Diagonal Representation for a Generic Matrix Valued Quantum Hamiltonian

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A general method to deduce the diagonal representation for a generic matrix valued quantum Hamiltonian is proposed. This method can be applied to any kind of quantum system which has an energy band spectrum. In particular it would be useful for the study of relativistic Dirac particles in strong external fields as well as for Bloch electrons in solids. In this approach the diagonal energy operator and the dynamical operators which depend on Berry phase terms can be expanded in power series in the planck constant. The connection with previous less general approaches is also presented. As an example, the case of a Dirac electron in an external electric field is considered.

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I. INTRODUCTION

The physical content of quantum systems is most often best revealed in the representation where the Hamiltonian is diagonal. The paradigmic 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 [1]. Actually even if several exact FW transformations have been found for some definite classes of potentials [2][3][4], the diagonalization (block-diagonalization for Dirac Hamiltonian) is a difficult mathematical problem requiring some approximations, essentially a perturbation expansion in weak fields. To overcome this limitation we have recently proposed a new method based on a formal expansion in powers of the Planck constant $\hbar$ which is not restricted to Dirac Hamiltonians (and thus very different from the FW method) but also applicable to a large class of quantum systems: as an example we carried out the diagonalization for the Hamiltonian of a spinless electron in magnetic Bloch bands [5][6]. It is worth mentioning that recently a variant of the FW transformation valid for strong fields and based also on an expansion in $\hbar$ of the Dirac Hamiltonian was presented [7]. The main advantage of the diagonalization procedure of [5] is that it embraces several different physical systems ranging from Bloch electrons in solid to Dirac particles interacting with any type of external fields (for instance in ref. [8] electrons and photons in a static gravitational field were considered). Another interesting feature of this approach is that it reveals the fundamental role played by Berry curvatures since it results in an effective diagonal Hamiltonian with Berry phase corrections as well as noncommutative (Berry connections dependent) coordinates and momentum operators. The resulting generic equations of motion are also corrected by Berry curvatures terms. One other advantage of an expansion in $\hbar$, apart the fact that it is valid for strong fields, is that the semiclassical limit of the relativistic quantum mechanics is readily obtained. Since semiclassical methods play a very important role in solid state physics too, in studying the dynamics of electrons to account for the various properties of metals, semiconductors and insulators, it is clear that a diagonalization method valid for a generic Hamiltonian is of a great interest.

In what follows we present an alternative method for the diagonalization of a generic matrix valued Hamiltonian which leads to a particulary compact and elegant exact diagonal energy operator. The philosophy behind this approach consists in a mapping of the initial quantum system to a classical one which can be diagonalized and then to return to the full quantum system. This method requires the introduction of some new mathematical objects like non-commuting operators which evolve with the planck constant promoted as a running variable. This construction forces to define a differential calculus on a non-commutative space which shows some similarities with the stochastic calculus. It is not our goal in this paper to deepens the mathematical aspect of our approach which might look sometimes formal but also shows to be very elegant and powerful. To check the validity of this new approach we show that the energy found in this paper is solution of the differential equation (with respect to $\hbar$) which is the base of the method presented in [5]. In the lack of exact solution for this differential equation, we resorted to a recursive method resulting in a series expansion in $\hbar$ of the solution. On the contrary the approach developed here allows us to find the exact solution of the differential equation of [5]. The derivation of the expansion of this solution into a power series in $\hbar$ appears to be much more simpler than in [5]. In particular we could derive a general expression for the diagonal Hamiltonian representation of any matrix valued Hamiltonian to the second order in $\hbar$. As a physical illustration of this result we derive the full relativistic energy of a spin 1/2 particle in an external electric field to the second order in $\hbar$. This allows us to recover the Darwin term when the non-relativistic limit is considered.

II. PRELIMINARIES:

A. Differential calculus on noncommutative space

Consider a quantum mechanical system whose state space is a tensor product $L^2\left(\mathcal{R}^3\right)\otimes V$ with V some internal space. In other words, the Hamiltonian can be written as a matrix $H\left(\mathbf{P},\mathbf{R}\right)$ of size $\dim V$ whose elements are operators depending on a couple of canonical operators $\left[R^i,P^i\right]=i\hbar$, 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. For that purpose we start with some definitions and notations.

1. Running coordinate and momentum operators

To begin with, we introduce a space of non commuting infinitesimal operators $dX^i_\alpha\equiv\left\{dR^i_\alpha,dP^i_\alpha\right\}\quad i=1,2,3$ indexed by a continuous parameter α, that satisfy the following infinitesimal Heisenberg algebra with a reversed sign :

$$\left[dR^i_\alpha,dP^j_{\alpha\prime}\right]=-id\alpha\delta_{\alpha,\alpha\prime}\delta_{ij}\quad\text{ and }\quad\left[dR^i_\alpha,dR^j_{\alpha\prime}\right]=\left[dP^i_\alpha,dP^j_{\alpha\prime}\right]=0. \tag{1}$$

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

$$R^i_\alpha=R^i-\int_\alpha^\hbar dR^i_\lambda,\quad\text{and}\quad P^i_\alpha=P^i-\int_\alpha^\hbar dP^i_\lambda \tag{2}$$

with the choice of convention : $dR^i_\alpha=R^i_\alpha-R^i_{\alpha-d\alpha}$ and $dP^i_\alpha=P^i_\alpha-P^i_{\alpha-d\alpha}$. For $\alpha=\hbar$ we recover the usual canonical operators $R^i\equiv R^i_\hbar$and $P^i\equiv P^i_\hbar$ which evidently satisfy the canonical Heisenberg algebra $\left[R^i,P^i\right]=i\hbar$, whereas the running operators satisfy

$$\left[R^i_\alpha,P^j_\alpha\right]=i\alpha\delta_{ij}\quad\text{ and }\quad\left[R^i_\alpha,R^j_\alpha\right]=\left[P^i_\alpha,P^j_\alpha\right]=0. \tag{3}$$

(Note that in this paper we will never consider the algebra of the operators R^i_α and $P^j_{\alpha\prime}$ 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 quantized 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, and then back from the formal classical one to the initial 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 the $d\mathbf{X}_\alpha$.

