The need for a flat higher gauge structure to describe a Berry phase associated with some resonance phenomena

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In the presence of a resonance crossing producing splitting of the base manifold (for example, a circle crossing in a plane), we show that the rigorous geometrical structure within which the Berry phase arises may be a 2-bundle (a structure related to gerbes and to category theory) rather than a fiber bundle. The Bloch wave operator plays an important role in the associated theory. © *2009 American Institute of Physics.* [DOI: 10.1063/1.3119004]

I. INTRODUCTION

Since the pioneering work of Berry[1] concerning the adiabatic dynamics of a conservative two-level system, several types of geometric phases for quantum systems have been studied, including non-Abelian geometric phases,[2] nonadiabatic geometric phases,[3] geometric phases associated with noncyclic evolutions,[4] and geometric phases associated with the Floquet theory.[5] The geometric structures within which the Berry phases arise have also been studied, e.g., the line bundle associated with an Abelian Berry phase,[6] the principal bundle associated with a non-Abelian Berry phase,[2] and the composite bundle associated with a Berry phase which does not commute with the dynamical phase.[7,8]

Some authors have also considered adiabatic Berry phases associated with non-self-adjoint Hamiltonians and, in particular, those associated with resonance states.[9–13] In these works the authors have not studied the geometric structure involved or have assumed that it is the same as for the self-adjoint case (as is the case in many situations). In Ref. 14 the authors studied the geometric structure involved in describing an exceptional crossing point where the definition of the base manifold is more subtle than for the usual case (a diabolic crossing point). In this paper we consider an eigenvalue which crosses another one with a crossing which produces splitting of the adiabatic base manifold (for example, a circle crossing in a plane). We show that the relevant geometric structure is not a fiber bundle but a higher degree fibered structure. Section II explains the particular difficulties with this case, and Sec. III sets out the appropriate geometrical treatment.

II. THE CONTEXT OF THE PROBLEM

Before describing the specific difficulties with some resonance crossings we briefly recall the usual situation.

A. The crossing point case

Let $\vec{R}\mapsto H(\vec{R})$ be a general parameter-dependent Hamiltonian matrix (not necessarily self-adjoint). We suppose for simplicity that the Hilbert space is finite dimensional. The set of all configurations of $\vec{R}$ is assumed to form a $\mathcal{C}^\infty$ manifold M. Let $M\ni\vec{R}\mapsto E_a(\vec{R})\in\mathbb{R}$ or $\mathbb{C}$ be a

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continuous eigenvalue of $H(\vec{R})$. We suppose that $E_a(\vec{R})$ is nondegenerate for all $\vec{R}$, except at a point $\vec{Q}$ where E_a crosses another eigenvalue E_b. Let $\{U^\alpha\}$ be a good cover of M (i.e., a set of contractible open sets of M such that $\cup_\alpha U^\alpha = M$) and let $|a,\vec{R}\rangle^\alpha$ be a $\mathcal{C}^2$-differentiable eigenvector of $H(\vec{R})$ associated with $E_a(\vec{R})$ on U^α. We then have

$$\forall \vec{R} \in U^\alpha, \quad H(\vec{R})|a,\vec{R}\rangle^\alpha = E_a(\vec{R})|a,\vec{R}\rangle^\alpha. \tag{1}$$

The eigenvector is locally defined (with one definition for each chart U^α) because in general it is impossible to define a globally $\mathcal{C}^2$ eigenvector or to keep the same normalization on the whole of M. This fact is due to the crossing and is intimately related to the Dirac–Wu–Yang magnetic monopole theory (see Chap. 10.6 in Ref. 15 and also Ref. 16).

Let $\vec{R} \mapsto |a*,\vec{R}\rangle^\alpha$ be a $\mathcal{C}^2$ eigenvector of $H(\vec{R})^\dagger$ associated with $E_a(\vec{R})^*$ (the star denoting complex conjugation), with the normalization condition

$$\forall \vec{R} \in U^\alpha, \quad {}^\alpha\langle a*,\vec{R}|a,\vec{R}\rangle^\alpha = 1. \tag{2}$$

We note moreover that

$$\forall \vec{R} \in U^\alpha, \quad \vec{R} \neq \vec{Q}, \quad \forall\, c \neq a, \quad {}^\alpha\langle c*,\vec{R}|a,\vec{R}\rangle^\alpha = 0. \tag{3}$$

If H is self-adjoint then $|a*,\vec{R}\rangle^\alpha = |a,\vec{R}\rangle^\alpha$. The set $\{|c,\vec{R}\rangle^\alpha; |c*,\vec{R}\rangle^\alpha\}_c$ forms a biorthogonal basis of the Hilbert space.

Passing from a chart U^α to a chart U^β such that $U^\alpha \cap U^\beta \neq \emptyset$, the transformation from $|a,\vec{R}\rangle^\alpha$ to $|a,\vec{R}\rangle^\beta$ is just a change of the norm convention (or a change of the phase convention if H is self-adjoint). The change is defined by the transition functions

$$\forall \vec{R} \in U^\alpha \cap U^\beta, \quad g^{\alpha\beta}(\vec{R}) = {}^\alpha\langle a*,\vec{R}|a,\vec{R}\rangle^\beta \in \mathbb{C}^* \tag{4}$$

(where $\mathbb{C}^*$ is the group of nonzero complex numbers). Indeed by using the closure relation we have

$$\forall \vec{R} \neq \vec{Q}, \quad |a,\vec{R}\rangle^\beta = \sum_c |c,\vec{R}\rangle^\alpha \underbrace{{}^\alpha\langle c*,\vec{R}|a,\vec{R}\rangle^\beta}_{\delta_{ca} g^{\alpha\beta}(\vec{R})}. \tag{5}$$

The transition functions satisfy the cocycle relations

$$\forall \vec{R} \in U^\alpha \cap U^\beta \cap U^\gamma, \quad \vec{R} \neq \vec{Q}, \quad g^{\alpha\beta}(\vec{R}) g^{\beta\gamma}(\vec{R}) g^{\gamma\alpha}(\vec{R}) = 1, \tag{6}$$

$$\forall \vec{R} \in U^\alpha \cap U^\beta, \quad \vec{R} \neq \vec{Q}, \quad g^{\alpha\beta}(\vec{R}) g^{\beta\alpha}(\vec{R}) = 1, \tag{7}$$

$$\forall \vec{R} \in U^\alpha, \quad g^{\alpha\alpha}(\vec{R}) = 1. \tag{8}$$

By again using the closure relation we have

$$1 = {}^\alpha\langle a*,\vec{R}|a,\vec{R}\rangle^\alpha = \sum_c \underbrace{{}^\alpha\langle a*,\vec{R}|c,\vec{R}\rangle^\beta}_{\delta_{ca} g^{\alpha\beta}} \underbrace{{}^\beta\langle c*,\vec{R}|a,\vec{R}\rangle^\alpha}_{\delta_{ca} g^{\beta\alpha}}, \tag{9}$$

$$\underbrace{{}^\alpha\langle a*,\vec{R}|a,\vec{R}\rangle^\gamma}_{g^{\alpha\gamma}} = \sum_c \underbrace{{}^\alpha\langle a*,\vec{R}|c,\vec{R}\rangle^\beta}_{\delta_{ca} g^{\alpha\beta}} \underbrace{{}^\beta\langle c*,\vec{R}|a,\vec{R}\rangle^\gamma}_{\delta_{ca} g^{\beta\gamma}}. \tag{10}$$

A good cover $\{U^\alpha\}_\alpha$ together with a set of transition functions $\{g^{\alpha\beta}\}_{\alpha,\beta}$ satisfying the cocycle relations (6)–(8) define a principal $\mathbb{C}^*$-bundle [or a $U(1)$-bundle if H is self-adjoint] over $M\backslash\{\vec{Q}\}$ (see Ref. 15). It is called the adiabatic bundle and is endowed with a connection defined by the connection potential

$$\forall \vec{R} \in U^\alpha, \quad A^\alpha(\vec{R}) = {}^\alpha\langle a*,\vec{R}|d|a,\vec{R}\rangle^\alpha \in \Omega^1(U^\alpha,\mathbb{C}), \tag{11}$$

where d is the exterior differential of M and $\Omega^n(U^\alpha,\mathbb{C})$ is the set of complex-valued differential n-forms of U^α. By using the closure relation, we see that the adiabatic potential satisfies the gluing relation

$$\forall \vec{R} \in U^\alpha \cap U^\beta, \quad \vec{R} \neq \vec{Q}, \quad A^\beta(\vec{R}) = A^\alpha(\vec{R}) + g^{\alpha\beta}(\vec{R})^{-1} dg^{\alpha\beta}(\vec{R}). \tag{12}$$

