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Diagonal Representation for a Generic Matrix Valued Quantum Hamiltonian

Pierre Gosselin¹ and Hervé Mohrbach²

*Institut Fourier, UMR 5582 CNRS-UJF UFR de Mathématiques,
Université Grenoble I, BP74, 38402 Saint Martin d'Hères, Cedex, France and
Laboratoire de Physique Moléculaire et des Collisions, ICPMB-FR CNRS 2843,
Université Paul Verlaine-Metz, 57078 Metz Cedex 3, France*

A general method to derive the diagonal representation for a generic matrix valued quantum Hamiltonian is proposed. In this approach new mathematical objects like non-commuting operators evolving with the Planck constant promoted as a running variable are introduced. This method leads to a formal compact expression for the diagonal Hamiltonian which can be expanded in a power series of the Planck constant. In particular, we provide an explicit expression for the diagonal representation of a generic Hamiltonian to the second order in the Planck constant. This last result is applied, as a physical illustration, to Dirac electrons and neutrinos in external fields.

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I. INTRODUCTION

The spacetime evolution of some important quantum systems is governed by a multicomponent Schrödinger like equation whose Hamiltonian is a matrix valued operators. In many cases, these systems are too complicated to be solved directly using the Schrödinger equation and some simplifications are required. For systems displaying a separation of scales in terms of slow and fast degrees of freedom a major simplification is to treat quantally the fast ones while the slow ones can be approximated classically or semiclassically. For a slow cyclic variation of the classical part, Berry has shown that the wave function of the quantum part gets an additional geometric phase factor [1]. It has also been understood, in the context of the Born-Oppenheimer theory of molecules [2][3][4] that the geometric phases induced by the quantum part of the system provide a correction, reacting on the classical part with

geometric Lorentz and electric forces [5][6]. Going beyond this first correction has proved extraordinarily difficult due to the intricate entanglement of noncommuting operators [7].

In fact, many physical systems share a very similar mathematical structure with molecular systems. For instance, the translational movement of a Dirac electron in a slowly varying external field can be separated from the spin evolution and therefore considered semiclassically.

In this paper, we address the question of the dynamics governing the slow part of an arbitrary quantum system and present a formalism for calculating the Hamiltonian of this slow part to all orders in the Planck's constant. Of course, we do not expect the convergence of the series in general, since for most quantum systems the limit $\hbar \rightarrow 0$ is singular, which means that an exact quantum behavior can not be approximated even by an infinite expansion.

The philosophy behind the approach developed here, consists in a mapping of the initial quantum system to a classical one which can be easily diagonalized and then to return to the full quantum system. The method requires the introduction of new mathematical objects like non-commuting operators evolving with the Planck constant promoted as a running variable. This leads to a differential calculus on a non-commutative space which shows some similarities with the stochastic calculus. This innovation is the clue to derive the formal exact diagonal representation for any arbitrary matrix valued Hamiltonian.

The results presented here extend the work presented in [8], where a differential equation with respect to $\hbar$ was proposed for the required diagonal Hamiltonian. The semiclassical limit, which is often enough to get physical insight for the problem considered, was obtained by a straightforward integration of this differential equation and a general semiclassical formula for an arbitrary diagonal Hamiltonian in terms of covariant operators and commutators between Berry connections was obtained. This formalism allowed to consider several straightforward applications. These ones included the deflection of light by the interaction between its polarization state and external inhomogeneities, such as a varying refractive index or a gravitational field [9]; Dirac electrons and Bloch electrons in crystals [10], leading to new effective geometrical forces and a clarification of the Peierls substitution [11] as well as to a generalization of the Bohr-Sommerfeld quantification rule [12]. In principle, one could solve the differential equation to the desired order in a series of $\hbar$, but although this was done for simple examples to order $\hbar^2$ (see [8]), we could not derive such an expression

for an arbitrary Hamiltonian.

The main advantage of the new method presented in this paper is that being not based on a differential equation, it directly leads to a formal exact diagonal representation for any arbitrary matrix valued Hamiltonian, which, as proven in this paper, is an exact solution of the differential equation of [8]. It appears also, as one could expect, that the expansion in series of $\hbar$ for the exact diagonal Hamiltonian derived here is much more easier to obtain than by the successive integration of the differential equation of [8]. In particular, we provide an explicit formula for the diagonal Hamiltonian to order $\hbar^2$ that can be directly applied in principle to any physical systems.

In this paper, for the sake of clarity and to keep the length reasonable, we will consider only two simple but still physically relevant examples. More applications can be found in [13], where interacting Bloch electrons are considered, and in [14] for a generalization of the Born-Oppenheimer approximation.

It is worth mentioning that some other diagonalization procedures exist, each of them having its range of validity, advantages and defects. The paradigmatic example is provided by the Foldy-Wouthuysen (FW) representation of the Dirac Hamiltonian for relativistic particles interacting with an external electromagnetic field. In this representation the positive and negative energy states are separately represented and the non-relativistic Pauli-Hamiltonian is obtained [15]. Actually even if several exact FW transformations have been found for some definite classes of potentials [16][17][18], the diagonalization is a difficult mathematical problem requiring approximations, essentially a perturbation expansion in weak fields. A generalisation of the FW transformation developed by Blount and also based on an expansion in weak electromagnetic fields, is in principle applicable to Bloch electrons and Dirac electrons [19]. But this method is limited by construction to weak external perturbations and provides a formal series expansion which leads to cumbersome calculations for practical applications. Recently a variant of the Foldy Wouthuysen transformation valid for strong fields and based also on an expansion in $\hbar$ of the Dirac Hamiltonian was presented [20].

Among other approaches, Weigert and Littlejohn developed a systematic method to diagonalize general quantum Hamiltonian in a series expansion in $\hbar$ [7]. It leads also to a formal series expansion written in terms of symbols of operators which also makes the method complicated for practical applications. In particular this method does not provide explicit formulas, but instead is an algorithm to compute case by case the series order by order.

To our knowledge, this approach was only used for Born-Oppenheimer molecular systems. Note also, that a different method based on a adiabatic perturbation theory was proposed in [21] (and references therein) and applied to the Dirac electron and electrons in a cristal at the first order.

Our approach, although similar in spirit to these methods, is technically very different and allows us for the first time to derive the expression of the diagonal representation at order $\hbar^2$ of an arbitrary quantum Hamiltonian. This efficiency could be explained by the fact that, unlike other approaches, no Weyl calculus and Moyal Algebra are required. Another interesting feature of our approach is that it confirms the fundamental role played by Berry curvatures since it leads to an effective diagonal Hamiltonian with Berry phase corrections as well as noncommutative (Berry connections dependent) coordinates and momentum co-variant operators as in previous approaches [8][10] (see also [22] for Dirac electrons in an electric field and [23] for the extension to the full electromagnetic field). The resulting generic equations of motion are also corrected by Berry curvatures terms.

The paper is organized as follows. In the next section we develop the differential calculus in noncommutative space. We then derive, in section 3, the diagonalization procedure and show the link with the differential equation in section 4. Section 5 is devoted to the discussion of the dynamical coordinate and momentum operators. In section 6, we give the general diagonal energy operator formula to the second order in $\hbar$ and in section 7, Dirac electron in an external electric field and neutrinos in a static symmetric gravitational field are considered as an illustration of the general formalism. Last section is for the conclusion.

II. PRELIMINARIES:

A. Differential calculus on noncommutative space

Consider a quantum mechanical system whose state space is a tensor product $L^2(\mathcal{R}^3) \otimes V$ with V some internal space. In other words, the Hamiltonian can be written as a matrix $H(\mathbf{P}, \mathbf{R})$ of size $\dim V$ whose elements are operators depending on a couple of canonical operators $[R^i, P^j] = i\hbar\delta_{ij}$, the archetype example being the Dirac Hamiltonian with $V = C^4$. Our goal is to derive the formal diagonal representation of this matrix valued quantum Hamiltonian. By diagonal Hamiltonian it is meant an effective in-band Hamiltonian which

has a matrix representation with block-diagonal matrix elements associated with energy band subspaces. As in paper [8] the procedure we propose for the removal of the interband matrix elements needs the use of some unconventional mathematics compared to the usual formalism of quantum mechanics. Since the Planck constant is here considered as a variable, operators do not satisfy the usual rules of quantum mechanics. Therefore before directly embarking on the diagonalization procedure we first introduce the required mathematical tools. For that purpose we start with some definitions and notations.

1. Running coordinates and momentum operators

To begin with, we introduce a formal space of non commuting infinitesimal operators $dX_\alpha^i \equiv \{dR_\alpha^i, dP_\alpha^i\}$ $i = 1, 2, 3$ indexed by a continuous parameter α , that satisfy the following infinitesimal Heisenberg algebra (with a reversed sign) :

$$[dR_\alpha^i, dP_{\alpha'}^j] = -id\alpha\delta_{\alpha,\alpha'}\delta_{ij} \quad \text{and} \quad [dR_\alpha^i, dR_{\alpha'}^j] = [dP_\alpha^i, dP_{\alpha'}^j] = 0. \quad (1)$$

Then, we define a set of running coordinate and momentum operators by witting the following formal sums :

$$R_\alpha^i = R^i - \int_\alpha^\hbar dR_\lambda^i, \quad \text{and} \quad P_\alpha^i = P^i - \int_\alpha^\hbar dP_\lambda^i \quad (2)$$

with the convention $dR_\alpha^i = R_\alpha^i - R_{\alpha-d\alpha}^i$ and $dP_\alpha^i = P_\alpha^i - P_{\alpha-d\alpha}^i$. This "downward" choice of the differential element notably implies the commutation rules $[R_\alpha^i, dP_\alpha^j] = [dR_\alpha^i, P_\alpha^j] = 0$ which turns out to be absolutely necessary to develop later on a differential calculus on this noncommutative space.

For $\alpha = \hbar$ we recover the usual canonical operators $R^i \equiv R_\hbar^i$ and $P^i \equiv P_\hbar^i$ which satisfy the canonical Heisenberg algebra $[R^i, P^j] = i\hbar\delta_{ij}$, whereas the running operators satisfy

$$[R_\alpha^i, P_\alpha^j] = i\alpha\delta_{ij} \quad \text{and} \quad [R_\alpha^i, R_\alpha^j] = [P_\alpha^i, P_\alpha^j] = 0. \quad (3)$$

Note that in this paper we will never consider the algebra of the operators R_α^i and $P_{\alpha'}^j$ for $\alpha \neq \alpha'$, which from the definition Eq. (2) is clearly not a Heisenberg one.

The variables $d\mathbf{X}_\alpha$ have to be understood as fictitious variables that make the link between quantal operators ($\alpha = \hbar$) and classical variables ($\alpha = 0$). As will be explicit later on, their role is to transport our quantum system to a formal classical one that can be in general

easily diagonalized, and then back from the formal classical one to the required quantized system. By writing $d\mathbf{X}_\alpha = \sqrt{d\alpha/\hbar}\hat{\mathbf{X}}_\alpha$ with $\hat{\mathbf{X}}_\alpha$ a normalized canonical operator we see that the infinitesimal quantities $d\mathbf{X}_\alpha$ are actually of order $\sqrt{d\alpha}$. However, having this in mind, we will never use the $\hat{\mathbf{X}}_\alpha$ notation and always work with $d\mathbf{X}_\alpha$.

2. Differential algebra

For the sequel, we need to define the differential $dF(\mathbf{X}_\alpha, \alpha)$ of an arbitrary function $F(\mathbf{X}_\alpha, \alpha)$ where $X_\alpha^i \equiv \{R_\alpha^i, P_\alpha^i\}$. For this purpose, consider the operators $R_\alpha^i - \int_\alpha^\hbar dR_\lambda^i$, and $P_\alpha^i = P^i - \int_\alpha^\hbar dP_\lambda^i$ as acting on a space $W = (V \otimes L^2(\mathcal{R}^3)) \otimes (\otimes_{\alpha < \hbar} L^2(\mathcal{R}^3)_\alpha)$ which is the tensor product of V and an infinite number of copies of $L^2(\mathcal{R}^3)$. The tensor product $V \otimes L^2(\mathcal{R}^3)$ and the space $L^2(\mathcal{R}^3)_\alpha$ refer respectively to the spaces on which the canonical operators (R^i, P^i) and the differential operators dX_α^i act.

Now to be consistent with our convention for the differential element dX_α^i , the differential of the function $F(\mathbf{X}_\alpha, \alpha)$ is defined in an unusual backward manner as $dF(\mathbf{X}_\alpha, \alpha) \equiv F(\mathbf{X}_\alpha, \alpha) - F(\mathbf{X}_{\alpha-d\alpha}, \alpha - d\alpha)$. This construction is essential as it permits the commutation between the non-differential and the differential elements dX_α^i . The differential will be written as a second order expansion plus some neglected terms:

$$\begin{aligned} dF(\mathbf{X}_\alpha, \alpha) &= \nabla_{R_i} F dR_\alpha^i + \nabla_{P_i} F dP_\alpha^i - \frac{1}{2} (\nabla_{R_i} \nabla_{R_j} F) dR_\alpha^i dR_\alpha^j - \frac{1}{2} (\nabla_{P_i} \nabla_{P_j} F) dP_\alpha^i dP_\alpha^j \\ &\quad - \frac{1}{2} (\nabla_{R_i} \nabla_{P_j} F) (dR_\alpha^i dP_\alpha^j + dP_\alpha^j dR_\alpha^i) + \langle F(\mathbf{X}_\alpha, \alpha) \rangle d\alpha + \frac{\partial F}{\partial \alpha} d\alpha \\ &\quad + \text{terms of order 3,} \end{aligned} \tag{4}$$

where all expressions in the r.h.s. are evaluated at $(\mathbf{X}_\alpha, \alpha)$. Note that here, we have kept the terms of order square in dX_α^i since they are of order $d\alpha$ and thus contribute to the differential, whereas higher orders can safely be disregarded as they are negligible when the integration over α is considered. These second order terms have been organized in a certain form that will be practical for us later. There is nothing to say about the usual $dR_\alpha^i dR_\alpha^j$ or $dP_\alpha^i dP_\alpha^j$ terms. The crossed terms involving products of dP_α^i and dR_α^j have to be taken with care since these two infinitesimal elements do not commute with each other. For this purpose we have decomposed the second order terms involving products such as $dP_\alpha^i dR_\alpha^j$ and $dR_\alpha^j dP_\alpha^i$ in a symmetric part proportional to $(dR_\alpha^i dP_\alpha^j + dP_\alpha^j dR_\alpha^i)$ giving the contribution $-\frac{1}{2} (\nabla_{R_i} \nabla_{P_j} F) (dR_\alpha^i dP_\alpha^j + dP_\alpha^j dR_\alpha^i)$, and an antisymmetric part proportional

to $(dR_\alpha^i dP_\alpha^j - dP_\alpha^j dR_\alpha^i) = -i\delta^{ij}d\alpha$ corresponding to the bracket $\langle F(\mathbf{X}_\alpha, \alpha) \rangle d\alpha$ that we now explain in details. The notation $\langle F(\mathbf{X}_\alpha, \alpha) \rangle$ (which in [8] was corresponding to the operation $-\frac{i}{2} \text{Asym} \nabla_{R_i} \nabla_{P^i} F(\mathbf{X}_\alpha, \alpha)$) is defined as a specific procedure on a series expansion of F in the variables R_α^i, P_α^i in the following way : let F be a sum of monomials of the kind $M_1(\mathbf{R}_\alpha) M_2(\mathbf{P}_\alpha) M_3(\mathbf{R}_\alpha) \dots$ the M_i being arbitrary monomials in R_α or P_α alternatively. The operator $\nabla_{R_i} \nabla_{P^j}$ acts on such an expression by deriving all combinations of one monomial in $\mathbf{R}_\alpha$ and one monomial in $\mathbf{P}_\alpha$. For each of these combinations, insert a dR_α^i at the place where the derivative ∇_{R_i} is acting and in a same manner a dP_α^j at the place where the derivative ∇_{P^j} is acting. This leads to an expression with two kind of terms, one kind being proportional to the $dR_\alpha^i dP_\alpha^j$, and the second proportional to $dP_\alpha^j dR_\alpha^i$. Then rewrite this expression in terms of $dR_\alpha^i dP_\alpha^j + dP_\alpha^j dR_\alpha^i$ and $dR_\alpha^i dP_\alpha^j - dP_\alpha^j dR_\alpha^i = -i\delta^{ij}d\alpha$. Then $\langle F(\mathbf{X}_\alpha, \alpha) \rangle$ is defined as minus the sum over i and j of all the terms proportional to $d\alpha$ in the computation procedure just considered. This definition implies a procedure which is clearly dependent of the symmetrization chosen for the expansion of F .

To make the definition of $\langle F(\mathbf{X}_\alpha, \alpha) \rangle$ clearer, consider some important practical examples. If the function F has the following form $F = \frac{1}{2} (A(\mathbf{R}_\alpha) B(\mathbf{P}_\alpha) + B(\mathbf{P}_\alpha) A(\mathbf{R}_\alpha))$ which corresponds to a frequent choice of symmetrization in R_α and P_α , then $\langle F(\mathbf{X}_\alpha, \alpha) \rangle = \frac{i}{4} \sum_i [\nabla_{R_i} A(\mathbf{R}_\alpha), \nabla_{P^i} B(\mathbf{P}_\alpha)]$. Another choice of symmetrization leads in general to a different result.

For instance, if we rewrite the same function F in a fully symmetrized form in R_α and P_α (that is invariant by all permutations in R_α and P_α) which is also often used, we now have a different result since $\langle F(\mathbf{X}_\alpha, \alpha) \rangle = 0$.

Nevertheless, this dependence of $\langle F(\mathbf{X}_\alpha, \alpha) \rangle$ in the symmetrization choice is not astonishing at all. Actually changing the symmetrization of a function $F(\mathbf{X}_\alpha, \alpha)$ introduces some explicit terms in α which changes also the term $\partial_\alpha F d\alpha$ present in the differential Eq. (4). As a consequence, neither the partial derivative with respect to α , nor the bracket are invariant by a change of form. But, what is invariant is the sum $\partial_\alpha F + \langle F \rangle$.

We show this assertion by first giving a useful formula for the differential of a product of

functions :

$$\begin{aligned}
d(F(\mathbf{X}_\alpha, \alpha) G(\mathbf{X}_\alpha, \alpha)) &= dFG + FdG - \nabla_{R_i} F \nabla_{R_j} G dR_\alpha^i dR_\alpha^j - \nabla_{P_i} F \nabla_{P_j} G dP_\alpha^i dP_\alpha^j \\
&\quad - (\nabla_{R_i} F \nabla_{P_j} G) dR_\alpha^i dP_\alpha^j - (\nabla_{P_j} F \nabla_{R_i} G) dP_\alpha^j dR_\alpha^i \\
&= dFG + FdG - \nabla_{R_i} F \nabla_{R_j} G dR_\alpha^i dR_\alpha^j - \nabla_{P_i} F \nabla_{P_j} G dP_\alpha^i dP_\alpha^j \\
&\quad - \frac{1}{2} (\nabla_{R_i} F \nabla_{P_j} G + \nabla_{P_j} F \nabla_{R_i} G) (dR_\alpha^i dP_\alpha^j + dP_\alpha^j dR_\alpha^i) \\
&\quad - \frac{i}{2} (\nabla_{P_i} F \nabla_{R_i} G - \nabla_{R_i} F \nabla_{P_i} G) d\alpha
\end{aligned} \tag{5}$$

Now, the invariance of $\partial_\alpha F + \langle F \rangle$ is the consequence of two facts. The first one is that the definition of the differential $dF(\mathbf{X}_\alpha, \alpha)$ is independent of the way the function $F(\mathbf{X}_\alpha, \alpha)$ has been symmetrized. Actually, considering $F(\mathbf{X}_\alpha, \alpha)$ as a monomial, a change of symmetrization amounts to move successively powers of the momentum on the right or the left of the position variable. Recursively, one just has to check that moving only one power of the momentum does not change the differential. Considering thus a monomial of the form $F(\mathbf{X}_\alpha, \alpha) = M_1 P_\alpha^i R_\alpha^i M_2$ with M_1 and M_2 arbitrary, move the momentum to rewrite $F(\mathbf{X}_\alpha, \alpha) = M_1 (R_\alpha^i P_\alpha^i - i\alpha) M_2$. Our formula for a product of differential, allows to assert that the differentials of the two terms $M_1 P_\alpha^i R_\alpha^i M_2$ and $M_1 (R_\alpha^i P_\alpha^i - i\alpha) M_2$ differ only by the contributions $M_1 d(P_\alpha^i R_\alpha^i) M_2$ and $M_1 d(R_\alpha^i P_\alpha^i - i\alpha) M_2$. As a consequence, the differential $dF(\mathbf{X}_\alpha, \alpha)$ is independent of the choice of symmetrization if and only if $d(P_\alpha^i R_\alpha^i) = d(R_\alpha^i P_\alpha^i - i\alpha)$. Given that

$$\begin{aligned}
d(P_\alpha^i R_\alpha^i) &= dP_\alpha^i R_\alpha^i + P_\alpha^i dR_\alpha^i - \frac{1}{2} (dR_\alpha^i dP_\alpha^j + dP_\alpha^j dR_\alpha^i) - \frac{i}{2} d\alpha \\
d(R_\alpha^i P_\alpha^i - i\alpha) &= R_\alpha^i dP_\alpha^i + dR_\alpha^i P_\alpha^i - \frac{1}{2} (dR_\alpha^i dP_\alpha^j + dP_\alpha^j dR_\alpha^i) + \frac{i}{2} d\alpha - id\alpha
\end{aligned}$$

and that the dP_α^i, dR_α^i commute with R_α^i, P_α^i the equality of the two previous lines holds as well as the assertion of symmetrization independence.

This result joined to the second fact that in the series expansion of $dF(\mathbf{X}_\alpha, \alpha)$, the variables $dX_\alpha^i, dX_\alpha^i dX_\alpha^j, d\alpha$, are independent, and thus that the coefficients of the expansion of $dF(\mathbf{X}_\alpha, \alpha)$ are uniquely defined, leads directly to the announced result that $\partial_\alpha F + \langle F \rangle$ which is the coefficient of $d\alpha$ in the expansion of $dF(\mathbf{X}_\alpha, \alpha)$ is independent of any symmetrization choice. Therefore it is convenient to introduce a symmetrization invariant derivative D_α as given by

$$D_\alpha F(\mathbf{X}_\alpha, \alpha) = \partial_\alpha F(\mathbf{X}_\alpha, \alpha) + \langle F(\mathbf{X}_\alpha, \alpha) \rangle \tag{6}$$

We end up this paragraph by introducing two formulas that will be convenient later. First, we still more compactify our notations for the differential by writing :

$$dF(\mathbf{X}_\alpha, \alpha) = \sum_{i=1}^6 \nabla_{X_\alpha^i} F(\mathbf{X}_\alpha, \alpha) dX_\alpha^i - \frac{1}{4} \sum_{i,j=1}^6 \nabla_{X_\alpha^i} \nabla_{X_\alpha^j} F(\mathbf{X}_\alpha, \alpha) (dX_\alpha^i dX_\alpha^j + dX_\alpha^j dX_\alpha^i) + D_\alpha F(\mathbf{X}_\alpha, \alpha) d\alpha \quad (7)$$

with $i, j = 1..6$. We also assume that $X_\alpha^i \equiv R_\alpha^i$ for $i = 1, 2, 3$ and $X_\alpha^i \equiv P_\alpha^i$ for $i = 4, 5, 6$. In fact, as we will show in the next sections the quantity of real importance for us in Eq. (7) is the term proportional to $d\alpha$. Note that in this notation, our previous formula for a product of differential Eq. (5) takes a compact form :

$$d(F(\mathbf{X}_\alpha, \alpha) G(\mathbf{X}_\alpha, \alpha)) = dFG + FdG - \sum_{i,j=1}^6 \nabla_{X_\alpha^i} (F) \nabla_{X_\alpha^j} (G) dX_\alpha^i dX_\alpha^j \quad (8)$$

where the last term could of course be developed as before in symmetric and antisymmetric parts.

Second, we also give the bracket formula $\langle . \rangle$ for a product of two functions. Using the procedure defined previously (see also ref. [8]) one obtains the following expression

$$\langle F(\mathbf{X}_\alpha, \alpha) G(\mathbf{X}_\alpha, \alpha) \rangle = \langle F \rangle G + F \langle G \rangle - \frac{i}{2} \nabla_{P_i} F \nabla_{R_i} G + \frac{i}{2} \nabla_{R_i} F \nabla_{P_i} G. \quad (9)$$

This formula shows that the bracket operation for a product $F(\mathbf{X}_\alpha, \alpha) G(\mathbf{X}_\alpha, \alpha)$ can also be seen as a sort of deformation of the Poisson bracket including some "internal" contributions $\langle F(\mathbf{X}_\alpha, \alpha) \rangle$ and $\langle G(\mathbf{X}_\alpha, \alpha) \rangle$.

Let us remark ultimately that the term $\langle F(\mathbf{X}_\alpha, \alpha) \rangle d\alpha$ in Eq. (4) which is of the second order in the derivatives ∇_{R_i} and ∇_{P_i} is very reminiscent of the bracket introduced in the stochastic calculus. Given the non commutativity of the operators at stake, one should in fact rather expect our formalism to be close to the quantum stochastic calculus [25]. However, it does not seem at first sight that our objects fit in such a framework which deals rather with a formalism of creation, annihilation and conservation operators. A full comparison is out of the scope of our paper.

3. Integration

Now, we will prove that the formula Eq. (4) allows to express a function $F(\mathbf{X}_\hbar, \hbar)$ which depends on the physical quantum operators $X_\hbar$ defined at the quantum scale $\alpha = \hbar$, as the

integration of a differential.

Proposition

$$F(\mathbf{X}_h, \hbar) = F(\mathbf{X}_0, 0) + \int_0^{\hbar} dF(\mathbf{X}_\alpha, \alpha). \quad (10)$$

Before proving Eq. (10), remark that this expression has the following immediate generalization :

$$F(\mathbf{X}_h, \hbar) = F(\mathbf{X}_\alpha, \alpha) + \int_\alpha^{\hbar} dF(\mathbf{X}_\beta, \beta)$$

Proof.

The proof of formula Eq. (10) is by recursion. Expanding $F(\mathbf{X}_\alpha, \alpha)$ as sum of monomials in the canonical variable, it is enough to prove our assertion for a monomial of a certain degree in the R_h^i, P_h^i . For monomials of degree one, that is linear expressions in the R_h^i, P_h^i , the result is trivial given our definitions. Now, assume that the result is true for all monomial M of, say, bidegree m, n in the R_h^i, P_h^i . We will show the result for a monomial whose degree has increased by one in one variable. Such a monomial can be written $X_h^i M$ or $M X_h^i$, with M of bidegree m, n (recall that $X_h^i = (R_h^i, P_h^i)$). We will concentrate on the first possibility, the proof being obviously the same for the other case. We compute directly $X_0^i M(\mathbf{X}_0, 0) + \int_0^{\hbar} dX_\alpha^i M(\mathbf{X}_\alpha, \alpha)$.

Given our formula for the differential of a product as well as the recurrence hypothesis which states that the integral formula is true for M we have :

$$\begin{aligned} X_0^i M(\mathbf{X}_0, 0) + \int_0^{\hbar} d(X_\alpha^i M(\mathbf{X}_\alpha, \alpha)) &= \left(X_h^i - \int_0^{\hbar} dX_\alpha^i \right) \left(M(X_h^i, \hbar) - \int_0^{\hbar} dM(\mathbf{X}_\alpha, \alpha) \right) \\ &\quad + \int_0^{\hbar} dX_\alpha^i M(\mathbf{X}_\alpha, \alpha) + \int_0^{\hbar} X_\alpha^i dM(\mathbf{X}_\alpha, \alpha) \\ &\quad - \sum_j \int_0^{\hbar} dX_\alpha^i dX_\alpha^j \nabla_{X_\alpha^j} M(\mathbf{X}_\alpha, \alpha) \end{aligned}$$

In the last line we have chosen (for the sake of simplicity) not to separate the product $dX_\alpha^i dX_\alpha^j$ into symmetric and antisymmetric part, but to keep the second order terms in a compact form. Note again the minus sign arising in front of this term due to our choice of

definition for the differential. As a consequence one has :

$$\begin{aligned}
& X_0^i M(\mathbf{X}_0, 0) + \int_0^{\hbar} d(X_\alpha^i M(\mathbf{X}_\alpha, \alpha)) \\
&= X_h^i M(X_h^i, \hbar) - \int_0^{\hbar} dX_\alpha^i M(X_h^i, \hbar) - X_h^i \int_0^{\hbar} dM(\mathbf{X}_\alpha, \alpha) + \int_0^{\hbar} dX_\alpha^i \int_0^{\hbar} dM(\mathbf{X}_\alpha, \alpha) \\
&\quad + \int_0^{\hbar} dX_\alpha^i M(\mathbf{X}_\alpha, \alpha) + \int_0^{\hbar} X_\alpha^i dM(\mathbf{X}_\alpha, \alpha) - \sum_j \int_0^{\hbar} dX_\alpha^i dX_\alpha^j \nabla_{X_\alpha^j} M(\mathbf{X}_\alpha, \alpha)
\end{aligned}$$

Now, due again to the recursion hypothesis, we rewrite $A = \int_0^{\hbar} dX_\alpha^i M(\mathbf{X}_\alpha, \alpha) + \int_0^{\hbar} X_\alpha^i dM(\mathbf{X}_\alpha, \alpha)$ in the following manner :

$$\begin{aligned}
A &= \int_0^{\hbar} dX_\alpha^i \left[M(X_h^i, \hbar) - \int_\alpha^{\hbar} dM(\mathbf{X}_{\alpha'}, \alpha') \right] + \int_0^{\hbar} \left(X_h^i - \int_\alpha^{\hbar} dX_{\alpha'}^i \right) dM(\mathbf{X}_\alpha, \alpha) \\
&= \int_0^{\hbar} dX_\alpha^i M(X_h^i, \hbar) + X_h^i \int_0^{\hbar} dM(\mathbf{X}_\alpha, \alpha) - \int_0^{\hbar} dX_\alpha^i \int_\alpha^{\hbar} dM(\mathbf{X}_{\alpha'}, \alpha') - \int_0^{\hbar} \int_\alpha^{\hbar} dX_{\alpha'}^i dM(\mathbf{X}_\alpha, \alpha)
\end{aligned}$$

Now, we have to take care about the meaning of the two last integrals. Actually, given our definition of the differential, in the first integral $\int_0^{\hbar} dX_\alpha^i \left[\int_\alpha^{\hbar} dM(\mathbf{X}_{\alpha'}, \alpha') \right]$, one has to consider that $\alpha' > \alpha$, since our differentials are pointing downward, and as a consequence when α' is getting closer to α , the "last" element of integration is $dM(\mathbf{X}_{\alpha+d\alpha}, \alpha+d\alpha) = M(\mathbf{X}_{\alpha+d\alpha}, \alpha+d\alpha) - M(\mathbf{X}_\alpha, \alpha)$. In the integral $\int_0^{\hbar} \int_\alpha^{\hbar} dX_{\alpha'}^i dM(\mathbf{X}_\alpha, \alpha)$ one has rather to consider $\alpha' < \alpha$. As a consequence, one has :

$$\begin{aligned}
& \int \int_{\alpha' < \alpha < \hbar} dX_\alpha^i dM(\mathbf{X}_{\alpha'}, \alpha') + \int \int_{\alpha < \alpha' < \hbar} dX_\alpha^i dM(\mathbf{X}_{\alpha'}, \alpha') \\
&= \int_0^{\hbar} dX_\alpha^i \int_0^{\hbar} dM(\mathbf{X}_\alpha, \alpha) - \int_0^{\hbar} dX_\alpha^i dM(\mathbf{X}_\alpha, \alpha)
\end{aligned}$$

the last term in the right cancelling the diagonal contribution that should not appear given our considerations just above. Note that this contribution would be negligible for an ordinary integral. As a consequence, we obtain :

$$\begin{aligned}
A &= \int_0^{\hbar} dX_\alpha^i M(X_h^i, \hbar) + X_h^i \int_0^{\hbar} dM(\mathbf{X}_\alpha, \alpha) - \iint_{\alpha' < \alpha < \hbar} dX_\alpha^i dM(\mathbf{X}_{\alpha'}, \alpha') - \iint_{\alpha < \alpha' < \hbar} dX_\alpha^i dM(\mathbf{X}_{\alpha'}, \alpha') \\
&= \int_0^{\hbar} dX_\alpha^i M(X_h^i, \hbar) + X_h^i \int_0^{\hbar} dM(\mathbf{X}_\alpha, \alpha) - \left(\int_0^{\hbar} dX_\alpha^i \int_0^{\hbar} dM(\mathbf{X}_\alpha, \alpha) - \int_0^{\hbar} dX_\alpha^i dM(\mathbf{X}_\alpha, \alpha) \right)
\end{aligned}$$

Gathering all the terms leads thus ultimately to :

$$\begin{aligned}
X_0^i M(\mathbf{X}_0, 0) + \int_0^{\hbar} d(X_\alpha^i M(\mathbf{X}_\alpha, \alpha)) &= X_h^i M(X_h^i, \hbar) \\
&\quad + \int_0^{\hbar} dX_\alpha^i dM(\mathbf{X}_\alpha, \alpha) - \sum_j \int_0^{\hbar} dX_\alpha^i dX_\alpha^j \nabla_{X_\alpha^j} M(\mathbf{X}_\alpha, \alpha)
\end{aligned}$$

Now, the integral on the diagonal $\int_0^{\hbar} dX_{\alpha}^i dM(\mathbf{X}_{\alpha}, \alpha)$ reduces to $\sum_j \int_0^{\hbar} dX_{\alpha}^i dX_{\alpha}^j \nabla_{X_{\alpha}^j} M(\mathbf{X}_{\alpha}, \alpha)$. Actually as explained before in the definition of the differential, the second order terms in $dM(\mathbf{X}_{\alpha}, \alpha)$, multiplied by dX_{α}^i contribute to the order $d\alpha^{\frac{3}{2}}$ which yields a zero contribution while summing over α . We thus end up with :

$$X_0^i M(\mathbf{X}_0, 0) + \int_0^{\hbar} d(X_{\alpha}^i M(\mathbf{X}_{\alpha}, \alpha)) = X_{\hbar}^i M(X_{\hbar}^i, \hbar) \quad (11)$$

which proves Eq. (10) ■.