2. Differential algebra

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

By considering the function $F\left(\mathbf{X}_\alpha,\alpha\right)$ as a series expansion in symmetrized products of the kind $\frac{1}{2}\left(\mathbf{R}^n_\alpha\mathbf{P}^m_\alpha+\mathbf{P}^m_\alpha\mathbf{R}^n_\alpha\right)$ with n and m the degrees of the monomials, we can write the differential $dF\left(\mathbf{X}_\alpha,\alpha\right)\equiv F\left(\mathbf{X}_\alpha,\alpha\right)-F\left(\mathbf{X}_{\alpha-d\alpha},\alpha-d\alpha\right)$ (note that this unusual definition fits with our convention for the dX^i_α) as :

$$\begin{aligned}dF\left(\mathbf{X}_\alpha,\alpha\right)\;=\;&\nabla_{R_i}FdR^i_\alpha+\nabla_{P_i}FdP^i_\alpha-\frac{1}{2}\left(\nabla_{R_i}\nabla_{R_j}F\right)dR^i_\alpha dR^j_\alpha-\frac{1}{2}\left(\nabla_{P_i}\nabla_{P_j}F\right)dP^i_\alpha dP^j_\alpha\\&-\frac{1}{2}\left(\nabla_{R_i}\nabla_{P^i}F\right)\left(dR^i_\alpha dP^j_\alpha+dP^j_\alpha dR^i_\alpha\right)-\frac{i}{2}Asym\left(\nabla_{R_i}\nabla_{P^i}F\right)d\alpha+\frac{\partial F}{\partial\alpha}d\alpha+\text{terms of order 3},\end{aligned} \tag{4}$$

all expression in the R.H.S. being evaluated at $\left(\mathbf{X}_\alpha,\alpha\right)$. We kept terms of order square in dX^i_α since they are of order $d\alpha$ and thus contribute to the differential, whereas higher orders can safely be disregarded as negligible when we do the summation over α.

The operation *Asym* already introduced in [5] acts on symmetrical functions and has the following meaning : $Asym\left\{\frac{1}{2}A\left(\mathbf{R}\right)B\left(\mathbf{P}\right)+\frac{1}{2}B\left(\mathbf{P}\right)A\left(\mathbf{R}\right)\right\}=\frac{1}{2}\left[B\left(\mathbf{P}\right),A\left(\mathbf{R}\right)\right]$. In Eq. (4) it is obtained by picking the coefficient of $\left[dR_\alpha^i,dP_\alpha^j\right]$ in the second order expansion of $dF\left(\mathbf{X}_\alpha,\alpha\right)$ in terms of $dR_\alpha^i dP_\alpha^j+dP_\alpha^j dR_\alpha^i$ and $dR_\alpha^i dP_\alpha^j-dP_\alpha^j dR_\alpha^i=id\alpha$.

Note that the appearance of a second order term proportional to $d\alpha$ in Eq. (4) is very reminiscent of the stochastic calculus. This analogy suggests us to call this term the bracket of F and we therefore introduce the notation

$$\left\langle F\left(\mathbf{X}_\alpha,\alpha\right)\right\rangle\equiv-\frac{i}{2}Asym\left(\nabla_{R_i}\nabla_{P^i}F\left(\mathbf{X}_\alpha,\alpha\right)\right). \tag{5}$$

This definition implies two remarks :

First, the bracket can be defined even if the function $F\left(\mathbf{X}_\alpha,\alpha\right)$ has not been put in a symmetric form. Indeed by developing $dF\left(\mathbf{X}_\alpha,\alpha\right)$ to the second order, the terms proportional to $dR_\alpha^i dP_\alpha^j$ can always be uniquely written as a sum of terms of the type $dR_\alpha^i dP_\alpha^j+dP_\alpha^j dR_\alpha^i$ and $dR_\alpha^i dP_\alpha^j-dP_\alpha^j dR_\alpha^i=id\alpha$. Picking the $id\alpha$ term yields then the bracket. However, and this is the second remark, the bracket thus defined is different from the one computed in the symmetric form of the function. This is not astonishing at all. Actually passing from a symmetric to a non symmetric form introduces some explicit terms in α which changes also the term $\partial_\alpha F d\alpha$ in the differential. 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 $\partial_\alpha F+\langle F\rangle$. This is the consequence of the fact that in the series expansion the variables dX_α^i, $dX_\alpha^i dX_\alpha^j$, $d\alpha$, are independent, and as a consequence the coefficients of the expansion are unique.

Formula Eq. (4) for the differential allows us to write formally :

$$F\left(\mathbf{X}_\hbar,\hbar\right)-F(\mathbf{X}_0,0)=\int_0^\hbar dF\left(\mathbf{X}_\alpha,\alpha\right) \tag{6}$$

The integral 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 $\boldsymbol{\nabla}_{\mathbf{R}_\alpha}F.d\mathbf{R}_\alpha=-\boldsymbol{\nabla}_{\mathbf{R}_\alpha}F\left(\mathbf{X}_\alpha,\alpha\right)\left(\mathbf{R}_{\alpha-d\alpha}-\mathbf{R}_\alpha\right)$. 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.

