

ABSTRACT ADIABATIC CHARGE PUMPING

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This paper is devoted to the analysis of an abstract formula describing quantum adiabatic charge pumping in a general context. We consider closed systems characterized by a slowly varying time-dependent Hamiltonian depending on an external parameter α . The current operator, defined as the derivative of the Hamiltonian with respect to α , once integrated over some time interval, gives rise to a charge pumped through the system over that time span. We determine the first two leading terms in the adiabatic parameter of this pumped charge under the usual gap hypothesis. In particular, in case the Hamiltonian is time periodic and has discrete non-degenerate spectrum, the charge pumped over a period is given to leading order by the derivative with respect to α of the corresponding dynamical and geometric phases.

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1. Introduction

1.1. Motivation

Many physical systems of interest can be described by means of a time-dependent Hamiltonian reflecting the action of external agents on the system or taking into account the variations of its environment, in an effective manner. In such generality, little can be said about the evolution of the system. However, when the Hamiltonian is a slowly varying function of time with respect to some fixed relevant time scale of the system, the adiabatic theorem of quantum mechanics provides a very useful tool to describe the evolution in an approximate way under certain hypotheses, see e.g. [8, 23]. The mathematical circumstances under which an adiabatic theorem

of quantum mechanics can be proven are diverse, starting with the well-known gap hypothesis in the spectrum of the Hamiltonian, see e.g. [19, 26, 4], which will be enough for our purposes. Note, however, that higher order approximations [27, 28, 18], generalizations to situations where the gap assumption fails [9, 2] or where self-adjointness does not hold [31, 17] or to a spacetime setting [33] have been carried out over the years; see also the review [15] and references therein.

In several physical systems, the Hamiltonian also depends on some external parameter, $\alpha \in \mathbb{R}$, associated with an instantaneous charge *current*. For instance, this is the case for models used in the study of the quantum Hall effect where the electric current is monitored by a magnetic flux, α , through the sample which appears as a parameter in the Hamiltonian $H_\alpha(s)$. The instantaneous current operator is given by $\partial_\alpha H_\alpha(s)$ see e.g. [29, 4]. A similar phenomenon holds in models of mesoscopic physics where the current across the device they describe is driven by a phase difference. Examples are superconducting systems used as Cooper pair pumps [30, 1, 13, 14, 24, 25, 10]. In both cases, the physical reason behind the interpretation of $\partial_\alpha H_\alpha(s)$ as a current comes from the fact that a variation of magnetic fluxes induces currents.

Accordingly, for an initial state ψ , the charge pumped through the system in that state between time 0 and τ is given by

$$\langle Q_\alpha(\tau) \rangle_\psi := \int_0^\tau \langle U_\alpha(\tau') \psi | (\partial_\alpha H_\alpha(\tau')) U_\alpha(\tau') \psi \rangle d\tau',$$

where $U_\alpha(\tau)$ is the evolution operator. It is often true in applications that the time variation of the Hamiltonian is periodic, in which case one considers the charge transported over a time period. For a slowly varying Hamiltonian H_α with an isolated part of spectrum and an initial state ψ in the corresponding spectral subspace, the pumped charge $\langle Q_\alpha(\tau) \rangle_\psi$ can be computed by making use of an adiabatic approximation. This yields the starting point of the analysis of the geometrical and topological properties of this quantity. In particular, when the dependence of the Hamiltonian is periodic in both the time and parameter α , it is well known that the pumped charge over a cycle suitably *averaged* over α is quantized and related to topological indices associated with the spectral projector, see e.g. [29, 5, 4]. However, in certain mesoscopic devices, the observed charge transfers do correspond to $\langle Q_\alpha(\tau) \rangle_\psi$ for fixed values of α [10], which is also known to differ significantly from the average value over α , [4].

Note that in contrast to other mathematical studies, see e.g. [3], the time-dependent adiabatic pumps we consider are not open systems in the following sense: their dynamics for frozen times is not characterized by an explicit scattering matrix between infinite reservoirs. Therefore, no formula is available to determine the charge transport in terms of matrix elements of the instantaneous scattering matrix [11, 12].

The purpose of this paper is to provide a mathematical derivation of the adiabatic pumped charge through the system in an abstract setting that covers the physical situations described above.

We focus on the derivation of a controlled approximate expression for $\langle Q_\alpha(\tau) \rangle_\psi$, the charge pumped through the system over a time span $[0, \tau]$ for fixed values of α up to vanishing corrections in the adiabatic regime. We work in a quite general framework, with arbitrary dependence of the Hamiltonian on time and α , assuming only the existence of an isolated part of spectrum in $H_\alpha(\tau)$. This allows us to recover as particular cases the time-periodic situations and, for an isolated eigenvalue in the spectrum, expressions for the charge pumped over a period used in several contexts, involving the geometric phase or its non-Abelian version [10].

Moreover, we hope the present analysis can provide an introduction to the mathematical methods used in the analysis of adiabatic phenomena beyond the matrix case.

1.2. Setup and results

Let us describe more precisely the mathematical setup and results we prove in the next section. The adiabatic regime is characterized by a dimensionless time scale $1/\epsilon$, which is assumed to be long, i.e. $\epsilon \ll 1$. The Hamiltonian is assumed to depend on ϵ as follows: $H_\alpha = H_\alpha(\epsilon\tau)$. This makes the Hamiltonian slowly varying since it takes a time of order $1/\epsilon$ for it to change significantly. Introducing the rescaled time variable $t = \epsilon\tau$, of order one, the corresponding evolution operator U_α also depends on the small parameter ϵ and satisfies

$$i\epsilon\partial_t U_\alpha(t) = H_\alpha(t)U_\alpha(t), \quad U_\alpha(0) = \mathbb{I}.$$

Accordingly, for any initial state ψ , the charge pumped over a time interval $[0, \tau = t/\epsilon]$ now reads

$$\langle Q_\alpha(t) \rangle_\psi = \frac{1}{\epsilon} \int_0^t \langle U_\alpha(s)\psi | (\partial_\alpha H_\alpha(s)) U_\alpha(s)\psi \rangle ds,$$

which is of order $1/\epsilon$. From here on, s is consistently the rescaled dummy integration time variable. In order to capture the leading term, up to a vanishing error in the adiabatic limit $\epsilon \rightarrow 0$, it is necessary to compute the next-to-leading order approximation of the evolution operator in ϵ . We do this in Theorem 2.2, under the sole gap hypothesis, after having recalled the usual leading order adiabatic approximation in Theorem 2.1. Then we focus on initial conditions that belong to the spectral projector corresponding to the isolated part of spectrum. The corresponding general expression for the charge operator is provided in Proposition 2.1. A far more tractable expression is obtained for an isolated eigenvalue, of arbitrary degeneracy, as Corollary 2.1. In case the Hamiltonian is periodic in time of period one, we recover in Corollary 2.2 the expressions used in [10]. The simplest instance being for a simple isolated eigenvalue $E_\alpha(t)$, such that $H_\alpha(t)\psi(t) = E_\alpha(t)\psi(t)$. The charge pumped over a cycle for the initial condition $\psi = \psi(0)$ then reads

$$\langle Q_\alpha(1) \rangle_\psi = \frac{1}{\epsilon} \int_0^1 \partial_\alpha E_\alpha(s) ds + \partial_\alpha \beta_\alpha + O(\epsilon).$$

Here the first term is the usual dynamic contribution, whereas the second one is of geometric nature [32, 34], β_α being the familiar geometric phase [6, 7]. In case the eigenvalue is degenerate, the matrix-valued non-Abelian generalization of this quantity, $B(1)$, to be used is of course also described in Corollary 2.1.

The last section of the paper is devoted to the study of a family of examples used in the physical application described in [10]. The Hamiltonians considered display a permanently degenerate isolated eigenvalue for which explicit computations of $B(1)$ can be performed. In case the dimension of the corresponding degenerate eigenspace is two, which corresponds to the applications considered in [10], we also provide a geometric interpretation of $B(1)$.

2. Analysis

In this section, we provide the abstract rigorous mathematical analysis behind the formulas used in the study of the physical phenomenon of adiabatic charge pumping. We feel such a rigorous analysis is useful because of the presence of a variety of formulations of geometric adiabatic charge pumping in the literature which have similar features. This allows us to make clear under which hypotheses we work. Also, we believe the analysis is interesting in itself because it applies under very general conditions and it might be of use in different frameworks.

