{d}l^2. \tag{A35}$$

Since $\cos \mathrm{dist}_{\mathrm{FS}}(Z,Z+\mathrm{d}Z) \simeq 1 - [\mathrm{dist}_{\mathrm{FS}}(Z,Z+dZ)^2]/2$, we have $\mathrm{dist}_{\mathrm{FS}}(Z,Z+\mathrm{d}Z)^2 = 2\mathrm{d}l^2$. ■

Letting C be a geodesic for $\mathrm{d}l^2$ in $G_M(\mathbb{C}^N)$ linking Z and W, then

$$\int_C \mathrm{d}l = \frac{1}{\sqrt{2}}\mathrm{dist}_{\mathrm{FS}}(Z,W). \tag{A36}$$

Moreover, we know that $G_M(\mathbb{C}^N) \subset \mathcal{M}_{N\times N}(\mathbb{C})$. $WW^\dagger$ is self-adjoint $\forall W \in V_M(\mathbb{C}^N)$, and then $G_M(\mathbb{C}^N) \subset \mathbb{R}^{N^2}$ [a vector $\mathbf{v}_W$ of $\mathbb{R}^{N^2}$ being the list of the real and the imaginary parts of the components $(WW^\dagger)^i_j$ with $j \leqslant i$]. $G_M(\mathbb{C}^N)$ is then a submanifold of $\mathbb{R}^{N^2}$. We endow $\mathbb{R}^{N^2}$ with the Euclidian metric. $\forall WW^\dagger \in G_M(\mathbb{C}^N)$, since $W^\dagger W = I_M$, we have

$$(WW^\dagger)^i_j (WW^\dagger)^j_i = W^\alpha_j \bar{W}^i_\alpha W^\beta_i \bar{W}^j_\beta \tag{A37}$$

$$= \bar{W}^i_\alpha W^\beta_i \bar{W}^j_\beta W^\alpha_j \tag{A38}$$

$$= \delta^\beta_\alpha \delta^\alpha_\beta \tag{A39}$$

$$=M. \tag{A40}$$

Then

$$\mathrm{dist}_{\mathrm{ch}}(WW^\dagger, ZZ^\dagger) = \sqrt{2}\sqrt{M - (W^\dagger ZZ^\dagger W)^\alpha_\alpha} \tag{A41}$$

$$= \sqrt{2}\sqrt{M - \bar{W}^i_\alpha Z^\beta_i \bar{Z}^j_\beta W^\alpha_j} \tag{A42}$$

$$= \sqrt{2M - 2(WW^\dagger)^i_j (ZZ^\dagger)^j_i} \tag{A43}$$

$$= \sqrt{(WW^\dagger)^i_j (WW^\dagger)^j_i + (ZZ^\dagger)^i_j (ZZ^\dagger)^j_i - 2(WW^\dagger)^i_j (ZZ^\dagger)^j_i} \tag{A44}$$

$$= \sqrt{(WW^\dagger - ZZ^\dagger)^j_i (WW^\dagger - ZZ^\dagger)^i_j} \tag{A45}$$

$$= \sqrt{(\mathbf{v}_W - \mathbf{v}_Z) \cdot (\mathbf{v}_W - \mathbf{v}_Z)} \tag{A46}$$

$$= \|\mathbf{v}_W - \mathbf{v}_Z\|. \tag{A47}$$

The chordal distance is then the distance through the space $\mathbb{R}^{N^2}$, whereas the Fubini-Stuty distance is the distance on the "surface" of $G_M(\mathbb{C}^N)$.

Remark: In practice, we consider a manifold $\mathcal{M}$ associated with the classical control parameters characterizing the environment of the quantum system. For example, if the quantum system is an atom driven by a laser field, then $\mathcal{M}$ is the manifold generated by the intensity, the polarization, and the frequency of the field. This control manifold is closer to the experimental situation than the active space manifold $G_M(\mathbb{C}^N)$. The relation between the control parameters and the active spaces is characterized by an immersion map from $\mathcal{M}$ to $G_M(\mathbb{C}^N)$ (or equivalently to $\mathbb{R}^{N^2}$). The role of this map is (locally) analyzed in the adiabatic case in Ref. 46.

The Kählerian structure of $G_M(\mathbb{C}^N)$ is particularly important, since the metric measures the variations of the evolutive active space and then measures the change of the quantum properties induced by the subdynamics of the evolutive active space.

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