For later convenience we still more compactify our notations by writing :

$$\begin{aligned}dF\left(\mathbf{X}_\alpha,\alpha\right) &= \sum_{i=1}^{6}\nabla_{X_\alpha^i}F\left(\mathbf{X}_\alpha,\alpha\right)dX_\alpha^i-\frac{1}{4}\sum_{i,j=1}^{6}\nabla_{X_\alpha^i}\nabla_{X_\alpha^j}F\left(\mathbf{X}_\alpha,\alpha\right)\left(dX_\alpha^i dX_\alpha^j+dX_\alpha^i dX_\alpha^j\right)\\ &+\left(\frac{\partial F\left(\mathbf{X}_\alpha,\alpha\right)}{\partial\alpha}+\left\langle F\left(\mathbf{X}_\alpha,\alpha\right)\right\rangle\right)d\alpha\end{aligned} \tag{7}$$

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 that really matters for us in Eq. (7) is the term proportional to $d\alpha$. For later use we now give the bracket formula Eq. (5) for a product of two symmetric functions (the product is not put in a symmetric form, only the functions are individually symmetric). Using the same rules as before (see also ref. [5]) one obtains the following expression

$$<F\left(\mathbf{X}_\alpha\right)G\left(\mathbf{X}_\alpha\right)>=\left\langle F\left(\mathbf{X}_\alpha\right)\right\rangle G\left(\mathbf{X}_\alpha\right)+F\left(\mathbf{X}_\alpha\right)\left\langle G\left(\mathbf{X}_\alpha\right)\right\rangle-\frac{i}{2}\left(\boldsymbol{\nabla}_{P_i}F\left(\mathbf{X}_\alpha\right)\boldsymbol{\nabla}_{R_i}G\left(\mathbf{X}_\alpha\right)-\boldsymbol{\nabla}_{R_i}F\left(\mathbf{X}_\alpha\right)\boldsymbol{\nabla}_{P_i}G\left(\mathbf{X}_\alpha\right)\right). \tag{8}$$

Before going to the diagonalization procedure we still need to defined an expectation operator in the next section.

B. Expectation operator

Having now a differential set up, we define a conditional expectation operator $\mathcal{E}\left(.\right)$ by the following set of formula :

$$\mathcal{E}\left(d\alpha\right)=d\alpha\quad\text{and}\quad\mathcal{E}\left(F\left(\mathbf{X}_\hbar,\hbar\right)\right)=F\left(\mathbf{X}_\hbar,\hbar\right) \tag{9}$$

which corresponds to the conditional part of the expectation as the starting point is fixed. We set also

$$\mathcal{E}\left(\prod_{i=1}^{n}dR_{\alpha_i}\right)=\mathcal{E}\left(\prod_{i=1}^{n}dP_{\alpha_i}\right)=0,\quad\mathcal{E}\left(\prod_{i=1}^{n}\left(dX_{\alpha_i}^i dX_{\alpha_i}^j+dX_{\alpha_i}^j dX_{\alpha_i}^i\right)\right)=0 \tag{10}$$

and

$$\mathcal{E}\left(\prod_{i=1}^{n}\prod_{j=1}^{p} dX_{\alpha_i}^i dX_{\alpha_j}^j\right) = 0 \quad \text{for} \quad \alpha_i \neq \alpha_j \tag{11}$$

The role of this operator is to pick up the initial term in a series of independent operators depending on $\prod_{i=1}^{n}\prod_{j=1}^{p} dX_{\alpha_i}^i dX_{\alpha_j}^j$, that is the term depending only on the physical operators $R^i \equiv R_\hbar^i$and $P^i \equiv P_\hbar^i$. This can include contributions proportional to $d\alpha$ which can thus be integrated.

From these results we can then see that the expectation of Eq. (7) gives

$$\mathcal{E}\left(dF\left(\mathbf{X}_\alpha,\alpha\right)\right) = \mathcal{E}\left(\left(\frac{\partial F\left(\mathbf{X}_\alpha,\alpha\right)}{\partial\alpha} + \left\langle F\left(\mathbf{X}_\alpha,\alpha\right)\right\rangle\right) d\alpha\right) \tag{12}$$

For later use we will need to relate $\mathcal{E}\left(F\left(\mathbf{X}_\alpha,\alpha\right)\right)$ to a function $F\left(\mathbf{X}_{\alpha\prime},\alpha\right)$ at a constant α. Given our previous definitions Eq. (7), one has

$$F\left(\mathbf{X}_{\alpha-d\alpha},\alpha\right) - F\left(\mathbf{X}_\alpha,\alpha\right) = -\sum_{i=1}^{6} \nabla_{X_\alpha^i} F\left(\mathbf{X}_\alpha,\alpha\right) dX_\alpha^i + \frac{1}{4}\sum_{i,j=1}^{6} \nabla_{X_\alpha^j}\nabla_{X_\alpha^i} F\left(\mathbf{X}_\alpha,\alpha\right)\left(dX_\alpha^i dX_\alpha^j + dX_\alpha^i dX_\alpha^j\right) - \left\langle F\left(\mathbf{X}_\alpha,\alpha\right)\right\rangle d\alpha \tag{13}$$