Let \mathcal{H} be a separable Hilbert space and $H_\alpha(t)$ be a bounded self-adjoint operator on \mathcal{H} . In order not to obscure the analysis by side issues regarding the technical difficulties related to the use of unbounded operators, we stick to the bounded case. For the same reason, we assume the parameter α is real-valued. We work under the

Regularity assumption. The map $(t, \alpha) \mapsto H_\alpha(t)$ is C^3 in the norm sense, as a bounded operator valued function, with $(t, \alpha) \in [0, 1] \times [0, 1]$.

Let $U_\alpha(t)$ be the solution to

$$i\epsilon \dot{U}_\alpha(t) = H_\alpha(t)U_\alpha(t), \quad U_\alpha(0) = \mathbb{I}, \quad (1)$$

where we rescaled time for convenience. Since $\mathcal{L}(\mathcal{H})$ is a Banach space, it follows from the general theory of differential equations, see e.g. [21] Chap. VI, that the solution to (1) is as regular in (t, α) as the Hamiltonian is, i.e.

$$(t, \alpha) \mapsto U_\alpha(t) \in C^3([0, 1] \times [0, 1], \mathcal{L}(\mathcal{H})). \quad (2)$$

The variable α is a parameter whose variations monitor fluxes or currents in the time-dependent physical device described by $H_\alpha(t)$. The *current* operator being defined as $\partial_\alpha H_\alpha(t)$, if $\psi \in \mathcal{H}$ is a normalized initial state, the average charge pumped by the system between the physical times 0 and t/ϵ is equal to

$$\langle Q_\alpha(t) \rangle_\psi = \frac{1}{\epsilon} \int_0^t \langle U_\alpha(s)\psi | (\partial_\alpha H_\alpha(s)) U_\alpha(s)\psi \rangle ds. \quad (3)$$

This leads us to study the charge operator $Q_\alpha(t)$, whose matrix elements carry the physical interpretation, defined by

$$Q_\alpha(t) = \frac{1}{\epsilon} \int_0^t U_\alpha^{-1}(s)(\partial_\alpha H_\alpha(s))U_\alpha(s)ds. \tag{4}$$

The geometrical properties of another *average* charge operator in the adiabatic limit have been investigated in [5] under the assumption that $(t, \alpha) \mapsto H_\alpha(t)$ is periodic in both variables. The average there is taken both over the period of the time-dependent Hamiltonian and over the flux variable α . By contrast, we analyze the adiabatic behavior of the charge operator for fixed values of α and t . In case of a time periodic Hamiltonian, the geometric content of the charge operator over a period is elucidated.

As already observed in [4] for example, an alternative exact expression for $Q_\alpha(t)$ reads as follows:

$$Q_\alpha(t) = iU_\alpha^{-1}(t)\partial_\alpha U_\alpha(t). \tag{5}$$

It is a consequence of the regularity of $U_\alpha(t)$ and the computation

$$\begin{aligned} i\epsilon\partial_t (U_\alpha^{-1}(t)\partial_\alpha U_\alpha(t)) &= -U_\alpha^{-1}(t)H_\alpha(t)\partial_\alpha U_\alpha(t) \\ &\quad + U_\alpha^{-1}(t)\partial_\alpha(H_\alpha(t)U_\alpha(t)) \\ &= U_\alpha^{-1}(t)(\partial_\alpha H_\alpha(t))U_\alpha(t), \end{aligned} \tag{6}$$

with $\partial_\alpha U_\alpha(0) = 0$. Note that we also deduce from (5) the general estimate

$$\partial_\alpha U_\alpha(t) = O(t/\epsilon), \tag{7}$$

which is sharp in the scalar case.

We proceed by considering the adiabatic limit $\epsilon \rightarrow 0$ under the familiar

Gap hypothesis. Assume the spectrum $\sigma(H_\alpha(t))$ consists in two disjoint parts $\sigma(H_\alpha(t)) = \sigma_\alpha(t) \cup \overline{\sigma_\alpha}(t)$ such that

$$\inf_{(t,\alpha) \in [0,1]^2} \text{dist}(\sigma_\alpha(t), \overline{\sigma_\alpha}(t)) = g > 0. \tag{8}$$

Let $P_\alpha(t)$ be the spectral projector of $H_\alpha(t)$ associated with $\sigma_\alpha(t)$ by means of the Riesz formula

$$P_\alpha(t) = -\frac{1}{2\pi i} \int_\gamma (H_\alpha(t) - z)^{-1} dz, \tag{9}$$

where γ is a loop in the complex plane encircling $\sigma_\alpha(t)$ only, which is locally independent of (t, α) and let $\overline{P_\alpha}(t) = \mathbb{I} - P_\alpha(t)$ be its complement. These projectors are as regular as the Hamiltonian is and moreover satisfy for any (t, α)

$$P_\alpha(t)\dot{P}_\alpha(t)P_\alpha(t) = P_\alpha(t)(\partial_\alpha P_\alpha(t))P_\alpha(t) \equiv 0, \tag{10}$$

as easily seen by differentiating the identity $P_\alpha(t)^2 = P_\alpha(t)$.

We introduce two unitary operators whose product will approach the true evolution in the adiabatic limit. Let $W_\alpha(t)$ and $\Phi_\alpha(t)$ be defined by

$$i\dot{W}_\alpha(t) = K_\alpha(t)W_\alpha(t), \quad W_\alpha(0) = \mathbb{I}, \tag{11}$$

$$i\epsilon\dot{\Phi}_\alpha(t) = W_\alpha^{-1}(t)H_\alpha(t)W_\alpha(t)\Phi_\alpha(t), \quad \Phi_\alpha(0) = \mathbb{I}, \tag{12}$$

where

$$K_\alpha(t) = i[\dot{P}_\alpha(t), P_\alpha(t)]. \tag{13}$$

It is a classical fact that the following relations hold,

$$W_\alpha(t)P_\alpha(0) = P_\alpha(t)W_\alpha(t), \tag{14}$$

$$\Phi_\alpha(t)P_\alpha(0) = P_\alpha(0)\Phi_\alpha(t). \tag{15}$$

The first identity is proven by showing that both operators satisfy the same differential equation with the same initial condition, exploiting the relation

$$P_\alpha(t)K_\alpha(t)P_\alpha(t) = 0, \tag{16}$$

which is a consequence of (10), see e.g. [19]. The second identity follows from the fact that, by construction, the generator of $\Phi_\alpha(t)$ commutes with $P_\alpha(0)$.

We have

Theorem 2.1. (Adiabatic Theorem) *Assuming the Regularity and Gap hypotheses above, we have for any $(t, \alpha) \in [0, 1] \times [0, 1]$,*

$$U_\alpha(t) = W_\alpha(t)\Phi_\alpha(t) + O(\epsilon), \tag{17}$$

where the error term is uniform in $\alpha \in [0, 1]$.

Remarks. (i) As stated, the theorem dates back to [26], [27] and was generalized by [4] to the unbounded case. The fact that the error term is uniform in $\alpha \in [0, 1]$ is a straightforward consequence of our Regularity Assumptions and of the Gap hypothesis which is uniform in $\alpha \in [0, 1]$.

(ii) In case $\sigma_\alpha(t)$ consists of a single eigenvalue $E_\alpha(t)$, the theorem says

$$U_\alpha(t)P_\alpha(0) = e^{-\frac{i}{\epsilon} \int_0^t E_\alpha(s) ds} P_\alpha(t)W_\alpha(t) + O(\epsilon). \tag{18}$$

This is the statement proven by Kato in [19].