Let $[0,T] \ni t \mapsto \vec{R}(t) \in M$ be a closed path $\mathcal{C}$ in M which does not pass through $\vec{Q}$ and which is followed sufficiently slowly such that the time-dependent Hamiltonian $t \mapsto H(\vec{R}(t))$ generates an adiabatic evolution. If the evolution starts from $|\psi(0)\rangle = |a,\vec{R}(0)\rangle^\alpha$, then at the end of the adiabatic evolution the wave function is given by

$$|\psi(T)\rangle = e^{-\imath\hbar^{-1}\int_0^T E_a(\vec{R}(t'))dt'} e^{\gamma_a(\mathcal{C})} |a,\vec{R}(0)\rangle^\alpha, \tag{13}$$

where $e^{\gamma_a(\mathcal{C})}$ is the geometric phase. If $\mathcal{C} \subset U^\alpha$ then

$$e^{\gamma_a(\mathcal{C})} = e^{-\oint_{\mathcal{C}} A^\alpha}. \tag{14}$$

However, if $\mathcal{C}$ passes through several charts, we have

$$e^{-\gamma_a(\mathcal{C})} = e^{\int_{\vec{R}(0)}^{\vec{R}^{\alpha\beta}} A^\alpha} g^{\alpha\beta}(\vec{R}^{\alpha\beta}) e^{\int_{\vec{R}^{\alpha\beta}}^{\vec{R}^{\beta\gamma}} A^\beta} g^{\beta\gamma}(\vec{R}^{\beta\gamma}) e^{\int_{\vec{R}^{\beta\gamma}}^{\vec{R}^{\gamma\delta}} A^\gamma} \cdots g^{\zeta\alpha}(\vec{R}^{\zeta\alpha}) e^{\int_{\vec{R}^{\zeta\alpha}}^{\vec{R}(0)} A^\alpha}, \tag{15}$$

where $\vec{R}^{\alpha\beta}$ is an arbitrary point in $U^\alpha \cap U^\beta \cap \mathcal{C}$, the integrations being along the path $\mathcal{C}$. This formula correctly defines the geometric phase, since the result is independent of the choice of arbitrary transition points $\{\vec{R}^{\alpha\beta}\}_{\alpha\beta}$ as is proved by Alvarez in Ref. 17 for a general Abelian gauge theory.

The adiabatic bundle is constructed on $M\backslash\{\vec{Q}\}$ because E_a is degenerate with E_b at $\vec{Q}$. If $\vec{Q} \in U^\alpha \cap U^\beta$, we have

$${}^\beta\langle b*,\vec{Q}|a,\vec{Q}\rangle^\alpha \neq 0 \tag{16}$$

because of the possible basis change in the eigenspace associated with $E_a = E_b$ between the conventions α and β.

The cocycle relations (6) and (7) then fail at the point $\vec{Q}$. Moreover, for the same reason, the gluing relation (12) fails and the expression (15) for the geometric phase is not well defined if $\mathcal{C}$ passes through $\vec{Q}$. A first approach to including $\vec{Q}$ in the description is to consider the principal $GL(2,\mathbb{C})$-bundle defined by the transition functions

$$\forall \vec{R} \in U^\alpha \cap U^\beta, \quad \begin{pmatrix} {}^\alpha\langle a*,\vec{R}|a,\vec{R}\rangle^\beta & {}^\alpha\langle a*,\vec{R}|b,\vec{R}\rangle^\beta \\ {}^\alpha\langle b*,\vec{R}|a,\vec{R}\rangle^\beta & {}^\alpha\langle b*,\vec{R}|b,\vec{R}\rangle^\beta \end{pmatrix} \in GL(2,\mathbb{C}) \tag{17}$$

and endowed with the matrix potential

$$\begin{pmatrix} {}^{\alpha}\langle a*,\vec{R}|d|a,\vec{R}\rangle^{\alpha} & {}^{\alpha}\langle a*,\vec{R}|d|b,\vec{R}\rangle^{\alpha} \\ {}^{\alpha}\langle b*,\vec{R}|d|a,\vec{R}\rangle^{\alpha} & {}^{\alpha}\langle b*,\vec{R}|d|b,\vec{R}\rangle^{\alpha} \end{pmatrix}, \tag{18}$$

generating a non-Abelian Berry phase. This bundle is used to described nonadiabatic transitions between the states a and b. However, if we are only interested in evolutions which are everywhere adiabatic except at $\vec{Q}$ then it is possible to regularize the point $\vec{Q}$. Indeed, since the cocycle relations (6) and (7) and the gluing relation (12) are true at all points of a neighborhood of $\vec{Q}$ except at $\vec{Q}$ itself, we will have the following limits:

$$\lim_{\vec{R}\to\vec{Q}} g^{\alpha\beta}(\vec{R})g^{\beta\alpha}(\vec{R}) = 1, \tag{19}$$

$$\lim_{\vec{R}\to\vec{Q}} g^{\alpha\beta}(\vec{R})g^{\beta\gamma}(\vec{R})g^{\gamma\alpha}(\vec{R}) = 1, \tag{20}$$

$$\lim_{\vec{R}\to\vec{Q}} (A^{\beta}(\vec{R}) - A^{\alpha}(\vec{R}) - g^{\alpha\beta}(\vec{R})^{-1}dg^{\alpha\beta}(\vec{R})) = 0. \tag{21}$$

By using the limit on $\vec{Q}$ the adiabatic bundle can be defined on the whole of M. For a path passing through $\vec{Q}$ at time t_Q and sufficiently slow to remain adiabatic except at $\vec{Q}$, where an adiabatic passage suddenly occurs (see Ref. 18), the wave function after the evolution is given by

$$|\psi(T)\rangle = e^{-\imath\hbar^{-1}\int_0^{t_Q} E_a(\vec{R}(t'))dt'} e^{-\imath\hbar^{-1}\int_{t_Q}^{T} E_b(\vec{R}(t'))dt'} e^{\gamma_a(\vec{R}(0)\to\vec{Q})} e^{\gamma_b(\vec{Q}\to\vec{R}(0))} |b,\vec{R}(0)\rangle^{\alpha}, \tag{22}$$

where the geometric phases $e^{\gamma_a(\vec{R}(0)\to\vec{Q})}$ and $e^{\gamma_b(\vec{Q}\to\vec{R}(0))}$ are defined as in Eq. (15). In fact we use two adiabatic bundles, one associated with E_a for the first part of the evolution until $\vec{R}(t_Q)=\vec{Q}$ and the other associated with E_b for the second part.

B. Difficulties with a splitting resonance crossing

To simplify the explanation we suppose that M is two dimensional (the generalization to more dimensions does not present any difficulty of principle). We consider the Hamiltonian matrix

$$H(\vec{R}) = \frac{\hbar}{2}\begin{pmatrix} 0 & x-\imath y \\ x+\imath y & 2\Delta - \frac{\imath}{2}\Gamma \end{pmatrix}, \tag{23}$$

with $\vec{R}=(x,y)$ and M being a plane. This is the Hamiltonian of a bound state coupled to a resonance state of width Γ, the coupling being realized by (for example) a laser field with $\Omega e^{\imath\phi}=x-\imath y$ (Ω being the amplitude of the laser and ϕ being its phase). Δ is equal to the energy gap between the bound state and the resonance minus the energy of one photon. Without loss of generality we can choose $\Delta=0$ since it plays no role in the present discussion. The eigenvalues of H are

$$\frac{\hbar}{2}\left(-\frac{\imath}{4}\Gamma \pm \sqrt{x^2+y^2-\frac{\Gamma^2}{16}}\right). \tag{24}$$

They cross on a circle $\mathbb{S}$ centered on zero with a radius equal to $\Gamma/4$. $\mathbb{S}$ then splits M in two distinct parts, the interior of the circle, M^{int}, and the exterior, M^{ext}. The first conceptual problem arising is that there is no natural link between the eigenstates in M^{int} and the eigenstates in M^{ext}. Indeed, we have