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

$$\begin{aligned}\mathcal{E}\left(F\left(\mathbf{X}_{\alpha-d\alpha},\alpha\right)\right) &= \mathcal{E}\left(F\left(\mathbf{X}_\alpha,\alpha\right) + \frac{i}{2} Asym\left(\nabla_{R_i}\nabla_{P_i} F\left(\mathbf{X}_\alpha,\alpha\right)\right) d\alpha\right) \\ &= \mathcal{E}\left(\left(1 - \left\langle .\right\rangle d\alpha\right) F\left(\mathbf{X}_\alpha,\alpha\right)\right)\end{aligned} \tag{14}$$

where $\langle . \rangle$ is the bracket operator defined in Eq. (5). The above differential equation can be easily integrated to get the required relation

$$\mathcal{E}\left(F\left(\mathbf{X}_{\alpha_2},\alpha_2\right)\right) = \mathcal{E}\left(\exp\left(\left(\alpha_2 - \alpha_1\right)\left\langle .\right\rangle\right) F\left(\mathbf{X}_{\alpha_1},\alpha_2\right)\right) \tag{15}$$

valid for $\alpha_1 > \alpha_2$. We can now exploit the mathematical construction developed in this section to consider the formal diagonalization of a generic matrix valued quantum Hamiltonian.

III. THE DIAGONALIZATION PROCEDURE

We now consider a generic matrix valued quantum Hamiltonian $H\left(\mathbf{R},\mathbf{P}\right)$ where $\mathbf{R}$ and $\mathbf{P}$ are the usual canonical coordinate and momentum operators satisfying the canonical Heisenberg algebra. Our goal is the find an unitary transformation U such that UHU^+ is a diagonal matrix valued operator $\varepsilon\left(\mathbf{R},\mathbf{P}\right)$ (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 $U_\alpha\left(\mathbf{X}_\alpha\right) \equiv U\left(\mathbf{X}_\alpha,\alpha\right)$ which diagonalizes the Hamiltonian $H\left(\mathbf{X}_\alpha\right)$ 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

$$U_\alpha\left(\mathbf{X}_\alpha\right) H\left(\mathbf{X}_\alpha\right) U_\alpha^+\left(\mathbf{X}_\alpha\right) = \varepsilon_\alpha\left(\mathbf{X}_\alpha\right) \tag{16}$$

Note that following [5] we choose to put $U_\alpha\left(\mathbf{X}_\alpha\right)$ and $H\left(\mathbf{X}_\alpha\right)$ in a symmetric form. With the help of the previous identities Eqs. (6) (9) (10), we can compute $\varepsilon_\hbar\left(\mathbf{X}_\hbar\right) \equiv \varepsilon\left(\mathbf{X}\right)$. Indeed as $\varepsilon\left(\mathbf{X}\right) = \mathcal{E}\left(\varepsilon\left(\mathbf{X}\right)\right)$ we can write

$$\varepsilon\left(\mathbf{X}\right) = \mathcal{E}\left(\varepsilon_0\left(\mathbf{X}_0\right) + \int_0^\hbar d\varepsilon_{\alpha_1}\left(\mathbf{X}_{\alpha_1}\right)\right). \tag{17}$$

Clearly $\varepsilon_0(\mathbf{X}_0)$ corresponds to the diagonal representation of the original Hamiltonian $H(X)$ where the canonical operators X have been replaced by the classical variables 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 $\mathcal{E}(d\varepsilon_{\alpha_1}) = \mathcal{E}\left(\left(\frac{\partial}{\partial\alpha_1} + \langle . \rangle\right)\varepsilon_{\alpha_1}(\mathbf{X}_{\alpha_1})\right)$ can be straightforwardly computed by using the rule previously given for the bracket of a product Eq. (8). Indeed we find

$$\begin{aligned}\left(\frac{\partial}{\partial\alpha_1} + \langle . \rangle\right)\varepsilon_{\alpha_1}(\mathbf{X}_{\alpha_1}) &= \partial_{\alpha_1}U_{\alpha_1}U_{\alpha_1}^+\varepsilon_{\alpha_1} + \varepsilon_{\alpha_1}U_{\alpha_1}\partial_{\alpha_1}U_{\alpha_1}^+ + U_{\alpha_1}\frac{\partial}{\partial\alpha_1}H(\mathbf{X}_{\alpha_1})U_{\alpha_1}^+ \\ &+ \langle U_{\alpha_1}\rangle U_{\alpha_1}^+\varepsilon_{\alpha_1} + U_{\alpha_1}\langle H(\mathbf{X}_{\alpha_1})\rangle U_{\alpha_1}^+ + \varepsilon_{\alpha_1}U_{\alpha_1}\langle U_{\alpha_1}^+\rangle \\ &- \frac{i}{2}\left(\nabla_{P_i}U_{\alpha_1}\nabla_{R_i}H(\mathbf{X}_{\alpha_1})U_{\alpha_1}^+ - \nabla_{R_i}U_{\alpha_1}\nabla_{P_i}H(\mathbf{X}_{\alpha_1})U_{\alpha_1}^+\right) \\ &- \frac{i}{2}\left(U_{\alpha_1}\nabla_{P_i}H(\mathbf{X}_{\alpha_1})\nabla_{R_i}U_{\alpha_1}^+ - U_{\alpha_1}\nabla_{R_i}H(\mathbf{X}_{\alpha_1})\nabla_{P_i}U_{\alpha_1}^+\right) \\ &- \frac{i}{2}\left(\nabla_{P_i}U_{\alpha_1}H(\mathbf{X}_{\alpha_1})\nabla_{R_i}U_{\alpha_1}^+ - \nabla_{R_i}U_{\alpha_1}H(\mathbf{X}_{\alpha_1})\nabla_{P_i}U_{\alpha_1}^+\right) \end{aligned} \quad (18)$$