(iii) Further assuming $E_\alpha(t)$ is nondegenerate and the time-dependent Hamiltonian is periodic in time, of period 1, we get the *geometric* or Berry phase out of this formula as follows:

Let $\varphi_\alpha(0) = P_\alpha(0)\varphi_\alpha(0)$, be a normalized eigenvector associated with $E_\alpha(0)$. Then, property (14) implies that $\forall (\alpha, t) \in [0, 1]^2$

$$\varphi_\alpha(t) = W_\alpha(t)\varphi_\alpha(0) \quad \text{satisfies } H_\alpha(t)\varphi_\alpha(t) = E_\alpha(t)\varphi_\alpha(t) \tag{19}$$

and (11) together with (16) yield

$$\langle \varphi_\alpha(t) | \dot{\varphi}_\alpha(t) \rangle = 0. \tag{20}$$

By periodicity, $\varphi_\alpha(0)$ and $\varphi_\alpha(1)$ differ only by a phase

$$\varphi_\alpha(1) = e^{-i\beta_\alpha} \varphi_\alpha(0), \tag{21}$$

where β_α is the geometric or Berry phase. Therefore we finally get

$$U_\alpha(1)\varphi_\alpha(0) = e^{-\frac{i}{\epsilon} \int_0^1 E_\alpha(s) ds} e^{-i\beta_\alpha} \varphi_\alpha(0) + O(\epsilon). \tag{22}$$

This shows concretely that the operator $W_\alpha(t)$ carries the geometrical content of the adiabatic theorem. Note finally that if $t \mapsto \psi_\alpha(t)$ is another choice of instantaneous normalized eigenvector associated with $E_\alpha(t)$ which is periodic in time, these vectors differ from $\varphi_\alpha(t)$ by a phase for any time

$$\varphi_\alpha(t) = e^{-ib_\alpha(t)} \psi_\alpha(t). \tag{23}$$

Using (20), we get an explicit expression for b_α

$$b_\alpha(t) = b_\alpha(0) - i \int_0^t \langle \psi_\alpha(s) | \dot{\psi}_\alpha(s) \rangle ds. \tag{24}$$

Therefore $\varphi_\alpha(1) = e^{-\int_0^1 \langle \psi_\alpha(s) | \dot{\psi}_\alpha(s) \rangle ds} \varphi_\alpha(0)$ and

$$\beta_\alpha = -i \int_0^1 \langle \psi_\alpha(s) | \dot{\psi}_\alpha(s) \rangle ds. \tag{25}$$

Coming back to the charge operator, we see that in order to estimate $Q_\alpha(t)$ up to errors of order $O(\epsilon)$ vanishing in the adiabatic limit, we need to control the evolution to order $O(\epsilon^2)$, see (4). This can be achieved as follows, see e.g. [27, 4, 18, 28], etc.

Let

$$H_\alpha^{(1)}(t) = H_\alpha(t) - \epsilon K_\alpha(t), \tag{26}$$

which satisfies the gap assumption (8) for ϵ small enough since $K_\alpha(t)$ is bounded, i.e.

$$\sigma(H_\alpha^{(1)}(t)) = \sigma_\alpha^{(1)}(t) \cup \overline{\sigma_\alpha^{(1)}(t)}. \tag{27}$$

Hence we can define the corresponding spectral projectors $P_\alpha^{(1)}(t)$ by (9) and $\overline{P_\alpha^{(1)}(t)} = \mathbb{I} - P_\alpha^{(1)}(t)$. By perturbation theory we have for ϵ small enough

$$(H_\alpha^{(1)}(t) - z)^{-1} = (H_\alpha(t) - z)^{-1} + (H_\alpha(t) - z)^{-1} \epsilon K_\alpha(t) (H_\alpha(t) - z)^{-1} + O(\epsilon^2), \tag{28}$$

where the remainder term is C^2 in (t, α) and of order ϵ^2 , as a uniformly convergent Neumann series. The same is true for the perturbed projector expressed using (9) with the same path γ for ϵ small enough,

$$P_\alpha^{(1)}(t) = P_\alpha(t) - \epsilon \mathcal{R}_\alpha(K_\alpha)(t) + O(\epsilon^2), \tag{29}$$

where, for any bounded operator B ,

$$\mathcal{R}_\alpha(B)(t) = \frac{1}{2i\pi} \oint_\gamma (H_\alpha(t) - z)^{-1} B (H_\alpha(t) - z)^{-1} dz \tag{30}$$

with γ is a loop encircling $\sigma_\alpha^{(1)}(t)$, which can be chosen locally independently of (t, α) . Let us also note here for future reference that

$$P_\alpha(t) \mathcal{R}_\alpha(K_\alpha)(t) P_\alpha(t) = 0, \tag{31}$$

as a consequence of the fact that the resolvent and the spectral projectors of $H_\alpha(t)$ commute and of (16). We set

$$K_\alpha^{(1)}(t) = i[\dot{P}_\alpha^{(1)}(t), P_\alpha^{(1)}(t)] = K_\alpha(t) + O(\epsilon), \tag{32}$$

where, again, the error term can be differentiated without harm. We define $W_\alpha^{(1)}(t)$ and $\Phi_\alpha^{(1)}(t)$ by

$$i\dot{W}_\alpha^{(1)}(t) = K_\alpha^{(1)}(t)W_\alpha^{(1)}(t), \quad W_\alpha^{(1)}(0) = \mathbb{I}, \tag{33}$$

$$i\epsilon\dot{\Phi}_\alpha^{(1)}(t) = W_\alpha^{(1)-1}(t) \left(H_\alpha^{(1)}(t) + \epsilon \mathcal{D}_\alpha^1(K_\alpha(t)) \right) W_\alpha^{(1)}(t) \Phi_\alpha^{(1)}(t), \tag{34}$$

$$\Phi_\alpha^{(1)}(0) = \mathbb{I},$$

where, for any bounded operator B , $\mathcal{D}_\alpha^1(B) = P_\alpha^{(1)} B P_\alpha^{(1)} + \overline{P_\alpha^{(1)}} B \overline{P_\alpha^{(1)}}$. One gets that the relations equivalent to (14), (15) hold with superscript “(1)” at the relevant operators.

The point of this construction is that it gives a

Theorem 2.2. (Second Order Adiabatic Theorem) *Under the hypotheses of Theorem 2.1, we have for any $(t, \alpha) \in [0, 1] \times [0, 1]$,*

$$U_\alpha(t) = W_\alpha^{(1)}(t) \Phi_\alpha^{(1)}(t) + O(\epsilon^2), \tag{35}$$

where the error term is uniform in $\alpha \in [0, 1]$.

Remarks. (i) If the Hamiltonian is regular enough in the t variable, it is possible to get arbitrary order adiabatic theorems.

(ii) These adiabatic theorems further yield the perturbative estimate

$$W_\alpha^{(1)}(t) \Phi_\alpha^{(1)}(t) = W_\alpha(t) \Phi_\alpha(t) + O(\epsilon). \tag{36}$$

(iii) This result can be found under various guises in [27, 4, 18, 28], As such, it is stated and proven in [16], Theorem 3.3.1, p. 38 (for α fixed). Again, the uniformity in α of the error term is easily checked.

As a consequence of this second theorem, we have the approximation

$$Q_\alpha(t) = \frac{1}{\epsilon} \int_0^t \Phi_\alpha^{(1)-1}(s) W_\alpha^{(1)-1}(s) \partial_\alpha H_\alpha(s) W_\alpha^{(1)}(s) \Phi_\alpha^{(1)}(s) ds + O(\epsilon). \quad (37)$$

We point out again that the analog of the formula above with operators W_α and Φ_α in place of $W_\alpha^{(1)}$ and $\Phi_\alpha^{(1)}$ yields an error term of order one, instead of $O(\epsilon)$.

We are interested in the matrix elements of $Q_\alpha(t)$ with vectors belonging to the spectral subspace $P_\alpha(0)\mathcal{H}$, so that from now on, we focus on the operator $P_\alpha(0)Q_\alpha(t)P_\alpha(0)$. The goal is to express the information in (37) in terms of more familiar quantities, like dynamical phases and geometric phases, in certain cases.

The next technical result says that we can express $P_\alpha(0)Q_\alpha(t)P_\alpha(0)$ as a leading term (of order $1/\epsilon$) that corresponds to the replacement of $U_\alpha(t)$ by its second order adiabatic approximation with $P_\alpha^{(1)}(0)$ in place of $P_\alpha(0)$ and $\partial_\alpha H_\alpha^{(1)}(t)$ in place of $\partial_\alpha H_\alpha(t)$ plus a term of order ϵ^0 which will give rise to the geometric contribution:

Proposition 2.1. *Under the hypotheses of Theorem 2.1, we have for any $(t, \alpha) \in [0, 1] \times [0, 1]$,*

$$\begin{aligned} & P_\alpha(0)Q_\alpha(t)P_\alpha(0) \\ &= P_\alpha(0) \left(\frac{1}{\epsilon} \int_0^t \Phi_\alpha^{(1)-1}(s) W_\alpha^{(1)-1}(s) \right. \\ &\quad \times P_\alpha^{(1)}(s) \partial_\alpha H_\alpha^{(1)}(s) P_\alpha^{(1)}(s) W_\alpha^{(1)}(s) \Phi_\alpha^{(1)}(s) ds \left. \right) P_\alpha(0) \\ &\quad + P_\alpha(0) \left(\int_0^t \Phi_\alpha^{-1}(s) W_\alpha^{-1}(s) \partial_\alpha K_\alpha(s) W_\alpha(s) \Phi_\alpha(s) ds \right) P_\alpha(0) + O(\epsilon). \end{aligned} \quad (38)$$