Now, we interpret Eq. (10) as follows. Starting from the classical regime the integration over α leads in continuous manner to the fully quantum regime. This original manner to achieve a sort of quantification is very reminiscent of the renormalization group technics in which the integration of the high energy modes leads to an effective low energy theory with all quantum fluctuations included.

Eq. (10) allows us to rewrite formally a function $F(\mathbf{X}_{\hbar}, \hbar)$ depending on the physical variables in terms of the same function evaluated at the classical variables $(\mathbf{X}_0, 0)$ plus an integral of a differential. This introduce apparently a useless complexity since the expansion of the right hand side of Eq. (10) around $\mathbf{X}_{\hbar}$ involve a infinite series of the infinitesimal increment of the $d\mathbf{X}_{\alpha}$. By construction, this expansion implies trivially that all terms of the series exactly vanishes except obviously the initial term which is equal to the function $F(\mathbf{X}_{\hbar}, \hbar)$. Although trivial, this decomposition will prove useful later.

Note again that the integral in Eq. (10) has to be understood as being computed downward as seen in the definition of $(\mathbf{R}_{\alpha}, \mathbf{P}_{\alpha})$: the starting point is at $\hbar$ and the differentials are pointed downward. For example $\nabla_{\mathbf{R}_{\alpha}} F d\mathbf{R}_{\alpha} = -\nabla_{\mathbf{R}_{\alpha}} F(\mathbf{X}_{\alpha}, \alpha) (\mathbf{R}_{\alpha-d\alpha} - \mathbf{R}_{\alpha})$. However, this equation has to be taken with some care. Actually the sum over the terms proportional to $d\mathbf{X}_{\alpha}$ being a sum of terms of magnitude $\sqrt{d\alpha}$, it converges only if the sum is discretized, and this will be implicitly assumed in this paper. Defining properly the continuous limit is out of the scope of this paper.

B. Expectation operator

Having now a differential set up, we aim at defining a linear conditional expectation operator $\mathcal{E}(\cdot)$. We first set the following formula :

$$\mathcal{E}(Gd\alpha) = \mathcal{E}(G)d\alpha, \text{ whatever } G \quad (12)$$

$$\mathcal{E}(F(\mathbf{X}_h, h)) = F(\mathbf{X}_h, h) \text{ and } \mathcal{E}(F(\mathbf{X}_\alpha, \alpha)) = F(\mathbf{X}_h, h) - \int_\alpha^h \mathcal{E}(dF(\mathbf{X}_\alpha, \alpha)) \quad (13)$$

The first equality will allow to define recursively expectations of integrals of a function $F(\mathbf{X}_\alpha, \alpha)$ with a deterministic increment $d\alpha$. The second one will make the expectation conditional by fixing the starting point $\mathbf{X}_h$ of the path $\mathbf{X}_\alpha$. The third equation allows to define the expectation of an arbitrary function $F(\mathbf{X}_\alpha, \alpha)$ with the help of its initial value $F(\mathbf{X}_h, h)$ and the integral of the expectation of a differential whose rule of computation is given below. Note that, due to the required linearity of the expectation operator, the expectation has to commute with the integration. This property is implied by the third equality which yields $\mathcal{E} \int_\alpha^h (dF(\mathbf{X}_\alpha, \alpha)) = \int_\alpha^h \mathcal{E}(dF(\mathbf{X}_\alpha, \alpha))$. By analogy with the stochastic calculus, $\mathbf{X}_\alpha$ will be seen as a random path whose infinitesimal increments $d\mathbf{X}_\alpha$ will have zero expectation. However, again as in stochastic calculus, the expectation of a quadratic term like $dX_\alpha^i dX_\alpha^j$ can not be set consistently to vanish since it can be written in terms of $\mathcal{E}(dR_\alpha^i dP_\alpha^j + dP_\alpha^j dR_\alpha^i)$ and $\mathcal{E}(dR_\alpha^i dP_\alpha^j - dP_\alpha^j dR_\alpha^i) = -i\delta^{ij}d\alpha$, and the last term can not vanish due to the first definition in Eq.(12), and only the symmetric part $\mathcal{E}(dR_\alpha^i dP_\alpha^j + dP_\alpha^j dR_\alpha^i)$ can be chosen to vanish.

Consequently we set the expectation rules for products at the same "time" α

$$\mathcal{E}\left(\prod_{i=1}^n dR_{\alpha_i}\right) = \mathcal{E}\left(\prod_{i=1}^n dP_{\alpha_i}\right) = 0, \quad \mathcal{E}\left(\prod_{i=1}^n (dX_{\alpha_i}^{k_i} dX_{\alpha_i}^{l_i} + dX_{\alpha_i}^{l_i} dX_{\alpha_i}^{k_i})\right) = 0 \quad (14)$$

and for different times

$$\mathcal{E}\left(\prod_{i=1}^n \prod_{j=1}^p dX_{\alpha_i}^{k_i} dX_{\alpha_j}^{l_j}\right) = 0 \quad \text{for } \alpha_i \neq \alpha_j \quad (15)$$

We need also the independence of the increments $d\mathbf{X}_\alpha$ with respect to a function evaluated at the corresponding $\mathbf{X}_\alpha$ or all the "previous ones" $\mathbf{X}_{\alpha'}$, $\alpha' \geq \alpha$, which is formulated as

$$\mathcal{E}(F(\mathbf{X}_{\alpha'}) d\mathbf{Z}_\alpha) = \mathcal{E}(F(\mathbf{X}_{\alpha'})) \mathcal{E}(d\mathbf{Z}_\alpha) = 0 \text{ for } \alpha' \geq \alpha \quad (16)$$

where $\alpha = (\alpha_1, \dots, \alpha_p)$ is an arbitrary number of values all different and all lower or equal to α' . $d\mathbf{Z}_\alpha$ is condensed notation for a product $\prod_{i=1}^p dZ_{\alpha_i}$ where the dZ_{α_i} can be $dX_{\alpha_i}^{k_i}$ or $(dX_{\alpha_i}^{k_i}dX_{\alpha_i}^{l_i} + dX_{\alpha_i}^{l_i}dX_{\alpha_i}^{k_i})$ with $k_i = 1..6$.

We could impose Eq. (16) directly, but this property is in fact the direct consequence of a single condition that we will thus enforce which is the independence of the increments $d\mathbf{X}_\alpha$ with respect to the initial value $\mathbf{X}_h$ of the path :

$$\mathcal{E}(F(\mathbf{X}_h) d\mathbf{Z}_\alpha) = \mathcal{E}(F(\mathbf{X}_h)) \mathcal{E}(d\mathbf{Z}_\alpha) = 0 \quad (17)$$

That Eq. (16) follows from this single condition is a direct recursive computation. Actually, Eq. (16) is trivially checked for $F(\mathbf{X}_{\alpha'})$ a polynomial of degree 0 in $(\mathbf{X}_{\alpha'}, \alpha')$ since $\mathcal{E}(ad\mathbf{X}_\alpha) = a\mathcal{E}(d\mathbf{X}_\alpha) = 0$ for a constant. If Eq. (16) is true for a polynomial of degree N in the variables $(\mathbf{X}_{\alpha'}, \alpha')$, then consider $F(\mathbf{X}_{\alpha'}, \alpha')$ to be of degree $N + 1$. As a consequence,

$$\begin{aligned} \mathcal{E}(F(\mathbf{X}_{\alpha'}) d\mathbf{Z}_\alpha) &= \mathcal{E}\left(\left(F(\mathbf{X}_h) - \int_{\alpha'}^h dF(\mathbf{X}_\beta, \beta)\right) d\mathbf{Z}_\alpha\right) \\ &= \mathcal{E}(F(\mathbf{X}_h) d\mathbf{Z}_\alpha) - \mathcal{E}\left(\int_{\alpha'}^h dF(\mathbf{X}_\beta, \beta) d\mathbf{Z}_\alpha\right) \\ &= -\mathcal{E}\left(\int_{\alpha'}^h dF(\mathbf{X}_\beta, \beta) d\mathbf{Z}_\alpha\right) \end{aligned}$$

the last equality being a consequence of (17). Now, since

$$\begin{aligned} \mathcal{E}(dF(\mathbf{X}_\beta, \beta)) &= \mathcal{E}\left(D_\beta F(\mathbf{X}_\beta, \beta) d\beta + \sum_{i=1}^6 \nabla_{X_\beta^i} F(\mathbf{X}_\beta, \beta) dX_\beta^i \right. \\ &\quad \left. - \frac{1}{4} \sum_{i,j=1}^6 \nabla_{X_\beta^i} \nabla_{X_\beta^j} F(\mathbf{X}_\beta, \beta) (dX_\beta^i dX_\beta^j + dX_\beta^j dX_\beta^i) \right) \end{aligned}$$

all terms in the integral are of degree lower or equal to N , so that the recurrence applies (recall that since the integration is downward, in the integral over β , $\beta > \alpha' \geq \alpha$ and thus in the set (β, α) all elements are different) and $\mathcal{E}(dF(\mathbf{X}_\beta, \beta)) d\mathbf{Z}_\alpha = 0$. Thus Eq. (16) is true for polynomials. Since all along the paper we consider functions $F(\mathbf{X}_{\alpha'}, \alpha')$ that are converging series in the variables $(\mathbf{X}_{\alpha'}, \alpha')$ (seen as classical commuting real variables), the density of the polynomial in that space of functions ends the proof.

A first consequence of the definitions and Eq. (16) is

$$\begin{aligned} \mathcal{E}(dF(\mathbf{X}_\alpha, \alpha)) &= \mathcal{E}(\partial_\alpha F(\mathbf{X}_\alpha, \alpha) + \langle F(\mathbf{X}_\alpha, \alpha) \rangle) d\alpha \\ &= \mathcal{E}(D_\alpha F(\mathbf{X}_\alpha, \alpha)) d\alpha \end{aligned}$$

This formula allows to compute the integral of $\mathcal{E}(dF(\mathbf{X}_\alpha, \alpha))$ set previously, as an "ordinary" integral since the integration element is only $d\alpha$.

The main interest of these definitions will show up later on when a function $F(\mathbf{X}_h, \hbar)$ will be written as an series expansion of iterated integrals along the path $\mathbf{X}_\alpha$. Indeed, as already said before, the expansion of the two terms in the right hand side of Eq. (10) around $\mathbf{X}_h$, implies a mechanism of cancellation of all contributions proportional to products of $dX_{\alpha_i}^{k_i}$. The expectation operator is built to cancel separately the contributions of products of $dX_{\alpha_i}^{k_i}$ at different times and symmetric products $(dX_{\alpha_i}^{k_i} dX_{\alpha_i}^{l_i} + dX_{\alpha_i}^{l_i} dX_{\alpha_i}^{k_i})$ at the same time, coming from the two terms of the right hand side of Eq. (10). The rest of the contributions form the right hand side of Eq. (10) proportional to $d\alpha$ cancel exactly. As a consequence of this, an arbitrary function can be written

$$\begin{aligned} F_h(\mathbf{X}_h) &= \mathcal{E}(F_h(\mathbf{X}_h)) = \mathcal{E}\left(F(\mathbf{X}_0, 0) + \int_0^h dF(\mathbf{X}_\alpha, \alpha)\right) \\ &= \mathcal{E}(F(\mathbf{X}_0, 0)) + \mathcal{E}\left(\int_0^h D_\alpha F(\mathbf{X}_\alpha, \alpha) d\alpha\right) \end{aligned}$$

Once again we have apparently introduced some useless complexity, since the function $F_h(\mathbf{X}_h)$ has been replaced by $\mathcal{E}(F(\mathbf{X}_0, 0))$ which cannot be computed directly, plus the integral $\mathcal{E}\left(\int_0^h D_\alpha F(\mathbf{X}_\alpha, \alpha) d\alpha\right)$. Irrelevant sums of infinitesimal increments have been introduced in both terms and thus ultimately have to cancel. However, this formulation presents the advantage of replacing $\mathbf{X}_h$ by $\mathbf{X}_0$ in the first contribution which will simplify some of our computations later. The integration over $d\alpha$ will allow to start a recursive expansion in the Planck constant. But to do so, we first need to introduce an other operator connecting a function evaluated at $\mathbf{X}_0$ to the same function evaluated at $\mathbf{X}_h$. This is the role of the EBS operation defined below that realizes a kind of connection between the spaces of operators at two different values of α .

A second consequence of our definitions is the factorization of the initial value in the expectation :

$$\mathcal{E}(F(\mathbf{X}_h, \hbar) G(\mathbf{X}_\alpha, \alpha)) = F(\mathbf{X}_h) \mathcal{E}(G(\mathbf{X}_\alpha, \alpha)), \alpha \leq h$$

This property is usually trivial in probability, but here has to be derived given we have started with expectations of infinitesimal increments. It comes from iterating the differentiation of

$G(\mathbf{X}_\alpha)$ similar to the chaotic expansion in stochastic calculus. Actually, we can write :

$$\mathcal{E}(F(\mathbf{X}_h, \hbar) G(\mathbf{X}_\alpha, \alpha)) = F(\mathbf{X}_h, \hbar) G(\mathbf{X}_h, \hbar) - \mathcal{E}\left(F(\mathbf{X}_h, \hbar) \int_\alpha^\hbar dG(\mathbf{X}_\alpha, \alpha) d\alpha\right)$$

given Eq. (16), this reduces to :

$$\begin{aligned} \mathcal{E}(F(\mathbf{X}_h, \hbar) G(\mathbf{X}_\alpha, \alpha)) &= F(\mathbf{X}_h, \hbar) G(\mathbf{X}_h, \hbar) - \mathcal{E}\left(F(\mathbf{X}_h, \hbar) \int_\alpha^\hbar D_\alpha G(\mathbf{X}_\alpha, \alpha) d\alpha\right) \\ &= F(\mathbf{X}_h, \hbar) G(\mathbf{X}_h, \hbar) - \int_\alpha^\hbar \mathcal{E}(F(\mathbf{X}_h, \hbar) D_\alpha G(\mathbf{X}_\alpha, \alpha)) d\alpha \end{aligned}$$

and once again the recurrence works recursively for polynomials. If $G(\mathbf{X}_\alpha, \alpha)$ is of degree N in $(\mathbf{X}_\alpha, \alpha)$, then $D_\alpha G(\mathbf{X}_\alpha, \alpha)$ is of degree $N - 1$, and thus the property can be assumed to be true for $D_\alpha G(\mathbf{X}_\alpha, \alpha)$, so that :

$$\begin{aligned} \mathcal{E}(F(\mathbf{X}_h, \hbar) G(\mathbf{X}_\alpha, \alpha)) &= F(\mathbf{X}_h, \hbar) G(\mathbf{X}_h, \hbar) - F(\mathbf{X}_h, \hbar) \mathcal{E}\left(\int_\alpha^\hbar D_\alpha G(\mathbf{X}_\alpha, \alpha) d\alpha\right) \\ &= F(\mathbf{X}_h, \hbar) \mathcal{E}(G(\mathbf{X}_\alpha, \alpha)) \end{aligned}$$

as needed.

We close this paragraph by a general remark about the nature of the expectation operation. Despite the formal similarities with the stochastic calculus, the expectation defined above is really different, since the expectation is in fact a function of operators evaluated at $\mathbf{X}_h$, not a number. This has some consequences concerning the cancellation of certain types of expectations that have no counterpart in usual probability theory. But to derive such consequences, we first need to define some more tools.

C. EBS operator

We now introduce a way to relate two expectations of the same function evaluated at two different variables namely $\mathcal{E}(F(\mathbf{X}_\alpha, \alpha))$ to $\mathcal{E}(F(\mathbf{X}_{\alpha'}, \alpha))$ but with constant explicit dependence in α . Given our previous definitions Eq. (7), one has

$$\begin{aligned} F(\mathbf{X}_{\alpha-d\alpha}, \alpha-d\alpha) - F(\mathbf{X}_\alpha, \alpha-d\alpha) &= -\langle F(\mathbf{X}_\alpha, \alpha-d\alpha) \rangle d\alpha - \sum_{i=1}^6 \nabla_{X_\alpha^i} F(\mathbf{X}_\alpha, \alpha-d\alpha) dX_\alpha^i \\ &\quad + \frac{1}{4} \sum_{i,j=1}^6 \nabla_{X_\alpha^j} \nabla_{X_\alpha^i} F(\mathbf{X}_\alpha, \alpha-d\alpha) (dX_\alpha^i dX_\alpha^j + dX_\alpha^j dX_\alpha^i) \end{aligned} \tag{18}$$

The absence of the $\partial/\partial\alpha$ term implies that this expression really depends on the choice of the symmetrization of the function $F(\mathbf{X}_\alpha, \alpha)$. As a consequence considering the expectation, one has :

$$\mathcal{E}(F(\mathbf{X}_{\alpha-d\alpha}, \alpha - d\alpha)) = \mathcal{E}((1 - \langle \cdot \rangle) d\alpha) F(\mathbf{X}_\alpha, \alpha - d\alpha) \quad (19)$$

where $\langle \cdot \rangle$ is the bracket operator defined previously. At this point we have to remark that, since the $\langle \cdot \rangle$ operation depends on the symmetrization procedure, the right hand side of Eq.(19) seems to depend on the choice of symmetrization in the variables $\mathbf{X}_\alpha$ in $F(\mathbf{X}_\alpha, \alpha - d\alpha)$. However, and this is the most important for us, the operation that sends $F(\mathbf{X}_{\alpha-d\alpha}, \alpha - d\alpha)$ to $(1 - \langle \cdot \rangle) d\alpha) F(\mathbf{X}_\alpha, \alpha - d\alpha)$ by first replacing $\mathbf{X}_{\alpha-d\alpha}$ by $\mathbf{X}_\alpha$ in F and then applying $(1 - \langle \cdot \rangle) d\alpha)$, is independent at the first order in $d\alpha$ of any choice of symmetrization for the operators in the series expansion of $F(\mathbf{X}_{\alpha-d\alpha}, \alpha - d\alpha)$. This is a trivial fact since $((1 - \langle \cdot \rangle) d\alpha) F(\mathbf{X}_\alpha, \alpha - d\alpha) = F(\mathbf{X}_\alpha, \alpha) - (\frac{\partial}{\partial\alpha} + \langle \cdot \rangle) d\alpha) F(\mathbf{X}_\alpha, \alpha)$, and this expression is independent of the symmetrization choice as explained before. This operation, that will be the only one relevant for us, is thus a consistent and independent of any symmetrization. The apparent trouble with the right hand side in Eq. (19) comes only from the fact that changing the order of operators $\mathbf{X}_{\alpha-d\alpha}$ is not the same operation as changing the order of operators $\mathbf{X}_\alpha$ due to different commutation relations. To avoid any confusion a subscript $\alpha - d\alpha$ should be added to F to remind that the symmetrization has to be considered for the variables $\mathbf{X}_{\alpha-d\alpha}$, but it would complicate the notations in a useless way for the present paper.

The meaning of our operator $1 - \langle \cdot \rangle d\alpha$ being now clarified, the above differential equation Eq. (19) can be integrated to get the following relation

Proposition

$$\mathcal{E}(F(\mathbf{X}_{\alpha_2}, \alpha_2)) = \mathcal{E}\left(S_{\mathbf{X}_{\alpha_1}} \left[T \exp\left(-\int_{\alpha_2}^{\alpha_1} [S_{\mathbf{X}_{\alpha_1}} \langle \cdot \rangle_\alpha S_{\mathbf{X}_\alpha}] d\alpha\right) F(\mathbf{X}_{\alpha_2}, \alpha_2) \right]\right) \quad (20)$$

valid for $\alpha_1 > \alpha_2$.

The bracket $\langle \cdot \rangle_\alpha$ reminds that all commutators between canonical variables have to be computed with values $i\alpha$. The operator $S_{\mathbf{X}_\alpha}$ is a shift operator that sets the dynamical variables to $\mathbf{X}_\alpha$. that is $S_{\mathbf{X}_\alpha} F(\mathbf{X}_\beta) = F(\mathbf{X}_\alpha)$. Its action does not depend on the relative values of α and β and $S_{\mathbf{X}_\alpha} S_{\mathbf{X}_\beta} = S_{\mathbf{X}_\alpha}$ whatever the values of α and β . In addition, T is the

notation for the ordered exponential, that is :

$$\begin{aligned} T e^{-\int_{\alpha_2}^{\alpha_1} S_{\mathbf{X}_{\alpha_1}} \langle \cdot \rangle_{\alpha} S_{\mathbf{X}_{\alpha}} d\alpha} &= \sum_{n=0}^{\infty} \int_{\alpha_2 < \beta_n < \dots \beta_1 < \alpha_1} \left[-S_{\mathbf{X}_{\alpha_1}} \langle \cdot \rangle_{\beta_n} S_{\mathbf{X}_{\beta_n}} \right] \dots \left[-S_{\mathbf{X}_{\alpha_1}} \langle \cdot \rangle_{\beta_1} S_{\mathbf{X}_{\beta_1}} \right] d\beta_1 \dots d\beta_n \\ &= \sum_{n=0}^{\infty} \int_{\alpha_2 < \beta_n < \dots \beta_1 < \alpha_1} \left[-S_{\mathbf{X}_{\alpha_1}} \langle \cdot \rangle_{\beta_n} S_{\mathbf{X}_{\beta_n}} \right] \dots \left[-\langle \cdot \rangle_{\beta_1} S_{\mathbf{X}_{\beta_1}} \right] d\beta_1 \dots d\beta_n \end{aligned}$$

Once again, the result is independent of the choice of initial symmetrization chosen in the variables $\mathbf{X}_{\alpha_2}$. The introduction of the shift $S_{\mathbf{X}_{\alpha}}$ is crucial and induced by our previous considerations since the bracket operation has to be accompanied by a shift of the variable all along the integration process, so that ultimately $\mathbf{X}_{\alpha_2}$ is replaced by $\mathbf{X}_{\alpha_1}$.

Proof.

The proof of Eq. (20) is as follows. Define the function :

$$G(\mathbf{X}_{\alpha_1}, \alpha_1) = S_{\mathbf{X}_{\alpha_1}} \left[T \exp \left(- \int_{\alpha_2}^{\alpha_1} [S_{\mathbf{X}_{\alpha_1}} \langle \cdot \rangle_{\alpha} S_{\mathbf{X}_{\alpha}}] d\alpha \right) F(\mathbf{X}_{\alpha_2}, \alpha_2) \right]$$

The dependence in the parameter α_2 has been skipped for the sake of convenience. Differentiating $G(\mathbf{X}_{\alpha_1}, \alpha_1)$ with respect to α_1 yields :

$$\begin{aligned} dG(\mathbf{X}_{\alpha_1}, \alpha_1) &= G(\mathbf{X}_{\alpha_1}, \alpha_1) - G(\mathbf{X}_{\alpha_1-d\alpha}, \alpha_1 - d\alpha) \\ &= S_{\mathbf{X}_{\alpha_1}} \left(T e^{-\int_{\alpha_2}^{\alpha_1} [S_{\mathbf{X}_{\alpha_1}} \langle \cdot \rangle_{\alpha} S_{\mathbf{X}_{\alpha}}] d\alpha} F(\mathbf{X}_{\alpha_2}, \alpha_2) \right) - G(\mathbf{X}_{\alpha_1-d\alpha}, \alpha_1 - d\alpha) \\ &= S_{\mathbf{X}_{\alpha_1}} (1 - \langle \cdot \rangle_{\alpha_1-d\alpha} d\alpha) S_{\mathbf{X}_{\alpha_1-d\alpha_1}} \left(T e^{-\int_{\alpha_2}^{\alpha_1-d\alpha_1} [S_{\mathbf{X}_{\alpha_1}} \langle \cdot \rangle_{\alpha} S_{\mathbf{X}_{\alpha}}] d\alpha} F(\mathbf{X}_{\alpha_2}, \alpha_2) \right) \\ &\quad - G(\mathbf{X}_{\alpha_1-d\alpha}, \alpha_1 - d\alpha) \\ &= (1 - \langle \cdot \rangle_{\alpha_1} d\alpha) S_{\mathbf{X}_{\alpha_1}} S_{\mathbf{X}_{\alpha_1-d\alpha_1}} \left[T e^{-\int_{\alpha_2}^{\alpha_1-d\alpha_1} [S_{\mathbf{X}_{\alpha_1}} \langle \cdot \rangle_{\alpha} S_{\mathbf{X}_{\alpha}}] d\alpha} F(\mathbf{X}_{\alpha_2}, \alpha_2) \right] \\ &\quad - G(\mathbf{X}_{\alpha_1-d\alpha}, \alpha_1 - d\alpha) \end{aligned}$$

where the last equality is taken at the lowest order in $d\alpha$. Considering the expectations of the quantities involved, and using Eq. (19), we are thus ultimately left with :

$$\begin{aligned} \mathcal{E} dG(\mathbf{X}_{\alpha_1}, \alpha_1) &= \mathcal{E} \left((1 - \langle \cdot \rangle_{\alpha_1} d\alpha) S_{\mathbf{X}_{\alpha_1}} G(\mathbf{X}_{\alpha_1-d\alpha}, \alpha_1 - d\alpha) - G(\mathbf{X}_{\alpha_1-d\alpha}, \alpha_1 - d\alpha) \right) \\ &= \mathcal{E} \left((1 - \langle \cdot \rangle_{\alpha_1} d\alpha) G(\mathbf{X}_{\alpha_1}, \alpha_1 - d\alpha) - G(\mathbf{X}_{\alpha_1-d\alpha}, \alpha_1 - d\alpha) \right) = 0 \end{aligned}$$

and as a consequence, using the properties of the expectation operator :

$$\mathcal{E} (G(\mathbf{X}_{\alpha_1}, \alpha_1) - G(\mathbf{X}_{\alpha_2}, \alpha_2)) = \mathcal{E} \int_{\alpha_1}^{\alpha_2} dG(\mathbf{X}_{\alpha_1}, \alpha_1) = \int_{\alpha_1}^{\alpha_2} \mathcal{E} dG(\mathbf{X}_{\alpha_1}, \alpha_1) = 0$$

The fact that $G(\mathbf{X}_{\alpha_2}, \alpha_2) = F(\mathbf{X}_{\alpha_2}, \alpha_2)$ ends the proof ■.

To gain some space in the sequel, we will define an abbreviation for the previous operation. We will denote ultimately :

$$\exp\left(-\langle.\rangle_{\alpha_2 \rightarrow \alpha_1}^S\right) \equiv S_{\mathbf{X}_{\alpha_1}} T \exp\left(-\int_{\alpha_2}^{\alpha_1} S_{\mathbf{X}_{\alpha_1}} \langle.\rangle_{\alpha} S_{\mathbf{X}_{\alpha}} d\alpha\right) \quad (21)$$

as the **exponentiated bracket plus shift**, called EBS operation. As a consequence, Eq. (20) rewrites as :

$$\mathcal{E}(F(\mathbf{X}_{\alpha_2}, \alpha_2)) = \mathcal{E}\left(\exp\left(-\langle.\rangle_{\alpha_2 \rightarrow \alpha_1}^S\right) F(\mathbf{X}_{\alpha_2}, \alpha_2)\right) \text{ for } \alpha_1 > \alpha_2 \quad (22)$$

This last formula can be understood intuitively as follows. since the EBS operation changes the function (by the action of the bracket defined above) but also changes progressively the variables from $\mathbf{X}_{\alpha_2}$ to $\mathbf{X}_{\alpha_1}$ (through the shift operator) both the bracket operation and the shift of variable compensate each other to produce the equality with the left hand side.

Let us ultimately insist on the fact that the expression in the right hand side $\exp\left(-\langle.\rangle_{\alpha_2 \rightarrow \alpha_1}^S\right) F(\mathbf{X}_{\alpha_2}, \alpha_2)$ is a function of $(\mathbf{X}_{\alpha_1}, \alpha_1)$ due to the action of the shift and is therefore a different function than $F(\mathbf{X}_{\alpha_2}, \alpha_2)$. Only the expectations of both expressions of Eq. (22) are equal.

In the particular case where $\alpha_1 = \hbar$, since the right hand side of Eq. (22) depends only on $(\mathbf{X}_{\hbar}, \hbar)$ the expectation can be safely removed so that

$$\mathcal{E}(F(\mathbf{X}_{\alpha_2}, \alpha_2)) = \exp\left(-\langle.\rangle_{\alpha_2 \rightarrow \hbar}^S\right) F(\mathbf{X}_{\alpha_2}, \alpha_2) \quad (23)$$

We end up this section by giving a full generalization of the previous formula to a product of n functions and show the

Proposition

$$\begin{aligned} & \mathcal{E}(H_1(\mathbf{X}_{\alpha_1}, \alpha_1) \dots H_n(\mathbf{X}_{\alpha_n}, \alpha_n)) \\ &= \mathcal{E}\left(e^{-\langle.\rangle_{\alpha_1 \rightarrow \alpha}^S} H_1(\mathbf{X}_{\alpha_1}, \alpha_1) e^{-\langle.\rangle_{\alpha_2 \rightarrow \alpha_1}^S} H_2(\mathbf{X}_{\alpha_2}, \alpha_2) \dots e^{-\langle.\rangle_{\alpha_n \rightarrow \alpha_{n-1}}^S} H_n(\mathbf{X}_{\alpha_n}, \alpha_n)\right) \end{aligned} \quad (24)$$

for $\alpha_n < \dots < \alpha_1 < \alpha$. This expression for $\alpha = \hbar$ becomes

$$\begin{aligned} & \mathcal{E}(H_1(\mathbf{X}_{\alpha_1}, \alpha_1) \dots H_n(\mathbf{X}_{\alpha_n}, \alpha_n)) \\ &= \mathcal{E}\left(e^{-\langle.\rangle_{\alpha_1 \rightarrow \hbar}^S} H_1(\mathbf{X}_{\alpha_1}, \alpha_1) e^{-\langle.\rangle_{\alpha_2 \rightarrow \alpha_1}^S} H_2(\mathbf{X}_{\alpha_2}, \alpha_2) \dots e^{-\langle.\rangle_{\alpha_n \rightarrow \alpha_{n-1}}^S} H_n(\mathbf{X}_{\alpha_n}, \alpha_n)\right) \end{aligned} \quad (25)$$

Note that the order of the functions in the product is irrelevant, and the formula is also true if some functions are permuted.