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

$$\left(\frac{\partial}{\partial\alpha_1} + \langle . \rangle\right)\varepsilon_{\alpha_1}(\mathbf{X}_{\alpha_1}) = \mathcal{P}_+(\text{R.H.S. of Eq. 18}) \quad (19)$$

$$0 = \mathcal{P}_-(\text{R.H.S. of Eq. 18}) \quad (20)$$

where $\mathcal{P}_+$ and $\mathcal{P}_-$ are the projection on the diagonal and off the diagonal respectively. As in [5] we now introduce the notations $\mathcal{A}_{\alpha_1}^{R_l} = iU_{\alpha_1}(\mathbf{X}_{\alpha_1})\nabla_{P_i}U_{\alpha_1}^+(\mathbf{X}_{\alpha_1})$ and $\mathcal{A}_{\alpha_1}^{P_l} = -iU_{\alpha_1}(\mathbf{X}_{\alpha_1})\nabla_{R_i}U_{\alpha_1}^+(\mathbf{X}_{\alpha_1})$ as well as $\mathcal{B}_{\alpha_1} = (Asym\left[\nabla_{R_k}\nabla_{P_l}U_{\alpha_1}(\mathbf{X}_{\alpha_1})\right])U_{\alpha_1}^+(\mathbf{X}_{\alpha_1})$ so that Eq. (19) can be written

$$\begin{aligned}\left(\frac{\partial}{\partial\alpha_1} + \langle . \rangle\right)\varepsilon_{\alpha_1}(\mathbf{X}_{\alpha_1}) &= \mathcal{P}_+\left(\partial_{\alpha_1}U_{\alpha_1}U_{\alpha_1}^+\varepsilon_{\alpha_1} + \varepsilon_{\alpha_1}U_{\alpha_1}\partial_{\alpha_1}U_{\alpha_1}^+ + U_{\alpha_1}\frac{\partial}{\partial\alpha_1}H(\mathbf{X}_{\alpha_1})U_{\alpha_1}^+\right) \\ &+ \mathcal{P}_+\left\{\frac{1}{2}\mathcal{A}_{\alpha_1}^{R_l}\nabla_{R_l}\varepsilon_{\alpha_1} + \nabla_{R_l}\varepsilon_{\alpha_1}\mathcal{A}_{\alpha_1}^{R_l} + \mathcal{A}_{\alpha_1}^{P_l}\nabla_{P_l}\varepsilon_{\alpha_1} + \nabla_{P_l}\varepsilon_{\alpha_1}\mathcal{A}_{\alpha_1}^{P_l}\right\} \\ &+ \frac{i}{2}\mathcal{P}_+\left\{\mathcal{A}_{\alpha_1}^{P_l}\varepsilon_{\alpha_1}\mathcal{A}_{\alpha_1}^{R_l} - \mathcal{A}_{\alpha_1}^{R_l}\varepsilon_{\alpha_1}\mathcal{A}_{\alpha_1}^{P_l} + \varepsilon_{\alpha_1}\left[\mathcal{A}_{\alpha_1}^{R_l}, \mathcal{A}_{\alpha_1}^{P_l}\right] + \left[\mathcal{A}_{\alpha_1}^{R_l}, \mathcal{A}_{\alpha_1}^{P_l}\right]\varepsilon_{\alpha_1}\right\} \\ &+ \frac{i}{2}\mathcal{P}_+\left\{-U_{\alpha_1}Asym\left\{\nabla_{P_l}\nabla_{R_l}H(\mathbf{X}_{\alpha_1})\right\}U_{\alpha_1}^+ - \left[\mathcal{B}_{\alpha_1}\varepsilon_{\alpha_1} - \varepsilon_{\alpha_1}\mathcal{B}_{\alpha_1}^+\right]\right\}. \end{aligned} \quad (21)$$

This action is of affine type in $\varepsilon_{\alpha_1}(\mathbf{X}_{\alpha_1})$ and will be denoted

$$\left(\frac{\partial}{\partial\alpha_1} + \langle . \rangle\right)\varepsilon_{\alpha_1}(\mathbf{X}_{\alpha_1}) = O_{\alpha_1}.\varepsilon_{\alpha_1}(\mathbf{X}_{\alpha_1}) \quad (22)$$

with O_{α_1} given by the r.h.s. expression of Eq. (21). Now similarly to Eq. (17) we can write :

$$\varepsilon_{\alpha_1}(\mathbf{X}_{\alpha_1}) = \varepsilon_0(\mathbf{X}_0) + \int_0^{\alpha_1} d\varepsilon_{\alpha_2}(\mathbf{X}_{\alpha_2}) = \varepsilon_0(\mathbf{X}_0) + \int_0^{\alpha_1} d\left(U(\mathbf{X}_{\alpha_2})H(\mathbf{X}_{\alpha_2})U^+(\mathbf{X}_{\alpha_2})\right) \quad (23)$$

which can be inserted in the expectation Eq. (17) to get the full quantum diagonal representation $\varepsilon(\mathbf{X}) \equiv \varepsilon_\hbar(\mathbf{X}_\hbar)$ as :

$$\begin{aligned}\varepsilon_\hbar(\mathbf{X}_\hbar) &= \mathcal{E}\left(\varepsilon_0(\mathbf{X}_0) + \int_0^\hbar d\varepsilon_{\alpha_1}(\mathbf{X}_{\alpha_1})\right) \quad (24) \\ &= \mathcal{E}\left(\varepsilon_0(\mathbf{X}_0) + \int_0^\hbar O_{\alpha_1}.\left[\varepsilon_0(\mathbf{X}_0) + \int_0^{\alpha_1} dU(\mathbf{X}_{\alpha_2})H(\mathbf{X}_{\alpha_2})U^+(\mathbf{X}_{\alpha_2})d\alpha_2\right]d\alpha_1\right)\end{aligned}$$