Proof. Plugging the relations

$$P_\alpha(t) = P_\alpha(t)^2 = P_\alpha(t)(P_\alpha^{(1)}(t) - \epsilon \mathcal{R}_\alpha(K_\alpha)(t)) + O(\epsilon^2) \quad (39)$$

and

$$\partial_\alpha H_\alpha(t) = \partial_\alpha H_\alpha^{(1)}(t) + \epsilon \partial_\alpha K_\alpha(t) \quad (40)$$

into the expression (37), and making use of the properties of $W_\alpha^{(1)}$ and $\Phi_\alpha^{(1)}$ together with (36), we get

$$\begin{aligned} & P_\alpha(0)Q_\alpha(t)P_\alpha(0) \\ &= P_\alpha(0) \left(\frac{1}{\epsilon} \int_0^t \Phi_\alpha^{(1)-1}(s) W_\alpha^{(1)-1}(s) P_\alpha^{(1)}(s) \right. \\ &\quad \times \partial_\alpha H_\alpha^{(1)}(s) P_\alpha^{(1)}(s) W_\alpha^{(1)}(s) \Phi_\alpha^{(1)}(s) ds \left. \right) P_\alpha(0) \\ &\quad + P_\alpha(0) \left(\int_0^t \Phi_\alpha^{-1}(s) W_\alpha^{-1}(s) \partial_\alpha K_\alpha(s) W_\alpha(s) \Phi_\alpha(s) ds \right) P_\alpha(0) \end{aligned}$$

$$\begin{aligned}
 & - P_\alpha(0) \left(\mathcal{R}_\alpha(K_\alpha)(0) \int_0^t \Phi_\alpha^{-1}(s) W_\alpha^{-1}(s) \partial_\alpha H_\alpha(s) W_\alpha(s) \Phi_\alpha(s) ds \right. \\
 & \left. + \int_0^t \Phi_\alpha^{-1}(s) W_\alpha^{-1}(s) \partial_\alpha H_\alpha(s) W_\alpha(s) \Phi_\alpha(s) ds \mathcal{R}_\alpha(K_\alpha)(0) \right) P_\alpha(0) + O(\epsilon).
 \end{aligned} \tag{41}$$

We want to show that the last two terms are actually of order ϵ , by integration by parts. We consider the last term only, since the previous one can be dealt with in a similar fashion. Using property (31), the integrand of this term is

$$P_\alpha(0) \Phi_\alpha^{-1}(s) W_\alpha^{-1}(s) P_\alpha(s) \partial_\alpha H_\alpha(s) \overline{P}_\alpha(s) W_\alpha(s) \Phi_\alpha(s) \overline{P}_\alpha(0). \tag{42}$$

Differentiating the following identity with respect to α

$$H_\alpha(s) = P_\alpha(s) H_\alpha(s) P_\alpha(s) + \overline{P}_\alpha(s) H_\alpha(s) \overline{P}_\alpha(s), \tag{43}$$

we get

$$\begin{aligned}
 P_\alpha(s) \partial_\alpha H_\alpha(s) \overline{P}_\alpha(s) &= P_\alpha(s) H_\alpha(s) \partial_\alpha P_\alpha(s) \overline{P}_\alpha(s) + P_\alpha(s) \partial_\alpha \overline{P}_\alpha(s) H_\alpha(s) \overline{P}_\alpha(s) \\
 &= P_\alpha(s) [H_\alpha(s), \partial_\alpha P_\alpha(s)] \overline{P}_\alpha(s).
 \end{aligned} \tag{44}$$

Hence, together with (11), we can write

$$\begin{aligned}
 (42) &= P_\alpha(0) \Phi_\alpha^{-1}(s) W_\alpha^{-1}(s) [H_\alpha(s), \partial_\alpha P_\alpha(s)] W_\alpha(s) \Phi_\alpha(s) \overline{P}_\alpha(0) \\
 &= P_\alpha(0) \Phi_\alpha^{-1}(s) [W_\alpha^{-1}(s) H_\alpha(s) W_\alpha(s), W_\alpha^{-1}(s) \partial_\alpha P_\alpha(s) W_\alpha(s)] \Phi_\alpha(s) \overline{P}_\alpha(0) \\
 &= -i\epsilon \partial_s (P_\alpha(0) \Phi_\alpha^{-1}(s) W_\alpha^{-1}(s) \partial_\alpha P_\alpha(s) W_\alpha(s) \Phi_\alpha(s) \overline{P}_\alpha(0)) \\
 &\quad + i\epsilon P_\alpha(0) \Phi_\alpha^{-1}(s) \partial_s (W_\alpha^{-1}(s) \partial_\alpha P_\alpha(s) W_\alpha(s)) \Phi_\alpha(s) \overline{P}_\alpha(0).
 \end{aligned} \tag{45}$$

Thus, since $W_\alpha(s)$ and $P_\alpha(s)$ are independent of ϵ , and $\Phi_\alpha(s)$ is unitary, when integrated between 0 and $t \in [0, 1]$, this yields a contribution of order ϵ . \square

Remark. We can get an alternative expression for the zeroth order term by making use of the identity

$$\begin{aligned}
 P_\alpha(s) \partial_\alpha K_\alpha(s) P_\alpha(s) &= iP_\alpha(s) \partial_\alpha [\dot{P}_\alpha(s), P_\alpha(s)] P_\alpha(s) \\
 &= iP_\alpha(s) [\dot{P}_\alpha(s), \partial_\alpha P_\alpha(s)] P_\alpha(s).
 \end{aligned} \tag{46}$$

We want to focus now on the situation $\sigma_\alpha(t) = \{E_\alpha(t)\}$, that is when $P_\alpha(t)$ corresponds to an isolated eigenvalue $E_\alpha(t)$, not necessarily simple, possibly associated with an infinite dimensional spectral subspace. Which means that

$$H_\alpha(t) = E_\alpha(t) P_\alpha(t) + \overline{P}_\alpha(t) H_\alpha(t) \overline{P}_\alpha(t), \tag{47}$$

$$(H_\alpha(t) - z)^{-1} = \frac{P_\alpha(t)}{E_\alpha(t) - z} + \overline{P}_\alpha(t) (H_\alpha(t) - z)^{-1} \overline{P}_\alpha(t), \tag{48}$$

where the reduced resolvent $\overline{P}_\alpha(t) (H_\alpha(t) - z)^{-1} \overline{P}_\alpha(t)$ is holomorphic for all z 's inside the loop γ of the definition (9) of $P_\alpha(t)$.

This case allows one to distinguish nicely contributions from the dynamical phase and from the geometric phase in the usual adiabatic language, in the periodic case. This comes as a simple

Corollary 2.1. *Assume $\sigma_\alpha(t) = \{E_\alpha(t)\}$, then*

$$P_\alpha(0)Q_\alpha(t)P_\alpha(0) = P_\alpha(0) \left(\frac{1}{\epsilon} \int_0^t \partial_\alpha E_\alpha(s) ds + iW_\alpha^{-1}(t)\partial_\alpha W_\alpha(t) \right) P_\alpha(0) + O(\epsilon). \tag{49}$$

Remarks. (i) We do not use periodicity in any of the variables yet.

(ii) The form of the order zero term is similar to (5), which allows one to interpret it as the geometrical charge transported in the adiabatic process. This is supported by the fact that this term is determined by the spectral projector $P_\alpha(t)$ only.