Proof. We start the proof with the following lemma:

Lemma

Let $F_1(\mathbf{X}_{\alpha_1}, \alpha_1)$, $F_2(\mathbf{X}_{\alpha_2}, \alpha_2)$ be two arbitrary functions with $\alpha_2 < \alpha_1$. We state that :

$$\mathcal{E}(dF_2(\mathbf{X}_{\alpha_2}, \alpha_2)) = 0 \Rightarrow \mathcal{E}(F_1(\mathbf{X}_{\alpha_1}, \alpha_1) dF_2(\mathbf{X}_{\alpha_2}, \alpha_2)) = 0 \quad (26)$$

This result has no counterpart in usual probability, and, as said in the previous section, this is the consequence of our definition of the expectation which sends an operator to an operator, not to a number.

Proof of the Lemma.

We first show that, for $\alpha < \hbar$ and every function $F(\mathbf{X}_\alpha, \alpha)$ that can be expanded in a series of $(\mathbf{X}_\alpha, \alpha)$ converging "in the classical sense, that is when the $(\mathbf{X}_\alpha, \alpha)$ are seen as commuting real variables, $\mathcal{E}(F(\mathbf{X}_\alpha, \alpha)) = 0$ implies that $F(\mathbf{X}_\alpha, \alpha) = 0$. This is trivially true for a polynomial of degree 0 or 1 in $\mathbf{X}_\alpha$ since $\mathbf{X}_\alpha = \mathbf{X}_\hbar - \int_\alpha^\hbar d\mathbf{X}_\beta$ and $\mathcal{E}\mathbf{X}_\alpha = \mathbf{X}_\hbar - \int_\alpha^\hbar \mathcal{E}d\mathbf{X}_\beta = \mathbf{X}_\hbar$ as derived from Eq. (16). As a consequence $\mathcal{E}(a\mathbf{X}_\alpha + b) = (a\mathbf{X}_\hbar + b)$ which is null only if $a = b = 0$.

Now, assume that $\mathcal{E}(F(\mathbf{X}_\alpha, \alpha)) = 0 \Rightarrow F(\mathbf{X}_\alpha, \alpha) = 0$ for all polynomial of degree lower or equal to N in the variables $\mathbf{X}_\alpha$. Consider then for $F(\mathbf{X}_\alpha, \alpha)$ a polynomial of degree $N+1$ (the coefficients depend on α). Then using the EBS operator, we can write :

$$\mathcal{E}(F(\mathbf{X}_\alpha, \alpha)) = \mathcal{E}\left(\exp\left(-\langle \cdot \rangle_{\alpha \rightarrow \alpha_1}^S\right) F(\mathbf{X}_\alpha, \alpha)\right)$$

given the bracket operation is defined through a derivative of second order, we thus have :

$$\mathcal{E}(F(\mathbf{X}_\alpha, \alpha)) = F(\mathbf{X}_\hbar, \alpha) + \text{Polynomial of degree } N-1 \text{ in } \mathbf{X}_\hbar$$

If this is 0, then necessarily the monomials of degree $N+1$ in $F(\mathbf{X}_\hbar, \alpha)$ have to be null. As a consequence $F(\mathbf{X}_\hbar, \alpha)$ is of degree N and thus null by hypothesis. As a consequence, the lemma to be shown is true for every polynomial, and by a density argument for all the kind of series considered.

In a second step, notice that a direct consequence of the above proposition is that

$$\mathcal{E}(dF(\mathbf{X}_\alpha, \alpha)) = 0 \Rightarrow D_\alpha F(\mathbf{X}_\alpha, \alpha) = 0$$

actually, $\mathcal{E}(dF(\mathbf{X}_\alpha, \alpha)) = \mathcal{E}(D_\alpha F(\mathbf{X}_\alpha, \alpha)) d\alpha = 0$, which implies that $D_\alpha F(\mathbf{X}_\alpha, \alpha) = 0$.

We can then prove the required proposition. Actually, by construction of our expectation operator, since $\alpha_2 < \alpha_1$,

$$\begin{aligned}
& \mathcal{E}(F_1(\mathbf{X}_{\alpha_1}, \alpha_1) dF_2(\mathbf{X}_{\alpha_2}, \alpha_2)) \\
&= \mathcal{E}\left(F_1(\mathbf{X}_{\alpha_1}, \alpha_1) \left(D_{\alpha_2} F_2(\mathbf{X}_{\alpha_2}, \alpha_2) d\alpha_2 + \nabla_{X_{\alpha_2}^i} F_2(\mathbf{X}_{\alpha_2}, \alpha_2) dX_{\alpha_2}^i\right)\right) \\
&\quad + \mathcal{E}\left(F_1(\mathbf{X}_{\alpha_1}, \alpha_1) \left(-\frac{1}{4} \nabla_{X_{\alpha_2}^j} \nabla_{X_{\alpha_2}^i} F_2(\mathbf{X}_{\alpha_2}, \alpha_2) dX_{\alpha_2}^i dX_{\alpha_2}^j + dX_{\alpha_2}^j dX_{\alpha_2}^i\right)\right) \\
&= \mathcal{E}(F_1(\mathbf{X}_{\alpha_1}, \alpha_1) D_{\alpha_2} F_2(\mathbf{X}_{\alpha_2}, \alpha_2)) d\alpha_2 \\
&= 0
\end{aligned}$$

the second equality is a consequence of Eq. (16). This last result shows the lemma ■.

The proof of the proposition is now in two steps. We first consider a product of two functions and show :

$$\begin{aligned}
\mathcal{E}(H_1(\mathbf{X}_{\alpha_1}, \alpha_1) H_2(\mathbf{X}_{\alpha_2}, \alpha_2)) &= \mathcal{E}\left(e^{-\langle \cdot \rangle_{\alpha_1 \rightarrow \alpha}^S} H_1(\mathbf{X}_{\alpha_1}, \alpha_1) e^{-\langle \cdot \rangle_{\alpha_2 \rightarrow \alpha_1}^S} H_2(\mathbf{X}_{\alpha_2}, \alpha_2)\right) \\
&\text{for } \alpha_1 > \alpha_2
\end{aligned} \tag{27}$$

To do so, let us start again with $G(\mathbf{X}_{\alpha_\gamma}, \gamma) = \exp\left(-\langle \cdot \rangle_{\alpha_2 \rightarrow \gamma}^S\right) H_2(\mathbf{X}_{\alpha_2}, \alpha_2)$, γ is an arbitrary parameter varying between α_1 and α_2 . The dependence in α_2 in $G(\mathbf{X}_{\alpha_\gamma}, \gamma)$ is forgotten here for the sake of simplicity. By differentiation with respect to γ we have, as before, at the lowest order in $d\alpha$:

$$\mathcal{E}(dG(\mathbf{X}_{\alpha_\gamma}, \gamma)) = \mathcal{E}(H_2(\mathbf{X}_{\alpha_\gamma}, \gamma) - H_2(\mathbf{X}_{\alpha_\gamma - d\gamma}, \gamma - d\gamma)) = 0$$

Now, multiply by $H_1(\mathbf{X}_{\alpha_1}, \alpha_1)$ and take the expectation. Since $\gamma < \alpha_1$, one has using Eq. (26) :

$$\mathcal{E}(H_1(\mathbf{X}_{\alpha_1}, \alpha_1) dG(\mathbf{X}_{\alpha_\gamma}, \gamma)) = 0$$

the integration of this last relation (recall that the integral and the expectation commute), yields :

$$\mathcal{E}\left(H_1(\mathbf{X}_{\alpha_1}, \alpha_1) \int_{\alpha_2}^{\alpha_1} dG(\mathbf{X}_\alpha, \alpha)\right) = 0$$

that is :

$$\mathcal{E}\left(H_1(\mathbf{X}_{\alpha_1}, \alpha_1) e^{-\langle \cdot \rangle_{\alpha_2 \rightarrow \alpha_1}^S} H_2(\mathbf{X}_{\alpha_2}, \alpha_2)\right) = \mathcal{E}(H_1(\mathbf{X}_{\alpha_1}, \alpha_1) H_2(\mathbf{X}_{\alpha_2}, \alpha_2))$$

Then, use Eq. (22) with $F(\mathbf{X}_{\alpha_1}, \alpha_1) = H_1(\mathbf{X}_{\alpha_1}, \alpha_1) \exp\left(-\langle \cdot \rangle_{\alpha_2 \rightarrow \alpha_1}^S\right) H_2(\mathbf{X}_{\alpha_2}, \alpha_2)$ between α_1 and $\hbar$ to get :

$$\begin{aligned} \mathcal{E}(H_1(\mathbf{X}_{\alpha_1}, \alpha_1) H_2(\mathbf{X}_{\alpha_2}, \alpha_2)) &= \mathcal{E}\left(H_1(\mathbf{X}_{\alpha_1}, \alpha_1) e^{-\langle \cdot \rangle_{\alpha_2 \rightarrow \alpha_1}^S} H_2(\mathbf{X}_{\alpha_2}, \alpha_2)\right) \\ &= \mathcal{E}\left(e^{-\langle \cdot \rangle_{\alpha_1 \rightarrow \alpha}^S} H_1(\mathbf{X}_{\alpha_1}, \alpha_1) e^{-\langle \cdot \rangle_{\alpha_2 \rightarrow \alpha_1}^S} H_2(\mathbf{X}_{\alpha_2}, \alpha_2)\right) \end{aligned}$$

which is the required result. In a second step, the generalization to a product of n arbitrary functions is shown recursively by starting from the right and replacing $H_1(\mathbf{X}_{\alpha_n}, \alpha_n)$ by $\exp\left(-\langle \cdot \rangle_{\alpha_n \rightarrow \alpha_{n-1}}^S\right) H_n(\mathbf{X}_{\alpha_n}, \alpha_n)$, then to do the same with $H_1(\mathbf{X}_{\alpha_{n-1}}, \alpha_{n-1}) \exp\left(-\langle \cdot \rangle_{\alpha_n \rightarrow \alpha_{n-1}}^S\right) H_n(\mathbf{X}_{\alpha_n}, \alpha_n)$ and so on ■.

We can now exploit the mathematical construction developed in this section to consider the formal diagonalization of an arbitrary matrix valued quantum Hamiltonian.

III. THE DIAGONALIZATION PROCEDURE

We now consider a generic matrix valued quantum Hamiltonian $H(\mathbf{R}, \mathbf{P})$ where $\mathbf{R}$ and $\mathbf{P}$ are the usual canonical coordinate and momentum operators satisfying the canonical Heisenberg algebra. Our goal is to find a unitary transformation U such that UHU^+ is a diagonal matrix valued operator $\varepsilon(\mathbf{R}, \mathbf{P})$ (block diagonal for the Dirac Hamiltonian). This is in general an excessively difficult mathematical problem. For this reason we consider this problem by dividing it in several steps.

A. The Hamiltonian

First we introduce the unitary matrix $U_\alpha(\mathbf{X}_\alpha) \equiv U(\mathbf{X}_\alpha, \alpha)$ which diagonalizes the Hamiltonian $H(\mathbf{X}_\alpha)$ where the canonical variables $\mathbf{X}_\hbar \equiv \mathbf{X}$ have been replaced by the running ones $\mathbf{X}_\alpha$, so that we can write

$$U_\alpha(\mathbf{X}_\alpha) H(\mathbf{X}_\alpha) U_\alpha^+(\mathbf{X}_\alpha) = \varepsilon_\alpha(\mathbf{X}_\alpha) \quad (28)$$

with $\varepsilon_\alpha(\mathbf{X}_\alpha) \equiv \varepsilon_\alpha(\mathbf{X}_\alpha, \alpha)$. With the help of the previous identities Eqs. (10) (12) (14), we can compute $\varepsilon_\hbar(\mathbf{X}_\hbar) \equiv \varepsilon(\mathbf{X})$. Indeed as $\varepsilon(\mathbf{X}) = \mathcal{E}(\varepsilon(\mathbf{X}))$ we can write

$$\varepsilon(\mathbf{X}) = \mathcal{E}\left(\varepsilon_0(\mathbf{X}_0) + \int_0^\hbar d\varepsilon_{\alpha_1}(\mathbf{X}_{\alpha_1})\right). \quad (29)$$

Clearly $\varepsilon_0(\mathbf{X}_0)$ corresponds to the diagonal representation of the original Hamiltonian $H(\mathbf{X})$ where the canonical operators $\mathbf{X}$ have been replaced by the classical variables $\mathbf{X}_0$. In practice, it is usually quite easy to diagonalize the Hamiltonian when the operators are commuting. This is the essence of the method. Starting with classical variables we can recursively introduce more and more "quantification" through the running parameter α until we get the full quantum Hamiltonian. This procedure is now described in the following.

The quantity $\mathcal{E}(d\varepsilon_{\alpha_1}) = \mathcal{E}\left(\left(\frac{\partial}{\partial\alpha_1} + \langle\cdot\rangle\right)\varepsilon_{\alpha_1}(\mathbf{X}_{\alpha_1})\right)d\alpha_1$ can be straightforwardly computed by using the rule previously given for the bracket of a product Eq. (9). Indeed we find

$$\begin{aligned} \left(\frac{\partial}{\partial\alpha_1} + \langle\cdot\rangle\right)\varepsilon_{\alpha_1}(\mathbf{X}_{\alpha_1}) &= \frac{\partial}{\partial\alpha_1}U_{\alpha_1}U_{\alpha_1}^+\varepsilon_{\alpha_1} + \varepsilon_{\alpha_1}U_{\alpha_1}\frac{\partial}{\partial\alpha_1}U_{\alpha_1}^+ + U_{\alpha_1}\frac{\partial}{\partial\alpha_1}H(\mathbf{X}_{\alpha_1})U_{\alpha_1}^+ \\ &\quad + \langle U_{\alpha_1}\rangle U_{\alpha_1}^+\varepsilon_{\alpha_1} + U_{\alpha_1}\langle H(\mathbf{X}_{\alpha_1})\rangle U_{\alpha_1}^+ + \varepsilon_{\alpha_1}U_{\alpha_1}\langle U_{\alpha_1}^+\rangle \\ &\quad - \frac{i}{2}(\nabla_{P_i}U_{\alpha_1}\nabla_{R_i}H(\mathbf{X}_{\alpha_1})U_{\alpha_1}^+ - \nabla_{R_i}U_{\alpha_1}\nabla_{P_i}H(\mathbf{X}_{\alpha_1})U_{\alpha_1}^+) \\ &\quad - \frac{i}{2}(U_{\alpha_1}\nabla_{P_i}H(\mathbf{X}_{\alpha_1})\nabla_{R_i}U_{\alpha_1}^+ - U_{\alpha_1}\nabla_{R_i}H(\mathbf{X}_{\alpha_1})\nabla_{P_i}U_{\alpha_1}^+) \\ &\quad - \frac{i}{2}(\nabla_{P_i}U_{\alpha_1}H(\mathbf{X}_{\alpha_1})\nabla_{R_i}U_{\alpha_1}^+ - \nabla_{R_i}U_{\alpha_1}H(\mathbf{X}_{\alpha_1})\nabla_{P_i}U_{\alpha_1}^+) \end{aligned} \quad (30)$$

As in [8] we now introduce the notations $\mathcal{A}_{\alpha_1}^{R_l} = iU_{\alpha_1}(\mathbf{X}_{\alpha_1})\nabla_{P_l}U_{\alpha_1}^+(\mathbf{X}_{\alpha_1})$ and $\mathcal{A}_{\alpha_1}^{P_l} = -iU_{\alpha_1}(\mathbf{X}_{\alpha_1})\nabla_{R_l}U_{\alpha_1}^+(\mathbf{X}_{\alpha_1})$ so that Eq. (30) can be written in a more useful form in terms of quantities of physical interest. Actually, replacing $H(\mathbf{X}_{\alpha_1})$ by $U_{\alpha_1}^+\varepsilon_{\alpha_1}U_{\alpha_1}$ everywhere, allows to write

$$\begin{aligned} &-\frac{i}{2}(\nabla_{P_i}U_{\alpha_1}\nabla_{R_i}H(\mathbf{X}_{\alpha_1})U_{\alpha_1}^+ - \nabla_{R_i}U_{\alpha_1}\nabla_{P_i}H(\mathbf{X}_{\alpha_1})U_{\alpha_1}^+) \\ &-\frac{i}{2}(U_{\alpha_1}\nabla_{P_i}H(\mathbf{X}_{\alpha_1})\nabla_{R_i}U_{\alpha_1}^+ - U_{\alpha_1}\nabla_{R_i}H(\mathbf{X}_{\alpha_1})\nabla_{P_i}U_{\alpha_1}^+) \\ &= \frac{1}{2}\mathcal{A}_{\alpha_1}^{R_l}\nabla_{R_l}\varepsilon_{\alpha_1} + \nabla_{R_l}\varepsilon_{\alpha_1}\mathcal{A}_{\alpha_1}^{R_l} + \mathcal{A}_{\alpha_1}^{P_l}\nabla_{P_l}\varepsilon_{\alpha_1} + \nabla_{P_l}\varepsilon_{\alpha_1}\mathcal{A}_{\alpha_1}^{P_l} \\ &\quad + \frac{i}{2}[\mathcal{A}_{\alpha_1}^{R_l}, \mathcal{A}_{\alpha_1}^{P_l}]\varepsilon_{\alpha_1} + \frac{i}{2}\varepsilon_{\alpha_1}[\mathcal{A}_{\alpha_1}^{R_l}, \mathcal{A}_{\alpha_1}^{P_l}] - i\mathcal{A}_{\alpha_1}^{R_l}\varepsilon_{\alpha_1}\mathcal{A}_{\alpha_1}^{P_l} + i\mathcal{A}_{\alpha_1}^{P_l}\varepsilon_{\alpha_1}\mathcal{A}_{\alpha_1}^{R_l} \end{aligned}$$

and

$$\begin{aligned} &-\frac{i}{2}(\nabla_{P_i}U_{\alpha_1}H(\mathbf{X}_{\alpha_1})\nabla_{R_i}U_{\alpha_1}^+ - \nabla_{R_i}U_{\alpha_1}H(\mathbf{X}_{\alpha_1})\nabla_{P_i}U_{\alpha_1}^+) \\ &= \frac{i}{2}\mathcal{A}_{\alpha_1}^{R_l}\varepsilon_{\alpha_1}\mathcal{A}_{\alpha_1}^{P_l} - \frac{i}{2}\mathcal{A}_{\alpha_1}^{P_l}\varepsilon_{\alpha_1}\mathcal{A}_{\alpha_1}^{R_l} \end{aligned}$$

so that ultimately, one has:

$$\begin{aligned}
\left(\frac{\partial}{\partial\alpha_1} + \langle.\rangle\right) \varepsilon_{\alpha_1}(\mathbf{X}_{\alpha_1}) &= \left(\left(\frac{\partial}{\partial\alpha_1} + \langle.\rangle\right) U_{\alpha_1}\right) U_{\alpha_1}^+ \varepsilon_{\alpha_1} + \varepsilon_{\alpha_1} U_{\alpha_1} \left(\frac{\partial}{\partial\alpha_1} + \langle.\rangle\right) U_{\alpha_1}^+ \\
&\quad + U_{\alpha_1} \left(\frac{\partial}{\partial\alpha_1} + \langle.\rangle\right) H(\mathbf{X}_{\alpha_1}) U_{\alpha_1}^+ \\
&\quad + \frac{1}{2} \mathcal{A}_{\alpha_1}^{R_l} \nabla_{R_l} \varepsilon_{\alpha_1} + \nabla_{R_l} \varepsilon_{\alpha_1} \mathcal{A}_{\alpha_1}^{R_l} + \mathcal{A}_{\alpha_1}^{P_l} \nabla_{P_l} \varepsilon_{\alpha_1} + \nabla_{P_l} \varepsilon_{\alpha_1} \mathcal{A}_{\alpha_1}^{P_l} \\
&\quad + \frac{i}{2} \left\{ \mathcal{A}_{\alpha_1}^{P_l} \varepsilon_{\alpha_1} \mathcal{A}_{\alpha_1}^{R_l} - \mathcal{A}_{\alpha_1}^{R_l} \varepsilon_{\alpha_1} \mathcal{A}_{\alpha_1}^{P_l} + \varepsilon_{\alpha_1} [\mathcal{A}_{\alpha_1}^{R_l}, \mathcal{A}_{\alpha_1}^{P_l}] + [\mathcal{A}_{\alpha_1}^{R_l}, \mathcal{A}_{\alpha_1}^{P_l}] \varepsilon_{\alpha_1} \right\}
\end{aligned} \tag{31}$$

We note that by construction $d\varepsilon_{\alpha_1}$ is a diagonal matrix and we obviously have the following identities

$$\left(\frac{\partial}{\partial\alpha_1} + \langle.\rangle\right) \varepsilon_{\alpha_1}(\mathbf{X}_{\alpha_1}) = \mathcal{P}_+ (\text{R.H.S. of Eq. 31}) \tag{32}$$

$$0 = \mathcal{P}_- (\text{R.H.S. of Eq. 31}) \tag{33}$$

where $\mathcal{P}_+$ and $\mathcal{P}_-$ are the projection on the diagonal and off the diagonal respectively.

$$\left(\frac{\partial}{\partial\alpha_1} + \langle.\rangle\right) \varepsilon_{\alpha_1}(\mathbf{X}_{\alpha_1}) = O_{\alpha_1} \cdot \varepsilon_{\alpha_1}(\mathbf{X}_{\alpha_1}) + \mathcal{P}_+ \{U_{\alpha_1} (D_{\alpha}(\mathbf{X}_{\alpha_1}, \alpha_1) H(\mathbf{X}_{\alpha_1})) U_{\alpha_1}^+\} \tag{34}$$

with O_{α_1} is given by the projected "linear part" of the r.h.s. expression of Eq. (31) :

$$\begin{aligned}
O_{\alpha_1} \varepsilon_{\alpha_1}(\mathbf{X}_{\alpha_1}) &= \mathcal{P}_+ \left((D_{\alpha}(\mathbf{X}_{\alpha_1}, \alpha_1) U_{\alpha_1}) U_{\alpha_1}^+ \varepsilon_{\alpha_1} + \varepsilon_{\alpha_1} U_{\alpha_1} D_{\alpha}(\mathbf{X}_{\alpha_1}, \alpha_1) U_{\alpha_1}^+ \right) \\
&\quad + \mathcal{P}_+ \left\{ \frac{1}{2} \mathcal{A}_{\alpha_1}^{R_l} \nabla_{R_l} \varepsilon_{\alpha_1} + \nabla_{R_l} \varepsilon_{\alpha_1} \mathcal{A}_{\alpha_1}^{R_l} + \mathcal{A}_{\alpha_1}^{P_l} \nabla_{P_l} \varepsilon_{\alpha_1} + \nabla_{P_l} \varepsilon_{\alpha_1} \mathcal{A}_{\alpha_1}^{P_l} \right\} \\
&\quad + \frac{i}{2} \mathcal{P}_+ \left\{ \mathcal{A}_{\alpha_1}^{P_l} \varepsilon_{\alpha_1} \mathcal{A}_{\alpha_1}^{R_l} - \mathcal{A}_{\alpha_1}^{R_l} \varepsilon_{\alpha_1} \mathcal{A}_{\alpha_1}^{P_l} + \varepsilon_{\alpha_1} [\mathcal{A}_{\alpha_1}^{R_l}, \mathcal{A}_{\alpha_1}^{P_l}] + [\mathcal{A}_{\alpha_1}^{R_l}, \mathcal{A}_{\alpha_1}^{P_l}] \varepsilon_{\alpha_1} \right\}.
\end{aligned}$$

Let us remark that the operator O_{α_1} is well defined since, as explained before, the operation $D_{\alpha}(\mathbf{X}_{\alpha_1}, \alpha_1) = \left(\frac{\partial}{\partial\alpha_1} + \langle.\rangle\right)$ is independent from any symmetrization scheme for $\varepsilon_{\alpha_1}(\mathbf{X}_{\alpha_1})$ and $H(\mathbf{X}_{\alpha_1})$, and so is $O_{\alpha_1} \cdot \varepsilon_{\alpha_1}(\mathbf{X}_{\alpha_1}) = D_{\alpha}(\mathbf{X}_{\alpha_1}, \alpha_1) \varepsilon_{\alpha_1}(\mathbf{X}_{\alpha_1}) - \mathcal{P}_+ \{U_{\alpha_1} (D_{\alpha}(\mathbf{X}_{\alpha_1}, \alpha_1) H(\mathbf{X}_{\alpha_1})) U_{\alpha_1}^+\}$.

Since in the applications of practical interest (Bloch electrons, Dirac Hamiltonian...), $(D_{\alpha}(\mathbf{X}_{\alpha_1}, \alpha_1) H(\mathbf{X}_{\alpha_1}))$ cancels, we will set this term to 0 for the sake of the exposition and will consider later its contribution. As a consequence, one has :

$$\varepsilon(\mathbf{X}) = \mathcal{E} \left(\varepsilon_0(\mathbf{X}_0) + \int_0^{\hbar} O_{\alpha_1} \cdot \varepsilon_{\alpha_1}(\mathbf{X}_{\alpha_1}) d\alpha_1 \right). \tag{35}$$

Now, similarly to Eq. (29) we can write :

$$\varepsilon_{\alpha_1}(\mathbf{X}_{\alpha_1}) = \varepsilon_0(\mathbf{X}_0) + \int_0^{\alpha_1} d\varepsilon_{\alpha_2}(\mathbf{X}_{\alpha_2}) = \varepsilon_0(\mathbf{X}_0) + \int_0^{\alpha_1} d[U(\mathbf{X}_{\alpha_2})H(\mathbf{X}_{\alpha_2})U^+(\mathbf{X}_{\alpha_2})] \quad (36)$$

which can be inserted in the expectation Eq. (29) to get the full quantum diagonal representation $\varepsilon(\mathbf{X}) \equiv \varepsilon_{\hbar}(\mathbf{X}_{\hbar})$ as :

$$\begin{aligned} \varepsilon_{\hbar}(\mathbf{X}_{\hbar}) &= \mathcal{E} \left(\varepsilon_0(\mathbf{X}_0) + \int_0^{\hbar} d\varepsilon_{\alpha_1}(\mathbf{X}_{\alpha_1}) d\alpha_1 \right) \\ &= \mathcal{E} \left(\varepsilon_0(\mathbf{X}_0) + \int_0^{\hbar} O_{\alpha_1} \cdot \varepsilon_{\alpha_1}(\mathbf{X}_{\alpha_1}) d\alpha_1 \right) \\ &= \mathcal{E} \left(\varepsilon_0(\mathbf{X}_0) + \int_0^{\hbar} O_{\alpha_1} \cdot \left[\varepsilon_0(\mathbf{X}_0) + \int_0^{\alpha_1} d[U(\mathbf{X}_{\alpha_2})H(\mathbf{X}_{\alpha_2})U^+(\mathbf{X}_{\alpha_2})] \right] d\alpha_1 \right) \quad (37) \end{aligned}$$

Now remark that since $\alpha_2 < \alpha_1$, the terms $\nabla_{\mathbf{X}_{\alpha_2}} \varepsilon_{\alpha_2}(\mathbf{X}_{\alpha_2}) d\mathbf{X}_{\alpha_2}$ and $\nabla_{X_{\alpha_2}^j} \nabla_{X_{\alpha_2}^i} \varepsilon_{\alpha_2}(\mathbf{X}_{\alpha_2}) (dX_{\alpha_2}^i dX_{\alpha_2}^j + dX_{\alpha_2}^j dX_{\alpha_2}^i)$ in $d\varepsilon(\mathbf{X}_{\alpha_2}) = d[U(\mathbf{X}_{\alpha_2})H(\mathbf{X}_{\alpha_2})U^+(\mathbf{X}_{\alpha_2})]$ do not recombine with anything coming from $O_{\alpha_1}(\mathbf{X}_{\alpha_1})$ to give a product of the type $d\mathbf{R}_{\alpha_2} d\mathbf{P}_{\alpha_2}$ that would induce a $d\alpha_2$ contribution to the expectation. They will thus cancel in the expectation. As a consequence, Eq. (37) can be written:

$$\varepsilon_{\hbar}(\mathbf{X}_{\hbar}) = \mathcal{E} \left(\varepsilon_0(\mathbf{X}_0) + \int_0^{\hbar} O_{\alpha_1} \cdot \left[\varepsilon_0(\mathbf{X}_0) + \int_0^{\alpha_1} O_{\alpha_2} \cdot \varepsilon_{\alpha_2}(\mathbf{X}_{\alpha_2}) d\alpha_2 \right] d\alpha_1 \right)$$

Repeating the procedure one can then show by iteration that :

$$\varepsilon_{\hbar}(\mathbf{X}_{\hbar}) = \mathcal{E} \left(\left[1 + \sum_{n=1}^{\infty} \int_{0 < \alpha_n < \dots < \alpha_1 < \hbar} O_{\alpha_1} \dots O_{\alpha_n} d\alpha_1 \dots d\alpha_n \right] \varepsilon_0(\mathbf{X}_0) \right) \quad (38)$$

At this point, two important comments have to be made, both related to the fact that the operators O_{α_i} have been designed to depend on $\mathbf{X}_{\alpha_i}$. First, notice that the gradient appearing in the definition of O_{α_i} have to be taken with respect to $\mathbf{X}_{\alpha_i}$, but that these operators act on functions of $\mathbf{X}_{\alpha_j}$ with $\alpha_j < \alpha_i$, such as $\varepsilon_0(\mathbf{X}_0)$. This is not a problem however, since $\mathbf{X}_{\alpha_j} = \mathbf{X}_{\alpha_i} - \int_{\alpha_j}^{\alpha_i} d\mathbf{X}_{\lambda}$ and thus the derivative of a function $F(\mathbf{X}_{\alpha_j})$ with respect to $\mathbf{X}_{\alpha_i}$ is just the same as the derivative with respect to $\mathbf{X}_{\alpha_j}$, that is the gradient of the function. This the reason why, in the definition of O_{α_i} we discarded any reference to the α_i 's in the gradients.

The second remark is that we can use the EBS operation defined in Eq. (21) and formula (25) to put the series appearing in the previous formula Eq. (38) at the same point. Once

again, since $0 < \alpha_n < \dots < \alpha_1$, we can write, inside the expectation :

$$\begin{aligned} & \left[\int_{0 < \alpha_n < \dots < \alpha_1 < \hbar} O_{\alpha_1} \dots O_{\alpha_n} d\alpha_1 \dots d\alpha_n \right] \varepsilon_0(\mathbf{X}_0) \\ &= \left[\int_{0 < \alpha_n < \dots < \alpha_1 < \hbar} e^{-\langle \cdot \rangle_{\alpha_1 \rightarrow \hbar}^S} O_{\alpha_1} \dots e^{-\langle \cdot \rangle_{\alpha_{n-1} \rightarrow \alpha_{n-2}}^S} O_{\alpha_{n-1}} e^{-\langle \cdot \rangle_{\alpha_n \rightarrow \alpha_{n-1}}^S} O_{\alpha_n} e^{-\langle \cdot \rangle_{0 \rightarrow \alpha_n}^S} \right] \varepsilon_0(\mathbf{X}_0) \quad (39) \end{aligned}$$

Note that this formula is a generalization of Eq. (25) since the O_{α_k} are not functions, but rather operators including derivatives with respect to the canonical variables. The part of O_{α_k} acting through some multiplication on the left or on the right or both on the left and on the right is not problematic and Eq. (25) applies (with the slight modification of an irrelevant change of order in the multiplication of the functions with respect to Eq. (25)). Likewise, the differential part of $O_{\alpha_k}(\mathbf{X}_{\alpha_k})$, such as $\frac{1}{2} \mathcal{A}_{\alpha_k}^{R_l}(\mathbf{X}_{\alpha_k}) \nabla_{R_{\alpha_k}^l}$ acting on some function say $F(\mathbf{X}_{\alpha_{k+1}})$, is not problematic since the operator $\exp\left(-\langle \cdot \rangle_{\alpha_{k+1} \rightarrow \alpha_k}^S\right)$ is a (complicate) function of the derivative with respect to the canonical variables and thus commute with $\nabla_{R_{\alpha_{k+1}}^l}$. As a consequence setting $\frac{1}{2} \mathcal{A}_{\alpha_k}^{R_l}(\mathbf{X}_{\alpha_k}) \nabla_{R_{\alpha_k}^l} F(\mathbf{X}_{\alpha_{k+1}})$ at the same point through the EBS operation, that is replacing it by $\left[\frac{1}{2} \mathcal{A}_{\alpha_k}^{R_l}(\mathbf{X}_{\alpha_k}) \exp\left(-\langle \cdot \rangle_{\alpha_{k+1} \rightarrow \alpha_k}^S\right) \nabla_{R_{\alpha_k}^l} F(\mathbf{X}_{\alpha_{k+1}}) \right]$ in the expectation really amounts to compute $\left[\frac{1}{2} \mathcal{A}_{\alpha_k}^{R_l}(\mathbf{X}_{\alpha_k}) \nabla_{R_{\alpha_k}^l} \exp\left(-\langle \cdot \rangle_{\alpha_{k+1} \rightarrow \alpha_k}^S\right) F(\mathbf{X}_{\alpha_{k+1}}) \right]$, that is to let the EBS operation act before the action of $O_{\alpha_k}(\mathbf{X}_{\alpha_{k+1}})$. This thus justifies formula Eq. (39).