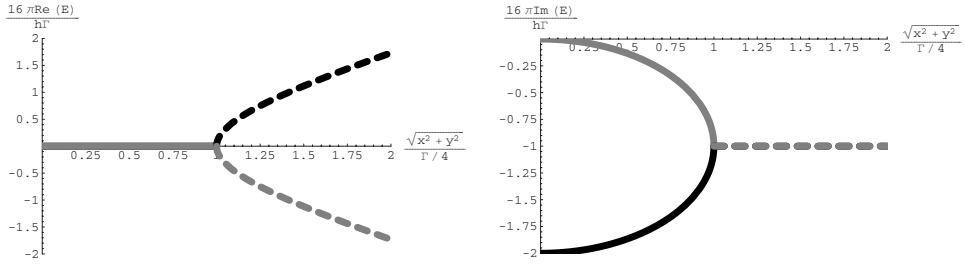

FIG. 1. Real (left) and imaginary (right) parts of the eigenvalues as a function of $\sqrt{x^2+y^2}/(\Gamma/4)$. Plain black line; the more dissipative. Plain gray line; the less dissipative. Dashed black line; the high energy state. Dashed gray line; the low energy state.

$$\forall \vec{R} \in M^{\text{int}}, \quad E_{\pm}(\vec{R}) = \frac{\hbar}{2}\left(-\frac{\imath}{4}\Gamma \mp \imath\sqrt{\frac{\Gamma^2}{16} - x^2 - y^2}\right), \tag{25}$$

where the label "−" signifies the less dissipative state and the label "+" signifies the more dissipative state, whereas we also have

$$\forall \vec{R} \in M^{\text{ext}}, \quad E_{\pm}(\vec{R}) = \frac{\hbar}{2}\left(-\frac{\imath}{4}\Gamma \pm \sqrt{x^2 + y^2 - \frac{\Gamma^2}{16}}\right), \tag{26}$$

where the label − signifies the low energy state and the label + signifies the high energy state. In M^{int} the two states have the same energy and in M^{ext} they are equally dissipative. As we see in Fig. 1, there is no natural continuation through the crossing circle. Let $\mathcal{C}$ be a closed path crossing the circle, for example, in Fig. 2.

We suppose that $\mathcal{C}$ is followed sufficiently slowly so that the evolution remains adiabatic. Since there is no natural continuation through $\mathbb{S}$ we can think that the adiabatic passage does not make a complete transfer from the less dissipative state to one exterior state but instead realizes a

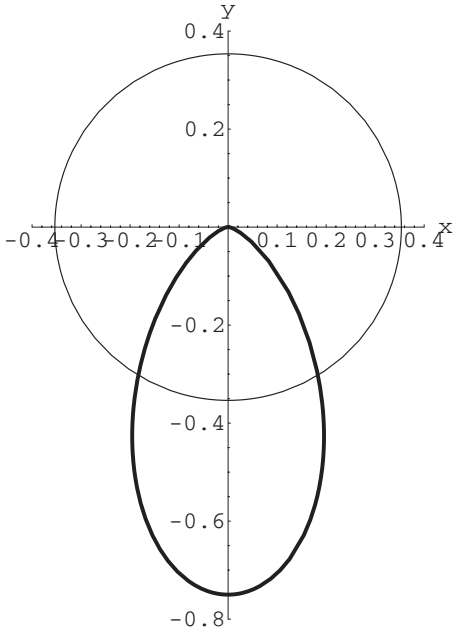

FIG. 2. A closed path in M starting from (0,0) and crossing the circle $\mathbb{S}$ ($\Gamma=\sqrt{2}$). This path corresponds to a laser pulse with $\Omega(t)=\Omega_0 e^{-(t-t_0)^2/\tau}$ and with a phase drift $\phi(t)=\pi/2+\alpha t$ ($\Omega_0=0.75$ a.u. and $\alpha=\pi/5$).

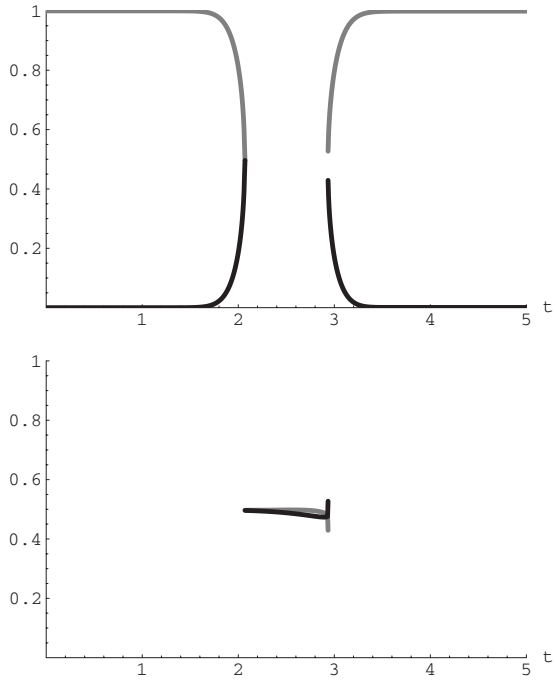

FIG. 3. Probabilities associated with a slow following of the path of Fig. 2. Upper: occupation probabilities of the interiorless (in gray) and more (in black) dissipative states. Lower: occupation probabilities of the exterior low (in gray) and high (in black) energy states. The circle is crossed at times $t \simeq 2$ and $t \simeq 3$ a.u. We see that the evolution is adiabatic (no transition occurs) except in the immediate neighborhood of the circle. At the passage through the circle the probability of transition from the interiorless dissipative state to the exterior low or high energy state is equal to 1/2 for both transitions.

transition to the symmetric superposition of the two exterior states. Finally we can think that after the second passage through $\mathbb{S}$ we recover completely the interiorless dissipative state. This is confirmed by the numerical integration of the Schrödinger equation, see Fig. 3.

After the evolution, the wave function depends on two geometric phases (associated with each continuation through the circle). If $\psi(0)=|-,(0,0)\rangle$ then we have

$$|\psi(T)\rangle = \frac{1}{\sqrt{2}}\Big(e^{-\imath\hbar^{-1}\left(\int_0^{t_1}E_-^{\mathrm{int}}(\vec{R}(t'))dt'+\int_{t_1}^{t_2}E_-^{\mathrm{ext}}(\vec{R}(t'))dt'+\int_{t_2}^{T}E_-^{\mathrm{int}}(\vec{R}(t'))dt'\right)}e^{\gamma_{--}(\mathcal{C})}$$
$$+ e^{-\imath\hbar^{-1}\left(\int_0^{t_1}E_-^{\mathrm{int}}(\vec{R}(t'))dt'+\int_{t_1}^{t_2}E_+^{\mathrm{ext}}(\vec{R}(t'))dt'+\int_{t_2}^{T}E_-^{\mathrm{int}}(\vec{R}(t'))dt'\right)}e^{\gamma_{-+}(\mathcal{C})}\Big)|-,(0,0)\rangle, \tag{27}$$

t_1 and t_2 being the times of the passages through the crossing circle $\mathbb{S}$. $\gamma_{--}(\mathcal{C})$ is the geometric phase associated with the continuation of the interiorless dissipative state by the exterior low energy state and $\gamma_{-+}(\mathcal{C})$ is the geometric phase associated with the continuation of the interiorless dissipative state by the exterior high energy state. As for an adiabatic passage through a point crossing, we need two fibered adiabatic structures, one for γ_{-+} and one for γ_{--}. In order to avoid repetition for the two cases, in the following discussion the label a denotes $-$ and the label b denotes + in M^{int}; a denotes $-$ and b denotes + in M^{ext} for the convention "$--$" and the contrary for the convention "$-+$."

Since $\mathbb{S}$ is associated with a discontinuity in the eigenvector definition [we note moreover that $H(\vec{R})$ is not diagonalizable on $\mathbb{S}$], we have some difficulty in considering a $\mathcal{C}^2$ eigenvector locally defined on an open set crossed by $\mathbb{S}$. To solve this problem, we consider a ring $\mathbb{T}$ centered on $\mathbb{S}$. We take $\mathbb{T}$ to be of width 2ϵ, with ϵ in the neighborhood of zero. We consider that E_a and E_b are approximately degenerate on $\mathbb{T}$, and then we can mix the eigenvectors on the whole of $\mathbb{T}$ in order

to define a $\mathcal{C}^2$ continuation of $|a,\vec{R}\rangle$ from M^{int} (M^{ext}) through $\mathbb{S}$ up to the border of $\mathbb{T}$ in M^{ext} (M^{int}). This is equivalent to defining $|a,\vec{R}\rangle$ not as an eigenvector but as a weak eigenvector:

$$\frac{\|(H(\vec{R})-E_a(\vec{R}))|a,\vec{R}\rangle\|}{\||a,\vec{R}\rangle\|}<\epsilon\hbar. \tag{28}$$

Indeed if $|E_a(\vec{R})-E_b(\vec{R})|>\hbar\epsilon$ (this is true if $\vec{R}\notin\mathbb{T}$ in our example) then $|a,\vec{R}\rangle$ is necessarily the single eigenvector associated with E_a, or else the weak eigenspace is two dimensional. This approximation is in fact appropriate to the physical situation because $\epsilon\hbar$ can model the experimental limitation on the energy measurement. Equation (28) is used in numerical simulations and, as we see it in Fig. 3, the strict adiabatic assumption fails on a small neighborhood of $\mathbb{S}$ (to rest in a strict adiabatic evolution the speed of the evolution in M must tend to zero when the path approaches $\mathbb{S}$).