Proof. We will approximate $P_\alpha^{(1)}(t)H_\alpha^{(1)}(t)$ by $E_\alpha(t)P_\alpha^{(1)}(t)$ by perturbation theory in ϵ . By means of the Riesz formula (9) for $P_\alpha^{(1)}(t)$ we can write

$$\begin{aligned} P_\alpha^{(1)}(t)(H_\alpha^{(1)}(t) - E_\alpha(t)) &= -\frac{1}{2\pi i} \int_\gamma (H_\alpha^{(1)}(t) - z)^{-1} (H_\alpha^{(1)}(t) - E_\alpha(t)) dz \\ &= -\frac{1}{2\pi i} \int_\gamma (z - E_\alpha(t))(H_\alpha^{(1)}(t) - z)^{-1} dz. \end{aligned} \tag{50}$$

We used $\int_\gamma \mathbb{1} dz = 0$. Introducing the perturbed resolvent (28), we get

$$\begin{aligned} P_\alpha^{(1)}(t)(H_\alpha^{(1)}(t) - E_\alpha(t)) &= -\frac{1}{2\pi i} \int_\gamma (z - E_\alpha(t))(H_\alpha(t) - z)^{-1} dz \\ &\quad - \frac{\epsilon}{2\pi i} \int_\gamma (z - E_\alpha(t))(H_\alpha(t) - z)^{-1} K_\alpha(t)(H_\alpha(t) - z)^{-1} + O(\epsilon^2), \end{aligned} \tag{51}$$

where the remainder keeps being of order ϵ^2 when differentiated. By making use of (48) and by the fact that the reduced resolvent is analytic inside γ , one gets from the Cauchy formula that the first term of the right-hand side is zero whereas the second yields

$$-\frac{\epsilon}{2\pi i} \int_\gamma (z - E_\alpha(t))(H_\alpha(t) - z)^{-1} K_\alpha(t)(H_\alpha(t) - z)^{-1} = \epsilon P_\alpha(t)K_\alpha(t)P_\alpha(t). \tag{52}$$

This term is zero due to (16), hence

$$P_\alpha^{(1)}(t)H_\alpha^{(1)}(t) = E_\alpha(t)P_\alpha^{(1)}(t) + O(\epsilon^2), \tag{53}$$

where the remainder term can be differentiated. Therefore

$$\partial_\alpha H_\alpha^{(1)}(t) = \partial_\alpha(E_\alpha(t)P_\alpha^{(1)}(t) + \overline{P_\alpha}(t)H_\alpha^{(1)}(t)\overline{P_\alpha}(t)) + O(\epsilon^2) \tag{54}$$

and we get

$$P_\alpha^{(1)}(t)\partial_\alpha H_\alpha^{(1)}(t)P_\alpha^{(1)}(t) = P_\alpha^{(1)}(t)\partial_\alpha E_\alpha(t) + O(\epsilon^2). \tag{55}$$

This allows us to further simplify the first term in the expression of Proposition 2.1, making use of (29) and (31) to get

$$\begin{aligned} P_\alpha(0) & \left(\frac{1}{\epsilon} \int_0^t \Phi_\alpha^{(1)-1}(s)W_\alpha^{(1)-1}(s)P_\alpha^{(1)}(s)\partial_\alpha H_\alpha^{(1)}(s)P_\alpha^{(1)}(s)W_\alpha^{(1)}(s)\Phi_\alpha^{(1)}(s)ds \right) P_\alpha(0) \\ & = P_\alpha(0)\frac{1}{\epsilon} \int_0^t \partial_\alpha E_\alpha(s)P_\alpha^{(1)}(0)ds P_\alpha(0) + O(\epsilon) \\ & = P_\alpha(0)\frac{1}{\epsilon} \int_0^t \partial_\alpha E_\alpha(s)ds + O(\epsilon). \end{aligned} \tag{56}$$

The last term in the expression of Proposition 2.1 is dealt with as follows. The condition (47) implies

$$\Phi_\alpha^{\pm 1}(t)P_\alpha(0) = P_\alpha(0)e^{\mp \frac{i}{\epsilon} \int_0^t E_\alpha(s)ds} \tag{57}$$

so that we are left with

$$P_\alpha(0) \left(\int_0^t W_\alpha^{-1}(s)\partial_\alpha K_\alpha(s)W_\alpha(s)ds \right) P_\alpha(0). \tag{58}$$

The argument leading from (4) to (5) depends only on the differential equation satisfied by $U_\alpha(t)$, and thus also applies, *mutatis mutandis*, to $W_\alpha(t)$, whose generator is $K_\alpha(t)$. This ends the proof of the corollary. \square

Further specializing to the periodic case we get

Corollary 2.2. *Assume $\sigma_\alpha(t) = \{E_\alpha(t)\}$ and suppose $t \mapsto H_\alpha(t)$ is periodic in t , of period 1. Then,*

(i) *if $E_\alpha(t)$ is nondegenerate*

$$\langle \varphi_\alpha(0) | Q_\alpha(1) \varphi_\alpha(0) \rangle = \frac{1}{\epsilon} \int_0^1 \partial_\alpha E_\alpha(s)ds + \partial_\alpha \beta_\alpha + O(\epsilon), \tag{59}$$

where $\varphi_\alpha(0)$ is any normalized eigenvector at $t = 0$ and β_α is the corresponding geometric or Berry phase,

(ii) *if $E_\alpha(t)$ is degenerate and $\{\varphi_\alpha^{(r)}(0) \mid r \in \mathbb{N}\}$ denotes an orthonormal basis of $P_\alpha(0)\mathcal{H}$, we have*

$$\langle \varphi_\alpha^{(r)}(0) | Q_\alpha(1) \varphi_\alpha^{(s)}(0) \rangle = \frac{1}{\epsilon} \int_0^1 \partial_\alpha E_\alpha(s)ds + i \langle \varphi_\alpha^{(r)}(t) | \partial_\alpha \varphi_\alpha^{(s)}(t) \rangle|_0^1 + O(\epsilon), \tag{60}$$

where $\varphi_\alpha^{(r)}(t) = W_\alpha(t)\varphi_\alpha^{(r)}(0)$, $r \in \mathbb{N}$,

(iii) if $E_\alpha(t)$ is finitely degenerate, and if $\{\psi_\alpha^{(r)}(t), | r \in \{1, 2, \dots, N\}\}$ denotes a C^1 , 1-periodic orthonormal basis of $P_\alpha(t)\mathcal{H}$, we can write

$$\begin{aligned} \langle \varphi_\alpha^{(r)}(0) | Q_\alpha(1) \varphi_\alpha^{(s)}(0) \rangle &= \frac{1}{\epsilon} \int_0^1 \partial_\alpha E_\alpha(s) ds \\ &+ i \left(\sum_{q, q'} \overline{B_\alpha^{q', r}}(1) B_\alpha^{q, s}(1) \langle \psi_\alpha^{(q')} (0) | \partial_\alpha \psi_\alpha^{(q)} (0) \rangle \right. \\ &\left. + \sum_q \overline{B_\alpha^{q, r}}(1) \partial_\alpha B_\alpha^{q, s}(1) - \langle \psi_\alpha^{(r)}(0) | \partial_\alpha \psi_\alpha^{(s)}(0) \rangle \right) + O(\epsilon), \end{aligned} \quad (61)$$

where $B_\alpha(t)$ solves the ODE

$$\dot{B}_\alpha(t) = \Gamma_\alpha(t) B_\alpha(t), \quad B_\alpha(0) = \mathbb{I}, \quad (62)$$

with $\Gamma_\alpha(t)$ defined by its matrix elements in the basis $\{\psi_\alpha^{(r)}(0)\}_{r=1, \dots, N}$

$$\langle \psi_\alpha^{(s)}(0) | \Gamma_\alpha(t) \psi_\alpha^{(r)}(0) \rangle = -\langle \psi_\alpha^{(s)}(t) | \dot{\psi}_\alpha^{(r)}(t) \rangle. \quad (63)$$

Remarks. (i) An explicit quantity for the geometric part of the charge transported is always available in the nondegenerate case only, see (25). In the degenerate case, the geometric part is determined by the solution to a (second order at least) ordinary differential equation. No explicit solution is available in general and, moreover, the equation is parameter free which forbids an asymptotic analysis. However, as we explain below, there are special cases of interest in which an explicit expression is available for this geometric contribution.

(ii) The third point is a mere restatement of the second one, making use of an *a priori* time-dependent basis of the eigenspace provided by an independent spectral analysis.