The computation of Eq. (39) derives directly from the definitions of the various operators involved and proceeds as follows : for $n > 0$, starting from $\varepsilon_0(\mathbf{X}_0)$, first apply $e^{-\langle \cdot \rangle_{0 \rightarrow \alpha_n}^S}$ on $\varepsilon_0(\mathbf{X}_0)$ that will shift $\mathbf{X}_0$ by $\mathbf{X}_{\alpha_n}$. Then make O_{α_n} acts on the result, apply $e^{-\langle \cdot \rangle_{\alpha_n \rightarrow \alpha_{n-1}}^S}$ which replaces $\mathbf{X}_{\alpha_n}$ by $\mathbf{X}_{\alpha_{n-1}}$ and so on. Ultimately at the end of the process, $\mathbf{X}_0$ is replaced by $\mathbf{X}_{\hbar}$, this last variable being independent from the integration variables, the various integrals can be computed easily, as the integral of a series expansion. This process of integration will be of course the same for all similar expressions in the sequel.

The case $n = 0$ corresponding to the first term in the series expansion : $\mathcal{E}(\varepsilon_0(\mathbf{X}_0))$ is of course easily handled by replacing it with $e^{-\langle \cdot \rangle_{0 \rightarrow \hbar}^S} \varepsilon_0(\mathbf{X}_0)$.

We can now deduce that (with the notation $\mathbf{X} \equiv \mathbf{X}_{\hbar}$):

$$\varepsilon(\mathbf{X}) \equiv \varepsilon_{\hbar}(\mathbf{X}_{\hbar}) = \mathcal{E} \left(\left[\mathcal{T} \exp \left[\int_{0 < \alpha < \hbar} e^{-\langle \cdot \rangle_{\alpha \rightarrow \hbar}^S} O_{\alpha} e^{-\langle \cdot \rangle_{0 \rightarrow \alpha}^S} d\alpha \right] \right] \varepsilon_0(\mathbf{X}_0) \right) \quad (40)$$

which is a compact expression for the diagonal Hamiltonian $\varepsilon(\mathbf{R}, \mathbf{P})$ in terms of the "classical" diagonal Hamiltonian $\varepsilon_0(\mathbf{R}, \mathbf{P})$ in which the classical variables $\mathbf{R}_0, \mathbf{P}_0$ have been now

replaced by the quantum ones $\mathbf{R}, \mathbf{P}$ due to the *EBS* action. Here $\mathcal{T}$ is the usual notation for the "time ordered product". Eq. (40) is the required expression and constitutes the main result of this paper.

We can now consider the additional contributions that would appear if we had considered a case such that $(D_\alpha(\mathbf{X}_{\alpha_1}, \alpha_1) H(\mathbf{X}_{\alpha_1})) \neq 0$. Let $C(\mathbf{X}_{\alpha_1}) = \mathcal{P}_+ \{U_{\alpha_1}(D_\alpha(\mathbf{X}_{\alpha_1}, \alpha_1) H(\mathbf{X}_{\alpha_1})) U_{\alpha_1}^+\}$. In such a case, the repeated application of $O_{\alpha_1} + C(\mathbf{X}_{\alpha_1})$ yields rather :

$$\begin{aligned} \varepsilon_{\hbar}(\mathbf{X}_{\hbar}) = & \mathcal{E} \left(\left[1 + \sum_{n=1}^{\infty} \int_{0 < \alpha_n < \dots < \alpha_1 < \alpha} O_{\alpha_1} \dots O_{\alpha_n} d\alpha_1 \dots d\alpha_n \right] \varepsilon_0(\mathbf{X}_0) \right) \\ & + \mathcal{E} \left(\left[1 + \sum_{n=1}^{\infty} \int_{0 < \alpha_n < \dots < \alpha_1 < \alpha} O_{\alpha_1} \dots O_{\alpha_{n-1}} d\alpha_1 \dots d\alpha_{n-1} \right] C(\mathbf{X}_{\alpha_n}) \right) \end{aligned}$$

Using the same tricks as before it leads directly to the following expression for the diagonalized energy operator :

$$\begin{aligned} & \mathcal{E} \left(\left[\mathcal{T} \exp \left[\int_{0 < \alpha < \hbar} e^{-\langle \cdot \rangle_{\alpha \rightarrow \hbar}^S} O_{\alpha} e^{-\langle \cdot \rangle_{0 \rightarrow \alpha}^S} d\alpha \right] \right] \varepsilon_0(\mathbf{X}_0) \right) \\ & + \mathcal{E} \int_{\alpha_0}^{\hbar} \left(\left[\mathcal{T} \exp \left[\int_{\alpha_0 < \alpha < \hbar} e^{-\langle \cdot \rangle_{\alpha \rightarrow \hbar}^S} O_{\alpha} e^{-\langle \cdot \rangle_{\alpha_0 \rightarrow \alpha}^S} d\alpha \right] \right] C(\mathbf{X}_{\alpha_0}) d\alpha_0 \right) \end{aligned}$$

Clearly the practical application of Eq. (40) requires the knowledge of the transformation matrices U_{α} which enter into the definition of the operators O_{α} .

B. The transformation matrix U

Note first that there is a certain arbitrariness in the choice of the unitary matrix $U_{\alpha}(\mathbf{X})$ as explained in [8] which reflects a kind of gauge invariance. Actually, multiplying the transformation matrix $U_{\alpha}(\mathbf{X})$ on the right by a diagonal unitary matrix yields an other diagonalization, equivalent to the previous one. In particular it allows to choose n conditions for the diagonal entries of $U_{\alpha}(\mathbf{X})$ ($n \times n$ being the size of $U_{\alpha}(\mathbf{X})$). An explicit choice will be done below to simplify our expressions.

To find the transformation matrix U we use the same approach as for the diagonalization

of the Hamiltonian, by writing :

$$\begin{aligned} U_{\hbar}(\mathbf{X}_{\hbar}) &= \mathcal{E} \left(U(\mathbf{X}_0) + \int_0^{\hbar} dU_{\alpha}(\mathbf{X}_{\alpha}) \right) \\ &= \mathcal{E} \left(\int_0^{\hbar} \left(\frac{\partial}{\partial \alpha} + \langle \cdot \rangle \right) U_{\alpha}(\mathbf{X}_{\alpha}) d\alpha \right) \end{aligned} \quad (41)$$

we can find $(\partial_{\alpha} + \langle \cdot \rangle) U_{\alpha}(\mathbf{X}_{\alpha})$ by using again the diagonalization process leading to Eq. (31). Indeed we had

$$\begin{aligned} \left(\frac{\partial}{\partial \alpha_1} + \langle \cdot \rangle \right) \varepsilon_{\alpha_1}(\mathbf{X}_{\alpha_1}) &= \left(\left(\frac{\partial}{\partial \alpha_1} + \langle \cdot \rangle \right) U_{\alpha_1} \right) U_{\alpha_1}^+ \varepsilon_{\alpha_1} + \varepsilon_{\alpha_1} U_{\alpha_1} \left(\frac{\partial}{\partial \alpha_1} + \langle \cdot \rangle \right) U_{\alpha_1}^+ \\ &\quad + U_{\alpha_1} \left(\frac{\partial}{\partial \alpha_1} + \langle \cdot \rangle \right) H(\mathbf{X}_{\alpha_1}) U_{\alpha_1}^+ \\ &\quad + \frac{1}{2} \{ \mathcal{A}_{\alpha_1}^{R_l} \nabla_{R_l} \varepsilon_{\alpha_1} + \nabla_{R_l} \varepsilon_{\alpha_1} \mathcal{A}_{\alpha_1}^{R_l} + \mathcal{A}_{\alpha_1}^{P_l} \nabla_{P_l} \varepsilon_{\alpha_1} + \nabla_{P_l} \varepsilon_{\alpha_1} \mathcal{A}_{\alpha_1}^{P_l} \} \\ &\quad + \frac{i}{2} \{ \mathcal{A}_{\alpha_1}^{P_l} \varepsilon_{\alpha_1} \mathcal{A}_{\alpha_1}^{R_l} - \mathcal{A}_{\alpha_1}^{R_l} \varepsilon_{\alpha_1} \mathcal{A}_{\alpha_1}^{P_l} + \varepsilon_{\alpha_1} [\mathcal{A}_{\alpha_1}^{R_l}, \mathcal{A}_{\alpha_1}^{P_l}] + [\mathcal{A}_{\alpha_1}^{R_l}, \mathcal{A}_{\alpha_1}^{P_l}] \varepsilon_{\alpha_1} \} \end{aligned} \quad (42)$$

In addition, the unitarity condition $U_{\alpha} U_{\alpha}^+ = 1$ implies the relation $(\partial_{\alpha} + \langle \cdot \rangle) (U_{\alpha} U_{\alpha}^+) = 0$ which reads :

$$0 = \left(\left(\frac{\partial}{\partial \alpha} + \langle \cdot \rangle \right) U_{\alpha} \right) U_{\alpha}^+ + U_{\alpha} \left(\frac{\partial}{\partial \alpha} + \langle \cdot \rangle \right) U_{\alpha}^+ - \frac{i}{2} (\nabla_{P_l} U_{\alpha} \nabla_{R_l} U_{\alpha}^+ - \nabla_{R_l} U_{\alpha} \nabla_{P_l} U_{\alpha}^+)$$

or, in a more compact way:

$$0 = \left(\left(\frac{\partial}{\partial \alpha} + \langle \cdot \rangle \right) U_{\alpha} \right) U_{\alpha}^+ + U_{\alpha} \left(\frac{\partial}{\partial \alpha} + \langle \cdot \rangle \right) U_{\alpha}^+ + \frac{i}{2} [\mathcal{A}_{\alpha}^{R_l}, \mathcal{A}_{\alpha}^{P_l}] \quad (43)$$

Mixing the two equations Eqs. (42) (43), we obtain that Eq. (42) after projection on the non diagonal part becomes the equality

$$\begin{aligned} \mathcal{P}_- \left[\left(\left(\frac{\partial}{\partial \alpha} + \langle \cdot \rangle \right) U_{\alpha} \right) U_{\alpha}^+, \varepsilon_{\alpha} \right] &= -\mathcal{P}_- \left(U_{\alpha} \left(\left(\frac{\partial}{\partial \alpha} + \langle \cdot \rangle \right) H(\mathbf{X}_{\alpha}) \right) U_{\alpha}^+ \right) \\ &\quad + \frac{i}{2} \varepsilon_{\alpha} \mathcal{P}_- [\mathcal{A}_{\alpha}^{R_l}, \mathcal{A}_{\alpha}^{P_l}] \\ &\quad - \frac{1}{2} \mathcal{P}_- \{ \mathcal{A}_{\alpha_1}^{R_l} \nabla_{R_l} \varepsilon_{\alpha_1} + \nabla_{R_l} \varepsilon_{\alpha_1} \mathcal{A}_{\alpha_1}^{R_l} + \mathcal{A}_{\alpha_1}^{P_l} \nabla_{P_l} \varepsilon_{\alpha_1} + \nabla_{P_l} \varepsilon_{\alpha_1} \mathcal{A}_{\alpha_1}^{P_l} \} \\ &\quad - \frac{i}{2} \mathcal{P}_- \{ \mathcal{A}_{\alpha_1}^{P_l} \varepsilon_{\alpha_1} \mathcal{A}_{\alpha_1}^{R_l} - \mathcal{A}_{\alpha_1}^{R_l} \varepsilon_{\alpha_1} \mathcal{A}_{\alpha_1}^{P_l} + \varepsilon_{\alpha_1} [\mathcal{A}_{\alpha_1}^{R_l}, \mathcal{A}_{\alpha_1}^{P_l}] + [\mathcal{A}_{\alpha_1}^{R_l}, \mathcal{A}_{\alpha_1}^{P_l}] \varepsilon_{\alpha_1} \} \end{aligned} \quad (44)$$

Both conditions Eqs. (43) (44) can be solved for $(\partial_{\alpha} + \langle \cdot \rangle) U_{\alpha}$. Actually, decomposing $[(\partial_{\alpha} + \langle \cdot \rangle) U_{\alpha}] U_{\alpha}^+ = hr + ahr$ in Hermitian hr and anti-Hermitian ahr part, Eq. (44) reads

$$\mathcal{P}_- [hr + ahr, \varepsilon_{\alpha}] = M(U_{\alpha}) \quad (45)$$

where $M(U_\alpha)$ is the r.h.s of Eq. (44). We can now use a particular choice of gauge. We fix our diagonalization process by setting $\mathcal{P}_+(ahr) = 0$. Practically it corresponds to multiply U_α on the right by a unitary diagonal matrix D_α (which has n degree of freedom) such that $\mathcal{P}_+((\frac{\partial}{\partial\alpha} + \langle.\rangle) U_\alpha D_\alpha) D_\alpha^\dagger U_\alpha^\dagger$ is Hermitian. This gives n conditions that determine D_α .

Now, from Eq. (45) and given our gauge choice for U_α , we deduce that $\mathcal{P}_-(ahr) = ahr$ and $[ahr, \varepsilon_\alpha] = \frac{1}{2}(M(U_\alpha) + M^+(U_\alpha))$. To find ahr we aim now at inverting the commutator $[\cdot, \varepsilon_\alpha]$ in the left hand side of this equation. First note that, since we have assumed the diagonalization is possible, we can safely assume that the right hand side $\frac{1}{2}(M(U_\alpha) + M^+(U_\alpha))$ lies in the image of the operator $[\cdot, \varepsilon_\alpha]$. It is in fact the case in all practical cases. Since both ahr and $M(U_\alpha)$ are anti-diagonal by construction, we just need to invert the commutator with ε_α , $[\cdot, \varepsilon_\alpha]$ on the space of anti-diagonal matrices. To do so, we first need to find the kernel of $[\cdot, \varepsilon_\alpha]$ on this space and check if it is null.

Assume first that the bands of the system are non degenerate, that is $(\varepsilon_\alpha)_n \neq (\varepsilon_\alpha)_m$ for $m \neq n$. As a consequence an element V in the kernel of the commutator satisfies

$$V_{nm} [(\varepsilon_\alpha)_m - (\varepsilon_\alpha)_n] = -i\alpha (\nabla_{P_i}(\varepsilon_\alpha)_n \nabla_{R_i} V_{nm} - \nabla_{R_i}(\varepsilon_\alpha)_n \nabla_{P_i} V_{nm})$$

that is :

$$V_{nm} = -i\alpha (\nabla_{P_i}(\varepsilon_\alpha)_n \nabla_{R_i} V_{nm} - \nabla_{R_i}(\varepsilon_\alpha)_n \nabla_{P_i} V_{nm}) \frac{1}{[(\varepsilon_\alpha)_n - (\varepsilon_\alpha)_m]}$$

Since the beginning, we have assumed that all the functions involved are regular in α and have a series expansion in this parameter (as well as in the canonical variables). Thus, iterating the last relation for V_{nm} yields that, for each V_{nm} expanded as a series expansion in α , at each order in α , $V_{nm} = 0$. As a consequence, the kernel of the commutator with ε_α is null and we can thus formally write ahr under the form :

$$ahr = \tilde{N}(\alpha) . U_\alpha \tag{46}$$

where we have defined :

$$\tilde{N}(\alpha) . U_\alpha = \frac{1}{2} ([\cdot, \varepsilon_\alpha]^{-1}) (M(U_\alpha) + M^+(U_\alpha)) \tag{47}$$

and the inverse of the commutator operation $[\cdot, \varepsilon_\alpha]$ satisfies obviously :

$$[[\cdot, \varepsilon_\alpha]^{-1} . M, \varepsilon_\alpha] = [\cdot, \varepsilon_\alpha]^{-1} . [M, \varepsilon_\alpha] = M \quad \text{for } M \text{ anti-diagonal}$$

If the Band are degenerate, we need to define the inverse of the commutator more carefully. Actually since some bands may be degenerate, the kernel of the commutator $[\cdot, \varepsilon_\alpha]$ has no reason to be null now. This operator is thus no more bijective and we will not be able to define its inverse uniquely. This non uniqueness will lead to a non unique definition of ahr . This is not astonishing. Actually, when the Band are degenerate, as in the Dirac case, we do not look for a diagonal Hamiltonian, but rather for a Block diagonal Hamiltonian. This leaves thus more freedom for the diagonalization process and as a consequence, for the definition of $[\cdot, \varepsilon_\alpha]^{-1}$. Practically, we proceed as follows. Decompose our space of non diagonal matrices of operators denoted AD in the following way. Write $AD = \ker([\cdot, \varepsilon_\alpha]) \oplus ad_1$ with ad_1 an arbitrary supplementary space of $\ker([\cdot, \varepsilon_\alpha])$. Now, given M an element of $\text{Im}([\cdot, \varepsilon_\alpha])$, chose an antecedent m_1 of M with respect to $[\cdot, \varepsilon_\alpha]$, and decompose m_1 with respect to the previous decomposition, $m_1 = m_2 + m_3$ where $m_2 \in \ker([\cdot, \varepsilon_\alpha])$, $m_3 \in ad_1$. Now set $[\cdot, \varepsilon_\alpha]^{-1} \cdot M = m_3$. Given a chosen decomposition $\ker([\cdot, \varepsilon_\alpha]) \oplus ad_1$, m_3 is unique since if $\hat{m}_1$ is another antecedent of M , $\hat{m}_1 - m_1 \in \ker([\cdot, \varepsilon_\alpha])$ and as a consequence $\hat{m}_1 = m_3 + (m_2 + \hat{m}_1 - m_1)$ is the decomposition of $\hat{m}_1$.

One can check that

$$\begin{aligned} [[\cdot, \varepsilon_\alpha]^{-1} \cdot M, \varepsilon_\alpha] &= [m_3, \varepsilon_\alpha] \\ &= [m_1 - m_2, \varepsilon_\alpha] \\ &= [m_1, \varepsilon_\alpha] = M \end{aligned}$$

as needed to solve Eq. (45). On the other hand, notice that $[\cdot, \varepsilon_\alpha]^{-1} [M, \varepsilon_\alpha]$ is not equal to M in general. Actually, choosing M as an antecedent of $[M, \varepsilon_\alpha]$ and decomposing it gives an element m_3 that a priori depends on the supplementary space chosen. As a consequence, the operation $[\cdot, \varepsilon_\alpha]^{-1}$ is only a right inverse to $[\cdot, \varepsilon_\alpha]$. This is not a problem, since it allows anyway to write our solution for Eq. (45) as :

$$ahr = \tilde{N}(\alpha) \cdot U_\alpha \quad (48)$$

where we have again defined :

$$\tilde{N}(\alpha) \cdot U_\alpha = \frac{1}{2} ([\cdot, \varepsilon_\alpha]^{-1}) (M(U_\alpha) + M^+(U_\alpha)) \quad (49)$$

The non unicity in the definition of $[\cdot, \varepsilon_\alpha]^{-1}$ is reflected in the choice of decomposition for the space AD . Let us insist on the fact that this choice is itself the consequence of the

Bands degeneracy that allows for a larger freedom of gauge choice for a block diagonal representation.

To complete the determination of U_α we still need to deduce hr which is readily obtained from the unitarity condition Eq. (43) as:

$$hr = -\frac{i}{4} [\mathcal{A}_\alpha^{R_l}, \mathcal{A}_\alpha^{P_l}] \quad (50)$$

Indeed, Eq. (50) follows easily from Eq. (43), when noting that $((\frac{\partial}{\partial\alpha} + \langle.\rangle) U_\alpha) U_\alpha^+ + U_\alpha (\frac{\partial}{\partial\alpha} + \langle.\rangle) U_\alpha^+$ is hermitian due to the fact that for any operator A , $\langle.\rangle A^+ = (\langle.\rangle A)^+$ (and this is true in particular for U_α). This assertion can be checked on an arbitrary expansion in $\mathbf{R}$ and $\mathbf{P}$ of A , since for an arbitrary monomial $R_l^n P_l^k A_{n,k}$ with $A_{n,k}$ an arbitrary coefficient matrix, $\langle.\rangle (R_l^n P_l^k) A_{n,k}^+ = \frac{i}{2} (nk R_l^{n-1} P_l^{k-1}) A_{n,k}^+ = (-\frac{i}{2} nk P_l^{k-1} R_l^{n-1} A_{n,k})^+$ and this last quantity is equal to $[\langle.\rangle (P_l^k R_l^n) A_{n,k}]^+$.

Gathering the results Eqs.(47) (50) allows us to introduce the operator N_α operating on U_α in the following manner $N_\alpha.U_\alpha = (hr + ahr) U_\alpha$, so that we can write

$$\left[\left(\frac{\partial}{\partial\alpha} + \langle.\rangle \right) U_\alpha \right] = N_\alpha.U_\alpha$$

with N_α given explicitly by the following expression

$$N_\alpha.U_\alpha = \frac{1}{2} ([., \varepsilon_\alpha]^{-1}) (M(U_\alpha) + M^+(U_\alpha)) U_\alpha - \frac{i}{4} [\mathcal{A}_\alpha^{R_l}, \mathcal{A}_\alpha^{P_l}] U_\alpha$$

As for the energy diagonalization, this expression can be rewritten in terms of physical quantities. Recall that $M(U_\alpha)$ is the r.h.s of Eq. (44), so that

$$\begin{aligned} \frac{1}{2} (M(U_\alpha) + M^+(U_\alpha)) &= -\frac{1}{2} \mathcal{P}_- \{ \mathcal{A}_{\alpha_1}^{R_l} \nabla_{R_l} \varepsilon_{\alpha_1} + \nabla_{R_l} \varepsilon_{\alpha_1} \mathcal{A}_{\alpha_1}^{R_l} + \mathcal{A}_{\alpha_1}^{P_l} \nabla_{P_l} \varepsilon_{\alpha_1} + \nabla_{P_l} \varepsilon_{\alpha_1} \mathcal{A}_{\alpha_1}^{P_l} \} \\ &\quad -\frac{i}{4} \mathcal{P}_- \{ \mathcal{A}_{\alpha_1}^{P_l} \varepsilon_{\alpha_1} \mathcal{A}_{\alpha_1}^{R_l} - \mathcal{A}_{\alpha_1}^{R_l} \varepsilon_{\alpha_1} \mathcal{A}_{\alpha_1}^{P_l} + \varepsilon_{\alpha_1} [\mathcal{A}_{\alpha_1}^{R_l}, \mathcal{A}_{\alpha_1}^{P_l}] + [\mathcal{A}_{\alpha_1}^{R_l}, \mathcal{A}_{\alpha_1}^{P_l}] \varepsilon_{\alpha_1} + H.C. \} \\ &\quad +\frac{i}{4} \mathcal{P}_- \varepsilon_\alpha [\mathcal{A}_\alpha^{R_l}, \mathcal{A}_\alpha^{P_l}] + \frac{i}{4} \mathcal{P}_- [\mathcal{A}_\alpha^{R_l}, \mathcal{A}_\alpha^{P_l}] \varepsilon_\alpha \\ &= -\frac{1}{2} \mathcal{P}_- \{ \mathcal{A}_{\alpha_1}^{R_l} \nabla_{R_l} \varepsilon_{\alpha_1} + \nabla_{R_l} \varepsilon_{\alpha_1} \mathcal{A}_{\alpha_1}^{R_l} + \mathcal{A}_{\alpha_1}^{P_l} \nabla_{P_l} \varepsilon_{\alpha_1} + \nabla_{P_l} \varepsilon_{\alpha_1} \mathcal{A}_{\alpha_1}^{P_l} \} \\ &\quad -\frac{i}{4} \mathcal{P}_- \{ [\varepsilon_\alpha, \mathcal{A}_\alpha^{R_l}] \mathcal{A}_\alpha^{P_l} - [\varepsilon_\alpha, \mathcal{A}_\alpha^{P_l}] \mathcal{A}_\alpha^{R_l} + H.C. \} \end{aligned} \quad (51)$$

where $H.C.$ stands for the Hermitian conjugate. Note also that $U_\alpha ((\frac{\partial}{\partial\alpha} + \langle.\rangle) H(\mathbf{X}_\alpha)) U_\alpha^+$ is hermitian, as a consequence both of the hermiticity of $H(\mathbf{X}_\alpha)$ and the fact that $(\langle.\rangle H(\mathbf{X}_\alpha))^+ = \langle.\rangle H(\mathbf{X}_\alpha)^+ = \langle.\rangle H(\mathbf{X}_\alpha)$ (see the assertion below Eq. (50)). Ultimately, we are led to the following expression for $N_\alpha.U_\alpha$:

$$\begin{aligned}
N_\alpha U_\alpha = & -[\cdot, \varepsilon_\alpha]^{-1} \cdot \left[\mathcal{P}_- \left\{ \frac{1}{2} \mathcal{A}_\alpha^{R_l} \nabla_{R_l} \varepsilon_\alpha + \nabla_{R_l} \varepsilon_\alpha \mathcal{A}_\alpha^{R_l} + \mathcal{A}_\alpha^{P_l} \nabla_{P_l} \varepsilon_\alpha + \nabla_{P_l} \varepsilon_\alpha \mathcal{A}_\alpha^{P_l} \right\} \right. \\
& + \mathcal{P}_- \left\{ U_\alpha \left(\left(\frac{\partial}{\partial \alpha} + \langle \cdot \rangle \right) H(\mathbf{X}_\alpha) \right) U_\alpha^+ \right\} + \frac{i}{4} \mathcal{P}_- \{ [\varepsilon_\alpha, \mathcal{A}_\alpha^{R_l}] \mathcal{A}_\alpha^{P_l} - [\varepsilon_\alpha, \mathcal{A}_\alpha^{P_l}] \mathcal{A}_\alpha^{R_l} \} + H.C. \Big] U_\alpha \\
& - \frac{i}{4} \mathcal{P}_- \{ [\mathcal{A}_\alpha^{R_l}, \mathcal{A}_\alpha^{P_l}] U_\alpha \}
\end{aligned} \tag{52}$$

where $\varepsilon_\alpha(\mathbf{X}_\alpha)$ is computed recursively as explained before.

As for $\varepsilon(\mathbf{X})$, we can therefore write for $U(\mathbf{X}) \equiv U_h(\mathbf{X}_h)$:

$$U(\mathbf{X}) = \mathcal{E} \left(\left[\mathcal{T} \exp \left[\int_{0 < \alpha < \hbar} e^{-\langle \cdot \rangle_{\alpha \rightarrow \hbar}^S} N_\alpha e^{-\langle \cdot \rangle_{0 \rightarrow \alpha}^S} d\alpha \right] \right] U_0(\mathbf{X}_0) \right) \tag{53}$$

This expression has a very similar structure as the solution for the energy Eq. (40) except that the operator O_α has to be replaced by N_α .

To end up this section, and given the solution derived for U_α , we can rewrite the operator O_α in an simpler form. Indeed starting again from Eq. (31) using the unitarity condition for U_α yields :

$$\begin{aligned}
\left(\frac{\partial}{\partial \alpha_1} + \langle \cdot \rangle \right) \varepsilon_{\alpha_1}(\mathbf{X}_{\alpha_1}) = & \mathcal{P}_+ \left[\left(\left(\frac{\partial}{\partial \alpha_1} + \langle \cdot \rangle \right) U_{\alpha_1} \right) U_{\alpha_1}^+, \varepsilon_{\alpha_1} \right] - \frac{i}{2} \varepsilon_\alpha \mathcal{P}_+ [\mathcal{A}_\alpha^{R_l}, \mathcal{A}_\alpha^{P_l}] \\
& + U_{\alpha_1} \left(\frac{\partial}{\partial \alpha_1} + \langle \cdot \rangle \right) H(\mathbf{X}_{\alpha_1}) U_{\alpha_1}^+ \\
& + \frac{1}{2} \mathcal{A}_{\alpha_1}^{R_l} \nabla_{R_l} \varepsilon_{\alpha_1} + \nabla_{R_l} \varepsilon_{\alpha_1} \mathcal{A}_{\alpha_1}^{R_l} + \mathcal{A}_{\alpha_1}^{P_l} \nabla_{P_l} \varepsilon_{\alpha_1} + \nabla_{P_l} \varepsilon_{\alpha_1} \mathcal{A}_{\alpha_1}^{P_l} \\
& + \frac{i}{2} \{ \mathcal{A}_{\alpha_1}^{P_l} \varepsilon_{\alpha_1} \mathcal{A}_{\alpha_1}^{R_l} - \mathcal{A}_{\alpha_1}^{R_l} \varepsilon_{\alpha_1} \mathcal{A}_{\alpha_1}^{P_l} + \varepsilon_{\alpha_1} [\mathcal{A}_{\alpha_1}^{R_l}, \mathcal{A}_{\alpha_1}^{P_l}] + [\mathcal{A}_{\alpha_1}^{R_l}, \mathcal{A}_{\alpha_1}^{P_l}] \varepsilon_{\alpha_1} \}
\end{aligned} \tag{54}$$

Now, recall our gauge condition which states that $\mathcal{P}_+ \left(\left(\frac{\partial}{\partial \alpha} + \langle \cdot \rangle \right) U_\alpha \right) U_\alpha^+$ is Hermitian, so that $\mathcal{P}_+ \left[\left(\left(\frac{\partial}{\partial \alpha_1} + \langle \cdot \rangle \right) U_{\alpha_1} \right) U_{\alpha_1}^+, \varepsilon_{\alpha_1} \right]$ is antihermitian, as the commutator of two hermitian quantities. As a consequence, $\mathcal{P}_+ \left[\left(\left(\frac{\partial}{\partial \alpha_1} + \langle \cdot \rangle \right) U_{\alpha_1} \right) U_{\alpha_1}^+, \varepsilon_{\alpha_1} \right] + H.C. = 0$. Then, use the fact that $\varepsilon_\alpha(\mathbf{X}_\alpha)$ is assumed to be an Hermitian operator, so that $\left(\frac{\partial}{\partial \alpha_1} + \langle \cdot \rangle \right) \varepsilon_{\alpha_1}(\mathbf{X}_{\alpha_1})$ is equal to half its sum with its hermitic conjugate. A computation similar to Eq. (51), leads

us directly to the expression :

$$\begin{aligned} \left(\frac{\partial}{\partial \alpha_1} + \langle . \rangle \right) \varepsilon_{\alpha_1}(\mathbf{X}_{\alpha_1}) &= \frac{1}{2} \mathcal{P}_+ \left\{ \mathcal{A}_\alpha^{R_l} \nabla_{R_l} \varepsilon_\alpha + \nabla_{R_l} \varepsilon_\alpha \mathcal{A}_\alpha^{R_l} + \mathcal{A}_\alpha^{P_l} \nabla_{P_l} \varepsilon_\alpha + \nabla_{P_l} \varepsilon_\alpha \mathcal{A}_\alpha^{P_l} \right\} \\ &+ \left[\frac{i}{4} \mathcal{P}_+ \left\{ [\varepsilon_\alpha, \mathcal{A}_\alpha^{R_l}] \mathcal{A}_\alpha^{P_l} - [\varepsilon_\alpha, \mathcal{A}_\alpha^{P_l}] \mathcal{A}_\alpha^{R_l} \right\} + H.C. \right] \\ &+ U_{\alpha_1} \left(\frac{\partial}{\partial \alpha_1} + \langle . \rangle \right) H(\mathbf{X}_{\alpha_1}) U_{\alpha_1}^+ \end{aligned}$$

The action of O_α is obtained by skipping $U_{\alpha_1} \left(\frac{\partial}{\partial \alpha_1} + \langle . \rangle \right) H(\mathbf{X}_{\alpha_1}) U_{\alpha_1}^+$ from the last term, so that :

$$\begin{aligned} O_\alpha \varepsilon_\alpha(\mathbf{X}_\alpha) &= \frac{1}{2} \mathcal{P}_+ \left\{ \mathcal{A}_\alpha^{R_l} \nabla_{R_l} \varepsilon_\alpha + \nabla_{R_l} \varepsilon_\alpha \mathcal{A}_\alpha^{R_l} + \mathcal{A}_\alpha^{P_l} \nabla_{P_l} \varepsilon_\alpha + \nabla_{P_l} \varepsilon_\alpha \mathcal{A}_\alpha^{P_l} \right\} \\ &+ \left[\frac{i}{4} \mathcal{P}_+ \left\{ [\varepsilon_\alpha, \mathcal{A}_\alpha^{R_l}] \mathcal{A}_\alpha^{P_l} - [\varepsilon_\alpha, \mathcal{A}_\alpha^{P_l}] \mathcal{A}_\alpha^{R_l} \right\} + H.C. \right] \end{aligned} \quad (55)$$

Let us ultimately recall, that in most of the physical applications of interest for us (in particular for Dirac and Bloch electrons) the term $\left(\frac{\partial}{\partial \alpha} + \langle . \rangle \right) H(\mathbf{X}_\alpha)$ will cancel. This simplification will be assumed for the rest of the paper.