Now remark that since $\alpha_2 < \alpha_1$, the terms $\boldsymbol{\nabla}_{\mathbf{X}_{\alpha_1}} \varepsilon_{\alpha_1}(\mathbf{X}_{\alpha_1})\, d\mathbf{X}_{\alpha_1}$ and $\boldsymbol{\nabla}_{X^j_{\alpha_1}} \boldsymbol{\nabla}_{X^i_{\alpha_1}} \varepsilon_{\alpha_1}(\mathbf{X}_{\alpha_1}) \left(dX^i_{\alpha_1} dX^j_{\alpha_1} + dX^i_{\alpha_1} dX^j_{\alpha_1}\right)$ in $d\varepsilon(\mathbf{X}_{\alpha_1})$ do not recombine with anything to give a product of the type $d\mathbf{R}_{\alpha_1} d\mathbf{P}_{\alpha_1}$ that would induce a $d\alpha_1$ contribution. They will thus cancel in the expectation. As a consequence, Eq. (24) can be written:

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

Repeating the procedure one can then show by iteration that :

$$\varepsilon_\hbar(\mathbf{X}_\hbar) = \mathcal{E}\left(\int_0^\hbar \left[\sum_{n=0}^{\infty} \int_{0<\alpha_n<\ldots<\alpha_1<\alpha} O_{\alpha_1} ... O_{\alpha_n} d\alpha_1 ... d\alpha_n\right] \varepsilon_0(\mathbf{X}_0)\right) \tag{25}$$

At this point, an important comment has to be made. The operator O_{α_i} have been designed to depend on $\mathbf{X}_{\alpha_i}$. We can use the connection operation defined in Eq. (15) to put the series appearing in the previous formula Eq. (25) at the same point. Once again, since $0 < \alpha_n < ... < \alpha_1$, we can write, inside the expectation :

$$\begin{aligned} & \left[\int_{0<\alpha_n<\ldots<\alpha_1<\hbar} O_{\alpha_1} ... O_{\alpha_n} d\alpha_1 ... d\alpha_n\right] \varepsilon_0(\mathbf{X}_0) \\ = & \left[\int_{0<\alpha_n<\ldots<\alpha_1<\hbar} e^{(\alpha_1-\hbar)\langle . \rangle} O_{\alpha_1} ... e^{(\alpha_{n-1}-\alpha_{n-2})\langle . \rangle} O_{\alpha_{n-1}} e^{(\alpha_n-\alpha_{n-1})\langle . \rangle} O_{\alpha_n} e^{-\alpha_n \langle . \rangle}\right] \varepsilon_0(\mathbf{X}_\hbar) \end{aligned}$$

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

$$\varepsilon(\mathbf{X}) \equiv \varepsilon_\hbar(\mathbf{X}_\hbar) = \mathcal{E}\left(\left[\exp(-\hbar \langle . \rangle)\, \mathcal{T} \exp\left[\int_{0<\alpha<\hbar} \exp(\alpha \langle . \rangle)\, O_\alpha \exp(-\alpha \langle . \rangle)\, d\alpha\right]\right] \varepsilon_0(\mathbf{X})\right) \tag{26}$$

which is 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 $\mathbf{R}$, $\mathbf{P}$. Here $\mathcal{T}$ is the usual notation for the "time ordered product". Eq. (26) is the required expression and constitutes the main result of this paper.

Clearly the practical application of Eq. (26) 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 [5] 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 :

$$U_\hbar(\mathbf{X}_\hbar) = \mathcal{E}\left(U(\mathbf{X}_0) + \int_0^\hbar dU_\alpha(\mathbf{X}_\alpha)\right) \tag{27}$$

$$= \mathcal{E}\left(\int_0^\hbar \left(\frac{\partial}{\partial\alpha} + \langle . \rangle\right) U_\alpha(\mathbf{X}_\alpha)\, d\alpha\right) \tag{28}$$

we can find $(\partial_\alpha + \langle . \rangle) U_\alpha(\mathbf{X}_\alpha)$ by using again the diagonalization process leading to Eq. (18). Indeed we have

$$\begin{aligned} \left(\frac{\partial}{\partial\alpha} + \langle . \rangle\right) \varepsilon_\alpha(\mathbf{X}_\alpha) = & \left(\left(\frac{\partial}{\partial\alpha} + \langle . \rangle\right) U_\alpha\right) U_\alpha^+ \varepsilon_\alpha + \varepsilon_\alpha U_\alpha \left(\frac{\partial}{\partial\alpha} + \langle . \rangle\right) U_\alpha^+ + U_\alpha \left(\left(\frac{\partial}{\partial\alpha} + \langle . \rangle\right) H(\mathbf{X}_\alpha)\right) U_\alpha^+ \\ & -\frac{i}{2}\left(\nabla_{P_i} U_\alpha \nabla_{R_i} H(\mathbf{X}_\alpha)\, U_\alpha^+ - \nabla_{R_i} U_\alpha \nabla_{P_i} H(\mathbf{X}_\alpha)\, U_\alpha^+\right) \\ & -\frac{i}{2}\left(U_\alpha \nabla_{P_i} H(\mathbf{X}_\alpha) \nabla_{R_i} U_\alpha^+ - U_\alpha \nabla_{R_i} H(\mathbf{X}_\alpha) \nabla_{P_i} U_\alpha^+\right) \\ & -\frac{i}{2}\left(\nabla_{P_i} U_\alpha H(\mathbf{X}_\alpha) \nabla_{R_i} U_\alpha^+ - \nabla_{R_i} U_\alpha H(\mathbf{X}_\alpha) \nabla_{P_i} U_\alpha^+\right) \end{aligned} \tag{29}$$