Proof. To get the second statement, we compute

$$\begin{aligned} &i \langle \varphi_\alpha^{(r)}(0) | W_\alpha^{-1}(t) (\partial_\alpha W_\alpha(t)) \varphi_\alpha^{(s)}(0) \rangle \\ &= i \langle \varphi_\alpha^{(r)}(0) | (W_\alpha^{-1}(t) (\partial_\alpha W_\alpha(t)) \varphi_\alpha^{(s)}(0)) - W_\alpha^{-1}(t) W_\alpha(t) \partial_\alpha \varphi_\alpha^{(s)}(0) \rangle \\ &= i \langle \varphi_\alpha^{(r)}(t) | \partial_\alpha \varphi_\alpha^{(s)}(t) \rangle - i \langle \varphi_\alpha^{(r)}(0) | \partial_\alpha \varphi_\alpha^{(s)}(0) \rangle. \end{aligned} \quad (64)$$

The first statement follows from $\varphi_\alpha^{(s)}(t) = \varphi_\alpha^{(r)}(t) = \varphi_\alpha(t)$ together with the expression (21). Finally, the third statement is proven as follows. Let us introduce

$$\varphi_\alpha^{(r)}(t) = W_\alpha(t) \psi_\alpha^{(r)}(0) \quad \text{and} \quad \psi_\alpha^{(r)}(t) = V_\alpha(t) \psi_\alpha^{(r)}(0), \quad r = 1, \dots, N, \quad (65)$$

which defines the unitary $V_\alpha(t)$. The link between these two bases will be made by means of the unitary operator $B_\alpha(t)$ defined by

$$B_\alpha(t) = V_\alpha^{-1}(t) W_\alpha(t). \quad (66)$$

By construction, $[B_\alpha(t), P_\alpha(0)] = 0$ for any $t \in [0, 1]$, so that $[\dot{B}_\alpha(t), P_\alpha(0)] = 0$ as well. We compute

$$\dot{B}_\alpha(t) = B_\alpha(t)W_\alpha^{-1}(t)\dot{W}_\alpha(t) + \dot{V}_\alpha^{-1}(t)V_\alpha(t)B_\alpha(t), \tag{67}$$

where the first term of the right-hand side is zero due to (16). Hence, introducing

$$\Gamma_\alpha(t) = \dot{V}_\alpha^{-1}(t)V_\alpha(t) = -V_\alpha^{-1}(t)\dot{V}_\alpha(t) \tag{68}$$

whose matrix elements in the basis $\{\psi_\alpha^{(r)}(0)\}_{r \in \{1, 2, \dots, N\}}$ read

$$\langle \psi_\alpha^{(s)}(0) | \Gamma_\alpha(t) \psi_\alpha^{(r)}(0) \rangle = -\langle \psi_\alpha^{(s)}(t) | \dot{\psi}_\alpha^{(r)}(t) \rangle, \tag{69}$$

we get that $B_\alpha(t)$ is indeed determined by the ODE

$$\dot{B}_\alpha(t) = \Gamma_\alpha(t)B_\alpha(t), \quad B_\alpha(0) = \mathbb{I}. \tag{70}$$

Writing $W_\alpha = V_\alpha B_\alpha$, we compute

$$\begin{aligned} \langle \varphi_\alpha^{(r)}(t) | \partial_\alpha \varphi_\alpha^{(s)}(t) \rangle &= \langle \varphi_\alpha^{(r)}(0) | \partial_\alpha \varphi_\alpha^{(s)}(0) \rangle \\ &\quad + \langle \psi_\alpha^{(r)}(0) | B_\alpha^{-1}(t) V_\alpha^{-1}(t) (\partial_\alpha V_\alpha(t)) B_\alpha(t) \psi_\alpha^{(s)}(0) \rangle \\ &\quad + \langle \psi_\alpha^{(r)}(0) | B_\alpha^{-1}(t) (\partial_\alpha B_\alpha(t)) \psi_\alpha^{(s)}(0) \rangle. \end{aligned} \tag{71}$$

With the short hand $B_\alpha^{q,r}(t) = \langle \psi_\alpha^{(q)}(0) | B_\alpha \psi_\alpha^{(r)}(0) \rangle$, we have

$$B_\alpha(t) \psi_\alpha^{(s)}(0) = \sum_q \psi_\alpha^{(q)}(0) B_\alpha^{q,s}(t), \tag{72}$$

$$V_\alpha(t) B_\alpha(t) \psi_\alpha^{(s)}(0) = \sum_q \psi_\alpha^{(q)}(t) B_\alpha^{q,s}(t) \tag{73}$$

and

$$\begin{aligned} (\partial_\alpha V_\alpha(t)) B_\alpha(t) \psi_\alpha^{(s)}(0) &= \sum_q B_\alpha^{q,s}(t) ((\partial_\alpha V_\alpha(t) \psi_\alpha^{(q)}(0)) - V_\alpha(t) \partial_\alpha \psi_\alpha^{(q)}(0)) \\ &= \sum_q B_\alpha^{q,s}(t) (\partial_\alpha \psi_\alpha^{(q)}(t) - V_\alpha(t) \partial_\alpha \psi_\alpha^{(q)}(0)), \tag{74} \\ (\partial_\alpha B_\alpha(t)) \psi_\alpha^{(s)}(0) &= \sum_q \partial_\alpha (B_\alpha^{q,s}(t) \psi_\alpha^{(q)}(0)) - B_\alpha(t) \partial_\alpha \psi_\alpha^{(s)}(0). \end{aligned}$$

Inserting these expressions in (71), we get

$$\begin{aligned} &\langle \varphi_\alpha^{(r)}(t) | \partial_\alpha \varphi_\alpha^{(s)}(t) \rangle - \langle \varphi_\alpha^{(r)}(0) | \partial_\alpha \varphi_\alpha^{(s)}(0) \rangle \\ &= \sum_{q,q'} \overline{B_\alpha^{q',r}}(t) B_\alpha^{q,s}(t) \langle \psi_\alpha^{(q')} (t) | \partial_\alpha \psi_\alpha^{(q)}(t) \rangle + \sum_q \overline{B_\alpha^{q,r}}(t) \partial_\alpha B_\alpha^{q,s}(t) \\ &\quad - \langle \psi_\alpha^{(r)}(0) | \partial_\alpha \psi_\alpha^{(s)}(0) \rangle, \end{aligned} \tag{75}$$

which yields the result. □

Note. The operator $B_\alpha(t)$ and its generator $\Gamma_\alpha(t)$ depend of course on the choice of orthonormal basis $\{\psi_\alpha^{(r)}(t)\}_{r=1,\dots,N}$. It is not difficult to check that if one makes another choice of orthonormal basis $\{\chi_\alpha^{(r)}(t)\}_{r=1,\dots,N}$ such that $\chi_\alpha^{(r)}(t) = S_\alpha(t)\psi_\alpha^{(r)}(0)$, then the corresponding generator denoted by $\Sigma_\alpha(t)$ is related to the previous one by means of $C_\alpha(t) = S_\alpha^{-1}(t)V_\alpha(t)$ according to

$$\Sigma_\alpha(t) = C_\alpha(t)\Gamma_\alpha(t)C_\alpha^{-1}(t) + \dot{C}_\alpha(t)C_\alpha^{-1}(t). \tag{76}$$

3. Example

We consider here an explicit class of Hamiltonians which, on the one hand, display permanent degeneracies, and, on the other hand, allow in some cases for explicit computations. Moreover, the physical situation considered in [10] is governed by a Hamiltonian of this class.

Let $\{z_1, z_2, \dots, z_n\}$ be a set of n complex numbers, which we denote by the vector $z = (z_1, \dots, z_n)^T \in \mathbb{C}^n$, and let $E \in \mathbb{R}$. Let us denote the standard scalar product in \mathbb{C}^n by $\langle \cdot | \cdot \rangle$. We consider the self-adjoint Hamiltonian

$$H(z) = \begin{pmatrix} E & \bar{z}_1 & \cdots & \bar{z}_n \\ z_1 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ z_n & 0 & \cdots & 0 \end{pmatrix} \equiv \begin{pmatrix} E & \langle z | \\ |z \rangle & 0 \end{pmatrix} \quad \text{on } \mathbb{C}^{n+1} \simeq \mathbb{C} \oplus \mathbb{C}^n, \tag{77}$$

relative to the canonical basis $\{e_0, e_1, \dots, e_n\}$ of \mathbb{C}^{n+1} . We made z explicit in the notation because these parameters will become time-dependent below.