A further problem for the case being considered is that the cocycle relations (6) and (7) and the gluing relation (12) fail on $\mathbb{T}$. Since $\mathbb{T}$ is not a set of isolated points, we cannot regularize these relations.

III. GEOMETRIC PHASE FOR A SPLITTING RESONANCE CROSSING

A. The geometric phase

Let $\{U^\alpha\}_\alpha$ be a good cover of M such that if $U^\alpha\cap\mathbb{S}\neq\emptyset$ then $U^\alpha\subset M^{\text{int}}\cup\mathbb{T}$ or $U^\alpha\subset M^{\text{ext}}\cup\mathbb{T}$. If $U^\alpha\cap\mathbb{S}=\emptyset$ we define $|a,\vec{R}\rangle^\alpha$ as being the $\mathcal{C}^2$ eigenvector associated with $E_a(\vec{R})$; otherwise we define $|a,\vec{R}\rangle^\alpha$ as being a weak eigenvector $\mathcal{C}^2$-continuation in $\mathbb{T}$ of the eigenvector associated with $E_a(\vec{R})$. If $U^\alpha\cup U^\beta\subset M^{\text{int}}$ or if $U^\alpha\cup U^\beta\subset M^{\text{ext}}$ the transition from U^α to U^β is just a change of the norm convention between $|a,\vec{R}\rangle^\alpha$ and $|a,\vec{R}\rangle^\beta$. However, if $(U^\alpha\cup U^\beta)\cap\mathbb{S}\neq\emptyset$ we have ${}^\beta\langle b*,\vec{R}|a,\vec{R}\rangle^\alpha\neq 0$ on $U^\alpha\cap U^\beta\cap\mathbb{T}$. We then need an operator to describe the transformation from $|a,\vec{R}\rangle^\alpha$ to $|a,\vec{R}\rangle^\beta$. Let $P^\alpha(\vec{R})=|a,\vec{R}\rangle^{\alpha\alpha}\langle a*,\vec{R}|$ be the projector on the space spanned by $|a,\vec{R}\rangle^\alpha$. We introduce the Bloch wave operator (see Refs. 19–21), formally defined by

$$\forall\vec{R}\in U^\alpha\cap U^\beta,\quad \Omega^{\alpha\beta}(\vec{R})=P^\alpha(\vec{R})(P^\beta(\vec{R})P^\alpha(\vec{R})P^\beta(\vec{R}))^{-1}, \tag{29}$$

where $(P^\beta(\vec{R})P^\alpha(\vec{R})P^\beta(\vec{R}))^{-1}$ is the inverse of $P^\beta(\vec{R})P^\alpha(\vec{R})P^\beta(\vec{R})$ within Ran $P^\beta(\vec{R})$. $\Omega^{\alpha\beta}$ is in fact a solution of the equations

$$H(\vec{R})\Omega^{\alpha\beta}(\vec{R})=\Omega^{\alpha\beta}(\vec{R})H(\vec{R})\Omega^{\alpha\beta}(\vec{R}),$$

$$P^\alpha(\vec{R})\Omega^{\alpha\beta}(\vec{R})=\Omega^{\alpha\beta}(\vec{R}),\quad \Omega^{\alpha\beta}(\vec{R})P^\beta(\vec{R})=\Omega^{\alpha\beta}(\vec{R}), \tag{30}$$

which can be regarded as a higher order eigenequation: $H\Omega^{\alpha\beta}=\Omega^{\alpha\beta}H^{\alpha\beta,\text{eff}}$ ($H^{\alpha\beta,\text{eff}}=P^\beta H\Omega^{\alpha\beta}$ playing the role of a generalized eigenvalue matrix and $\Omega^{\alpha\beta}$ playing the role of a generalized eigenvector). Moreover an eigenprojector satisfies $[H,P^\alpha]=0$ with $(P^\alpha)^2=P^\alpha$ whereas the Bloch wave operator satisfies $[H,\Omega^{\alpha\beta}]\Omega^{\alpha\beta}=0$ with $(\Omega^{\alpha\beta})^2=\Omega^{\alpha\beta}$. Clearly $\Omega^{\alpha\beta}$ measures the difference between $|a,\vec{R}\rangle^\alpha$ and $|a,\vec{R}\rangle^\beta$, since if the two vectors are collinear then $\Omega^{\alpha\beta}=P^\alpha=P^\beta$, and $\|\Omega^{\alpha\beta}\|=1$. If the two vectors are orthogonal then $\Omega^{\alpha\beta}$ is singular (this situation is excluded in the present case) and otherwise $\Omega^{\alpha\beta}$ is not singular and $\|\Omega^{\alpha\beta}\|\neq 1$ [in a similar way, Bloch wave operators can be used to measure the adiabaticity of a quantum dynamical system (see Ref. 22)]. A straightforward calculation gives

$$\Omega^{\alpha\beta}(\vec{R})=\frac{|a,\vec{R}\rangle^{\alpha\beta}\langle a*,\vec{R}|}{{}^\beta\langle a*,\vec{R}|a,\vec{R}\rangle^\alpha}. \tag{31}$$

Let $\eta^\alpha(\vec{R}) = {}^\alpha\langle a*,\vec{R}|d|a,\vec{R}\rangle^\alpha$ be the usual adiabatic potential and let $g^{\alpha\beta}(\vec{R}) = 1/{}^\beta\langle a*,\vec{R}\,|\,a,\vec{R}\rangle^\alpha$; $g^{\alpha\beta}$ and η^α do not satisfy the cocycle relations (6) and (7) and the gluing relation (12) but we have the results

$$\forall \vec{R} \in U^\alpha \cap U^\beta, \quad \eta^\beta(\vec{R}) = \eta^\alpha(\vec{R}) + g^{\alpha\beta}(\vec{R})^{-1} dg^{\alpha\beta}(\vec{R}) + A^{\alpha\beta}(\vec{R}), \tag{32}$$

where

$$A^{\alpha\beta}(\vec{R}) = {}^\alpha\langle a*,\vec{R}|\Omega^{\alpha\beta}(\vec{R})d(\Omega^{\alpha\beta}(\vec{R}))^{-1}|a,\vec{R}\rangle^\alpha \in \Omega^1(U^\alpha \cap U^\beta, \mathbb{C}). \tag{33}$$

$(\Omega^{\alpha\beta})^{-1} = P^\beta P^\alpha$ denotes the operator such that $\Omega^{\alpha\beta}(\Omega^{\alpha\beta})^{-1} = P^\alpha$ and $(\Omega^{\alpha\beta})^{-1}\Omega^{\alpha\beta} = P^\beta$. We deduce the results

$$\eta^\beta = {}^\beta\langle a*,\vec{R}|d|a,\vec{R}\rangle^\beta \tag{34}$$

$$= ({}^\alpha\langle a*,\vec{R}|\Omega^{\alpha\beta\beta}\langle a*,\vec{R}|a,\vec{R}\rangle^\alpha) d\left(\frac{(\Omega^{\alpha\beta})^{-1}}{{}^\beta\langle a*,\vec{R}|a,\vec{R}\rangle^\alpha}|a,\vec{R}\rangle^\alpha\right) \tag{35}$$

$$= {}^\alpha\langle a*,\vec{R}|\Omega^{\alpha\beta}d(\Omega^{\alpha\beta})^{-1}|a,\vec{R}\rangle^\alpha + {}^\beta\langle a*,\vec{R}|a,\vec{R}\rangle^\alpha d({}^\beta\langle a*,\vec{R}|a,\vec{R}\rangle^\alpha)^{-1} + {}^\alpha\langle a*,\vec{R}|d|a,\vec{R}\rangle^\alpha. \tag{36}$$

$A^{\alpha\beta}$ measures the deviation from the usual gluing relation. It is interesting to see that, since $\Omega^{\alpha\beta}$ is a higher order generalization of an eigenvector, the definition of $A^{\alpha\beta}$, Eq. (33), is a higher order generalization of Eq. (11).