C. The full system $\mathbf{H}$ and $\mathbf{U}$

We can now write the solution of our diagonalization procedure for a general matrix valued Hamiltonian through an unitary transformation U as the solution of the following system of differential equations

$$\varepsilon(\mathbf{X}) = \mathcal{E} \left(\left[\mathcal{T} \exp \left[\int_{0 < \alpha < \hbar} e^{-\langle . \rangle_\alpha^S / \hbar} O_\alpha e^{-\langle . \rangle_{0 \rightarrow \alpha}^S} d\alpha \right] \right] \varepsilon_0(\mathbf{X}_0) \right) \quad (56)$$

$$U(\mathbf{X}) = \mathcal{E} \left(\left[\mathcal{T} \exp \left[\int_{0 < \alpha < \hbar} e^{-\langle . \rangle_\alpha^S / \hbar} N_\alpha e^{-\langle . \rangle_{0 \rightarrow \alpha}^S} d\alpha \right] \right] U_0(\mathbf{X}_0) \right) \quad (57)$$

where O_α and N_α are given respectively by Eqs.(55) and (52). The only pre-requirement is that the diagonal form at $\alpha = 0$, $\varepsilon_0(\mathbf{R}_0, \mathbf{P}_0)$ is known, i.e., when $\mathbf{R}$ and $\mathbf{P}$ are considered as classical commuting variables (which means that $U_0(\mathbf{X}_0)$ is known). Of course these equations do not allow to find directly $\varepsilon(\mathbf{X})$, $U(\mathbf{X})$ since those quantities are involved on the R.H.S. of these relations. However, they allow us to produce solutions for $\varepsilon(\mathbf{X})$ and $U(\mathbf{X})$ recursively in a series expansion in $\hbar$. Moreover, and as needed, the results of our previous sections show that the matrices $\varepsilon(\mathbf{X})$ and $U(\mathbf{X})$ obtained through this process are

independent of any choice of symmetrization. A particular choice in the way of arranging the variables for $U(\mathbf{X}) = 0$ will lead to differently symmetrized, but identical, operators.

As it will appear clearly later on, having both $\varepsilon(\mathbf{X})$ and $U(\mathbf{X})$ at order n in $\hbar$, and reinserting in the exponential of Eqs. (56) (57) allows us to find $\varepsilon(\mathbf{X})$ and $U(\mathbf{X})$ at order $n+1$ in $\hbar$. But before solving recursively the set of equations Eqs.(56) (57), we first compare the present approach with the one developed in article [8].

IV. LINK WITH THE DIFFERENTIAL EQUATION OF REF. [8]

In [8] we developed a different less general approach which led to the differential equation

$$\begin{aligned} \frac{\partial}{\partial \alpha} \varepsilon_\alpha(\mathbf{X}_\alpha, \alpha) = & [\partial_\alpha U_\alpha(\mathbf{X}_\alpha) U_\alpha^\dagger(\mathbf{X}_\alpha), \varepsilon_\alpha(\mathbf{X}_\alpha)] + \frac{1}{2} \{ \mathcal{A}_\alpha^{R_l} \nabla_{R_l} \varepsilon_\alpha + \nabla_{R_l} \varepsilon_\alpha \mathcal{A}_\alpha^{R_l} + \mathcal{A}_\alpha^{P_l} \nabla_{P_l} \varepsilon_\alpha + \nabla_{P_l} \varepsilon_\alpha \mathcal{A}_\alpha^{P_l} \} \\ & + \frac{i}{2} \{ [\varepsilon_\alpha, \mathcal{A}_\alpha^{R_l}] \mathcal{A}_\alpha^{P_l} - [\varepsilon_\alpha, \mathcal{A}_\alpha^{P_l}] \mathcal{A}_\alpha^{R_l} \} - \frac{i}{2} [\varepsilon_\alpha, [\mathcal{A}_\alpha^{R_l}, \mathcal{A}_\alpha^{P_l}]] \\ & + \left\{ U_\alpha \langle H(\mathbf{X}_\alpha) \rangle U_\alpha^\dagger - \frac{i}{2} [\mathcal{B}_\alpha \varepsilon_\alpha - \varepsilon_\alpha \mathcal{B}_\alpha] - \langle \varepsilon_\alpha \rangle \right\} \end{aligned} \quad (58)$$

(in the right hand side we have skipped the explicit dependence in α for the sake of simplicity) which was coupled to the evolution of the transformation matrix $U_\alpha(\mathbf{X}_\alpha)$ as a function of α [8] :

$$0 = \partial_\alpha U_\alpha(\mathbf{X}_\alpha) U_\alpha^\dagger(\mathbf{X}_\alpha) + U_\alpha(\mathbf{X}_\alpha) \partial_\alpha U_\alpha^\dagger(\mathbf{X}_\alpha) - \frac{i}{2} (\mathcal{B}_\alpha - \mathcal{B}_\alpha^\dagger) + \frac{i}{2} [\mathcal{A}_\alpha^{R_l}, \mathcal{A}_\alpha^{P_l}] \quad (59)$$

where $-\frac{i}{2} \mathcal{B}_\alpha = (Asym[\nabla_{R_l} \nabla_{P_l} U_\alpha(\mathbf{X}_\alpha)]) U_\alpha^\dagger(\mathbf{X}_\alpha) = \langle U_\alpha \rangle U_\alpha^\dagger$. With these two equations Eqs. (58) and (59) at hand, the diagonalization process can be performed. Actually, since all quantities are matrix valued and since $\varepsilon_\alpha(\mathbf{X}_\alpha)$ is by definition a diagonal matrix, we can separate the energy equation Eq. (58) in a diagonal and a off-diagonal part such that we are led to the following two equations

$$\frac{\partial}{\partial \alpha} \varepsilon_\alpha(\mathbf{X}_\alpha) = \mathcal{P}_+[\text{R.H.S. of Eq. 58}] \quad (60)$$

$$0 = \mathcal{P}_-[\text{R.H.S. of Eq. 58}] \quad (61)$$

In [8] it was claimed that those three Eqs. (59) (60) (61) allow us to determine recursively in powers of α the energy of the quantum system in question. Actually, the integration over α of Eq. (60) gives $\varepsilon_\alpha(\mathbf{X}_\alpha)$ at order n in α when knowing all quantities at order $n-1$. By the same token, Eqs. (61) and (59) (whose meaning is that $U_\alpha(\mathbf{X}_\alpha)$ is unitary at each order in

α) involve $\partial_\alpha U_\alpha(\mathbf{X}_\alpha)$, and allow to recover $U_\alpha(\mathbf{X}_\alpha)$ at order n by integration over α . As a consequence, the diagonalization process is perfectly controlled order by order in the series expansion in α . In [8] we also provided two physical examples at the order $\hbar^2$.

Now we want to show that our solution Eq. (40) satisfies the differential equation Eq. (58).

To do so, we first rewrite (58) and (59) with the notation of this paper. First, (59), is in fact (43). Actually, $-\frac{i}{2}(\mathcal{B}_\alpha - \mathcal{B}_\alpha^+) = \langle U_\alpha \rangle U_\alpha^+ + U_\alpha \langle U_\alpha^+ \rangle$.

Second, (61) is identical to (44). It can be seen by starting with (61), and noting that in (61)

$$\begin{aligned} & [\partial_\alpha U_\alpha(\mathbf{X}_\alpha) U_\alpha^+(\mathbf{X}_\alpha), \varepsilon_\alpha(\mathbf{X}_\alpha)] - \frac{i}{2} [\mathcal{B}_\alpha \varepsilon_\alpha - \varepsilon_\alpha \mathcal{B}_\alpha] \\ &= [\partial_\alpha U_\alpha(\mathbf{X}_\alpha) U_\alpha^+(\mathbf{X}_\alpha), \varepsilon_\alpha(\mathbf{X}_\alpha)] + \langle U_\alpha \rangle U_\alpha^+ \varepsilon_\alpha - \varepsilon_\alpha \langle U_\alpha \rangle U_\alpha^+ \\ &= \left[\left(\left(\frac{\partial}{\partial \alpha} + \langle \cdot \rangle \right) U_\alpha \right) U_\alpha^+, \varepsilon_\alpha \right] \end{aligned}$$

which, reinserted in (61) and projected on the non diagonal subspace through $\mathcal{P}_-$ leads to (44) after some rearrangements. Note that the term proportionnal to $\frac{\partial}{\partial \alpha} H(\mathbf{X}_\alpha)$ is missing in (61) compared to (44), since it was assumed to be nul in [8].

Now, we show that $\varepsilon_\alpha(\mathbf{X}_\alpha)$ as defined in (56), satisfies (60). We will use the hermiticity of $\varepsilon_\alpha(\mathbf{X}_\alpha, \alpha)$ as well as the previous gauge condition stating that $\mathcal{P}_+ \left(\left(\frac{\partial}{\partial \alpha} + \langle \cdot \rangle \right) U_\alpha \right) U_\alpha^+$ is hermitian. As proved in the previous section, it implies that $\left[\left(\left(\frac{\partial}{\partial \alpha} + \langle \cdot \rangle \right) U_\alpha \right) U_\alpha^+, \varepsilon_\alpha \right]$ is antihermitian. We also assume $\langle H(\mathbf{X}_\alpha) \rangle = 0$, to be consistent with the previous sections, but including it would not harm. We are led to:

$$\begin{aligned} \frac{\partial}{\partial \alpha} \varepsilon_\alpha(\mathbf{X}_\alpha) &= \frac{1}{2} \mathcal{P}_+ [\text{R.H.S. of Eq. 58} + H.C.] \\ &= \frac{1}{2} \mathcal{P}_+ \{ \mathcal{A}_\alpha^{R_l} \nabla_{R_l} \varepsilon_\alpha + \nabla_{R_l} \varepsilon_\alpha \mathcal{A}_\alpha^{R_l} + \mathcal{A}_\alpha^{P_l} \nabla_{P_l} \varepsilon_\alpha + \nabla_{P_l} \varepsilon_\alpha \mathcal{A}_\alpha^{P_l} \} \\ &\quad + \frac{i}{4} \{ [\varepsilon_\alpha, \mathcal{A}_\alpha^{R_l}] \mathcal{A}_\alpha^{P_l} - [\varepsilon_\alpha, \mathcal{A}_\alpha^{P_l}] \mathcal{A}_\alpha^{R_l} - [\varepsilon_\alpha, [\mathcal{A}_\alpha^{R_l}, \mathcal{A}_\alpha^{P_l}]] + H.C. \} - \langle \varepsilon_\alpha \rangle \\ &= O_\alpha \varepsilon_\alpha(\mathbf{X}_\alpha) - \langle \varepsilon_\alpha \rangle \end{aligned}$$

Now, from Eq. (56) we can write the partial differential with respect to $\hbar$:

$$\begin{aligned}
\frac{\partial}{\partial \hbar} \varepsilon(\mathbf{X}_{\hbar}) &= \frac{\partial}{\partial \hbar} \mathcal{E} \left(\left[\mathcal{T} \exp \left[\int_{0 < \alpha_1 < \hbar} e^{-\langle \cdot \rangle_{\alpha_1 \rightarrow \hbar}^S} O_{\alpha_1} e^{-\langle \cdot \rangle_{0 \rightarrow \alpha_1}^S} d\alpha_1 \right] \right] \varepsilon_0(\mathbf{X}_0) \right) \\
&= -\langle \cdot \rangle \varepsilon_{\hbar}(\mathbf{X}_{\hbar}) \\
&+ \mathcal{E} \left(\sum_n \int_{0 < \alpha_n < \dots < \alpha_2 < \hbar} O_{\hbar} e^{-\langle \cdot \rangle_{\alpha_2 \rightarrow \hbar}^S} O_{\alpha_2} \dots e^{-\langle \cdot \rangle_{\alpha_{n-1} \rightarrow \alpha_{n-2}}^S} O_{\alpha_{n-1}} e^{-\langle \cdot \rangle_{\alpha_n \rightarrow \alpha_{n-1}}^S} O_{\alpha_n} e^{-\langle \cdot \rangle_{0 \rightarrow \alpha_n}^S} \varepsilon_0(\mathbf{X}_0) \right) \\
&= -\langle \cdot \rangle \varepsilon_{\hbar}(\mathbf{X}_{\hbar}) + \\
&O_{\hbar} \mathcal{E} \left(\sum_n \int_{0 < \alpha_n < \dots < \alpha_2 < \hbar} e^{-\langle \cdot \rangle_{\alpha_2 \rightarrow \hbar}^S} O_{\alpha_2} \dots e^{-\langle \cdot \rangle_{\alpha_{n-1} \rightarrow \alpha_{n-2}}^S} O_{\alpha_{n-1}} e^{-\langle \cdot \rangle_{\alpha_n \rightarrow \alpha_{n-1}}^S} O_{\alpha_n} e^{-\langle \cdot \rangle_{0 \rightarrow \alpha_n}^S} \varepsilon_0(\mathbf{X}_0) \right) \\
&= -\langle \cdot \rangle \varepsilon_{\hbar}(\mathbf{X}_{\hbar}) + O_{\hbar} \varepsilon_{\hbar}(\mathbf{X}_{\hbar})
\end{aligned} \tag{62}$$

The first equality has been obtained by using that by construction, $\frac{\partial}{\partial \hbar} e^{-\langle \cdot \rangle_{\alpha_1 \rightarrow \hbar}^S} = -S_{\mathbf{X}_{\hbar}} \langle \cdot \rangle_{\hbar} S_{\mathbf{X}_{\hbar}}$ and by remarking that in computation of the partial derivative $\frac{\partial}{\partial \hbar}$, the canonical variables and the expectation operator remain unchanged (that is $\mathbf{X}_{\hbar}$ is seen as a constant). We have given previously the expression for $O_{\hbar} \varepsilon_{\hbar}(\mathbf{Y}_{\hbar})$. Using moreover Eq. (59) one gets directly that $(\varepsilon(\mathbf{R}, \mathbf{P}) - \varepsilon_0(\mathbf{R}, \mathbf{P}))$ is a solution of the differential (58).

V. DYNAMICAL OPERATORS AND COMMUTATION ALGEBRA

In this section we will see that new non-commuting position and momentum operators which have contributions from Berry connections emerge during the diagonalization and are more suitably to correspond to physical operators (for the physical discussion of this point see [9][11][8][22]). This discussion may be skipped, and the reader can directly move to the next section dealing with the general expressions for the diagonalized Hamiltonian to the first and second order.

From Eq.(31) one sees that the operator $O_{\alpha} = (\partial_{\alpha} + \langle \cdot \rangle)$ acting on $\varepsilon_0(\mathbf{X}_{\alpha})$ can be decomposed as a sum of a "translation" operator T and a "magnetization" M operator (this terminology is explained in [8])

$$O_{\alpha} \varepsilon_0(\mathbf{X}_{\alpha}) = (T_{\alpha} + M_{\alpha}) \varepsilon_0(\mathbf{X}_{\alpha}). \tag{63}$$

where the "magnetization" operator acts as

$$M_\alpha \varepsilon_0(\mathbf{X}_\alpha) = \frac{i}{2} \mathcal{P}_+ \left\{ [\varepsilon_\alpha, \mathcal{A}_\alpha^{R_l}] \mathcal{A}_\alpha^{P_l} - [\varepsilon_\alpha, \mathcal{A}_\alpha^{P_l}] \mathcal{A}_\alpha^{R_l} \right\} + \mathcal{P}_+ \left[U_\alpha \left(\left(\frac{\partial}{\partial \alpha} + \langle \cdot \rangle \right) H(\mathbf{X}_\alpha) \right) U_\alpha^+ \right] \quad (64)$$

and

$$T_\alpha \varepsilon_0(\mathbf{X}_\alpha) = \frac{1}{2} \mathcal{P}_+ \left\{ \mathcal{A}_\alpha^{R_l} \nabla_{R_l} \varepsilon_0(\mathbf{X}_\alpha) + \nabla_{R_l} \varepsilon_0 \mathcal{A}_\alpha^{R_l}(\mathbf{X}_\alpha) + \mathcal{A}_\alpha^{P_l} \nabla_{P_l} \varepsilon_0(\mathbf{X}_\alpha) + \nabla_{P_l} \varepsilon_0 \mathcal{A}_\alpha^{P_l}(\mathbf{X}_\alpha) \right\} \quad (65)$$

To inspect the action of T_α , let us skip the magnetization contribution M_α for the sake of clarity, and consider the following relevant contribution for the computation of the diagonalized Hamiltonian :

$$\mathcal{ET} \exp \left[\int_{0 < \alpha < \hbar} e^{-\langle \cdot \rangle_{\alpha \rightarrow \hbar}^S} T_\alpha e^{-\langle \cdot \rangle_{0 \rightarrow \alpha}^S} d\alpha \right] \varepsilon_0(\mathbf{X}_0)$$

When developed in series, as explained in the previous sections, it is given by

$$\mathcal{E} \sum_{n=0}^n \left[\int_{0 < \alpha_n < \dots < \alpha_1 < \hbar} e^{-\langle \cdot \rangle_{\alpha_1 \rightarrow \hbar}^S} T_{\alpha_1} \dots e^{-\langle \cdot \rangle_{\alpha_{n-1} \rightarrow \alpha_{n-2}}^S} T_{\alpha_{n-1}} e^{-\langle \cdot \rangle_{\alpha_n \rightarrow \alpha_{n-1}}^S} T_{\alpha_n} e^{-\langle \cdot \rangle_{0 \rightarrow \alpha_n}^S} \right] \varepsilon_0(\mathbf{X}_0) \quad (66)$$

Recall that each operation of the kind $e^{-\langle \cdot \rangle_{\alpha_i \rightarrow \alpha_{i-1}}^S}$ is going along with a change of variable $\mathbf{X}_{\alpha_i} \rightarrow \mathbf{X}_{\alpha_{i-1}}$.

We find $\mathcal{ET} \exp \left[\int_{0 < \alpha < \hbar} e^{-\langle \cdot \rangle_{\alpha \rightarrow \hbar}^S} T_\alpha e^{-\langle \cdot \rangle_{0 \rightarrow \alpha}^S} d\alpha \right] \varepsilon_0(\mathbf{X})$ by the following ansatz. We assume that $\mathcal{ET} \exp \left[\int_{0 < \alpha < \hbar} e^{-\langle \cdot \rangle_{\alpha \rightarrow \hbar}^S} T_\alpha e^{-\langle \cdot \rangle_{0 \rightarrow \alpha}^S} d\alpha \right] \varepsilon_0(\mathbf{X}) = \varepsilon_0(\mathbf{X}_\hbar + A_\hbar^{\mathbf{X}})$ where $A_\hbar^{\mathbf{X}} \equiv A_\hbar^{\mathbf{X}}(\mathbf{X}_\hbar, \hbar)$ has to be determined and a particular (arbitrary) choice of symmetrization of the variables $\mathbf{X}$ has been made. Due to the form of the left hand side in the previous relation Eq. (66), $A_\hbar^{\mathbf{X}}$ is of order $\hbar$. We choose to write ε_0 and $A_\hbar^{\mathbf{X}}$ such that the powers of $\mathbf{R}$ and $\mathbf{P}$ are in a completely symmetrized form, that is we sum over all equally weighted permutations of the canonical variables in the series expansion of $\varepsilon_0(\mathbf{X})$ (and $A_\hbar^{\mathbf{X}}$). Then, $\varepsilon_0(\mathbf{X} + A_\hbar^{\mathbf{X}})$ is obtained by replacing $\mathbf{X}$ by $\mathbf{X} + A_\hbar^{\mathbf{X}}$ in the series expansion of ε_0 . Note that, for later purposes $\langle \cdot \rangle_\hbar \varepsilon_0(\mathbf{X} + A_\hbar^{\mathbf{X}})$ is of order $\hbar^2$. To differentiate the right hand side of Eq. (66) with respect to $\hbar$ we proceed in the following way.

On one hand, assuming that ε_0 does not depends explicitly on $\hbar$, $\frac{\partial}{\partial \hbar} \varepsilon_0(\mathbf{X} + A_\hbar^{\mathbf{X}})$ is equal to :

$$\frac{\partial}{\partial \hbar} \varepsilon_0(\mathbf{X} + A_\hbar^{\mathbf{X}}) = \frac{\partial A_\hbar^{\mathbf{X}}}{\partial \hbar} \nabla_{\mathbf{X}} \varepsilon_0(\mathbf{X} + A_\hbar^{\mathbf{X}})$$

Note that in the last expression, the product $\frac{\partial A_h^{\mathbf{X}}}{\partial h} \nabla_{\mathbf{X}} \varepsilon_0 (\mathbf{X} + A_h^{\mathbf{X}})$ has to be understood in the sense that $\frac{\partial A_h^{\mathbf{X}}}{\partial h}$ replaces $\mathbf{X} + A_h^{\mathbf{X}}$ at each place the gradient is acting on the series expansion of ε_0 .

On the other hand, the same infinitesimal variation can be computed through the left hand side of Eq. (66) :

$$\begin{aligned}
& \frac{\partial}{\partial h} \varepsilon_0 (\mathbf{X}_h + A_h^{\mathbf{X}_h}) \\
&= \frac{\partial}{\partial h} \mathcal{E} \sum_{n=0}^n \left[\int_{0 < \alpha_n < \dots < \alpha_1 < h} e^{-\langle \cdot \rangle_{\alpha_1 \rightarrow h}^S} T_{\alpha_1} \dots e^{-\langle \cdot \rangle_{\alpha_{n-1} \rightarrow \alpha_{n-2}}^S} T_{\alpha_{n-1}} e^{-\langle \cdot \rangle_{\alpha_n \rightarrow \alpha_{n-1}}^S} T_{\alpha_n} e^{-\langle \cdot \rangle_{0 \rightarrow \alpha_n}^S} \right] \varepsilon_0 (\mathbf{X}_0) \\
&= -\langle \cdot \rangle_h \mathcal{E} \sum_{n=0}^n \left[\int_{0 < \alpha_n < \dots < \alpha_1 < h} e^{-\langle \cdot \rangle_{\alpha_1 \rightarrow h}^S} T_{\alpha_1} \dots e^{-\langle \cdot \rangle_{\alpha_{n-1} \rightarrow \alpha_{n-2}}^S} T_{\alpha_{n-1}} e^{-\langle \cdot \rangle_{\alpha_n \rightarrow \alpha_{n-1}}^S} T_{\alpha_n} e^{-\langle \cdot \rangle_{0 \rightarrow \alpha_n}^S} \right] \varepsilon_0 (\mathbf{X}_0) \\
&+ \mathcal{E} \left(\sum_n \left[\int_{0 < \alpha_n < \dots < \alpha_2 < h} T_h e^{-\langle \cdot \rangle_{\alpha_2 \rightarrow h}^S} T_{\alpha_2} \dots e^{-\langle \cdot \rangle_{\alpha_{n-1} \rightarrow \alpha_{n-2}}^S} T_{\alpha_{n-1}} e^{-\langle \cdot \rangle_{\alpha_n \rightarrow \alpha_{n-1}}^S} T_{\alpha_n} e^{-\langle \cdot \rangle_{0 \rightarrow \alpha_n}^S} \right] \varepsilon_0 (\mathbf{X}_0) \right) \\
&(-\langle \cdot \rangle_h + T_h) \varepsilon_0 (\mathbf{X}_h + A_h^{\mathbf{X}_h})
\end{aligned}$$

As a consequence, one is left ultimately with :

$$[-\langle \cdot \rangle_h + T_h] \varepsilon_0 (\mathbf{X} + A_h^{\mathbf{X}}) = \frac{\partial A_h^{\mathbf{X}}}{\partial h} \nabla_{\mathbf{X}} \varepsilon_0 (\mathbf{X} + A_h^{\mathbf{X}}) \quad (67)$$

Now consider $\mathcal{P}_+ [\mathcal{A}_\alpha^{\mathbf{R}}]$ and $\mathcal{P}_+ [\mathcal{A}_\alpha^{\mathbf{P}}]$, with the following definitions for the "non-projected" Berry connections $\mathcal{A}_\alpha^{\mathbf{R}} = i [U_\alpha \nabla_{\mathbf{P}} U_\alpha^\dagger]$ and $\mathcal{A}_\alpha^{\mathbf{P}} = -i [U_\alpha \nabla_{\mathbf{R}} U_\alpha^\dagger]$. Define also for convenience $\mathcal{P}_+ [\mathcal{A}_\alpha^{\mathbf{X}}] = (\mathcal{P}_+ [\mathcal{A}_\alpha^{\mathbf{R}}], \mathcal{P}_+ [\mathcal{A}_\alpha^{\mathbf{P}}])$. Our last equation Eq. (67) is thus equivalent to :

$$\begin{aligned}
& \frac{1}{2} \mathcal{P}_+ [\mathcal{A}_h^{\mathbf{X}}] \cdot \left[\nabla_{\mathbf{X}} \varepsilon_0 (\mathbf{X} + A_h^{\mathbf{X}}) + \nabla_{\mathbf{X}} (A_h^{\mathbf{X}})^i (\mathbf{X}) \nabla_{\mathbf{X}_i} \varepsilon_0 (\mathbf{X} + A_h^{\mathbf{X}}) \right] + H.C. - \langle \cdot \rangle_h \varepsilon_0 (\mathbf{X} + A_h^{\mathbf{X}}) \\
&= \frac{\partial A_h^{\mathbf{X}}}{\partial h} \nabla_{\mathbf{X}} \varepsilon_0 (\mathbf{X} + A_h^{\mathbf{X}})
\end{aligned}$$

where $H.C.$ stands for the Hermitian conjugate. The term $\nabla_{\mathbf{X}} \varepsilon_0 (\mathbf{X} + A_h^{\mathbf{X}})$ stems from the gradient of $\varepsilon_0 (\mathbf{X})$ evaluated at $(\mathbf{X} + A_h^{\mathbf{X}})$. As before $\nabla_{\mathbf{X}} (A_h^{\mathbf{X}})^i (\mathbf{X}) \nabla_{\mathbf{X}_i} \varepsilon_0 (\mathbf{X} + A_h^{\mathbf{X}})$ has to be understood in the sense that $\nabla_{\mathbf{X}} (A_h^{\mathbf{X}})^i$ replaces $\mathbf{X} + A_h^{\mathbf{X}}$ at each place the gradient is acting on the series expansion of ε_0 . To be able to compare both sides of this equation, one has to symmetrize both expressions in the same way. As a consequence the left hand side

has to be rewritten in the same symmetrized form as the right hand side :

$$\begin{aligned} & \frac{1}{2} \mathcal{P}_+ [\mathcal{A}_h^{\mathbf{X}}] \cdot \left[\nabla_{\mathbf{X}} \varepsilon_0 (\mathbf{X} + A_h^{\mathbf{X}}) + \nabla_{\mathbf{X}} (A_h^{\mathbf{X}})^i (\mathbf{X}) \nabla_{\mathbf{X}_i} \varepsilon_0 (\mathbf{X} + A_h^{\mathbf{X}}) \right] + H.C. \\ &= \frac{1}{2} \left\{ \mathcal{P}_+ [\mathcal{A}_h^{\mathbf{X}}] \cdot \left[\nabla_{\mathbf{X}} \varepsilon_0 (\mathbf{X} + A_h^{\mathbf{X}}) + \nabla_{\mathbf{X}} (A_h^{\mathbf{X}})^i (\mathbf{X}) \nabla_{\mathbf{X}_i} \varepsilon_0 (\mathbf{X} + A_h^{\mathbf{X}}) \right] \right\}_S + H.C. + C(\mathbf{X}) \end{aligned}$$

This formula requires some explanation. In the left hand side, the multiplication by $\mathcal{P}_+ [\mathcal{A}_\alpha^{\mathbf{X}}]$ is performed half on the left and half on the right, as implied by definition of the translation operator. On the right hand side, all expressions are seen as symmetrized in a way that $\mathcal{P}_+ [\mathcal{A}_\alpha^{\mathbf{X}}]$ has been inserted at each place where the $\nabla_{\mathbf{X}}$ is acting (exactly as for $\frac{\partial A_h^{\mathbf{X}}(\mathbf{X})}{\partial \hbar} \nabla_{\mathbf{X}} \varepsilon_0 (\mathbf{X} + A_h^{\mathbf{X}})$). The $\{\}_S$ is there to recall this full symmetrization in the variables. The term $C(\mathbf{X})$ is the correction due to this change of symmetrization while moving the $\mathcal{P}_+ [\mathcal{A}_\alpha^{\mathbf{X}}]$ inside the series expansion of ε_0 . By construction, it involves the powers of gradients of $\mathcal{P}_+ [\mathcal{A}_\alpha^{\mathbf{X}}]$ and ε_0 and is of order $\hbar^2$. In practice, this term depends specifically on the problem at hand (that is on the form of the Hamiltonian) and can be computed order by order in $\hbar$. Since later on, we will consider only the order $\hbar^2$, it will turn out that this term will be negligible due to an integration.