If $z \neq 0$, the rank of $H(z)$ is equal to two, so that its kernel is of dimension $n - 1$, for any value of the parameters. If $z = 0$, the kernel of $H(0)$ is of dimension n . Actually, it is easy to see that

$$\sigma(H(z)) = \left\{ \frac{1}{2}(E - \sqrt{E^2 + 4\|z\|^2}), 0, \frac{1}{2}(E + \sqrt{E^2 + 4\|z\|^2}) \right\}, \tag{78}$$

where $\|z\|^2 = \sum_{j=1}^n |z_j|^2$, and where the eigenspace corresponding to the $(n-1)$ -fold degenerate eigenvalue 0 is given by

$$\ker(H(z)) = \left\{ \begin{pmatrix} a_0 \\ a_1 \\ \vdots \\ a_n \end{pmatrix} \in \mathbb{C}^{n+1} \text{ s.t. } a_0 = 0 \text{ and } \sum_{j=1}^n \bar{z}_j a_j = 0 \right\}. \tag{79}$$

We can rewrite with $a = (a_1, \dots, a_n)^T \in \mathbb{C}^n$

$$\ker(H(z)) = \{0\} \oplus \{a \in \mathbb{C}^n \text{ s.t. } \langle z | a \rangle = 0\} = \{0\} \oplus z^\perp, \tag{80}$$

where z^\perp denotes the subspace orthogonal to $z \in \mathbb{C}^n$. It is now easy to express the projector $P(z)$ on the degenerate spectral subspace $\ker(H(z))$ in \mathbb{C}^{n+1} . Let $\hat{z} = z/\|z\| \in \mathbb{C}^n$ and $|\hat{z}\rangle\langle\hat{z}|$ be the projector on the vector \hat{z} in \mathbb{C}^n . Hence,

$$P_\perp(z) = \mathbb{I}_{\mathbb{C}^n} - |\hat{z}\rangle\langle\hat{z}| \tag{81}$$

is the projector on z^\perp in \mathbb{C}^n . Thus, expressed in block diagonal form in $\mathbb{C}^{n+1} \simeq \mathbb{C} \oplus \mathbb{C}^n$, we can write $P(z)$ as

$$P(z) = \begin{pmatrix} 0 & 0 \\ 0 & P_\perp(z) \end{pmatrix}. \tag{82}$$

Hence, with the same notations, $\overline{P}(z)$ can be written as

$$\overline{P}(z) = \begin{pmatrix} 1 & 0 \\ 0 & |\hat{z}\rangle\langle\hat{z}| \end{pmatrix}, \tag{83}$$

so that the range of $\overline{P}(z)$ is generated by the orthonormal basis

$$\text{Ran } \overline{P}(z) = \text{span} \left\{ \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ \hat{z} \end{pmatrix} \right\} \equiv \text{span} \{e_0, \tilde{z}\}. \tag{84}$$

Let us assume now that $z = z(t)$ is time-dependent, in such a way that $[0, 1] \ni t \mapsto z(t) \in \mathbb{C}^n$ is C^3 . By changing the phase of $z(t)$ if necessary, we can assume

$$\langle \hat{z}(t) | \dot{\hat{z}}(t) \rangle = \langle \tilde{z}(t) | \dot{\tilde{z}}(t) \rangle \equiv 0. \tag{85}$$

It is now straightforward to check that the parallel transport operator $W(t)$ is generated by the self-adjoint operator $K(t) = i[\dot{P}(z(t)), P(z(t))]$, with

$$K(t) = i(|\dot{\tilde{z}}(t)\rangle\langle\tilde{z}(t)| - |\tilde{z}(t)\rangle\langle\dot{\tilde{z}}(t)|). \tag{86}$$

Recall that $\tilde{z} = (0, \hat{z})^T$ is a normalized a vector of \mathbb{C}^{n+1} . Note that condition (85) is equivalent to saying

$$\tilde{z}(t) = W(t)\tilde{z}(0) \quad \text{and} \quad \begin{pmatrix} 1 \\ 0 \end{pmatrix} = W(t) \begin{pmatrix} 1 \\ 0 \end{pmatrix}. \tag{87}$$

Thus the determination of W restricted to $\text{Ran } \overline{P}$ is complete. With these preliminaries behind us, we can turn to the interesting task from our point of view, i.e. the determination of W restricted to $\text{Ran } P$. From (84) above, it is clear that we can restrict attention to $\mathbb{C}^n \simeq e_0^\perp$, where $\text{Ran } \overline{P}(z) \cup e_0^\perp \simeq \mathbb{C}\hat{z}$.

Let $\{\varphi_1, \varphi_2, \dots, \varphi_{n-1}\}$ be an orthonormal basis in \mathbb{C}^n of $\hat{z}(0)^\perp$. Then, using the same notation for $\varphi_j \in \mathbb{C}^n$ and $(0, \varphi_j)^T \in \mathbb{C}^{n+1}$, we have for any $j = 1, \dots, n$, and any $t \in [0, 1]$,

$$\varphi_j(t) = W(t)\varphi_j \in \mathbb{C}^{n+1} \Leftrightarrow \begin{cases} \dot{\varphi}_j(t) = -|\hat{z}(t)\rangle\langle\dot{\hat{z}}(t)|\varphi_j(t) \in \mathbb{C}^n \\ \varphi_j(0) = \varphi_j \in \mathbb{C}^n. \end{cases} \tag{88}$$

Actually, computing the parallel transport operator $W(t)$ restricted to $\ker(H(z(t)))$ for the model (77) where $z(t) \in \mathbb{C}^n$ is given, amounts to determining

$n - 1$ vectors $\varphi_j(t)$ in \mathbb{C}^n such that for all $j, k = \{1, \dots, n - 1\}^2$ and all $t \in [0, 1]$,

$$\langle \varphi_j(t) | \hat{z}(t) \rangle \equiv 0, \tag{89}$$

$$\langle \varphi_j(t) | \varphi_k(t) \rangle \equiv \delta_{jk}, \tag{90}$$

$$\langle \varphi_j(t) | \dot{\varphi}_k(t) \rangle \equiv 0. \tag{91}$$

Indeed, if (88) is satisfied, the conditions above are met. Conversely, if the first two conditions above are satisfied, we get that $\{\hat{z}(t), \varphi_1(t), \dots, \varphi_{n-1}\}$ form an orthonormal basis, for all t 's. Moreover, the third condition implies that $\dot{\varphi}_j = c_0(t)\hat{z}(t)$, for some coefficient $c_0(t) \in \mathbb{C}$. Differentiation of $\langle \varphi_j(t) | \hat{z}(t) \rangle \equiv 0$ yields $a_0(t) = -\langle \dot{\hat{z}}(t) | \varphi_j(t) \rangle$, so that Eq. (88) is true.

Even though the generator of W restricted to $P(z(t))$ is rather simple, these equations cannot be explicitly integrated in general. We present some special cases of interest which allow for explicit formulas.

3.1. Special case

We consider here a special case for $n = 3$ that is of interest for the physics of charge pumping, [10]. Let us consider the Hamiltonian

$$H(z_0, z_1, z_2) = \begin{pmatrix} E & \bar{z}_0 & \bar{z}_1 & \bar{z}_2 \\ z_0 & 0 & 0 & 0 \\ z_1 & 0 & 0 & 0 \\ z_2 & 0 & 0 & 0 \end{pmatrix} \quad \text{with } z = (z_0, z_1, z_2), \tag{92}$$

in the canonical basis. We assume that

$$|z_1|^2 + |z_2|^2 > 0, \tag{93}$$

so that a set of normalized eigenvectors corresponding to the degenerate subspace of energy zero is given by

$$\overline{|\psi_1\rangle} = N_1(z_2 e_2 - z_1 e_3), \tag{94}$$

$$\overline{|\psi_2\rangle} = N_1 [(z_1^2 + z_2^2) e_1 - z_0(z_1 e_2 + z_2 e_3)], \tag{95}$$

with

$$N_1 = 1/\sqrt{|z_1|^2 + |z_2|^2}, \tag{96}$$

$$N_2 = 1/\sqrt{|z_1^2 + z_2^2|^2 + |z_0|^2(|z_1|^2 + |z_2|^2)}. \tag{97}$$

We now compute the differentials of these eigenvectors, in order to get the generator of the non-Abelian transformation. At this level, we allow all parameters to vary, with the condition that (93) holds. Straightforward computations yield the (negative of) the matrix elements of the matrix Γ_ψ , with respect to this

instantaneous basis of eigenvectors of $\ker H$

$$\begin{aligned} \langle \psi_1 | d\psi_1 \rangle &= iN_1^2 \text{Im} (z_1 d\bar{z}_1 + z_2 d\bar{z}_2), \\ \langle \psi_2 | d\psi_2 \rangle &= iN_2^2 \text{Im} \{ 2(z_1^2 + z_2^2)(\bar{z}_1 d\bar{z}_1 + \bar{z}_2 d\bar{z}_2) \\ &\quad + |z_0|^2(z_1 d\bar{z}_1 + z_2 d\bar{z}_2) + (|z_1|^2 + |z_2|^2)z_0 d\bar{z}_0 \}, \\ \langle \psi_2 | d\psi_1 \rangle &= N_1 N_2 z_0 (z_2 d\bar{z}_1 - z_1 d\bar{z}_2), \\ \langle \psi_1 | d\psi_2 \rangle &= -\overline{\langle \psi_2 | d\psi_1 \rangle}. \end{aligned} \tag{98}$$