We introduce a higher order transition function, defined as the measure of the deviation from the usual cocycle relation (6):

$$\forall \vec{R} \in U^\alpha \cap U^\beta \cap U^\gamma, \quad h^{\alpha\beta\gamma}(\vec{R}) = g^{\beta\gamma}(\vec{R})g^{\alpha\gamma}(\vec{R})^{-1}g^{\alpha\beta}(\vec{R}). \tag{37}$$

After some algebra, we can prove that the $h^{\alpha\beta\gamma}$ satisfy the following higher order cocycle relations:

$$\forall \vec{R} \in U^\alpha \cap U^\beta \cap U^\gamma \cap U^\delta, \quad h^{\beta\gamma\delta}(\vec{R})h^{\alpha\gamma\delta}(\vec{R})^{-1}h^{\alpha\beta\delta}(\vec{R})h^{\alpha\beta\gamma}(\vec{R})^{-1} = 1, \tag{38}$$

$$\forall \vec{R} \in U^\alpha \cap U^\beta \cap U, ^\gamma \quad h^{\alpha\beta\gamma}(\vec{R})h^{\alpha\gamma\beta}(\vec{R}) = h^{\beta\gamma\alpha}(\vec{R})h^{\gamma\beta\alpha}(\vec{R}) = h^{\beta\gamma\beta}(\vec{R}), \tag{39}$$

$$\forall \vec{R} \in U^\alpha \cap U^\beta, \quad h^{\alpha\alpha\beta}(\vec{R}) = h^{\alpha\beta\beta}(\vec{R}) = 1, \tag{40}$$

$$\forall \vec{R} \in U^\alpha, \quad h^{\alpha\alpha\alpha}(\vec{R}) = 1. \tag{41}$$

We note that

$$\Omega^{\beta\gamma}(\vec{R})\Omega^{\alpha\gamma}(\vec{R})^{-1}\Omega^{\alpha\beta}(\vec{R}) = h^{\alpha\beta\gamma}(\vec{R})P^\beta(\vec{R}). \tag{42}$$

From this last equation, we can derive a higher gluing equation for $A^{\alpha\beta}$:

$$\Omega^{\beta\gamma}(\Omega^{\alpha\gamma})^{-1}\Omega^{\alpha\beta}d(\Omega^{\beta\gamma}(\Omega^{\alpha\gamma})^{-1}\Omega^{\alpha\beta})^{-1} = h^{\alpha\beta\gamma}d(h^{\alpha\beta\gamma})^{-1}P^\beta + P^\beta dP^\beta. \tag{43}$$

Since $(P^\beta)^2 = P^\beta \Rightarrow dP^\beta P^\beta + P^\beta dP^\beta = dP^\beta \Rightarrow P^\beta dP^\beta P^\beta = 0$ we have

$$\Omega^{\beta\gamma}(\Omega^{\alpha\gamma})^{-1}\Omega^{\alpha\beta}d(\Omega^{\beta\gamma}(\Omega^{\alpha\gamma})^{-1}\Omega^{\alpha\beta})^{-1}P^\beta = h^{\alpha\beta\gamma}d(h^{\alpha\beta\gamma})^{-1}P^\beta. \tag{44}$$

Moreover

$$\Omega^{\beta\gamma}(\Omega^{\alpha\gamma})^{-1}\Omega^{\alpha\beta}d(\Omega^{\beta\gamma}(\Omega^{\alpha\gamma})^{-1}\Omega^{\alpha\beta})^{-1} = \Omega^{\beta\gamma}(\Omega^{\alpha\gamma})^{-1}\Omega^{\alpha\beta}d(\Omega^{\alpha\beta})^{-1}\Omega^{\alpha\gamma}(\Omega^{\beta\gamma})^{-1} + \Omega^{\beta\gamma}(\Omega^{\alpha\gamma})^{-1}d\Omega^{\alpha\gamma}(\Omega^{\beta\gamma})^{-1}\Omega^{\beta\gamma}d(\Omega^{\beta\gamma})^{-1}. \quad (45)$$

Since

$$(\Omega^{\alpha\gamma})^{-1}\Omega^{\alpha\gamma} = P^{\gamma} \Rightarrow d(\Omega^{\alpha\gamma})^{-1}\Omega^{\alpha\gamma} + (\Omega^{\alpha\gamma})^{-1}d\Omega^{\alpha\gamma} = dP^{\gamma} \quad (46)$$

we then obtain

$$P^{\gamma}d(\Omega^{\alpha\gamma})^{-1}\Omega^{\alpha\gamma} + (\Omega^{\alpha\gamma})^{-1}d\Omega^{\alpha\gamma}P^{\gamma} = 0 \quad (47)$$

and so

$$\Omega^{\beta\gamma}(\Omega^{\alpha\gamma})^{-1}\Omega^{\alpha\beta}d(\Omega^{\beta\gamma}(\Omega^{\alpha\gamma})^{-1}\Omega^{\alpha\beta})^{-1} = \Omega^{\beta\gamma}(\Omega^{\alpha\gamma})^{-1}\Omega^{\alpha\beta}d(\Omega^{\alpha\beta})^{-1}\Omega^{\alpha\gamma}(\Omega^{\beta\gamma})^{-1} - \Omega^{\beta\gamma}(\Omega^{\alpha\gamma})^{-1}\Omega^{\alpha\gamma}d(\Omega^{\alpha\gamma})^{-1}\Omega^{\alpha\gamma}(\Omega^{\beta\gamma})^{-1} + \Omega^{\beta\gamma}d(\Omega^{\beta\gamma})^{-1}. \quad (48)$$

We conclude that

$$-(h^{\alpha\beta\gamma})^{-1}dh^{\alpha\beta\gamma}P^{\beta} = \Omega^{\beta\gamma}(\Omega^{\alpha\gamma})^{-1}\Omega^{\alpha\beta}d(\Omega^{\alpha\beta})^{-1}\Omega^{\alpha\gamma}(\Omega^{\beta\gamma})^{-1} - \Omega^{\beta\gamma}(\Omega^{\alpha\gamma})^{-1}\Omega^{\alpha\gamma}d(\Omega^{\alpha\gamma})^{-1}\Omega^{\alpha\gamma}(\Omega^{\beta\gamma})^{-1} + \Omega^{\beta\gamma}d(\Omega^{\beta\gamma})^{-1}P^{\beta}. \quad (49)$$

Finally, by projection from the right on $|a,\vec{R}\rangle^{\beta}$ and from the left on ${}^{\beta}\langle a*,\vec{R}|$ we have

$$-(h^{\alpha\beta\gamma})^{-1}dh^{\alpha\beta\gamma} = \frac{g^{\beta\gamma}}{g^{\alpha\gamma}}{}^{\alpha}\langle a*,\vec{R}|\Omega^{\alpha\beta}d(\Omega^{\alpha\beta})^{-1}|a,\vec{R}\rangle^{\alpha}\frac{g^{\alpha\gamma}}{g^{\beta\gamma}} - \frac{g^{\beta\gamma}}{g^{\alpha\gamma}}{}^{\alpha}\langle a*,\vec{R}|\Omega^{\alpha\gamma}d(\Omega^{\alpha\gamma})^{-1}|a,\vec{R}\rangle^{\alpha}\frac{g^{\alpha\gamma}}{g^{\beta\gamma}} + {}^{\beta}\langle a*,\vec{R}|\Omega^{\beta\gamma}d(\Omega^{\beta\gamma})^{-1}|a,\vec{R}\rangle^{\beta} \quad (50)$$

and so arrive at the higher degree gluing equation:

$$\forall \vec{R} \in U^{\alpha}\cap U^{\beta}\cap U^{\gamma}, \quad A^{\alpha\beta}(\vec{R}) - A^{\alpha\gamma}(\vec{R}) + A^{\beta\gamma}(\vec{R}) = -h^{\alpha\beta\gamma}(\vec{R})^{-1}dh^{\alpha\beta\gamma}(\vec{R}) \quad (51)$$

Finally, setting $B^{\alpha}=d\eta^{\alpha}\in\Omega^{2}(U^{\alpha},\mathbb{C})$ and using Eq. (32) we find a gluing equation for B^{α}:

$$\forall \vec{R} \in U^{\alpha}\cap U^{\beta}, \quad B^{\beta}(\vec{R}) = B^{\alpha}(\vec{R}) + dA^{\alpha\beta}(\vec{R}). \quad (52)$$