We can now write the differential equation :

$$\begin{aligned} \frac{\partial A_h^{\mathbf{X}}(\mathbf{X})}{\partial \hbar} \nabla_{\mathbf{X}} \varepsilon_0 (\mathbf{X} + A_h^{\mathbf{X}}) &= \frac{1}{2} \left\{ \mathcal{P}_+ [\mathcal{A}_\alpha^{\mathbf{X}}] \cdot \left[\nabla_{\mathbf{X}} \varepsilon_0 (\mathbf{X} + A_h^{\mathbf{X}}) + \nabla_{\mathbf{X}} (A_h^{\mathbf{X}})^i (\mathbf{X}) \nabla_{\mathbf{X}_i} \varepsilon_0 (\mathbf{X} + A_h^{\mathbf{X}}) \right] \right\}_S \\ &+ H.C. + C(\mathbf{X}) - \langle \cdot \rangle_{\hbar} \varepsilon_0 (\mathbf{X} + A_h^{\mathbf{X}}) \end{aligned}$$

where all expressions are now symmetrized in the same way. Now, remark that, given our previous remarks, $C(\mathbf{X}) - \langle \cdot \rangle_{\hbar} \varepsilon_0 (\mathbf{X} + A_h^{\mathbf{X}})$ is of order $\hbar^2$. It implies that, after integration, it will contribute only to the third order in $\hbar$ to $A_h^{\mathbf{X}}$. As a consequence, neglecting this term in first approximation (that will be indeed the case in our applications) we thus deduce that $A_h^{\mathbf{X}}$ satisfies the following differential equation :

$$\mathcal{P}_+ [\mathcal{A}_h^{\mathbf{X}}] + \frac{1}{2} (\mathcal{P}_+ [\mathcal{A}_h^{\mathbf{X}}] \cdot \nabla_{\mathbf{X}}) A_h^{\mathbf{X}} + H.C. = \frac{\partial A_h^{\mathbf{X}}}{\partial \hbar} \quad (68)$$

Given that for $\hbar = 0$, one has $A_h^{\mathbf{X}} = \mathbf{0}$, the solution of this equation can be written recursively as:

$$A_h^{\mathbf{X}} = \int_{0 < \alpha < \hbar} S_{\mathbf{X}_h} \left[\mathcal{P}_+ [\mathcal{A}_\alpha^{\mathbf{X}}] + \frac{1}{2} ((\mathcal{P}_+ [\mathcal{A}_\alpha^{\mathbf{X}}] \cdot \nabla_{\mathbf{X}}) A_\alpha^{\mathbf{X}} + H.C.) \right] d\alpha \quad (69)$$

$$\begin{aligned} &= \int_{0 < \alpha < \hbar} S_{\mathbf{X}_h} \mathcal{P}_+ [\mathcal{A}_\alpha^{\mathbf{X}}] d\alpha + \int_{0 < \alpha < \hbar} S_{\mathbf{X}_h} \frac{1}{2} \left[\left[\mathcal{P}_+ [\mathcal{A}_\alpha^{\mathbf{X}}] \cdot \nabla_{\mathbf{X}} \int_{0 < \alpha_1 < \alpha} \mathcal{P}_+ [\mathcal{A}_{\alpha_1}^{\mathbf{X}}] \right] + H.C. \right] d\alpha_1 d\alpha \\ &+ \dots \end{aligned} \quad (70)$$

Recall that $S_{\mathbf{X}_h}$ is the shift of variable $\mathbf{X}_\alpha \rightarrow \mathbf{X}_h = \mathbf{X}$, so that in the integrals, the variables $\mathbf{X}$ are inert, only the explicit dependence in α is integrated on. Let us also stress that in the previous integrals, the variables $\mathbf{X}_\alpha$ in $A_\alpha^{\mathbf{R}}$ and $A_\alpha^{\mathbf{P}}$ have been replaced by $\mathbf{X}$ and are thus constant with respect to the α integrations. The reason is that in the differential equation Eq. (68), $\mathbf{X}$ is seen as constant, only $\hbar$ is running. Actually, the equation involves only the partial derivative $\frac{\partial A_h^{\mathbf{X}}}{\partial \hbar}$. Having now the solution for $A_h^{\mathbf{X}}$ as a function of the Berry phases we can write our solution for the exponentiated action of the translation operator. Dividing $A_h^{\mathbf{X}}$ in two components with respect to $\mathbf{R}$ and $\mathbf{P}$, $A_h^{\mathbf{X}} \equiv (A_{\mathbf{R}}, A_{\mathbf{P}})$, one has :

$$\mathcal{ET} \exp \left[\int_{0 < \alpha < \hbar} e^{-\langle \cdot \rangle_\alpha^S} T_\alpha e^{-\langle \cdot \rangle_{\hbar-\alpha}^S} d\alpha \right] \varepsilon_0(\mathbf{X}) = \varepsilon_0(\mathbf{x}) \quad (71)$$

with $\mathbf{x} = (\mathbf{r}, \mathbf{p})$ and $\mathbf{r}$ and $\mathbf{p}$ are new coordinate and momentum operators corrected by Berry connections terms in the following way :

$$\begin{aligned} \mathbf{r} &\equiv \mathbf{R} + A_{\mathbf{R}} \\ \mathbf{p} &\equiv \mathbf{P} + A_{\mathbf{P}} \end{aligned} \quad (72)$$

justifying the name translation operator for T_α . The inclusion of the corrections due to $C(\mathbf{X})$ can be performed in the following way. Shifting $A_h^{\mathbf{X}}$ by a correction $A_h^{\mathbf{X}} + \delta A_h^{\mathbf{X}}$ with $A_h^{\mathbf{X}}$ the solution previously found for Eq. (68), gives the following equation for $\delta A_h^{\mathbf{X}}$:

$$\begin{aligned} &\frac{1}{2} \mathcal{P}_+ [A_h^{\mathbf{X}}] \cdot \left[\nabla_{\mathbf{X}} (\delta A_h^{\mathbf{X}})^i(\mathbf{X}) \nabla_{\mathbf{X}_i} \varepsilon_0(\mathbf{X} + A_h^{\mathbf{X}} + \delta A_h^{\mathbf{X}}) \right] + H.C. + C(\mathbf{X}) - \langle \cdot \rangle_h \varepsilon_0(\mathbf{X} + A_h^{\mathbf{X}}) \\ &= \frac{\partial \delta A_h^{\mathbf{X}}(\mathbf{X})}{\partial \hbar} \nabla_{\mathbf{X}} \varepsilon_0(\mathbf{X} + A_h^{\mathbf{X}} + \delta A_h^{\mathbf{X}}) \end{aligned}$$

Note that $C(\mathbf{X})$ is computed using the derivatives of $A_h^{\mathbf{X}} + \delta A_h^{\mathbf{X}}$. Expanding $\delta A_h^{\mathbf{X}}(\mathbf{X})$ as an $\hbar$ series expansion of completely symmetrized function $\delta A_h^{\mathbf{X}^{(n)}}(\mathbf{X})$ of $\mathbf{R}$ and $\mathbf{P}$ (starting with $n = 3$) allows, at least theoretically to find the $\delta A_h^{\mathbf{X}^{(n)}}$ recursively by solving an equation of the kind :

$$\frac{\partial \delta A_h^{\mathbf{X}^{(n+1)}}(\mathbf{X})}{\partial \hbar} = F\left(\mathbf{X}, \delta A_h^{\mathbf{X}^{(n)}}(\mathbf{X}), \dots, \delta A_h^{\mathbf{X}^{(n)}}(\mathbf{X})\right)$$

where $F\left(\mathbf{X}, \delta A_h^{\mathbf{X}^{(n)}}(\mathbf{X}), \dots, \delta A_h^{\mathbf{X}^{(n)}}(\mathbf{X})\right)$ is determined by replacing ε_0 , $A_h^{\mathbf{X}}$, $\mathcal{P}_+[A_h^{\mathbf{X}}]$ by their expressions at the n -th order. As said before, in our practical considerations the term $\delta A_h^{\mathbf{X}}(\mathbf{X})$ will always be neglected.

The variables $\mathbf{x} = \mathbf{X} + A_h^{\mathbf{X}}$ we have defined seem thus to be the natural ones arising in the diagonalization process.

Note that at the lowest order we have :

$$\begin{aligned}\mathbf{r} &= \mathbf{R} + \hbar \mathcal{P}_+ [\mathcal{A}_0^{\mathbf{R}}] \equiv \mathbf{R} + A_0^{\mathbf{R}} \\ \mathbf{p} &= \mathbf{P} + \hbar \mathcal{P}_+ [\mathcal{A}_0^{\mathbf{P}}] \equiv \mathbf{P} + A_0^{\mathbf{P}}\end{aligned}\quad (73)$$

where $A_0^{\mathbf{R}}$ and $A_0^{\mathbf{P}}$ are the usual "semiclassical Berry connections" defined previously [8].

From equations Eq. (72) we readily deduce the following non trivial algebra

$$\begin{aligned}[r_i, r_j] &= i\hbar^2 \Theta_{ij}^{rr} = i\hbar^2 (\nabla_{P_i} A_{R_j} - \nabla_{P_j} A_{R_i}) + \hbar^2 [A_{R_j}, A_{R_i}] \\ [p_i, p_j] &= i\hbar^2 \Theta_{ij}^{pp} = -i\hbar^2 (\nabla_{R_i} A_{P_j} - \nabla_{R_j} A_{P_i}) + \hbar^2 [A_{P_i}, A_{P_j}] \\ [p_i, r_j] &= -i\hbar \delta_{ij} + i\hbar^2 \Theta_{ij}^{pr} = -i\hbar \delta_{ij} - i\hbar^2 (\nabla_{R_i} A_{R_j} + \nabla_{P_j} A_{P_i}) + \hbar^2 [A_{P_i}, A_{R_j}]\end{aligned}\quad (74)$$

where the terms Θ_{ij} are the definitions of Berry curvatures. Of course these non trivial commutation relations also give new contributions to the equations of motion and thus lead to new phenomena [8] [11][9]. The commutation relations are valid to any order in $\hbar$, but in practice we can compute them as well as the energy $\varepsilon(\mathbf{X})$ in a series expansion in $\hbar$. Relations Eqs. (64)(71) will be helpful when writing the explicit expression of $\varepsilon(\mathbf{X})$ in a series expansion in $\hbar$ in the following section.

VI. SERIES EXPANSION IN $\hbar$

The exact expression Eq. (40), can now be expanded in a series expansion in $\hbar$. Note that we will always identify $\varepsilon_{\hbar}(\mathbf{R}_{\hbar}, \mathbf{P}_{\hbar})$ with $\varepsilon(\mathbf{R}, \mathbf{P})$. We also implicitly assume for convenience that all expressions are symmetrized in $\mathbf{R}$ and $\mathbf{P}$, in such a way that for all expression depending on $\mathbf{R}$ and $\mathbf{P}$, in the series expansion of this expression, all powers of the momentum are put half on the left and half on the right. Any other choice of symmetrization would be of course suitable. Recall at this point some previous notations : $\mathcal{A}_{\alpha}^{\mathbf{R}} = i[U_{\alpha}(\mathbf{X}_{\alpha}) \nabla_{\mathbf{P}_{\alpha}} U_{\alpha}^+(\mathbf{X}_{\alpha})]$ and $\mathcal{A}_{\alpha}^{\mathbf{P}} = -i[U_{\alpha}(\mathbf{X}_{\alpha}) \nabla_{\mathbf{R}_{\alpha}} U_{\alpha}^+(\mathbf{X}_{\alpha})]$, as well as $\mathcal{A}_{\alpha}^{\mathbf{X}} = (\mathcal{A}_{\alpha}^{\mathbf{R}}, \mathcal{A}_{\alpha}^{\mathbf{P}})$ and $\mathcal{A}_{\alpha}^{\mathbf{X}} = \mathcal{A}_{\hbar}^{\mathbf{X}}$. We will also denote $\mathcal{A}_0^{\mathbf{R}\alpha}$, and $\mathcal{A}_0^{\mathbf{P}\alpha}$ the zeroth order Berry connections evaluated at $\mathbf{X}_{\alpha}$, that is $\mathcal{A}_0^{\mathbf{R}\alpha} \equiv \mathcal{A}_0^{\mathbf{R}\alpha}(\mathbf{X}_{\alpha}) = i[U_0(\mathbf{X}_{\alpha}) \nabla_{\mathbf{P}_{\alpha}} U_0^+(\mathbf{X}_{\alpha})]$, $\mathcal{A}_0^{\mathbf{P}\alpha} \equiv \mathcal{A}_0^{\mathbf{P}\alpha}(\mathbf{X}_{\alpha}) = -i[U_0(\mathbf{X}_{\alpha}) \nabla_{\mathbf{R}_{\alpha}} U_0^+(\mathbf{X}_{\alpha})]$, and $\mathcal{A}_0^{\mathbf{X}\alpha} = (\mathcal{A}_0^{\mathbf{R}\alpha}, \mathcal{A}_0^{\mathbf{P}\alpha})$.

A. First order in $\hbar$

At the first order we obviously get the following expression :

$$\varepsilon(\mathbf{X}) = \varepsilon_0(\mathbf{X}) + \int_0^{\hbar} S_{\mathbf{X}_h} [O_\alpha \varepsilon_0(\mathbf{X}_\alpha)] d\alpha$$

This expression requires some explanations. The action of O_α on $\varepsilon_0(\mathbf{X}_\alpha)$ leads to an expression $F(\mathbf{X}_\alpha, \alpha)$ which depends both on $\mathbf{X}_\alpha$ and α . The shift operation replaces $\mathbf{X}_\alpha$ by $\mathbf{X}_h \equiv \mathbf{X}$ so that the integration is (trivially) performed on the variable α only. To stress this point, let us first introduce a convenient notation. Recall that at the lowest order :

$$\begin{aligned} O_\alpha \varepsilon_0(\mathbf{X}_\alpha) = & \mathcal{P}_+ \left\{ \frac{1}{2} \left(\mathcal{A}_\alpha^{R_l} \nabla_{R_l} \varepsilon_0(\mathbf{X}_\alpha) + \nabla_{R_l} \varepsilon_0(\mathbf{X}_\alpha) \mathcal{A}_\alpha^{R_l}(\mathbf{X}_\alpha) + \mathcal{A}_\alpha^{P_l} \nabla_{P_l} \varepsilon_0(\mathbf{X}_\alpha) + \nabla_{P_l} \varepsilon_0(\mathbf{X}_\alpha) \mathcal{A}_\alpha^{P_l} \right) \right. \\ & \left. \mathcal{P}_+ \left\{ \frac{i}{4} [\varepsilon_0(\mathbf{X}_\alpha), \mathcal{A}_\alpha^{R_l}] \mathcal{A}_\alpha^{P_l} - \frac{i}{4} [\varepsilon_0(\mathbf{X}_\alpha), \mathcal{A}_\alpha^{P_l}] \mathcal{A}_\alpha^{R_l} + H.C. \right\} \right\} \end{aligned}$$

where the Berry phases can be replaced by their value at zeroth order (evaluated at $\mathbf{X}_\alpha$), that is :

$$\begin{aligned} O_\alpha \varepsilon_0(\mathbf{X}_\alpha) = & \mathcal{P}_+ \left\{ \frac{1}{2} \left(\mathcal{A}_0^{R_{\alpha l}} \nabla_{R_{\alpha l}} \varepsilon_0(\mathbf{X}_\alpha) + \nabla_{R_{\alpha l}} \varepsilon_0(\mathbf{X}_\alpha) \mathcal{A}_0^{R_{\alpha l}} + \mathcal{A}_0^{P_{\alpha l}} \nabla_{P_l} \varepsilon_0(\mathbf{X}_\alpha) + \nabla_{P_l} \varepsilon_0(\mathbf{X}_\alpha) \mathcal{A}_0^{P_{\alpha l}} \right) \right\} \\ & \mathcal{P}_+ \left\{ \frac{i}{4} [\varepsilon_0(\mathbf{X}_\alpha), \mathcal{A}_0^{R_{\alpha l}}] \mathcal{A}_0^{P_{\alpha l}} - \frac{i}{4} [\varepsilon_0(\mathbf{X}_\alpha), \mathcal{A}_0^{P_{\alpha l}}] \mathcal{A}_0^{R_{\alpha l}} + H.C. \right\} \end{aligned}$$

since $[U_\alpha ((\frac{\partial}{\partial \alpha} + \langle . \rangle) H(\mathbf{X}_\alpha)) U_\alpha^+] = 0$, at that order.

Now, let define the "covariant derivative" operator : $\mathcal{D}_{\mathbf{X}_\alpha} = (\mathcal{D}_{\mathbf{R}_\alpha}, \mathcal{D}_{\mathbf{P}_\alpha})$

$$\begin{aligned} \mathcal{D}_{\mathbf{R}_\alpha} &= \left[\nabla_{\mathbf{R}_\alpha} + \frac{i}{2} \mathcal{A}_0^{\mathbf{P}_\alpha}, . \right] \\ \mathcal{D}_{\mathbf{P}_\alpha} &= \left[\nabla_{\mathbf{P}_\alpha} - \frac{i}{2} \mathcal{A}_0^{\mathbf{R}_\alpha}, . \right] \end{aligned}$$

and as usual $\mathcal{D}_{\mathbf{X}} \equiv \mathcal{D}_{\mathbf{X}_h}$, so that we can write directly :

$$O_\alpha \varepsilon_0(\mathbf{X}_\alpha) = \frac{1}{2} \mathcal{P}_+ [(\mathcal{D}_{\mathbf{X}_\alpha} \varepsilon_0(\mathbf{X}_\alpha)) \mathcal{A}_0^{\mathbf{X}_\alpha} + H.C.]$$

Therefore, at this order we have

$$\begin{aligned} \varepsilon(\mathbf{X}) &= \varepsilon_0(\mathbf{X}) + \int_0^{\hbar} S_{\mathbf{X}_h} \left[\frac{1}{2} \mathcal{P}_+ [(\mathcal{D}_{\mathbf{X}_\alpha} \varepsilon_0(\mathbf{X}_\alpha)) \mathcal{A}_0^{\mathbf{X}_\alpha} + H.C.] \right] d\alpha + O(\hbar^2) \\ &= \varepsilon_0(\mathbf{X}) + \frac{1}{2} \int_0^{\hbar} \mathcal{P}_+ [(\mathcal{D}_{\mathbf{X}} \varepsilon_0(\mathbf{X})) \mathcal{A}_0^{\mathbf{X}} + H.C.] d\alpha + O(\hbar^2) \\ &= \varepsilon_0(\mathbf{X}) + \frac{1}{2} \mathcal{P}_+ [(\mathcal{D}_{\mathbf{X}} \varepsilon_0(\mathbf{X})) \mathcal{A}_0^{\mathbf{X}} + H.C.] \int_0^{\hbar} d\alpha + O(\hbar^2) \\ &= \varepsilon_0(\mathbf{X}) + \frac{\hbar}{2} \mathcal{P}_+ [(\mathcal{D}_{\mathbf{X}} \varepsilon_0(\mathbf{X})) \mathcal{A}_0^{\mathbf{X}} + H.C.] + O(\hbar^2) \end{aligned} \tag{75}$$

In the three last lines, we have introduced a slight abuse of notation. Consistently with our conventions, we should have written $\mathcal{A}_0^{\mathbf{X}_h}$ rather than $\mathcal{A}_0^{\mathbf{X}}$. However, since in the final expression, all terms have to be expressed at $\mathbf{X}_h = \mathbf{X}$ and not at $\mathbf{X}_0$, no confusion should arise and $\mathcal{A}_0^{\mathbf{X}}$ will, from now, always stand for $\mathcal{A}_0^{\mathbf{X}_h}$ in the final results. Note that, as stated before, the integral over α in the previous computations is trivial once the shift of variable has been performed.

The previous formula can be expanded in several ways. one has,

$$\begin{aligned} \varepsilon(\mathbf{X}) = \varepsilon_0(\mathbf{X}) + \mathcal{P}_+ \left\{ \frac{\hbar}{2} \left(\mathcal{A}_0^{X_l} \nabla_{X_l} \varepsilon_0(\mathbf{X}) + \nabla_{X_l} \varepsilon_0(\mathbf{X}) \mathcal{A}_0^{X_l} \right) \right\} \\ + \frac{i\hbar}{2} \mathcal{P}_+ \left\{ \left[\varepsilon_0(\mathbf{X}), \mathcal{A}_0^{R_l} \right] \mathcal{A}_0^{P_l} - \left[\varepsilon_0(\mathbf{X}), \mathcal{A}_0^{P_l} \right] \mathcal{A}_0^{R_l} \right\} + O(\hbar^2) \end{aligned} \quad (76)$$

or, in terms of covariant variables:

$$\varepsilon(\mathbf{X}) = \varepsilon_0(\mathbf{x}) + \frac{i\hbar}{2} \mathcal{P}_+ \left\{ \left[\varepsilon_0(\mathbf{X}), \mathcal{A}_0^{R_l} \right] \mathcal{A}_0^{P_l} - \left[\varepsilon_0(\mathbf{X}), \mathcal{A}_0^{P_l} \right] \mathcal{A}_0^{R_l} \right\} + O(\hbar^2)$$

One then recover the formula first derived in ref. [8] where $x = (\mathbf{r}, \mathbf{p})$ are given by the expression Eq. (72). As previously mentioned, we only need to know $U_0(\mathbf{X})$ and thus the zeroth order Berry phases to get the energy expansion at the first order.

We end up this paragraph by providing the first order expansion for U that will be used for the second order diagonalization:

$$\begin{aligned} U(\mathbf{X}) = U_0(\mathbf{X}) + \int_0^{\hbar} S_{\mathbf{X}_h} [N_\alpha U_0(\mathbf{X}_\alpha)] d\alpha \equiv U_0(\mathbf{X}) + \hbar U_1(\mathbf{X}) U_0(\mathbf{X}) \\ = \left(1 - \hbar [\cdot, \varepsilon_0]^{-1} \cdot \left[\mathcal{P}_- \left\{ \frac{1}{2} \left(\mathcal{A}_0^{R_l} \nabla_{R_l} \varepsilon_0(\mathbf{X}) + \nabla_{R_l} \varepsilon_0(\mathbf{X}) \mathcal{A}_0^{R_l} + \mathcal{A}_0^{P_l} \nabla_{P_l} \varepsilon_0(\mathbf{X}) + \nabla_{P_l} \varepsilon_0(\mathbf{X}) \mathcal{A}_0^{P_l} \right) \right\} \right. \right. \\ \left. \left. - \frac{i}{2} \left\{ \left[\varepsilon_0(\mathbf{X}), \mathcal{A}_0^{R_l} \right] \mathcal{A}_0^{P_l} - \left[\varepsilon_0(\mathbf{X}), \mathcal{A}_0^{P_l} \right] \mathcal{A}_0^{R_l} \right\} \right] - \frac{i}{4} [\mathcal{A}_0^{R_l}, \mathcal{A}_0^{P_l}] \right) U_0(\mathbf{X}) \end{aligned} \quad (77)$$

B. Second order

Given our choice of symmetrization $\langle \varepsilon_0(\mathbf{X}_\alpha) \rangle_\alpha$ is of order 1 in α , so that. $\langle \cdot \rangle_{0 \rightarrow \hbar}^S \cdot \varepsilon_0(\mathbf{X}) = \int_0^{\hbar} S_{\mathbf{X}_h} \langle \varepsilon_0(\mathbf{X}_\alpha) \rangle_\alpha d\alpha$ is of order 2. As a consequence, expanding the compact form of the energy operator to the second order, leads to :

$$\begin{aligned} \varepsilon(\mathbf{X}) = \varepsilon_0(\mathbf{X}) + \int_0^{\hbar} S_{\mathbf{X}_h} [O_\alpha \varepsilon_0(\mathbf{X}_\alpha)] d\alpha + \int_0^{\hbar} \int_0^{\alpha_1} S_{\mathbf{X}_h} [O_{\alpha_1} S_{\mathbf{X}_{\alpha_1}} [O_{\alpha_2} \varepsilon_0(\mathbf{X}_{\alpha_2})]] d\alpha_2 d\alpha_1 \\ - \int_0^{\hbar} S_{\mathbf{X}_h} \langle \varepsilon_0(\mathbf{X}_\alpha) \rangle_\alpha d\alpha \end{aligned}$$

The last contribution can be computed easily. At the lowest order in α , $S_{\mathbf{X}_h} \langle \varepsilon_0(\mathbf{X}_\alpha) \rangle_\alpha = \frac{\alpha}{\hbar} \langle \varepsilon_0(\mathbf{X}) \rangle_\hbar$ (actually, $S_{\mathbf{X}_h} \langle \varepsilon_0(\mathbf{X}_\alpha) \rangle_\alpha$ is a function of $\mathbf{X}$ times α and $\langle \varepsilon_0(\mathbf{X}) \rangle_\hbar$ is the same function times $\hbar$). As a consequence, $\int_0^\hbar S_{\mathbf{X}_h} \langle \varepsilon_0(\mathbf{X}_\alpha) \rangle_\alpha d\alpha = \int_0^\hbar \frac{\alpha}{\hbar} \langle \varepsilon_0(\mathbf{X}) \rangle_\hbar d\alpha = \frac{\hbar}{2} \langle \varepsilon_0(\mathbf{X}) \rangle$ (with the convention $\langle \varepsilon_0(\mathbf{X}) \rangle = \langle \varepsilon_0(\mathbf{X}) \rangle_\hbar$).

The first contribution $\int_0^\hbar O_\alpha d\alpha \varepsilon_0(\mathbf{X}_\alpha)$ can be expanded as before as:

$$\begin{aligned} & \int_0^\hbar S_{\mathbf{X}_h} [O_\alpha \varepsilon_0(\mathbf{X}_\alpha)] d\alpha \\ &= \int_0^\hbar S_{\mathbf{X}_h} \mathcal{P}_+ \left\{ \frac{1}{2} (\mathcal{A}_\alpha^{R_l} \nabla_{R_l} \varepsilon_0(\mathbf{X}_\alpha) + \nabla_{R_l} \varepsilon_0(\mathbf{X}_\alpha) \mathcal{A}_\alpha^{R_l} + \mathcal{A}_\alpha^{P_l} \nabla_{P_l} \varepsilon_0(\mathbf{X}_\alpha) + \nabla_{P_l} \varepsilon_0(\mathbf{X}_\alpha) \mathcal{A}_\alpha^{P_l}) \right\} d\alpha \\ &+ \int_0^\hbar S_{\mathbf{X}_h} \mathcal{P}_+ \left\{ \frac{i}{4} [\varepsilon_0(\mathbf{X}_\alpha), \mathcal{A}_\alpha^{R_l}] \mathcal{A}_\alpha^{P_l} - \frac{i}{4} [\varepsilon_0(\mathbf{X}_\alpha), \mathcal{A}_\alpha^{P_l}] \mathcal{A}_\alpha^{R_l} + H.C. \right. \\ &\left. + \left[U_\alpha \left(\left(\frac{\partial}{\partial \alpha} + \langle \cdot \rangle \right) H(\mathbf{X}_\alpha) \right) U_\alpha^+ \right] \right\} d\alpha \end{aligned}$$

but now, the Berry connections have to be expanded to the first order in α . Note that in the second order contribution, due to the double integral,

$$\int_0^\hbar \int_0^{\alpha_1} S_{\mathbf{X}_h} [O_{\alpha_1} S_{\mathbf{X}_{\alpha_1}} [O_{\alpha_2} \varepsilon_0(\mathbf{X}_{\alpha_2})]] d\alpha_2 d\alpha_1 - \frac{\hbar}{2} \langle \varepsilon_0(\mathbf{X}) \rangle$$

the Berry connections need only to be expanded to the zeroth order in α .

To go further, we thus need to give first some expanded formula at the first order in α for the Berry phases $\mathcal{A}_\alpha^{\mathbf{X}}$ intervening in the definition of the diagonalized Hamiltonian and the dynamical variables.

1. Berry connections at the first order

To obtain $\mathcal{A}_\alpha^{\mathbf{X}}$ we only need the matrix U at the first order as computed before : $U(\mathbf{X}) \equiv U_h(\mathbf{X}) = U_0(\mathbf{X}) + \hbar U_1(\mathbf{X}) U_0(\mathbf{X})$ with $U_1(\mathbf{X})$ given by (Eq. (77))

$$\begin{aligned} U_1(\mathbf{X}) = & -[\cdot, \varepsilon_0]^{-1} \cdot \left[\mathcal{P}_- \left\{ \frac{1}{2} (\mathcal{A}_0^{R_l} \nabla_{R_l} \varepsilon_0(\mathbf{X}) + \nabla_{R_l} \varepsilon_0(\mathbf{X}) \mathcal{A}_0^{R_l} + \mathcal{A}_0^{P_l} \nabla_{P_l} \varepsilon_0(\mathbf{X}) + \nabla_{P_l} \varepsilon_0(\mathbf{X}) \mathcal{A}_0^{P_l}) \right\} \right. \\ & \left. + \frac{i}{2} \left\{ [\varepsilon_0(\mathbf{X}), \mathcal{A}_0^{R_l}] \mathcal{A}_0^{P_l} - [\varepsilon_0(\mathbf{X}), \mathcal{A}_0^{P_l}] \mathcal{A}_0^{R_l} \right\} \right] - \frac{i}{4} [\mathcal{A}_0^{R_l}, \mathcal{A}_0^{P_l}] \end{aligned} \quad (78)$$

At the same order the (non-diagonal) Berry connections $\mathcal{A}_\alpha^{\mathbf{X}} = (\mathcal{A}_\alpha^{\mathbf{R}}, \mathcal{A}_\alpha^{\mathbf{P}})$ are again given by

$$\begin{aligned} \mathcal{A}_\alpha^{\mathbf{R}}(\mathbf{X}_\alpha) &= i [U_\alpha(\mathbf{X}_\alpha) \nabla_{\mathbf{P}} U_\alpha^+(\mathbf{X}_\alpha)] = \frac{1}{\alpha} U_\alpha(\mathbf{X}_\alpha) \mathbf{R}_\alpha U_\alpha^+(\mathbf{X}_\alpha) \\ \text{and } \mathcal{A}_\alpha^{\mathbf{P}}(\mathbf{X}_\alpha) &= -i [U_\alpha(\mathbf{X}_\alpha) \nabla_{\mathbf{R}} U_\alpha^+(\mathbf{X}_\alpha)] = \frac{1}{\alpha} U_\alpha(\mathbf{X}_\alpha) \mathbf{P}_\alpha U_\alpha^+(\mathbf{X}_\alpha) \end{aligned}$$

where now $U_\alpha(\mathbf{X}_\alpha)$ is the transformation to the first order in α i.e. $U_0(\mathbf{X}_\alpha) + \alpha U_1(\mathbf{X}_\alpha)$, in which $\mathbf{X}$ is replaced by the running operator $\mathbf{X}_\alpha$. Using the hermiticity of $\mathcal{A}_\alpha^\mathbf{X}$, so that one has $\mathcal{A}_\alpha^\mathbf{X} = \left(\mathcal{A}_\alpha^\mathbf{X} + (\mathcal{A}_\alpha^\mathbf{X})^\dagger \right) / 2$ we can expand $\mathcal{A}_\alpha^\mathbf{X}$ as :

$$\mathcal{A}_\alpha^\mathbf{X} = \left(\frac{1}{2} ([1 + \alpha U_1(\mathbf{X}_\alpha)] U_0(\mathbf{X}_\alpha)) \frac{\mathbf{X}_\alpha}{\alpha} (U_0^\dagger(\mathbf{X}_\alpha) [1 + \alpha U_1^\dagger(\mathbf{X}_\alpha)]) + \frac{1}{2} H.C. \right) - \frac{\mathbf{X}_\alpha}{\alpha}$$

(the $\frac{1}{\alpha}$ factor reminds that in our definition of $\mathcal{A}_\alpha^\mathbf{X}$ the gradient with respect to $\mathbf{X}_\alpha$ is normalized, i.e. divided by α). After some recombinations, the previous expression can be written in a more convenient form :

$$\begin{aligned} \mathcal{A}_\alpha^\mathbf{X} &= \frac{1}{2\alpha} U_0(\mathbf{X}_\alpha) [\mathbf{X}_\alpha, U_0^\dagger(\mathbf{X}_\alpha)] + H.C. \\ &+ \frac{1}{2} [U_1(\mathbf{X}_\alpha) [U_0(\mathbf{X}_\alpha) \mathbf{X}_\alpha U_0^\dagger(\mathbf{X}_\alpha)] + [U_0(\mathbf{X}_\alpha) \mathbf{X}_\alpha U_0^\dagger(\mathbf{X}_\alpha)] U_1^\dagger(\mathbf{X}_\alpha)] + H.C. - \mathbf{X}_\alpha \end{aligned}$$

using now the fact that at the lowest order $U_0(\mathbf{X}_\alpha) \left[\frac{\mathbf{X}_\alpha}{\alpha}, U_0^\dagger(\mathbf{X}_\alpha) \right] = \mathcal{A}_0^\mathbf{X}(\mathbf{X}_\alpha)$, one has :

$$\begin{aligned} \mathcal{A}_\alpha^\mathbf{X} &= \frac{1}{2\alpha} [U_0(\mathbf{X}_\alpha) [\mathbf{X}_\alpha, U_0^\dagger(\mathbf{X}_\alpha)] + H.C.] \\ &+ \frac{1}{2} \left[\alpha U_1(\mathbf{X}_\alpha) \mathcal{A}_0^\mathbf{X}(\mathbf{X}_\alpha) + \alpha \mathcal{A}_0^\mathbf{X}(\mathbf{X}_\alpha) U_1^\dagger(\mathbf{X}_\alpha) + \frac{1}{2} [\mathbf{X}_\alpha, U_1^\dagger(\mathbf{X}_\alpha)] + H.C. \right] \end{aligned}$$

decomposing $U_1^\dagger(\mathbf{X}_\alpha)$ into Hermitian and anti-Hermitian part we are thus led to :

$$\begin{aligned} \mathcal{A}_\alpha^\mathbf{X} &= \frac{1}{2\alpha} (U_0(\mathbf{X}_\alpha) [\mathbf{X}_\alpha, U_0^\dagger(\mathbf{X}_\alpha)] + H.C.) + [\mathbf{X}_\alpha + \alpha \mathcal{A}_0^\mathbf{X}, ahr(U_1^\dagger(\mathbf{X}_\alpha))] \\ &+ \frac{\alpha}{2} (\mathcal{A}_0^\mathbf{X} hr(U_1^\dagger(\mathbf{X}_\alpha)) + hr(U_1^\dagger(\mathbf{X}_\alpha)) \mathcal{A}_0^\mathbf{X}) \end{aligned} \quad (79)$$

where $ahr(Z)$ and $hr(Z)$ denote the anti-Hermitian and Hermitian part of an operator Z respectively. Now using Eq. (42), we are led to the following expressions :

$$[\mathbf{X}_\alpha + \alpha \mathcal{A}_0^\mathbf{X}, ahr(U_1^\dagger(\mathbf{X}_\alpha))] = [B_\alpha, \mathbf{X}_\alpha + \alpha \mathcal{A}_0^\mathbf{X}]$$

and

$$\begin{aligned} &\frac{\alpha}{2} (\mathcal{A}_0^\mathbf{X} hr(U_1^\dagger(\mathbf{X}_\alpha)) + hr(U_1^\dagger(\mathbf{X}_\alpha)) \mathcal{A}_0^\mathbf{X}) + H.C. \\ &= \alpha (\mathcal{A}_0^\mathbf{X} hr(U_1^\dagger(\mathbf{X}_\alpha)) + hr(U_1^\dagger(\mathbf{X}_\alpha)) \mathcal{A}_0^\mathbf{X}) \\ &= -\frac{i}{4} \mathcal{A}_0^\mathbf{X} [\mathcal{A}_0^{R_l}, \mathcal{A}_0^{P_l}] + H.C. \end{aligned}$$

with B_α given by the following relation

$$\begin{aligned}
B_\alpha &= -[\cdot, \varepsilon_0(\mathbf{X}_\alpha)]^{-1} \cdot \left(\mathcal{P}_- \left\{ \frac{1}{2} \mathcal{A}_0^{R\alpha l} \nabla_{R\alpha l} \varepsilon_0(\mathbf{X}_\alpha) + \frac{1}{2} \mathcal{A}_0^{P\alpha l} \nabla_{P\alpha l} \varepsilon_0(\mathbf{X}_\alpha) + H.C. \right\} \right. \\
&\quad \left. - \frac{i}{4} \left\{ [\varepsilon_0(\mathbf{X}_\alpha), \mathcal{A}_0^{R\alpha l}] \mathcal{A}_0^{P\alpha l} - [\varepsilon_0(\mathbf{X}_\alpha), \mathcal{A}_0^{P\alpha l}] \mathcal{A}_0^{R\alpha l} + H.C. \right\} \right) \\
&= -[\cdot, \varepsilon_0(\mathbf{X}_\alpha)]^{-1} \cdot \left(\mathcal{P}_- \left\{ \frac{1}{2} \mathcal{A}_0^{R\alpha l} \nabla_{R\alpha l} \varepsilon_0(\mathbf{X}_\alpha) + \frac{1}{2} \mathcal{A}_0^{P\alpha l} \nabla_{P\alpha l} \varepsilon_0(\mathbf{X}_\alpha) + H.C. \right\} \right) \\
&\quad + \frac{i}{4} \left\{ \mathcal{P}_- \mathcal{A}_0^{R\alpha l} \mathcal{P}_+ \mathcal{A}_0^{P\alpha l} - \mathcal{P}_- \mathcal{A}_0^{P\alpha l} \mathcal{P}_+ \mathcal{A}_0^{R\alpha l} + H.C. \right\} \tag{80}
\end{aligned}$$

Note that given our previous notations, we can write:

$$B_\alpha = -[\cdot, \varepsilon_0(\mathbf{X}_\alpha)]^{-1} \cdot \{(\mathcal{D}_{\mathbf{X}_\alpha} \varepsilon_0(\mathbf{X}_\alpha)) \mathcal{A}_0^{\mathbf{X}_\alpha} + H.C.\}$$

The two last expressions will allow to rewrite $\mathcal{A}_\alpha^{\mathbf{X}}$: To do so, we need to express carefully $\frac{1}{2\alpha} [U_0(\mathbf{X}_\alpha) [\mathbf{X}_\alpha, U_0^+(\mathbf{X}_\alpha)] + H.C.]$.