In addition we have from the unitarity condition $U_\alpha U_\alpha^+ = 1$ the relation $(\partial_\alpha + \langle . \rangle)(U_\alpha U_\alpha^+) = 0$ which reads :

$$0 = \left(\left(\frac{\partial}{\partial\alpha} + \langle . \rangle\right) U_\alpha\right) U_\alpha^+ + U_\alpha \left(\frac{\partial}{\partial\alpha} + \langle . \rangle\right) U_\alpha^+ - \frac{i}{2}\left(\nabla_{P_i} U_\alpha \nabla_{R_i} U_\alpha^+ - \nabla_{R_i} U_\alpha \nabla_{P_i} U_\alpha^+\right) \tag{30}$$

Mixing the two equations Eqs. (29) (30), we obtain that Eq. (29) after projection on the non diagonal part becomes the equality

$$\begin{aligned}
\mathcal{P}_-\left[\left(\left(\frac{\partial}{\partial\alpha} + \langle . \rangle\right) U_\alpha\right) U_\alpha^+, \varepsilon_\alpha\right] \;=\; & -\mathcal{P}_-\left(U_\alpha \left(\left(\frac{\partial}{\partial\alpha} + \langle . \rangle\right) H(\mathbf{X}_\alpha)\right) U_\alpha^+\right) \\
& -\frac{i}{2}\varepsilon_\alpha \mathcal{P}_-\left(\nabla_{P_i} U_\alpha \nabla_{R_i} U_\alpha^+ - \nabla_{R_i} U_\alpha \nabla_{P_i} U_\alpha^+\right) \\
& +\frac{i}{2}\mathcal{P}_-\left(\nabla_{P_i} U_\alpha \nabla_{R_i} H(\mathbf{X}_\alpha) U_\alpha^+ - \nabla_{R_i} U_\alpha \nabla_{P_i} H(\mathbf{X}_\alpha) U_\alpha^+\right) \\
& +\frac{i}{2}\mathcal{P}_-\left(U_\alpha \nabla_{P_i} H(\mathbf{X}_\alpha) \nabla_{R_i} U_\alpha^+ - U_\alpha \nabla_{R_i} H(\mathbf{X}_\alpha) \nabla_{P_i} U_\alpha^+\right) \\
& +\frac{i}{2}\mathcal{P}_-\left(\nabla_{P_i} U_\alpha H(\mathbf{X}_\alpha) \nabla_{R_i} U_\alpha^+ - \nabla_{R_i} U_\alpha H(\mathbf{X}_\alpha) \nabla_{P_i} U_\alpha^+\right)
\end{aligned} \tag{31}$$

Both conditions Eqs. (30) (31) can be solved for $(\partial_\alpha + \langle . \rangle) U_\alpha$. Actually, decomposing $[(\partial_\alpha + \langle . \rangle) U_\alpha] U_\alpha^+ = hr + ahr$ in hermitian hr and anti-hermitian ahr part, Eq. (31) reads

$$\mathcal{P}_-\left[hr + ahr, \varepsilon_\alpha\right] = M(U_\alpha) \tag{32}$$

where $M(U_\alpha)$ is the r.h.s of Eq. (31). We can now use a particular choice of gauge. We fix our diagonalization process by setting $P_+(ahr) = 0$. 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 : $P_+\left(\left(\frac{\partial}{\partial\alpha} + \langle . \rangle\right) U_\alpha D_\alpha\right) D_\alpha^+ U_\alpha^+$ is hermitian. This gives n conditions that determine D_α.

Now, from Eq. (32) and given our gauge choice for U_α, we deduce that $\mathcal{P}_-(ahr) = ahr$ and $[ahr, \varepsilon_\alpha] = \frac{1}{2}\left(M(U_\alpha) + M^+(U_\alpha)\right)$. Then we can formally write ahr under the form

$$ahr = \widetilde{N}(\alpha) . U_\alpha \tag{33}$$

where we have defined :

$$\widetilde{N}(\alpha) . U_\alpha = \frac{1}{2}\left([., \varepsilon_\alpha]^{-1}\right)\left(M(U_\alpha) + M^+(U_\alpha)\right) \tag{34}$$

and the inverse of the commutator operation $[, \varepsilon_\alpha]$ has the following meaning

$$\begin{aligned}
\left[[., \varepsilon_\alpha]^{-1} . M, \varepsilon_\alpha\right] \;&=\; [., \varepsilon_\alpha]^{-1} . [M, \varepsilon_\alpha] = M \quad \text{for} \quad [M, \varepsilon_\alpha] \neq 0 \\
[., \varepsilon_\alpha]^{-1} . M \;&=\; 0 \quad \text{if} \quad [M, \varepsilon_\alpha] = 0
\end{aligned}$$

To complete the determination of U_α we still need to deduce hr which is readily obtained from the unitarity condition Eq. (30) as:

$$hr = -\frac{i}{4}\left(\nabla_{P_i} U_\alpha \nabla_{R_i} U_\alpha^+ - \nabla_{R_i} U_\alpha \nabla_{P_i} U_\alpha^+\right) \tag{35}$$