Equipped with $(h^{\alpha\beta\gamma},A^{\alpha\beta},B^{\alpha})$ we can go back to the problem of constructing a geometric phase expression. For a closed path $\mathcal{C}\subset M^{\text{int}}$ the usual formula, Eq. (15), can be used, and applying the Stokes theorem and the fact that $B^{\alpha}(\vec{R})=B^{\beta}(\vec{R})$ if $\vec{R}\notin\mathbb{T}$, we have

$$e^{-\gamma_a(\mathcal{C})} = e^{\int_{\vec{R}(0)}^{\vec{R}^{\alpha\beta}}\eta^{\alpha}}g^{\alpha\beta}(\vec{R}^{\alpha\beta})e^{\int_{\vec{R}^{\alpha\beta}}^{\vec{R}^{\beta\gamma}}\eta^{\gamma}}g^{\beta\gamma}(\vec{R}^{\beta\gamma})\cdots g^{\zeta\alpha}(\vec{R}^{\zeta\alpha})e^{\int_{\vec{R}^{\zeta\alpha}}^{\vec{R}(0)}\eta^{\alpha}} \quad (53)$$

$$= e^{\iint_{\mathcal{S}}B}, \quad (54)$$

where $\mathcal{S}$ is the surface on M having $\mathcal{C}$ as border. However, for a path crossing the circle (as in Fig. 2) we know that the expression in Eq. (54) is not well defined. Alvarez in Ref. 17 and various authors in Refs. 23–25 proposed a formula analogous to Eq. (15) but for the case of integration on a surface of a 2-form satisfying the gluing relation $B^{\beta}-B^{\alpha}=dA^{\alpha\beta}$. We can use it, by analogy with the Stokes theorem:

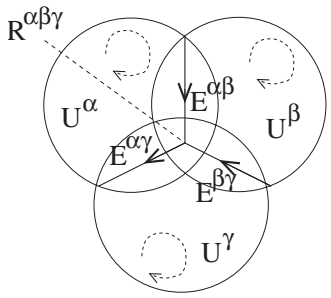

FIG. 4. Scheme of three charts, with their transition paths and their transition point. We have also indicated the orientations of the surfaces and of the paths.

$$e^{-\gamma_a(\mathcal{C})} = e^{\int_{\vec{R}(0)}^{\vec{R}^{\alpha\beta}} \eta^\alpha} g^{\alpha\beta}(\vec{R}^{\alpha\beta}) e^{\int_{\vec{R}^{\alpha\beta}}^{\vec{R}^{\beta\gamma}} \eta^\gamma} g^{\beta\gamma}(\vec{R}^{\beta\gamma}) \cdots g^{\zeta\alpha}(\vec{R}^{\zeta\alpha}) e^{\int_{\vec{R}^{\zeta\alpha}}^{\vec{R}(0)} \eta^\alpha} \tag{55}$$

$$= \prod_\alpha e^{\int\int_{\sigma^\alpha} B^\alpha} \prod_{\alpha,\beta} e^{\int_{E^{\alpha\beta}} A^{\alpha\beta}} \prod_{\alpha,\beta,\gamma} h^{\alpha\beta\gamma}(\vec{R}^{\alpha\beta\gamma}). \tag{56}$$

Here the orientation of the surfaces $\sigma^\alpha \subset U^\alpha$ ($\cup_\alpha \sigma^\alpha = \mathcal{S}$) is coherent with the orientation of $\mathcal{C}$, $E^{\alpha\beta}$ is an arbitrary path in $U^\alpha \cap U^\beta$ oriented coherently with the orientation of σ^α, and $\vec{R}^{\alpha\beta\gamma}$ is an arbitrary point in $U^\alpha \cap U^\beta \cap U^\gamma$, such that the different geometric objects are organized following the scheme of Fig. 4. The products are such that each $E^{\alpha\beta}$ and each $\vec{R}^{\alpha\beta\gamma}$ appear only once. $\vec{R}^{\alpha\beta}$ is an arbitrary point on $U^\alpha \cap U^\beta \cap \mathcal{C}$. Alvarez has shown in Ref. 17 that formula (56) is invariant under a change of the arbitrary paths $E^{\alpha\beta}$ and is then well defined [as is still the case even if $A^{\alpha\beta}$ and $h^{\alpha\beta\gamma}$ are not antisymmetric, since $A^{\alpha\beta} = -A^{\beta\alpha} + d\ln(g^{\alpha\beta} g^{\beta\alpha})$]. Nevertheless, formulas (55) and (56) are not invariant under a change of the arbitrary points $\vec{R}^{\alpha\beta} \in U^\alpha \cap U^\beta \cap \mathbb{T} \cap \mathcal{C}$. In other words, the Berry phase expression depends on the choice of the transition points between M^{int} and M^{ext} on $\mathcal{C}$ (the neighbor of $\mathcal{S}$). This pathology is not really a problem, since the width ϵ of $\mathbb{T}$ obeys $\epsilon \ll 1$, and the difference between two arbitrary choices of transition points can be absorbed within the approximation in Eq. (28).

B. The fibered structure

We suppose that $h^{\alpha\beta\gamma}$ and $A^{\alpha\beta}$ are antisymmetric with respect to the exchange of two chart indices and that $h^{\beta\gamma\delta}(h^{\alpha\gamma\delta})^{-1} h^{\alpha\beta\delta}(h^{\alpha\beta\gamma})^{-1} = 1$, $A^{\beta\alpha} - A^{\alpha\delta} + A^{\alpha\beta} = -(h^{\alpha\beta\gamma})^{-1} dh^{\alpha\beta\gamma}$, and $B^\beta - B^\alpha = dA^{\alpha\beta}$. The three kinds of data $(h^{\alpha\beta\gamma}, A^{\alpha\beta}, B^\beta)$ then define Abelian gerbes (i.e., a sheaf of groupoids) with a connective structure[26,27] (they can also define a twisted bundle[28] or a bundle gerbes[29]). However, in the present case $h^{\alpha\beta\gamma}$ and $A^{\alpha\beta}$ are not antisymmetric. We need then a more general structure, a 2-bundle, introduced by Baez and Schreiber in Refs. 30–32.

First, we suppose that the cover $\{U^\alpha\}_\alpha$ can be decomposed into three subsets $\{U^\alpha\}_{\alpha \in I^{\text{int}}}$, $\{U^\alpha\}_{\alpha \in I^{\text{ext}}}$, and $\{U^\alpha\}_{\alpha \in I^{\text{trans}}}$ such that $\cup_{\alpha \in I^{\text{int}}} U^\alpha = M^{\text{int}}$, $\cup_{\alpha \in I^{\text{ext}}} U^\alpha = M^{\text{ext}}$, and $\mathbb{T} \subset \cup_{\alpha \in I^{\text{trans}}} U^\alpha$ (if this is not the case, it is always possible to refine the cover). We can then define two principal $\mathbb{C}^*$-bundles: One of them, P^{int}, is defined on M^{int} with cover $\{U^\alpha\}_{\alpha \in I^{\text{int}}}$ and transition functions $g^{\alpha\beta}(\vec{R}) = 1/{}^\beta\langle a*, \vec{R} | a, \vec{R}\rangle^\alpha$ [the transition functions satisfy the cocycle relations (6)–(8) since $\mathbb{T}$ is not in M^{int}]. The other, P^{ext}, is defined in the same manner on M^{ext}.

To define the 2-bundle we need to reformulate the different structures in the language of category theory (see Ref. 33). At each open set U^α we associate a category $\mathcal{U}^\alpha$ with

$$\text{Obj}(\mathcal{U}^\alpha) = \{\vec{R}, \vec{R} \in U^\alpha\}, \tag{57}$$

$$\mathrm{Morph}(\mathcal{U}^\alpha) = \{\mathrm{id}_{\vec{R}}:\vec{R} \to \vec{R}; \vec{R} \in U^\alpha\}. \tag{58}$$

Obj denotes the set of objects in the category and Morph denotes the set of morphisms (so-called arrows) in the category. $\mathrm{id}_{\vec{R}}$ is the identity arrow on $\vec{R}$. In the same way we introduce the category $\mathcal{M}$ such that

$$\mathrm{Obj}(\mathcal{M}) = \{\vec{R}, \vec{R} \in M\}, \tag{59}$$

$$\mathrm{Morph}(\mathcal{M}) = \{\mathrm{id}_{\vec{R}}:\vec{R} \to \vec{R}; \vec{R} \in M\}. \tag{60}$$

In Refs. 30 and 32 $\mathcal{M}$ and $\mathcal{U}^\alpha$ are called trivial 2-spaces. $\{\mathcal{U}^\alpha\}_\alpha$ constitutes a 2-cover of $\mathcal{M}$ in the sense defined by Baez and Schreiber in Refs. 30 and 32. We introduce the groupoid $\mathcal{G}$ defined by

$$\mathrm{Obj}(\mathcal{G}) = \{\mathbb{C}^*\}, \tag{61}$$

$$\mathrm{Morph}(\mathcal{G}) = \{R(g), g \in \mathbb{C}^*\}, \tag{62}$$

where R is the canonical right action of the group $\mathbb{C}^*$ on itself, i.e., $\forall g, h \in \mathbb{C}^*$, $R(g)h = hg$. Note that the category $\mathcal{G}$ has only one object: $\mathbb{C}^*$; the identity arrow is $R(1)$ and the arrow composition is $R(g)R(h) = R(hg)$.