Actually, given our choice of symmetrization, at the second order this term is not equal to $\mathcal{A}_0^{\mathbf{X}}$ but also includes some second order corrections to symmetrize properly the product $U_0(\mathbf{X}_\alpha) \times [\mathbf{X}_\alpha, U_0^+(\mathbf{X}_\alpha)]$ (see [10] for this fact). Moving powers of $\mathbf{P}_\alpha$ and $\mathbf{R}_\alpha$ on the left or on the right yields:

$$\begin{aligned}
&\frac{1}{2\alpha} (U_0(\mathbf{X}_\alpha) [\mathbf{X}_\alpha, U_0^+(\mathbf{X}_\alpha)] + H.C.) \\
&= \mathcal{A}_0^{\mathbf{X}} + \frac{i}{4\alpha} \nabla_{R\alpha l} U_0(\mathbf{X}_\alpha) \nabla_{P\alpha l} ([\mathbf{X}_\alpha, U_0^+(\mathbf{X}_\alpha)]) - \frac{i}{4\alpha} \nabla_{P\alpha l} U_0(\mathbf{X}_\alpha) \nabla_{R\alpha l} ([\mathbf{X}_\alpha, U_0^+(\mathbf{X}_\alpha)]) + H.C. \\
&= \mathcal{A}_0^{\mathbf{X}} + \frac{1}{4\alpha} \mathcal{A}_0^{P\alpha l} U_0(\mathbf{X}_\alpha) \nabla_{P\alpha l} ([\mathbf{X}_\alpha, U_0^+(\mathbf{X}_\alpha)]) + \frac{1}{4\alpha} \mathcal{A}_0^{R\alpha l} U_0(\mathbf{X}_\alpha) \nabla_{R\alpha l} ([\mathbf{X}_\alpha, U_0^+(\mathbf{X}_\alpha)]) \\
&= \mathcal{A}_0^{\mathbf{X}} + \frac{\alpha}{4} \left(\mathcal{A}_0^{R\alpha l} U_0(\mathbf{X}_\alpha) \nabla_{R\alpha l} \mathcal{A}_0^{\mathbf{X}} + \mathcal{A}_0^{P\alpha l} U_0(\mathbf{X}_\alpha) \nabla_{P\alpha l} \mathcal{A}_0^{\mathbf{X}_\alpha} + H.C. \right) \\
&\quad - \frac{1}{4\alpha} \mathcal{A}_0^{P\alpha l} (\nabla_{P\alpha l} U_0(\mathbf{X}_\alpha)) ([\mathbf{X}_\alpha, U_0^+(\mathbf{X}_\alpha)]) - \frac{1}{4\alpha} \mathcal{A}_0^{R\alpha l} (\nabla_{R\alpha l} U_0(\mathbf{X}_\alpha)) ([\mathbf{X}_\alpha, U_0^+(\mathbf{X}_\alpha)]) + H.C. \\
&= \mathcal{A}_0^{\mathbf{X}} + \frac{\alpha}{4} \left(\mathcal{A}_0^{R\alpha l} \nabla_{R\alpha l} \mathcal{A}_0^{\mathbf{X}} + \mathcal{A}_0^{P\alpha l} \nabla_{P\alpha l} \mathcal{A}_0^{\mathbf{X}_\alpha} + H.C. \right) \\
&\quad - \frac{i}{4} \mathcal{A}_0^{P\alpha l} \mathcal{A}_0^{R\alpha l} \mathcal{A}_0^{\mathbf{X}} + \frac{i}{4} \mathcal{A}_0^{R\alpha l} \mathcal{A}_0^{P\alpha l} \mathcal{A}_0^{\mathbf{X}} + H.C. \\
&= \mathcal{A}_0^{\mathbf{X}} + \frac{\alpha}{4} \left(\mathcal{A}_0^{R\alpha l} \nabla_{R\alpha l} \mathcal{A}_0^{\mathbf{X}} + \mathcal{A}_0^{P\alpha l} \nabla_{P\alpha l} \mathcal{A}_0^{\mathbf{X}_\alpha} + H.C. \right) + \left(\frac{i}{4} \mathcal{A}_0^{\mathbf{X}} [\mathcal{A}_0^{Rl}, \mathcal{A}_0^{Pl}] + H.C. \right)
\end{aligned}$$

And as consequence, we can regroup the various terms of Eq. (79), to obtain ultimately :

$$\mathcal{A}_\alpha^{\mathbf{X}} = \mathcal{A}_0^{\mathbf{X}_\alpha} \left(\mathbf{R}_\alpha + \frac{\alpha}{2} \mathcal{A}_0^{R\alpha}, \mathbf{P}_\alpha + \frac{\alpha}{2} \mathcal{A}_0^{P\alpha} \right) + [B_\alpha, \mathbf{X}_\alpha + \alpha \mathcal{A}_0^{\mathbf{X}_\alpha}]$$

where we introduced the notations

$$\mathcal{A}_0^{\mathbf{X}_\alpha} \left(\mathbf{R}_\alpha + \frac{\alpha}{2} \mathcal{A}_0^{R\alpha}, \mathbf{P}_\alpha + \frac{\alpha}{2} \mathcal{A}_0^{P\alpha} \right) \equiv \mathcal{A}_0^{\mathbf{X}_\alpha} + \frac{\alpha}{4} \left\{ \mathcal{A}_0^{R\alpha l} \nabla_{R\alpha l} \mathcal{A}_0^{\mathbf{X}_\alpha} + \mathcal{A}_0^{P\alpha l} \nabla_{P\alpha l} \mathcal{A}_0^{\mathbf{X}_\alpha} + H.C. \right\}$$

2. Hamiltonian diagonalization at the second order

We can now turn to the expression of the diagonalized Hamiltonian. Focusing first on the double integral term :

$$\begin{aligned}
& \int_0^{\hbar} \int_0^{\alpha_1} S_{\mathbf{X}_h} [O_{\alpha_1} S_{\mathbf{X}_{\alpha_1}} [O_{\alpha_2} \varepsilon_0 (\mathbf{X}_{\alpha_2})]] d\alpha_2 d\alpha_1 - \frac{\hbar}{2} \langle \varepsilon_0 (\mathbf{X}) \rangle \\
&= \int_0^{\hbar} \int_0^{\alpha_1} S_{\mathbf{X}_h} \left[O_{\alpha_1} S_{\mathbf{X}_{\alpha_1}} \left[\frac{\alpha_2}{2} \mathcal{P}_+ \left[(\mathcal{D}_{\mathbf{X}_{\alpha_2}} \varepsilon_0 (\mathbf{X}_{\alpha_2})) \mathcal{A}_0^{\mathbf{X}_{\alpha_2}} + H.C. \right] \right] \right] d\alpha_2 d\alpha_1 - \frac{\hbar}{2} \langle \varepsilon_0 (\mathbf{X}) \rangle \\
&= \int_0^{\hbar} \int_0^{\alpha_1} \frac{S_{\mathbf{X}_h}}{2} \mathcal{P}_+ \left\{ \left(\mathcal{D}_{\mathbf{X}_{\alpha_1}} \left(\frac{1}{2} S_{\mathbf{X}_{\alpha_1}} \mathcal{P}_+ \left[(\mathcal{D}_{\mathbf{X}_{\alpha_2}} \varepsilon_0 (\mathbf{X}_{\alpha_2})) \mathcal{A}_0^{\mathbf{X}_{\alpha_2}} + H.C. \right] \right) \right) \mathcal{A}_0^{\mathbf{X}_{\alpha_1}} + H.C. \right\} \alpha_2 d\alpha_2 d\alpha_1 \\
&\quad - \frac{\hbar}{2} \langle \varepsilon_0 (\mathbf{X}) \rangle
\end{aligned}$$

due to the action of the shift operators, $\mathbf{X}_{\alpha_1}$ and $\mathbf{X}_{\alpha_2}$ are shifted to $\mathbf{X}_h = \mathbf{X}$ at that order.

As a consequence,

$$\begin{aligned}
& \int_0^{\hbar} \int_0^{\alpha_1} S_{\mathbf{X}_h} [O_{\alpha_1} S_{\mathbf{X}_{\alpha_1}} [O_{\alpha_2} \varepsilon_0 (\mathbf{X}_{\alpha_2})]] d\alpha_2 d\alpha_1 - \frac{\hbar}{2} \langle \varepsilon_0 (\mathbf{X}) \rangle \\
&= \int_0^{\hbar} \int_0^{\alpha_1} \frac{\alpha_2}{4} d\alpha_2 d\alpha_1 [\mathcal{P}_+ \{ (\mathcal{D}_{\mathbf{X}} [\mathcal{P}_+ [(\mathcal{D}_{\mathbf{X}} \varepsilon_0 (\mathbf{X})) \mathcal{A}_0^{\mathbf{X}} + H.C.]]) \mathcal{A}_0^{\mathbf{X}} \} + H.C.] - \frac{\hbar}{2} \langle \varepsilon_0 (\mathbf{X}) \rangle \\
&= \frac{\hbar^2}{8} [\mathcal{P}_+ \{ (\mathcal{D}_{\mathbf{X}} [\mathcal{P}_+ [(\mathcal{D}_{\mathbf{X}} \varepsilon_0 (\mathbf{X})) \mathcal{A}_0^{\mathbf{X}} + H.C.]]) \mathcal{A}_0^{\mathbf{X}} \} + H.C.] - \frac{\hbar}{2} \langle \varepsilon_0 (\mathbf{X}) \rangle
\end{aligned}$$

We can now turn to the determination of the single integral term. For the sake of simplicity, we consider the case $[U_{\alpha} ((\frac{\partial}{\partial \alpha} + \langle \cdot \rangle) H(\mathbf{X}_{\alpha})) U_{\alpha}^+] = 0$, which is in fact satisfied in the usual examples of interest..

$$\begin{aligned}
& \int_0^{\hbar} S_{\mathbf{X}_h} [O_{\alpha} \varepsilon_0 (\mathbf{X}_{\alpha})] d\alpha \\
&= \int_0^{\hbar} S_{\mathbf{X}_h} \mathcal{P}_+ \left\{ \frac{1}{2} (\mathcal{A}_{\alpha}^{R_l} \nabla_{R_l} \varepsilon_0 (\mathbf{X}_{\alpha}) + \nabla_{R_l} \varepsilon_0 (\mathbf{X}_{\alpha}) \mathcal{A}_{\alpha}^{R_l} + \mathcal{A}_{\alpha}^{P_l} \nabla_{P_l} \varepsilon_0 (\mathbf{X}_{\alpha}) + \nabla_{P_l} \varepsilon_0 (\mathbf{X}_{\alpha}) \mathcal{A}_{\alpha}^{P_l}) \right\} d\alpha \\
&+ \int_0^{\hbar} S_{\mathbf{X}_h} \mathcal{P}_+ \left\{ \frac{i}{4} [\varepsilon_0 (\mathbf{X}_{\alpha}), \mathcal{A}_{\alpha}^{R_l}] \mathcal{A}_{\alpha}^{P_l} - \frac{i}{4} [\varepsilon_0 (\mathbf{X}_{\alpha}), \mathcal{A}_{\alpha}^{P_l}] \mathcal{A}_{\alpha}^{R_l} + H.C. \right\} d\alpha
\end{aligned}$$

Introduce now the correction to the covariant derivatives at this order: $\hat{\mathcal{D}}_{\mathbf{X}_{\alpha}} \equiv (\hat{\mathcal{D}}_{\mathbf{R}_{\alpha}}, \hat{\mathcal{D}}_{\mathbf{P}_{\alpha}})$ with

$$\begin{aligned}
\hat{\mathcal{D}}_{\mathbf{R}_{\alpha}} &= \left[\nabla_{\mathbf{R}_{\alpha}} + \frac{i}{2} \mathcal{A}_{\alpha}^{\mathbf{P}}, \cdot \right] \\
\hat{\mathcal{D}}_{\mathbf{P}_{\alpha}} &= \left[\nabla_{\mathbf{P}_{\alpha}} - \frac{i}{2} \mathcal{A}_{\alpha}^{\mathbf{R}}, \cdot \right]
\end{aligned}$$

Then, one can write :

$$\int_0^{\hbar} S_{\mathbf{X}_h} [O_{\alpha} \varepsilon_0 (\mathbf{X}_{\alpha})] d\alpha = \int_0^{\hbar} S_{\mathbf{X}_h} \left[\frac{1}{2} \mathcal{P}_+ \left[\left(\hat{\mathcal{D}}_{\mathbf{X}_{\alpha}} \varepsilon_0 (\mathbf{X}_{\alpha}) \right) \mathcal{A}_{\alpha}^{\mathbf{X}} + H.C. \right] \right] d\alpha$$

which can be expanded as :

$$\begin{aligned} & \int_0^{\hbar} S_{\mathbf{X}_h} [O_{\alpha} \varepsilon_0 (\mathbf{X}_{\alpha})] d\alpha \\ &= \frac{1}{2} \int_0^{\hbar} S_{\mathbf{X}_h} [\mathcal{P}_+ [(\mathcal{D}_{\mathbf{X}_{\alpha}} \varepsilon_0 (\mathbf{X}_{\alpha})) \mathcal{A}_0^{\mathbf{X}_{\alpha}} + H.C.]] d\alpha \\ &+ \frac{1}{2} \int_0^{\hbar} S_{\mathbf{X}_h} \mathcal{P}_+ \left(\left(\frac{\alpha}{4} \mathcal{A}_0^{X_{\alpha l}} \nabla_{X_{\alpha l}} \mathcal{A}_0^{X_{\alpha j}} + H.C. + \left[B_{\alpha}, X_{\alpha j} + \alpha \mathcal{A}_0^{X_{\alpha j}} \right] \right) \nabla_{X_{\alpha j}} \varepsilon_0 (\mathbf{X}_{\alpha}) + H.C. \right) d\alpha \\ &+ \frac{i}{2} \int_0^{\hbar} S_{\mathbf{X}_h} \mathcal{P}_+ \left(\left[\varepsilon_0 (\mathbf{X}_{\alpha}), \frac{\alpha}{4} \mathcal{A}_0^{X_{\alpha l}} \nabla_{X_{\alpha l}} \mathcal{A}_0^{\mathbf{R}_{\alpha}} + H.C. + \left[B_{\alpha}, \mathbf{R}_{\alpha} + \alpha \mathcal{A}_0^{\mathbf{R}_{\alpha}} \right] \right] \mathcal{A}_0^{\mathbf{P}_{\alpha}} + H.C. \right) d\alpha \\ &- \frac{i}{2} \int_0^{\hbar} S_{\mathbf{X}_h} \mathcal{P}_+ \left(\left[\varepsilon_0 (\mathbf{X}_{\alpha}), \frac{\alpha}{4} \mathcal{A}_0^{X_{\alpha l}} \nabla_{X_{\alpha l}} \mathcal{A}_0^{\mathbf{P}_{\alpha}} + H.C. + \left[B_{\alpha}, \mathbf{P}_{\alpha} + \alpha \mathcal{A}_0^{\mathbf{P}_{\alpha}} \right] \right] \mathcal{A}_0^{\mathbf{R}_{\alpha}} + H.C. \right) d\alpha \\ &= \frac{\hbar}{2} \mathcal{P}_+ [(\mathcal{D}_{\mathbf{X}} \varepsilon_0 (\mathbf{X})) \mathcal{A}_0^{\mathbf{X}} + H.C.] \\ &+ \frac{\hbar^2}{4} \mathcal{P}_+ \left(\left(\frac{1}{4} \mathcal{A}_0^{X_l} \nabla_{X_l} \mathcal{A}_0^{X_i} + H.C. + \left[B, \frac{X_{\alpha j}}{\hbar} + \mathcal{A}_0^{X_{\alpha j}} \right] \right) \nabla_{X_j} \varepsilon_0 (\mathbf{X}) + H.C. \right) \\ &+ i \frac{\hbar^2}{4} \mathcal{P}_+ \left\{ \left(\varepsilon_0 (\mathbf{X}), \frac{1}{4} \mathcal{A}_0^{X_l} \nabla_{X_l} \mathcal{A}_0^{\mathbf{R}} + H.C. + \left[B, \frac{\mathbf{R}}{\hbar} + \mathcal{A}_0^{\mathbf{R}} \right] \right) \mathcal{A}_0^{\mathbf{P}} + H.C. \right\} \\ &- i \frac{\hbar^2}{4} \mathcal{P}_+ \left\{ \left(\varepsilon_0 (\mathbf{X}_{\alpha}), \mathcal{A}_0^{X_{\alpha l}} \nabla_{X_{\alpha l}} \mathcal{A}_0^{\mathbf{P}} + H.C. + \left[B, \frac{\mathbf{P}}{\hbar} + \mathcal{A}_0^{\mathbf{P}} \right] \right) \mathcal{A}_0^{\mathbf{R}} + H.C. \right\} \\ &= \frac{\hbar}{2} \mathcal{P}_+ \left[\left(\tilde{\mathcal{D}}_{\mathbf{X}} \varepsilon_0 (\mathbf{X}) \right) \mathcal{A}^{\mathbf{X}} + H.C. \right] \end{aligned} \tag{81}$$

with $B \equiv B_h$ and

$$\mathcal{A}^{\mathbf{X}} = \mathcal{A}_0^{\mathbf{X}} + \frac{\hbar}{4} \left(\frac{1}{2} \mathcal{A}_0^{X_l} \nabla_{X_l} \mathcal{A}_0^{\mathbf{X}} + \left[B, \frac{\mathbf{X}}{\hbar} + \mathcal{A}_0^{\mathbf{X}} \right] + H.C. \right) \tag{82}$$

We also introduced the notation $\tilde{\mathcal{D}}_{\mathbf{X}} \equiv (\tilde{\mathcal{D}}_{\mathbf{R}}, \tilde{\mathcal{D}}_{\mathbf{P}})$ with

$$\begin{aligned} \tilde{\mathcal{D}}_{\mathbf{R}} &= \left[\nabla_{\mathbf{R}_{\alpha}} + \frac{i}{2} \mathcal{A}^{\mathbf{P}}, \cdot \right] \\ \hat{\mathcal{D}}_{\mathbf{P}} &= \left[\nabla_{\mathbf{P}_{\alpha}} - \frac{i}{2} \mathcal{A}^{\mathbf{R}}, \cdot \right] \end{aligned}$$

Ultimately, one can gather the various terms to obtain the energy at the second order in $\hbar$ as a function of the canonical variables

$$\begin{aligned} \varepsilon (\mathbf{X}) &= \varepsilon_0 (\mathbf{X}) + \frac{\hbar}{2} \mathcal{P}_+ \left[\left(\hat{\mathcal{D}}_{\mathbf{X}} \varepsilon_0 (\mathbf{X}) \right) \mathcal{A}^{\mathbf{X}} + H.C. \right] \\ &+ \frac{\hbar^2}{8} [\mathcal{P}_+ \{ (\mathcal{D}_{\mathbf{X}} [\mathcal{P}_+ [(\mathcal{D}_{\mathbf{X}} \varepsilon_0 (\mathbf{X})) \mathcal{A}_0^{\mathbf{X}} + H.C.]] \mathcal{A}_0^{\mathbf{X}} \} + H.C.] - \frac{\hbar}{2} \langle \varepsilon_0 (\mathbf{X}) \rangle \end{aligned}$$

This formula is still compact and can be, for practical purposes, expanded in several ways. We first start by developing $\varepsilon(\mathbf{X})$ as a function of the zeroth order diagonalization data, that is $\varepsilon_0(\mathbf{X})$ and $\mathcal{A}_0^{\mathbf{X}}$. Starting first by expanding $\mathcal{A}^{\mathbf{X}}$, we are led to :

$$\begin{aligned} \varepsilon(\mathbf{X}) = & \varepsilon_0(\mathbf{X}) + \frac{\hbar}{2} \mathcal{P}_+ [\mathcal{D}_{\mathbf{X}} \varepsilon_0 \mathcal{A}_0^{\mathbf{X}} + H.C.] + \frac{\hbar^2}{8} [\mathcal{P}_+ \{ (\mathcal{D}_{\mathbf{X}} [[\mathcal{D}_{\mathbf{X}} \varepsilon_0 \mathcal{A}_0^{\mathbf{X}} + H.C.]]) \mathcal{A}_0^{\mathbf{X}} \} + H.C.] \\ & + \frac{\hbar^2}{4} \mathcal{P}_+ \left(\left(\frac{1}{4} \mathcal{A}_0^{X_l} \nabla_{X_l} \mathcal{A}_0^{X_i} + H.C. + [B, \mathcal{A}_0^{X_{\alpha j}}] \right) \nabla_{X_j} \varepsilon_0 + H.C. \right) \\ & + i \frac{\hbar^2}{4} \mathcal{P}_+ \left\{ \left[\varepsilon_0, \frac{1}{4} \mathcal{A}_0^{X_l} \nabla_{X_{\alpha l}} \mathcal{A}_0^{\mathbf{R}} + H.C. \right] \mathcal{A}_0^{\mathbf{P}} - \left[\varepsilon_0, \frac{1}{4} \mathcal{A}_0^{X_{\alpha l}} \nabla_{X_{\alpha l}} \mathcal{A}_0^{\mathbf{P}} + H.C. \right] \mathcal{A}_0^{\mathbf{R}} + H.C. \right\} \\ & + i \frac{\hbar^2}{4} \mathcal{P}_+ \left\{ \left[\varepsilon_0, \left[B, \frac{\mathbf{R}}{\hbar} + \mathcal{A}_0^{\mathbf{R}} \right] \right] \mathcal{A}_0^{\mathbf{P}} - \left[\varepsilon_0, \left[B, \frac{\mathbf{P}}{\hbar} + \mathcal{A}_0^{\mathbf{P}} \right] \right] \mathcal{A}_0^{\mathbf{R}} + H.C. \right\} \end{aligned} \quad (83)$$

Or, if we expand B fully,

$$\begin{aligned} \varepsilon(\mathbf{X}) = & \varepsilon_0(\mathbf{X}) + \frac{\hbar}{2} \mathcal{P}_+ \left[(\mathcal{A}_0^{\mathbf{X}} \nabla_{\mathbf{X}} \varepsilon_0(\mathbf{X})) + \frac{i}{2} [\varepsilon_0(\mathbf{X}), \mathcal{A}_0^{R_l}] \mathcal{A}_0^{P_l} - \frac{i}{2} [\varepsilon_0(\mathbf{X}), \mathcal{A}_0^{P_l}] \mathcal{A}_0^{R_l} + H.C. \right] \\ & + \frac{\hbar^2}{8} \mathcal{P}_+ \left\{ \left[\mathcal{A}_0^{\mathbf{X}} \nabla_{\mathbf{X}} \mathcal{P}_+ \left(\mathcal{A}_0^{\mathbf{X}} \nabla_{\mathbf{X}} \varepsilon_0(\mathbf{X}) + i [\varepsilon_0(\mathbf{X}), \mathcal{A}_0^{R_l}] \mathcal{A}_0^{P_l} + H.C. \right) \right] + H.C. \right\} \\ & + i \frac{\hbar^2}{8} \mathcal{P}_+ \left\{ \left[\mathcal{P}_+ \left((\mathcal{A}_0^{\mathbf{X}} \nabla_{\mathbf{X}} \varepsilon_0(\mathbf{X})) + i [\varepsilon_0(\mathbf{X}), \mathcal{A}_0^{R_l}] \mathcal{A}_0^{P_l} + H.C. \right), \mathcal{A}_0^{R_l} \right] \mathcal{A}_0^{P_l} \right\} \\ & - i \frac{\hbar^2}{8} \mathcal{P}_+ \left\{ \left[\mathcal{P}_+ \left((\mathcal{A}_0^{\mathbf{X}} \nabla_{\mathbf{X}} \varepsilon_0(\mathbf{X})) + i [\varepsilon_0(\mathbf{X}), \mathcal{A}_0^{R_l}] \mathcal{A}_0^{P_l} + H.C. \right), \mathcal{A}_0^{P_l} \right] \mathcal{A}_0^{R_l} \right\} \\ & + \frac{\hbar^2}{4} \mathcal{P}_+ \left(\left(\frac{1}{4} \mathcal{A}_0^{X_l} \nabla_{X_l} \mathcal{A}_0^{X_i} + H.C. + [\varepsilon_0, \cdot]^{-1} \left[\mathcal{A}_0^{\mathbf{X}} \nabla_{\mathbf{X}} \varepsilon_0 + i [\varepsilon_0, \mathcal{A}_0^{R_l}] \mathcal{A}_0^{P_l} + H.C. \right] \right) \nabla_{X_j} \varepsilon_0 + H.C. \right) \\ & + \frac{i \hbar^2}{4} \mathcal{P}_+ \left\{ \left[\varepsilon_0, \frac{1}{4} \mathcal{A}_0^{X_l} \nabla_{X_{\alpha l}} \mathcal{A}_0^{\mathbf{R}} + H.C. \right] \mathcal{A}_0^{\mathbf{P}} - \left[\varepsilon_0, \frac{1}{4} \mathcal{A}_0^{X_{\alpha l}} \nabla_{X_{\alpha l}} \mathcal{A}_0^{\mathbf{P}} + H.C. \right] \mathcal{A}_0^{\mathbf{R}} + H.C. \right\} \\ & - \frac{i \hbar^2}{4} \mathcal{P}_+ \left\{ \left[\varepsilon_0, \left[i \nabla_{\mathbf{P}} + \mathcal{A}_0^{\mathbf{R}}, [\varepsilon_0, \cdot]^{-1} \left[\mathcal{A}_0^{\mathbf{X}} \nabla_{\mathbf{X}} \varepsilon_0 + i [\varepsilon_0, \mathcal{A}_0^{R_l}] \mathcal{A}_0^{P_l} + H.C. \right] \right] \right] \mathcal{A}_0^{\mathbf{P}} + H.C. \right\} \\ & + \frac{i \hbar^2}{4} \mathcal{P}_+ \left\{ \left[\varepsilon_0, \left[-i \nabla_{\mathbf{R}} + \mathcal{A}_0^{\mathbf{P}}, [\varepsilon_0, \cdot]^{-1} \left[\mathcal{A}_0^{\mathbf{X}} \nabla_{\mathbf{X}} \varepsilon_0 + i [\varepsilon_0, \mathcal{A}_0^{R_l}] \mathcal{A}_0^{P_l} + H.C. \right] \right] \right] \mathcal{A}_0^{\mathbf{R}} + H.C. \right\} \end{aligned} \quad (84)$$

The last expansion is useful for practical purpose, since it yields directly the $\hbar$ expansion for the diagonalized Hamiltonian. However, it seems more elegant and relevant to rewrite $\varepsilon(\mathbf{X})$ as a function of the covariant variables $\mathbf{x} = (\mathbf{r}, \mathbf{p})$ defined in the preceding section. Note first that the Berry phases Eq. 82, $\mathcal{A}^{\mathbf{X}} = (\mathcal{A}^{\mathbf{R}}(\mathbf{X}), \mathcal{A}^{\mathbf{P}}(\mathbf{X}))$ with $\mathcal{A}^{\mathbf{X}} = \mathcal{A}_0^{\mathbf{X}} + \frac{\hbar}{4} \left(\mathcal{A}_0^{X_l} \nabla_{X_l} \mathcal{A}_0^{\mathbf{X}} + [B, \mathbf{X} + \mathcal{A}_0^{\mathbf{X}}] + H.C. \right)$, satisfy, by construction :

$$\begin{aligned} \mathcal{A}^{R_l}(\mathbf{X}) &= \frac{1}{\hbar} \int_{\alpha}^{\hbar} S_{\mathbf{X}_h} \mathcal{A}_{\alpha}^{R_l} d\alpha \\ \mathcal{A}^{P_l}(\mathbf{X}) &= \frac{1}{\hbar} \int_{\alpha}^{\hbar} S_{\mathbf{X}_h} \mathcal{A}_{\alpha}^{P_l} d\alpha \end{aligned}$$

So that, recalling our previous definition of the variables $\mathbf{x} = \mathbf{X} + A^{\mathbf{X}}$ (see Eq. 69), we can write for $\mathbf{r}$,

$$\begin{aligned}
\mathbf{r} &= \mathbf{R} + \int_0^{\hbar} S_{\mathbf{X}_h} \mathcal{P}_+ \mathcal{A}_{\alpha_1}^{\mathbf{R}}(\mathbf{R}, \mathbf{P}) d\alpha_1 + \int_{0 < \alpha < \hbar} S_{\mathbf{X}_h} \frac{1}{2} \left[\left[\mathcal{P}_+ [\mathcal{A}_{\alpha}^{\mathbf{X}}] \cdot \nabla_{\mathbf{X}} \int_{0 < \alpha_1 < \alpha} \mathcal{P}_+ [\mathcal{A}_{\alpha_1}^{\mathbf{R}}] \right] + H.C. \right] d\alpha_1 d\alpha \\
&= \mathbf{R} + \hbar \mathcal{P}_+ \mathcal{A}^{\mathbf{R}}(\mathbf{X}) + \frac{\hbar^2}{4} ((\mathcal{P}_+ \mathcal{A}_0^{\mathbf{R}} \cdot \nabla_{\mathbf{R}}) \mathcal{P}_+ \mathcal{A}_0^{\mathbf{R}} + (\mathcal{P}_+ \mathcal{A}_0^{\mathbf{P}} \cdot \nabla_{\mathbf{P}}) \mathcal{P}_+ \mathcal{A}_0^{\mathbf{R}} + H.C.) \\
&= \mathbf{R} + \hbar \mathcal{P}_+ \mathcal{A}_0^{\mathbf{R}} + \frac{\hbar^2}{4} \mathcal{P}_+ \left(\frac{1}{2} \mathcal{A}_0^{X_l} \nabla_{X_l} \mathcal{A}_0^{\mathbf{R}} + \left[B, \frac{\mathbf{R}}{\hbar} + \mathcal{A}_0^{\mathbf{R}} \right] + H.C. \right) \\
&\quad + \frac{\hbar^2}{4} ((\mathcal{P}_+ \mathcal{A}_0^{\mathbf{R}} \cdot \nabla_{\mathbf{R}}) \mathcal{P}_+ \mathcal{A}_0^{\mathbf{R}} + (\mathcal{P}_+ \mathcal{A}_0^{\mathbf{P}} \cdot \nabla_{\mathbf{P}}) \mathcal{P}_+ \mathcal{A}_0^{\mathbf{R}} + H.C.) \\
&\equiv \mathbf{R} + \hbar A_0^{\mathbf{R}} + \frac{\hbar^2}{2} A_1^{\mathbf{R}}
\end{aligned} \tag{85}$$

For $\mathbf{p}$, we have in the same manner the following expansion

$$\begin{aligned}
\mathbf{p} &= \mathbf{P} + \int_0^{\hbar} S_{\mathbf{X}_h} \mathcal{P}_+ \mathcal{A}_{\alpha_1}^{\mathbf{P}}(\mathbf{R}, \mathbf{P}) d\alpha_1 + \int_{0 < \alpha < \hbar} S_{\mathbf{X}_h} \frac{1}{2} \left[\left[\mathcal{P}_+ [\mathcal{A}_{\alpha}^{\mathbf{X}}] \cdot \nabla_{\mathbf{X}} \int_{0 < \alpha_1 < \alpha} \mathcal{P}_+ [\mathcal{A}_{\alpha_1}^{\mathbf{P}}] \right] + H.C. \right] d\alpha_1 d\alpha \\
&= \mathbf{P} + \hbar \mathcal{P}_+ \mathcal{A}^{\mathbf{P}}(\mathbf{X}) + \frac{\hbar^2}{4} ((\mathcal{P}_+ \mathcal{A}_0^{\mathbf{R}} \cdot \nabla_{\mathbf{R}}) \mathcal{P}_+ \mathcal{A}_0^{\mathbf{P}} + (\mathcal{P}_+ \mathcal{A}_0^{\mathbf{P}} \cdot \nabla_{\mathbf{P}}) \mathcal{P}_+ \mathcal{A}_0^{\mathbf{P}} + H.C.) \\
&= \mathbf{P} + \hbar \mathcal{P}_+ \mathcal{A}_0^{\mathbf{P}} + \frac{\hbar^2}{4} \mathcal{P}_+ \left(\frac{1}{2} \mathcal{A}_0^{X_l} \nabla_{X_l} \mathcal{A}_0^{\mathbf{P}} + \left[B, \frac{\mathbf{P}}{\hbar} + \mathcal{A}_0^{\mathbf{P}} \right] + H.C. \right) \\
&\quad + \frac{\hbar^2}{4} \left(\frac{1}{2} (\mathcal{P}_+ \mathcal{A}_0^{\mathbf{R}} \cdot \nabla_{\mathbf{R}}) \mathcal{P}_+ \mathcal{A}_0^{\mathbf{P}} + (\mathcal{P}_+ \mathcal{A}_0^{\mathbf{P}} \cdot \nabla_{\mathbf{P}}) \mathcal{P}_+ \mathcal{A}_0^{\mathbf{P}} + H.C. \right) \\
&\equiv \mathbf{P} + \hbar A_0^{\mathbf{P}} + \frac{\hbar^2}{2} A_1^{\mathbf{P}}
\end{aligned} \tag{86}$$

As before. $\mathbf{x} = (\mathbf{r}, \mathbf{p})$ satisfy of course an algebra Eq. (74).