We can simplify this matrix further by passing to the time-dependent basis

$$\chi_j(t) = \psi_j(\gamma(t)) e^{i\beta_j(t)}, \quad \beta_j(t) = i \int_0^t \langle \psi_j | d\psi_j \rangle (\gamma(s)) ds, \tag{99}$$

where the integral is taken along a path $[0, 1] \ni t \mapsto \gamma(t)$ in the parameters space. The matrix Γ_χ corresponding to the basis $\{\chi_1, \chi_2\}$ of eigenvectors of $\ker H$ now reads

$$\Gamma_\chi = \begin{pmatrix} 0 & -e^{i(\beta_2 - \beta_1)} \langle \psi_1 | d\psi_2 \rangle \\ e^{-i(\beta_2 - \beta_1)} \overline{\langle \psi_1 | d\psi_2 \rangle} & 0 \end{pmatrix}. \tag{100}$$

Setting

$$x(t) = e^{-i(\beta_2(t) - \beta_1(t))} \overline{\langle \psi_1 | d\psi_2 \rangle} (\gamma(t)), \tag{101}$$

so that

$$\Gamma_\chi(t) = \begin{pmatrix} 0 & -\overline{x(t)} \\ x(t) & 0 \end{pmatrix}, \tag{102}$$

we have to solve the ODE $\dot{B}(t) = \Gamma_\chi(t)B(t)$, see (70), to determine $W(t)$. In general, no explicit solution to (70) with such a matrix can be obtained.

However, in case $x(t) = \rho(t)e^{i\vartheta}$, where ϑ is constant in time, $\Gamma_\chi(t) = \rho(t)M$, where $M = \begin{pmatrix} 0 & -e^{-i\vartheta} \\ e^{i\vartheta} & 0 \end{pmatrix}$ and $B(t)$ is explicitly given by

$$B(t) = e^{\int_0^t \rho(s) ds} M = \begin{pmatrix} \cos \left(\int_0^t \rho(s) ds \right) & -\sin \left(\int_0^t \rho(s) ds \right) e^{-i\vartheta} \\ \sin \left(\int_0^t \rho(s) ds \right) e^{i\vartheta} & \cos \left(\int_0^t \rho(s) ds \right) \end{pmatrix}. \tag{103}$$

We consider below a case of this type, which allows us to determine explicitly the geometric part of the charge transported over a period. Moreover, we express the geometric content if the parallel transport within the *permanently degenerate* kernel of H as a solid angle in the space of parameters, in a similar fashion to what is done for the Berry phase, in case of *nondegenerate* eigenvalues.

Let us assume that

$$z_j = e^{i\theta_j} r_j \quad \text{and} \quad dz_j = e^{i\theta_j} dr_j, \tag{104}$$

that is, only the moduli of the complex numbers z_j vary with time. Plugging this into (98) yields

$$\begin{aligned} \langle \psi_1 | d\psi_1 \rangle &= 0, \\ \langle \psi_2 | d\psi_2 \rangle &= 2iN_2^2 \sin(2(\theta_1 - \theta_2))r_1r_2(r_1dr_2 - r_2dr_1), \\ \langle \psi_2 | d\psi_1 \rangle &= N_1N_2r_0e^{i\theta_0} \left(e^{-i(\theta_1 - \theta_2)}r_2dr_1 - e^{i(\theta_1 - \theta_2)}r_2dr_2 \right), \end{aligned} \quad (105)$$

with

$$N_1 = \frac{1}{\sqrt{r_1^2 + r_2^2}}, \quad N_2 = \frac{1}{\sqrt{(r_1^2 + r_2^2)r_0^2 + (r_1^4 + r_2^4 + 2r_1^2r_2^2 \cos(2(\theta_1 - \theta_2)))}}. \quad (106)$$

Further assuming

$$\theta_1 = \theta_2 = 0, \quad (107)$$

we finally get

$$\Gamma_\psi = \frac{r_0(r_1dr_2 - r_2dr_1)}{(r_1^2 + r_2^2)\sqrt{r_0^2 + r_1^2 + r_2^2}} \begin{pmatrix} 0 & -e^{-i\theta_0} \\ e^{i\theta_0} & 0 \end{pmatrix}, \quad (108)$$

which is of the form (102). The argument of the sines and cosines in (103) after a period characterized by a loop γ in the space of parameters is denoted by

$$\Omega = \int_\gamma \frac{-r_0(r_1dr_2 - r_2dr_1)}{(r_1^2 + r_2^2)\sqrt{r_0^2 + r_1^2 + r_2^2}} \quad (109)$$

so that

$$B(1) = \begin{pmatrix} \cos(\Omega) & \sin(\Omega)e^{-i\theta_0} \\ -\sin(\Omega)e^{i\theta_0} & \cos(\Omega) \end{pmatrix}. \quad (110)$$

Similarly, if z_1 and z_2 are as above and $z_0 = t_1e^{i\theta_0} + t_2$ with t_1, t_2 real and $dr_1 = dr_2 = d\theta_0 \equiv 0$, with $r_1^2 + r_2^2 > 0$, we have

$$\Gamma_\psi = i \sin(\theta_0)(t_1dt_2 - t_2dt_1)/(t_1^2 + t_2^2 + 2t_1t_2 \cos(\theta_0)) \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}. \quad (111)$$

3.2. Geometric interpretation of Ω

The explicit computation of Ω possesses a nice geometric interpretation, see (119), as we now explain.

For notational convenience, let us introduce Cartesian coordinates $(x, y, z) = (r_0, r_1, r_2)$. At the end of the loop γ , we have

$$\Gamma = \int_\gamma \frac{-z(xdy - ydx)}{(x^2 + y^2)\sqrt{x^2 + y^2 + z^2}} \quad (112)$$

$$= \int_\gamma \frac{-z}{(x^2 + y^2)\sqrt{x^2 + y^2 + z^2}} \begin{pmatrix} -y \\ x \\ 0 \end{pmatrix} \cdot \begin{pmatrix} dx \\ dy \\ dz \end{pmatrix}. \quad (113)$$

Applying Stokes' theorem, we can replace the curvilinear integral above by the flux of the curl of the corresponding vector through any surface Σ such that $\partial\Sigma = \gamma$, oriented consistently with the orientation of γ .

We compute

$$\mathbf{curl} \frac{-z}{(x^2 + y^2)\sqrt{x^2 + y^2 + z^2}} \begin{pmatrix} -y \\ x \\ 0 \end{pmatrix} = (x^2 + y^2 + z^2)^{-3/2} \begin{pmatrix} x \\ y \\ z \end{pmatrix} \quad (114)$$

$$= \frac{\mathbf{r}}{r^3}, \quad (115)$$

where

$$\mathbf{r} = \begin{pmatrix} x \\ y \\ z \end{pmatrix} \quad \text{and} \quad r = \sqrt{x^2 + y^2 + z^2}.$$

Hence we can write,

$$\int_{\gamma} \frac{-z(xdy - ydx)}{(x^2 + y^2)\sqrt{x^2 + y^2 + z^2}} = \int_{\Sigma} \frac{\mathbf{r}}{r^3} \cdot d\boldsymbol{\sigma}. \quad (116)$$

Consider the projection $\hat{\gamma}$ of the loop γ on the sphere \mathbb{S}^2 described by the unit vector $\hat{r} = \mathbf{r}/r$ along γ , and define $\hat{\Sigma} \subset \mathbb{S}^2$ such that $\partial\hat{\Sigma} = \hat{\gamma}$. Now, we can choose for Σ the surface which coincides with $\hat{\Sigma}$, and joins $\hat{\gamma}$ and γ along rays parallel to the unit vector. Since the flux of \mathbf{r}/r^3 through the latter portions of Σ is zero, we finally get

$$\int_{\gamma} \frac{-z(xdy - ydx)}{(x^2 + y^2)\sqrt{x^2 + y^2 + z^2}} = \int_{\hat{\Sigma}} \frac{\mathbf{r}}{r^3} \cdot d\boldsymbol{\sigma} \quad (117)$$

$$= \int_{\hat{\Sigma}} d\omega, \quad (118)$$

where we used the fact that on \mathbb{S}^2 , $d\boldsymbol{\sigma} = d\omega \hat{r}$, with $d\omega$ the differential of the solid angle.

Therefore, we have obtained

$$\Omega = \Omega(\hat{\Sigma}), \quad (119)$$

where $\Omega(\hat{\Sigma})$ is the oriented solid angle described by γ through \mathbb{S}^2 . If $\hat{\gamma}$ is oriented positively, $\Omega(\hat{\Sigma}) \geq 0$, and, in any case, $0 \leq |\Omega(\hat{\Sigma})| \leq 4\pi$.

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