A principal 2-bundle defined on $\mathcal{M}$ with structure groupoid $\mathcal{G}$ is, following Refs. 30 and 32, a category $\mathcal{Q}$ and a surjective functor $\pi_{\mathcal{Q}}: \mathcal{Q} \to \mathcal{M}$ such that $\forall \alpha$ there exists an equivalence $\phi^\alpha: \pi_{\mathcal{Q}}^{-1}(\mathcal{U}^\alpha) \to \mathcal{U}^\alpha \times \mathcal{G}$ [a functor ϕ^α is an equivalence if there exists a functor $\bar{\phi}^\alpha: \mathcal{U}^\alpha \times \mathcal{G} \to \pi_{\mathcal{Q}}^{-1}(\mathcal{U}^\alpha)$ and natural transformations between $\phi^\alpha \bar{\phi}^\alpha$ and $\mathrm{id}_{\mathcal{U}^\alpha \times \mathcal{G}}$ and between $\bar{\phi}^\alpha \phi^\alpha$ and $\mathrm{id}_{\pi_{\mathcal{Q}}^{-1}(\mathcal{U}^\alpha)}$]. If $U^\alpha \cap U^\beta \neq \emptyset$, there exists a natural transformation $\mathfrak{g}^{\alpha\beta}$ between the functors $\phi^\alpha_{|\mathcal{U}^\alpha \cap \mathcal{U}^\beta}$ and $\phi^\beta_{|\mathcal{U}^\alpha \cap \mathcal{U}^\beta}$, that we can write

$$\mathfrak{g}^{\alpha\beta}: \begin{array}{ccc} \mathrm{Obj}(\mathcal{U}^\alpha \cap \mathcal{U}^\beta) & \to & \mathrm{Morph}(\mathcal{U}^\alpha \cap \mathcal{U}^\beta \times \mathcal{G}) \\ \vec{R} & \mapsto & \mathrm{id}_{\vec{R}} \times R(g^{\alpha\beta}(\vec{R})) \end{array}. \tag{63}$$

In Refs. 30 and 32 it is shown that $g^{\alpha\beta}$ must satisfy

$$h^{\alpha\beta\gamma} g^{\alpha\gamma} = g^{\alpha\beta} g^{\beta\gamma} \tag{64}$$

for some $h^{\alpha\beta\gamma}$ which define the principal 2-bundle. In a more general context, Baez and Schreiber called the higher cocycle relation (38) the associative law and the higher cocycle relation (40) and (41) the left and right unit laws.

The Berry phase then arises in the 2-bundle $\mathcal{Q}$ defined by transition functions $g^{\alpha\beta}$ and transition tranformations $h^{\alpha\beta\gamma}$. Moreover by construction, $\mathcal{Q}$ satisfies

$$\forall \alpha \in I^{\mathrm{int}}, \quad \pi_{\mathcal{Q}}^{-1}(\mathcal{U}^\alpha) = \mathcal{P}^{\mathrm{int}}_{|U^\alpha}, \tag{65}$$

$$\forall \alpha \in I^{\mathrm{ext}}, \quad \pi_{\mathcal{Q}}^{-1}(\mathcal{U}^\alpha) = \mathcal{P}^{\mathrm{ext}}_{|U^\alpha}, \tag{66}$$

where the categories $\mathcal{P}^{\mathrm{int}}_{|U^\alpha}$ and $\mathcal{P}^{\mathrm{ext}}_{|U^\alpha}$ are defined by the principal 1-bundles P^{int} and P^{ext} with

$$\mathrm{Obj}(\mathcal{P}^{\mathrm{int/ext}}_{|U^\alpha}) = \{\pi^{-1}_{P^{\mathrm{int/ext}}}(\vec{R}), \vec{R} \in U^\alpha\}, \tag{67}$$

$$\mathrm{Morph}(\mathcal{P}^{\mathrm{int/ext}}_{|U^\alpha}) = \{R^{\mathrm{int/ext}}_{\vec{R}}(g), g \in \mathbb{C}^*, \vec{R} \in U^\alpha\}, \tag{68}$$

where $R^{\mathrm{int/ext}}_{\vec{R}}$ is the canonical right action of $\mathbb{C}^*$ on $P^{\mathrm{int/ext}}$ and where $\pi_{P^{\mathrm{int/ext}}}$ is the projection map of $P^{\mathrm{int/ext}}$. The functor between $\mathcal{P}^{\mathrm{int/ext}}_{|U^\alpha}$ and $\mathcal{U}^\alpha \times \mathcal{G}$ is defined by using the fiber diffeomorphisms φ^α of $P^{\mathrm{int/ext}}$ for the objects:

$$\mathrm{Obj}(\mathcal{P}^{\mathrm{int/ext}}_{|U^\alpha}) \ni \pi^{-1}_{P^{\mathrm{int/ext}}}(\vec{R}) \xrightarrow{\varphi^\alpha} (\vec{R}, \mathbb{C}^*) \in \mathrm{Obj}(\mathcal{U}^\alpha \times \mathcal{G}), \tag{69}$$

and by the following map for the arrows:

$$\mathrm{Morph}(\mathcal{P}^{\mathrm{int/ext}}_{|U^\alpha}) \ni R^{\mathrm{int/ext}}_{\vec{R}}(g) \to (\mathrm{id}_{\vec{R}}, R(g)) \in \mathrm{Morph}(\mathcal{U}^\alpha \times \mathcal{G}). \tag{70}$$

$(\eta^\alpha, A^{\alpha\beta}, B^\alpha)$ constitutes a flat 2-connection of $\mathcal{Q}$ (flat because $dB^\alpha = 0$), and the Berry phase defined by Eq. (56) is related to the horizontal lift of the surface $\mathcal{S}$ (viewed as a trivial 2-space) in the 2-bundle $\mathcal{Q}$.

C. The transitional gerbe

We have seen that $\mathcal{Q}$ is characterized on M^{int} and on M^{ext} by two principal 1-bundles. In this paragraph we characterize the geometric structure on $\mathbb{T}$. For all $\alpha, \beta \in I^{\mathrm{trans}}$ such that $U^\alpha \cap U^\beta \neq \emptyset$, let $\widetilde{\Omega}^{\alpha\beta}$ be the renormalized wave operator:

$$\forall \vec{R} \in U^\alpha \cap U^\beta, \quad \widetilde{\Omega}^{\alpha\beta}(\vec{R}) = \Omega^{\alpha\beta}(\vec{R})(\Omega^{\beta\alpha}(\vec{R})\Omega^{\alpha\beta}(\vec{R}))^{-1/2} = \sqrt{\frac{g^{\alpha\beta}(\vec{R})}{g^{\beta\alpha}(\vec{R})}} |a, \vec{R}\rangle^{\alpha\beta}\langle a*, \vec{R}|. \tag{71}$$

The renormalized wave operator $\Omega^{\alpha\beta}(\Omega^{\beta\alpha}\Omega^{\alpha\beta})^{-1/2}$ is constructed following a similar procedure as for the des Cloizeaux wave operator [see (19)]. The interest of this operator is that it is antisymmetric under chart index exchange:

$$\widetilde{\Omega}^{\alpha\beta}\widetilde{\Omega}^{\beta\alpha} = P^\alpha. \tag{72}$$