Now, come back to the compact form of $\varepsilon(\mathbf{X})$:

$$\begin{aligned}
\varepsilon(\mathbf{X}) &= \varepsilon_0(\mathbf{X}) + \frac{\hbar}{2} \mathcal{P}_+ \left[\left(\hat{\mathcal{D}}_{\mathbf{X}} \varepsilon_0(\mathbf{X}) \right) \mathcal{A}^{\mathbf{X}} + H.C. \right] \\
&\quad + \frac{\hbar^2}{8} \left[\mathcal{P}_+ \left\{ (\mathcal{D}_{\mathbf{X}} [\mathcal{P}_+ [(\mathcal{D}_{\mathbf{X}} \varepsilon_0(\mathbf{X})) \mathcal{A}_0^{\mathbf{X}} + H.C.]]) \mathcal{A}_0^{\mathbf{X}} \right\} + H.C. \right] - \frac{\hbar}{2} \langle \varepsilon_0(\mathbf{X}) \rangle
\end{aligned}$$

expanded as :

$$\begin{aligned}
\varepsilon(\mathbf{X}) = & \varepsilon_0(\mathbf{X}) + \mathcal{P}_+ \left\{ \frac{\hbar}{2} (\mathcal{A}^{X_l} \nabla_{X_l} \varepsilon_0(\mathbf{X}) + \nabla_{X_l} \varepsilon_0(\mathbf{X}) \mathcal{A}^{X_l}) \right\} \\
& + \frac{i\hbar}{4} [\mathcal{P}_+ \{ [\varepsilon_0(\mathbf{X}), \mathcal{A}^{R_l}] \mathcal{A}^{P_l} - [\varepsilon_0(\mathbf{X}), \mathcal{A}^{P_l}] \mathcal{A}^{R_l} \} + H.C.] \\
& + \frac{\hbar^2}{8} \mathcal{P}_+ \left\{ \left[\mathcal{A}_0^{\mathbf{X}} \nabla_{\mathbf{X}} \mathcal{P}_+ \left(\mathcal{A}_0^{\mathbf{X}} \nabla_{\mathbf{X}} \varepsilon_0(\mathbf{X}) + i [\varepsilon_0(\mathbf{X}), \mathcal{A}_0^{R_l}] \mathcal{A}_0^{P_l} + H.C. \right) \right] + H.C. \right\} \\
& + i \frac{\hbar^2}{8} \mathcal{P}_+ \left\{ \left[\mathcal{P}_+ \left((\mathcal{A}_0^{\mathbf{X}} \nabla_{\mathbf{X}} \varepsilon_0(\mathbf{X})) + i [\varepsilon_0(\mathbf{X}), \mathcal{A}_0^{R_l}] \mathcal{A}_0^{P_l} + H.C. \right), \mathcal{A}_0^{R_l} \right] \mathcal{A}_0^{P_l} \right\} \\
& - i \frac{\hbar^2}{8} \mathcal{P}_+ \left\{ \left[\mathcal{P}_+ \left((\mathcal{A}_0^{\mathbf{X}} \nabla_{\mathbf{X}} \varepsilon_0(\mathbf{X})) + i [\varepsilon_0(\mathbf{X}), \mathcal{A}_0^{R_l}] \mathcal{A}_0^{P_l} + H.C. \right), \mathcal{A}_0^{P_l} \right] \mathcal{A}_0^{R_l} \right\}
\end{aligned}$$

To the second order, and given our choice of symmetrization, the contributions

$$\varepsilon_0(\mathbf{X}) + \mathcal{P}_+ \left\{ \frac{\hbar}{2} (\mathcal{A}^{X_l} \nabla_{X_l} \varepsilon_0(\mathbf{X}) + \nabla_{X_l} \varepsilon_0(\mathbf{X}) \mathcal{A}^{X_l}) \right\} + \frac{\hbar^2}{4} \mathcal{P}_+ \{ \mathcal{A}_0^{\mathbf{X}} \nabla_{\mathbf{X}} \mathcal{P}_+ (\mathcal{A}_0^{\mathbf{X}} \nabla_{\mathbf{X}} \varepsilon_0(\mathbf{X})) + H.C. \}$$

can be recombined as :

$$\varepsilon_0 \left(\mathbf{X} + \hbar \mathcal{P}_+ \mathcal{A}^{X_l} + \frac{\hbar^2}{4} ((\mathcal{P}_+ \mathcal{A}_0^{\mathbf{R}} \cdot \nabla_{\mathbf{R}}) \mathcal{P}_+ \mathcal{A}_0^{\mathbf{R}} + (\mathcal{P}_+ \mathcal{A}_0^{\mathbf{P}} \cdot \nabla_{\mathbf{P}}) \mathcal{P}_+ \mathcal{A}_0^{\mathbf{R}} + H.C.) \right) = \varepsilon_0(\mathbf{x})$$

On the other hand, one has also at the same order:

$$\begin{aligned}
& \frac{i\hbar}{4} \mathcal{P}_+ \{ [\varepsilon_0(\mathbf{X}), \mathcal{A}^{R_l}] \mathcal{A}^{P_l} - [\varepsilon_0(\mathbf{X}), \mathcal{A}^{P_l}] \mathcal{A}^{R_l} + H.C. \} \\
& + i \frac{\hbar^2}{8} \mathcal{P}_+ \left\{ \left[\mathcal{A}_0^{\mathbf{X}} \nabla_{\mathbf{X}} \mathcal{P}_+ \left([\varepsilon_0(\mathbf{X}), \mathcal{A}_0^{R_l}] \mathcal{A}_0^{P_l} + H.C. \right) \right] + H.C. \right\} \\
& + i \frac{\hbar^2}{8} \mathcal{P}_+ \left\{ \left[\mathcal{P}_+ ((\mathcal{A}_0^{\mathbf{X}} \nabla_{\mathbf{X}} \varepsilon_0(\mathbf{X})) + H.C.), \mathcal{A}_0^{R_l} \right] \mathcal{A}_0^{P_l} \right\} \\
& - i \frac{\hbar^2}{8} \mathcal{P}_+ \left\{ \left[\mathcal{P}_+ ((\mathcal{A}_0^{\mathbf{X}} \nabla_{\mathbf{X}} \varepsilon_0(\mathbf{X})) + H.C.), \mathcal{A}_0^{P_l} \right] \mathcal{A}_0^{R_l} \right\} \\
& = \frac{i\hbar}{2} \mathcal{P}_+ \left\{ \left[\varepsilon_0(\mathbf{X} + \mathcal{P}_+ \mathcal{A}_0^{\mathbf{X}}), \mathcal{A}^{R_l} \left(X + \frac{\mathcal{P}_+ \mathcal{A}_0^{\mathbf{X}}}{2} \right) \right] \mathcal{A}^{P_l} \left(X + \frac{\mathcal{P}_+ \mathcal{A}_0^{\mathbf{X}}}{2} \right) \right\} \\
& - \frac{i\hbar}{2} \mathcal{P}_+ \left\{ \left[\varepsilon_0(\mathbf{X} + \mathcal{P}_+ \mathcal{A}_0^{\mathbf{X}}), \mathcal{A}^{P_l} \left(X + \frac{\mathcal{P}_+ \mathcal{A}_0^{\mathbf{X}}}{2} \right) \right] \mathcal{A}^{R_l} \left(X + \frac{\mathcal{P}_+ \mathcal{A}_0^{\mathbf{X}}}{2} \right) \right\} \\
& = \frac{i}{2} \hbar \mathcal{P}_+ \left\{ [\varepsilon_0(\mathbf{x}), \hat{\mathcal{A}}^{R_l}] \hat{\mathcal{A}}^{P_l} - [\varepsilon_0(\mathbf{x}), \hat{\mathcal{A}}^{P_l}] \hat{\mathcal{A}}^{R_l} - [\varepsilon_0(\mathbf{x}), [\hat{\mathcal{A}}^{R_l}, \hat{\mathcal{A}}^{P_l}]] \right\}
\end{aligned}$$

where we introduced the notations

$$\begin{aligned}
\hat{\mathcal{A}}^{R_l} &= \frac{1}{2} \left[1 - \frac{1}{2} (\mathcal{P}_+ \mathcal{A}_0^{\mathbf{X}} \cdot \nabla_{\mathbf{X}}) \right] \mathcal{A}^{R_l}(\mathbf{x}) + H.C. \\
\hat{\mathcal{A}}^{P_l} &= \frac{1}{2} \left[1 - \frac{1}{2} (\mathcal{P}_+ \mathcal{A}_0^{\mathbf{X}} \cdot \nabla_{\mathbf{X}}) \right] \mathcal{A}^{P_l}(\mathbf{x}) + H.C.
\end{aligned}$$

Ultimately, the contributions to the Hamiltonian can be recombined to yield :

$$\begin{aligned}
\varepsilon(\mathbf{X}) = & \varepsilon_0(\mathbf{x}) + \frac{i}{4}\hbar\mathcal{P}_+ \left\{ \left[\varepsilon_0(\mathbf{x}), \hat{\mathcal{A}}^{R_l} \right] \hat{\mathcal{A}}^{P_l} - \left[\varepsilon_0(\mathbf{x}), \hat{\mathcal{A}}^{P_l} \right] \hat{\mathcal{A}}^{R_l} - \left[\varepsilon_0(\mathbf{x}), \left[\mathcal{A}_0^{R_l}, \mathcal{A}_0^{P_l} \right] \right] + H.C. \right\} \\
& - \frac{\hbar^2}{8}\mathcal{P}_+ \left\{ \left[\left[\varepsilon_0(\mathbf{x}), \mathcal{A}_0^{R_l} \right] \mathcal{A}_0^{P_l} - \left[\varepsilon_0(\mathbf{x}), \mathcal{A}_0^{P_l} \right] \mathcal{A}_0^{R_l}, \mathcal{A}_0^{R_k} \right] \mathcal{A}_0^{P_k} \right\} \\
& + \frac{\hbar^2}{8}\mathcal{P}_+ \left\{ \left[\left[\varepsilon_0(\mathbf{x}), \mathcal{A}_0^{R_l} \right] \mathcal{A}_0^{P_l} - \left[\varepsilon_0(\mathbf{x}), \mathcal{A}_0^{P_l} \right] \mathcal{A}_0^{R_l}, \mathcal{A}_0^{P_k} \right] \mathcal{A}_0^{R_k} \right\} - \frac{\hbar}{2} \langle \varepsilon_0(\mathbf{x}) \rangle
\end{aligned} \tag{87}$$

Note that in the all Hamiltonian, including the Berry connections A^{R_l} and A^{P_l} , we have replaced the operators $(\mathbf{R}, \mathbf{P})$ by $\mathbf{x} = (\mathbf{r}, \mathbf{p})$ at each order of the expansion.

VII. PHYSICAL APPLICATIONS

A. The Dirac electron in an electric field

To illustrate our general theory we consider the case of a Dirac electron in an external electric field. We will obtain the block diagonal Hamiltonian to the second order in $\hbar$ and will compare with the FW transformation obtained in [19]. Note that contrary to the FW which is not an expansion in $\hbar$, the new method is valid for strong external fields (actually a FW transformation expanded into a power series in $\hbar$ was also recently proposed [20]).

Let consider the following Dirac Hamiltonian ($c = 1$)

$$H_1 = \boldsymbol{\alpha} \cdot \mathbf{P} + \beta m + eV(\mathbf{R})$$

To compute the diagonalized Hamiltonian to the second order in $\hbar$ we first need the zeroth order diagonalization transformation, which is the usual FW transformation for a free particle:

$$U_0 = \frac{E + m + \beta \boldsymbol{\alpha} \mathbf{P}}{\sqrt{2E(E + m)}}$$

where $E = \sqrt{\mathbf{P}^2 + m^2}$. In this case, we have (with $\boldsymbol{\Sigma} = \mathbf{1} \otimes \boldsymbol{\sigma}$)

$$\mathcal{A}_0^R = iU_0 \boldsymbol{\nabla}_{\mathbf{P}} U_0^{-1} = i \frac{-\beta \boldsymbol{\alpha} \cdot \mathbf{P} \mathbf{P} + E(E + m) \beta \boldsymbol{\alpha} - iE \mathbf{P} \times \boldsymbol{\Sigma}}{2E^2(E + m)}$$

$$\mathcal{A}_0^P = -iU_0^i \boldsymbol{\nabla}_{\mathbf{R}} U_0^{-1} = 0$$

which leads to the first order projected Berry connections:

$$A_0^{\mathbf{R}} = \mathcal{P}_+ \mathcal{A}_0^R = \frac{\mathbf{P} \times \boldsymbol{\Sigma}}{2E(E + m)}$$

$$A_0^{\mathbf{P}} = \mathcal{P}_+ \mathcal{A}_0^P = 0$$

The zeroth order diagonalized energy is $\varepsilon_0(\mathbf{R}, \mathbf{P}) = E = \sqrt{\mathbf{P}^2 + m^2}$

Now, to complete the diagonalization process, we need the matrix B Eq. (80) that enters in the definition of the covariant variables:

$$B = \frac{\beta e}{2E} \mathcal{P}_- (\mathcal{A}_0^R) \cdot \nabla_R V$$

From B and Eq.(82) we can then compute the Berry connections to the second order in $\hbar$. Here expressions simplify greatly. Actually, one has :

$$\begin{aligned} \mathcal{A}^R &= \mathcal{A}_0^R + \frac{1}{2} [B, \mathbf{R} + \hbar \mathcal{A}_0^X] \\ &= \hbar \frac{\mathbf{P} \times \Sigma}{2E(E+m)} + \frac{\hbar e}{2} \beta \frac{E^2 \nabla_R V - [\mathbf{P} \cdot \nabla_R V] \mathbf{P}}{4E^5} \\ &\quad + \hbar e \nabla_P \frac{-\alpha \cdot \mathbf{P} \mathbf{P} + E(E+m) \alpha}{8E^3(E+m)} \nabla_R V \\ &\quad + \hbar e \frac{E(E+m) \mathbf{P} \times (\nabla_R V \times \alpha) - (\mathbf{P} \times (\mathbf{P} \times \alpha)) \mathbf{P} \cdot \nabla_R V}{4E^4(E+m)^2} \end{aligned}$$

and

$$\mathcal{A}^P = \frac{1}{2} [B, \mathbf{P}] = i\hbar \frac{\beta e}{4E} (\mathcal{P}_- (\mathcal{A}_0^R) \cdot \nabla_R) \nabla_R V$$

we can also write the dynamical operators as:

$$\mathbf{r} = \mathbf{R} + \hbar \mathcal{P}_+ \mathcal{A}_0^R + \frac{\hbar^2}{2} \mathcal{P}_+ [B, \mathcal{A}_0^R] = \mathbf{R} + \hbar \frac{\mathbf{P} \times \Sigma}{2E(E+m)} + \frac{\hbar^2 e}{2} \beta \frac{E^2 \nabla_R V - [\mathbf{P} \cdot \nabla_R V] \mathbf{P}}{4E^5}$$

and

$$\mathbf{p} = \mathbf{P}$$

Now using expression Eq. (87), we arrive at the following expression for the diagonal representation of the energy operator as a function of the covariant variables $(\mathbf{r}, \mathbf{p})$:

$$\begin{aligned} \varepsilon(\mathbf{X}) &= \varepsilon_0(\mathbf{x}) + \frac{i}{2} \hbar \mathcal{P}_+ \left\{ \left[\varepsilon_0(\mathbf{x}), \hat{\mathcal{A}}^{R_l} \right] \hat{\mathcal{A}}^{P_l} - \left[\varepsilon_0(\mathbf{x}), \hat{\mathcal{A}}^{P_l} \right] \hat{\mathcal{A}}^{R_l} \right\} \\ &= \varepsilon_0(\mathbf{x}) + \frac{i}{2} \hbar \mathcal{P}_+ \left\{ \left[\varepsilon_0(\mathbf{x}), \mathcal{A}_0^{R_l} \right] \mathcal{A}^{P_l} - \left[\varepsilon_0(\mathbf{x}), \mathcal{A}^{P_l} \right] \mathcal{A}_0^{R_l} \right\} \end{aligned}$$

which, once developped, leads to:

$$\varepsilon = \beta \sqrt{\mathbf{p}^2 + m^2} + \frac{\hbar^2 e}{2} \nabla_{\mathbf{r}} \cdot \frac{E^2 \nabla_{\mathbf{r}} V - [\mathbf{p} \cdot \nabla_{\mathbf{r}} V] \mathbf{p}}{4E^4} + eV(\mathbf{r}) \quad (88)$$

Here we have made the choice of fully symmetrizing in $\mathbf{r}$ and $\mathbf{p}$, that is to weight equally all permutations in $\mathbf{r}$ and $\mathbf{p}$ in the series expansions of our expressions. One can now check that

developing the variables $\mathbf{r}$ as a function of the canonical variables $\mathbf{R}$ and $\mathbf{P}$ yields the same expression for the Hamiltonian as in [19] (apart from a small sign mistake for the spin-orbit coupling in that reference)

$$\begin{aligned} \varepsilon = & \beta\sqrt{\mathbf{P}^2 + m^2} + eV(\mathbf{R}) + \hbar \frac{\mathbf{P} \times \boldsymbol{\Sigma}}{2E(E+m)} \cdot \boldsymbol{\nabla}_R V \\ & + \hbar^2 e \beta \frac{E^2 (\boldsymbol{\nabla}_R V)^2 - (\mathbf{P} \cdot \boldsymbol{\nabla}_R V)^2}{8E^5} \\ & + \hbar^2 e \left(\frac{\boldsymbol{\nabla}_R^2 V}{4E(E+m)} - \frac{(2E^2 + 2Em + m^2) (\mathbf{P} \cdot \boldsymbol{\nabla}_R)^2 V}{8E^4 (E+m)^2} \right) \end{aligned} \quad (89)$$

Note that this result can also be found directly by using the expression Eq. (84) for the diagonalized Hamiltonian as a function of the canonical variables. Eq. (88) being fully relativistic, to compare with the usual FW [15] approach we consider the non-relativistic limit and expand our result to second order in $\frac{1}{mc}$. We readily obtain the well known diagonal representation of the positive energy (expressed in coordinates R and P) [15] :

$$\varepsilon = \frac{\mathbf{P}^2}{2m} - \frac{\mathbf{P}^4}{8m^3 c^2} + eV(\mathbf{R}) + \frac{e\hbar}{4m^2 c^2} \boldsymbol{\sigma} \cdot (\boldsymbol{\nabla}_R V \times \mathbf{P}) + \frac{e\hbar^2}{8m^2 c^2} \boldsymbol{\nabla}^2 V \quad (90)$$

with $\boldsymbol{\sigma}$ the Pauli matrices. Note that it is the term order $\hbar^2$ in Eq. (88) which, in the non relativistic limit, leads to the Darwin term.

B. Massless Dirac particle in a static symmetric gravitational field

We consider here the Hamiltonian of a massless neutrino propagating in an isotropic inhomogeneous curved space of metric $g^{ij}(\mathbf{R}) = n^{-1}(\mathbf{R}) \delta^{ij}$. (with the convention $c = 1$)

$$H_0 = \frac{1}{2} (\boldsymbol{\alpha} \cdot \mathbf{P} F(\mathbf{R}) + F(\mathbf{R}) \boldsymbol{\alpha} \cdot \mathbf{P}) \quad (91)$$

with $F(\mathbf{R}) = n^{-1}(\mathbf{R})$.

As for the electron in an electric field, we start by giving the zeroth order diagonalization matrix as well as the effective energy $\varepsilon_0(\mathbf{R}, \mathbf{P})$. Since at that order, $(\mathbf{R}, \mathbf{P})$ can be thought as commuting variables, one finds easily that the Hamiltonian diagonalization is performed through the following Foldy-Wouthuysen unitary matrix :

$$U_0(\mathbf{P}) = \frac{\sqrt{\mathbf{P}^2} + \beta \boldsymbol{\alpha} \cdot \mathbf{P}}{\sqrt{2\mathbf{P}^2}} \quad (92)$$

and

$$\varepsilon_0(\mathbf{P}, \mathbf{R}) = U_0 H_0(\mathbf{P}, \mathbf{R}) U_0^+ = \frac{1}{2} \beta \left(F(\mathbf{R}) \sqrt{\mathbf{P}^2} + \sqrt{\mathbf{P}^2} F(\mathbf{R}) \right) \quad (93)$$

We also need the Berry phases at the lowest order:

$$\begin{aligned} \mathcal{A}_0^{\mathbf{R}} &= i [U_0 \nabla_{\mathbf{P}} U_0^+] = i \frac{-\beta \boldsymbol{\alpha} \cdot \mathbf{P} \mathbf{P} + E^2 \beta \boldsymbol{\alpha} - i E \mathbf{P} \times \boldsymbol{\Sigma}}{2E^3} \\ \mathcal{A}_0^{\mathbf{P}} &= -i [U \nabla_{\mathbf{R}} U^+] = 0 \end{aligned}$$

The matrix B Eq. (80) needed to obtain the corrections to the energy at the second order is even simpler than for the electron in an electric field since here (see Eq. (82)):

$$B = -[\cdot, \varepsilon_0(\mathbf{X}_\alpha)]^{-1} \cdot \mathcal{P}_- \left\{ \frac{1}{2} \mathcal{A}_0^{R\alpha_l} \nabla_{R\alpha_l} \varepsilon_0(\mathbf{X}) + \frac{1}{2} \nabla_{R\alpha_l} \varepsilon_0(\mathbf{X}) \mathcal{A}_0^{R\alpha_l} \right\} = 0$$

Therefore Berry connections and covariant variables to the second order reduce to $\mathcal{A}^{\mathbf{R}} = \mathcal{A}_0^{\mathbf{R}}$ and $\mathcal{A}^{\mathbf{P}} = 0$ as well as $\mathbf{r} = \mathbf{R} + \hbar \mathcal{P}_+ \mathcal{A}_0^{\mathbf{R}} = \mathbf{R} + \hbar \frac{\mathbf{P} \times \boldsymbol{\Sigma}}{2E^2}$, $\mathbf{p} = \mathbf{P}$.

Now, using expression Eq. (87), we ultimately obtain the energy operator:

$$\begin{aligned} \varepsilon(\mathbf{P}, \mathbf{r}) &= \frac{1}{2} \beta \left(F(\mathbf{r}) \sqrt{\mathbf{P}^2} + \sqrt{\mathbf{P}^2} F(\mathbf{r}) \right) - \frac{\hbar}{2} \langle \varepsilon_0(\mathbf{X}) \rangle \\ &= \frac{1}{2} \beta \left(F(\mathbf{r}) \sqrt{\mathbf{P}^2} + \sqrt{\mathbf{P}^2} F(\mathbf{r}) \right) - \frac{1}{4} \hbar \left[\sqrt{\mathbf{P}^2}, F(\mathbf{R}) \right] \\ &= \frac{1}{2} \beta \left(F(\mathbf{r}) \sqrt{\mathbf{P}^2} + \sqrt{\mathbf{P}^2} F(\mathbf{r}) \right) - \frac{1}{4} \frac{\hbar^2}{\sqrt{\mathbf{P}^2}} \mathbf{P} \nabla F(\mathbf{r}) \end{aligned} \quad (94)$$

From the last formula, we can deduce the equations of motion to the second order approximation. Indeed, for a particle of positive energy only $\varepsilon(\mathbf{P}, \mathbf{r}) = \frac{1}{2} \left(F(\mathbf{r}) \sqrt{\mathbf{P}^2} + \sqrt{\mathbf{P}^2} F(\mathbf{r}) \right) - \frac{1}{4} \frac{\hbar^2}{\sqrt{\mathbf{P}^2}} \mathbf{P} \nabla F(\mathbf{r})$ with now $\mathbf{r} = \mathbf{R} + i \frac{\mathbf{P} \times \mathbf{S}}{\mathbf{P}^2}$ a 2×2 matrix (the spin matrix is $\mathbf{S} = \hbar \boldsymbol{\sigma} / 2$), the usual relations $\dot{\mathbf{r}} = -\frac{i}{\hbar} [\mathbf{r}, \varepsilon(\mathbf{P}, \mathbf{r})]$ and $\dot{\mathbf{P}} = -\frac{i}{\hbar} [\mathbf{P}, \varepsilon(\mathbf{P}, \mathbf{r})]$, lead to the equations of motion

$$\begin{aligned} \dot{\mathbf{r}} &= \nabla_{\mathbf{P}} \varepsilon + \hbar \dot{\mathbf{P}} \times \Theta^{rr} \\ \dot{\mathbf{P}} &= \nabla_{\mathbf{r}} \varepsilon \end{aligned} \quad (95)$$

Note that the anomalous velocity term $\hbar \dot{\mathbf{P}} \times \Theta^{rr}$ in Eq. (95) has to be understood as a symmetrized expression of $\mathbf{P}$ and $\mathbf{r}$. Here, $[r_i, r_j] = i \hbar^2 \Theta_{ij}^{rr} = i \hbar^2 \varepsilon_{ijk} \Theta_k^{rr} = -i \hbar^2 \varepsilon_{ijk} \lambda \frac{P^k}{P^3}$, and $\lambda = \boldsymbol{\sigma} \cdot \mathbf{P} / P$ the helicity. In addition helicity is conserved $d\lambda/dt = 0$. Eqs (95) imply the spin Hall effect of light (for the photon one just has to replace the Pauli matrices $\boldsymbol{\sigma}$ by the spin one matrices) as a consequence of the anomalous velocity term $\hbar \dot{\mathbf{P}} \times \Theta^{rr}$ (see also [26] and [27] for the experimental confirmation of this effect)

From the Eq. (95) we deduce the following expression for the velocity components

$$v^i = \frac{1}{2} \left(\frac{c}{n(\mathbf{r})} \frac{P^i}{P} + \frac{P^i}{P} \frac{c}{n(\mathbf{r})} \right) + \frac{\lambda \hbar}{2P^2} \varepsilon_{ijk} \left(P^k \frac{\partial \ln n}{\partial x^i} \frac{c}{n(\mathbf{r})} + \frac{\partial \ln n}{\partial x^i} \frac{c}{n(\mathbf{r})} P^k \right) + \frac{\hbar^2}{4} \frac{c}{n(\mathbf{r})} \left(\frac{1}{P} \partial_i \ln n - \frac{P_i P_j}{P^3} \partial_j \ln n \right) \quad (96)$$

from which we compute the modulus of the velocity

$$v = \frac{c}{n(\mathbf{r})} \left(1 + \hbar^2 \frac{\lambda^2}{P^2} \left((\nabla \ln n)^2 - \frac{1}{P^2} (\mathbf{P} \cdot \nabla \ln n)^2 \right) \right)^{1/2} + O(\hbar^3) \quad (97)$$

This expression shows a very small correction to the usual expression $v = c/n(\mathbf{r})$ of order $\hbar^2$ due to the interaction between the polarization state and external inhomogeneities.

VIII. CONCLUSION

In this paper, we presented a new diagonalization method for a generic matrix valued Hamiltonian which leads to a diagonal representation where the operator energy takes an elegant and compact form. This approach requires the introduction of some new mathematical objects like non-commuting operators evolving with the Planck constant promoted as a running variable and thus reveals a mathematical structure reminiscent of the stochastic calculus. It also shows once more the very important role played by Berry phases in these systems as the energy operator is written in terms of covariant dynamical operators containing Berry connections and satisfying a non-commutative algebra.

It was also found that the diagonal representation of the energy is solution of a differential equation in $\hbar$ presented previously in [8] and which could only be solved recursively in a series expansion in $\hbar$. Actually the formal exact solution presented here can also be written explicitly as a series expansion in $\hbar$, but it appears that the derivation of the coefficients of this expansion is now much more easier. Indeed we could give the expression of the energy and the dynamical variables to the second order in $\hbar$ for a generic matrix valued Hamiltonian. We then applied this method, first to the simple case of a Dirac electron in an external electric field which allowed to recover the usual Pauli Hamiltonian in the non relativistic limit including the Darwin term of order $\hbar^2$, and second to the neutrino in a gravitational field. This is obviously a good check for the validity of the proposed method. We leave for subsequent work its application to more complicated systems in condensed

matter or relativistic particle physics such as Bloch and Dirac electrons in interaction.

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