We can set $\tilde{g}^{\alpha\beta}(\vec{R}) = \sqrt{g^{\alpha\beta}(\vec{R})/g^{\beta\alpha}(\vec{R})}$ and we have

$$\widetilde{\Omega}^{\beta\gamma}(\widetilde{\Omega}^{\alpha\gamma})^{-1}\widetilde{\Omega}^{\alpha\beta} = \sqrt{\frac{h^{\alpha\beta\gamma}}{h^{\gamma\beta\alpha}}} P^\beta \tag{73}$$

and set $\tilde{h}^{\alpha\beta\gamma} = \sqrt{h^{\alpha\beta\gamma}/h^{\gamma\beta\alpha}}$ satisfying

$$\forall \vec{R} \in U^\alpha \cap U^\beta \cap U^\gamma \cap U^\delta, \quad \tilde{h}^{\beta\gamma\delta}(\vec{R})\tilde{h}^{\alpha\gamma\delta}(\vec{R})^{-1}\tilde{h}^{\alpha\beta\delta}(\vec{R})\tilde{h}^{\alpha\beta\gamma}(\vec{R})^{-1} = 1, \tag{74}$$

$$\forall \vec{R} \in U^\alpha \cap U^\beta \cap U^\gamma, \quad \tilde{h}^{\alpha\beta\gamma}(\vec{R})\tilde{h}^{\beta\alpha\gamma}(\vec{R}) = \tilde{h}^{\alpha\beta\gamma}(\vec{R})\tilde{h}^{\alpha\gamma\beta}(\vec{R}) = \tilde{h}^{\alpha\beta\gamma}(\vec{R})\tilde{h}^{\gamma\beta\alpha}(\vec{R}) = 1, \tag{75}$$

$$\forall \vec{R} \in U^\alpha \cap U^\beta, \quad \tilde{h}^{\alpha\alpha\beta}(\vec{R}) = \tilde{h}^{\alpha\beta\beta}(\vec{R}) = \tilde{h}^{\alpha\beta\alpha}(\vec{R}) = 1, \tag{76}$$

$$\forall \vec{R} \in U, \quad \tilde{h}^{\alpha\alpha\alpha}(\vec{R}) = 1. \tag{77}$$

$\tilde{h}^{\alpha\beta\gamma}$ is then antisymmetric under chart index exchange. Let $\tilde{A}^{\alpha\beta} = {}^\alpha\langle a*, \vec{R}|\widetilde{\Omega}^{\alpha\beta}d(\widetilde{\Omega}^{\alpha\beta})^{-1}|a, \vec{R}\rangle^\alpha$. By the same calculation as in the previous paragraph we have

$$\eta^\beta = \eta^\alpha + (\tilde{g}^{\alpha\beta})^{-1}d\tilde{g}^{\alpha\beta} + \tilde{A}^{\alpha\beta}, \tag{78}$$

$$\tilde{A}^{\alpha\beta} - \tilde{A}^{\alpha\gamma} + \tilde{A}^{\beta\gamma} = -(\tilde{h}^{\alpha\beta\gamma})^{-1} d\tilde{h}^{\alpha\beta\gamma}, \tag{79}$$

$$B^{\beta} - B^{\alpha} = d\tilde{A}^{\alpha\beta}. \tag{80}$$

We also have

$$\tilde{A}^{\beta\alpha} = {}^{\beta}\langle a*, \vec{R} | \tilde{\Omega}^{\beta\alpha} d(\tilde{\Omega}^{\beta\alpha})^{-1} | a, \vec{R} \rangle^{\beta} \tag{81}$$

$$= {}^{\beta}\langle a*, \vec{R} | (\tilde{\Omega}^{\alpha\beta})^{-1} d\tilde{\Omega}^{\alpha\beta} | a, \vec{R} \rangle^{\beta} \tag{82}$$

$$= - {}^{\beta}\langle a*, \vec{R} | d(\tilde{\Omega}^{\alpha\beta})^{-1} \tilde{\Omega}^{\alpha\beta} | a, \vec{R} \rangle^{\beta} \tag{83}$$

$$= - {}^{\alpha}\langle a*, \vec{R} | \tilde{\Omega}^{\alpha\beta} d(\tilde{\Omega}^{\alpha\beta})^{-1} | a, \vec{R} \rangle^{\alpha} \tag{84}$$

$$= - \tilde{A}^{\alpha\beta}. \tag{85}$$

The three kinds of data $(\tilde{h}^{\alpha\beta\gamma}, \tilde{A}^{\alpha\beta}, B^{\alpha})$ define then a flat Abelian gerbe with connection on $\cup_{\alpha \in I^{\text{trans}}} U^{\alpha}$. Note that $(\tilde{h}^{\alpha\beta\gamma}, \tilde{A}^{\alpha\beta}, B^{\alpha})$ and $(h^{\alpha\beta\gamma}, A^{\alpha\beta}, B^{\alpha})$ are related by

$$\tilde{h}^{\alpha\beta\gamma} = h^{\alpha\beta\gamma} f^{\beta\gamma} (f^{\alpha\gamma})^{-1} f^{\alpha\beta}, \tag{86}$$

$$\tilde{A}^{\alpha\beta} = A^{\alpha\beta} - (f^{\alpha\beta})^{-1} df^{\alpha\beta}, \tag{87}$$

where $f^{\alpha\beta}(\vec{R}) = 1/\sqrt{g^{\alpha\beta}(\vec{R}) g^{\beta\alpha}(\vec{R})}$. These formulas are analogous to the gauge change formulas, except that $f^{\alpha\beta}$ is symmetric rather than antisymmetric under chart index exchange.

IV. CONCLUSION

We have seen that Berry phases induced by paths passing through a resonance crossing splitting the base manifold are associated with a higher gauge theory. They take place in a 2-bundle defined by transition functions and transition transformations:

$$g^{\alpha\beta} = ({}^{\beta}\langle a*, \vec{R} | a, \vec{R} \rangle^{\alpha})^{-1}, \tag{88}$$

$$h^{\alpha\beta\gamma} P^{\beta} = \Omega^{\beta\gamma} (\Omega^{\alpha\gamma})^{-1} \Omega^{\alpha\beta}, \tag{89}$$

$|a, \vec{R}\rangle^{\alpha}$ being an eigenvector and $\Omega^{\alpha\beta}$ being a Bloch wave operator (a higher degree generalization of an eigenvector). The 2-bundle is endowed with a 2-connection defined by

$$\eta^{\alpha} = {}^{\alpha}\langle a*, \vec{R} | d | a, \vec{R} \rangle^{\alpha}, \tag{90}$$

$$A^{\alpha\beta} = {}^{\alpha}\langle a*, \vec{R} | \Omega^{\alpha\beta} d(\Omega^{\alpha\beta})^{-1} | a, \vec{R} \rangle^{\alpha}, \tag{91}$$

$$B^{\alpha} = {}^{\alpha}\langle a*, \vec{R} | P^{\alpha} dP^{\alpha} \wedge dP^{\alpha} P^{\alpha} | a, \vec{R} \rangle^{\alpha}. \tag{92}$$

The structure is characterized by the higher order cocycle relations:

$$h^{\beta\gamma\delta} (h^{\alpha\gamma\delta})^{-1} h^{\alpha\beta\delta} (h^{\alpha\beta\gamma})^{-1} = 1, \tag{93}$$

$$h^{\alpha\beta\gamma}h^{\alpha\gamma\beta}(h^{\beta\gamma\beta})^{-1} = h^{\alpha\beta\gamma}h^{\beta\alpha\gamma}(h^{\alpha\beta\alpha})^{-1} = 1, \tag{94}$$

$$h^{\alpha\alpha\beta} = h^{\alpha\beta\beta} = 1, \tag{95}$$

$$h^{\alpha\alpha\alpha} = 1, \tag{96}$$

and by the higher order gluing relations:

$$\eta^{\beta} - \eta^{\alpha} = A^{\alpha\beta} + (g^{\alpha\beta})^{-1}dg^{\alpha\beta}, \tag{97}$$

$$A^{\alpha\beta} - A^{\alpha\gamma} + A^{\beta\gamma} = -(h^{\alpha\beta\gamma})^{-1}dh^{\alpha\beta\gamma}, \tag{98}$$

$$B^{\beta} - B^{\alpha} = dA^{\alpha\beta}. \tag{99}$$

The Berry phase associated with a closed path $\mathcal{C}$ is associated with the horizontal lift in the 2-bundle of $\mathcal{S}$ (a surface having $\mathcal{C}$ as border):

$$e^{-\gamma_a(\mathcal{S})} = \prod_{\alpha} e^{\int\int_{\sigma^{\alpha}} B^{\alpha}} \prod_{\alpha,\beta} e^{\int\int_{E^{\alpha\beta}} A^{\alpha\beta}} \prod_{\alpha,\beta,\gamma} h^{\alpha\beta\gamma}(\vec{R}^{\alpha\beta\gamma}). \tag{100}$$

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