Gathering the results Eqs.(34) (35) 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

$$N_\alpha . U_\alpha = \frac{1}{2}\left([., \varepsilon_\alpha]^{-1}\right)\left(M(U_\alpha) + M^+(U_\alpha)\right) U_\alpha + \frac{i}{4}\left(\nabla_{P_i} U_\alpha \nabla_{R_i} U_\alpha^+ - \nabla_{R_i} U_\alpha \nabla_{P_i} U_\alpha^+\right) U_\alpha$$

As for the energy diagonalization, this expression can be rewritten in terms of physical quantities

$$N_\alpha.U_\alpha = -\left[.,\varepsilon_\alpha\right]^{-1}.\left[\mathcal{P}_-\left\{\frac{1}{2}\mathcal{A}_\alpha^{R_l}\nabla_{R_l}\varepsilon_\alpha+\nabla_{R_l}\varepsilon_\alpha\mathcal{A}_\alpha^{R_l}+\mathcal{A}_\alpha^{P_l}\nabla_{P_l}\varepsilon_\alpha+\nabla_{P_l}\varepsilon_\alpha\mathcal{A}_\alpha^{P_l}\right\}\right.$$
$$\left.+\frac{i}{4}\mathcal{P}_-\left\{\left[\varepsilon_\alpha,\mathcal{A}_\alpha^{R_l}\right]\mathcal{A}_\alpha^{P_l}-\left[\varepsilon_\alpha,\mathcal{A}_\alpha^{P_l}\right]\mathcal{A}_\alpha^{R_l}\right\}+H.C.\right]-\frac{i}{4}\mathcal{P}_-\left\{\left[\mathcal{A}_\alpha^{R_l},\mathcal{A}_\alpha^{P_l}\right]U_\alpha\right\} \quad (36)$$

where $H.C.$ stands for the hermitic conjugate of the right hand side and $\varepsilon_\alpha\left(\mathbf{X}_\alpha\right)$ is computed recursively as explained before.

As for $\varepsilon\left(\mathbf{X}\right)$, we can therefore write for $U\left(\mathbf{X}\right)\equiv U_\hbar\left(\mathbf{X}_\hbar\right)$:

$$U\left(\mathbf{X}\right)=\mathcal{E}\left(\left[\exp\left(-\hbar\left\langle.\right\rangle\right)\mathcal{T}\exp\left[\int_{0<\alpha<\hbar}\exp\left(\alpha\left\langle.\right\rangle\right)N_\alpha\exp\left(-\alpha\left\langle.\right\rangle\right)d\alpha\right]\right]U_0\left(\mathbf{X}\right)\right) \quad (37)$$

This expression has a very similar structure as the solution for the energy Eq. (26) except that the operator O_α has to be replaced by N_α.

Note that given the solution derived for U_α we can now rewrite the operator O_α in an simpler form. Indeed starting again from

$$O_\alpha = \left(\frac{\partial}{\partial\alpha}+\left\langle.\right\rangle\right)\varepsilon_\alpha\left(\mathbf{X}_\alpha\right)=\mathcal{P}_+\left[\left(\left(\frac{\partial}{\partial\alpha}+\left\langle.\right\rangle\right)U_\alpha\right)U_\alpha^+\varepsilon_\alpha+\varepsilon_\alpha U_\alpha\left(\frac{\partial}{\partial\alpha}+\left\langle.\right\rangle\right)U_\alpha^+ + U_\alpha\left(\left(\frac{\partial}{\partial\alpha}+\left\langle.\right\rangle\right)H\left(\mathbf{X}_\alpha\right)\right)U_\alpha^+\right]$$
$$-\frac{i}{2}\mathcal{P}_+\left(\nabla_{P_i}U_\alpha\nabla_{R_i}H\left(\mathbf{X}_\alpha\right)U_\alpha^+-\nabla_{R_i}U_\alpha\nabla_{P_i}H\left(\mathbf{X}_\alpha\right)U_\alpha^+\right)$$
$$-\frac{i}{2}\mathcal{P}_+\left(U_\alpha\nabla_{P_i}H\left(\mathbf{X}_\alpha\right)\nabla_{R_i}U_\alpha^+-U_\alpha\nabla_{R_i}H\left(\mathbf{X}_\alpha\right)\nabla_{P_i}U_\alpha^+\right)$$
$$-\frac{i}{2}\mathcal{P}_+\left(\nabla_{P_i}U_\alpha H\left(\mathbf{X}_\alpha\right)\nabla_{R_i}U_\alpha^+-\nabla_{R_i}U_\alpha H\left(\mathbf{X}_\alpha\right)\nabla_{P_i}U_\alpha^+\right) \quad (38)$$

using the unitarity condition for U_α yields :

$$O_\alpha\varepsilon_\alpha\left(\mathbf{X}_\alpha\right) = \mathcal{P}_+\left[\left[\left(\left(\frac{\partial}{\partial\alpha}+\left\langle.\right\rangle\right)U_\alpha\right)U_\alpha^+,\varepsilon_\alpha\right]+U_\alpha\left(\left(\frac{\partial}{\partial\alpha}+\left\langle.\right\rangle\right)H\left(\mathbf{X}_\alpha\right)\right)U_\alpha^+\right]$$
$$+\frac{i}{2}\varepsilon_\alpha\mathcal{P}_+\left(\nabla_{P_i}U_\alpha\nabla_{R_i}U_\alpha^+-\nabla_{R_i}U_\alpha\nabla_{P_i}U_\alpha^+\right)$$
$$-\frac{i}{2}\mathcal{P}_+\left(\nabla_{P_i}U_\alpha\nabla_{R_i}H\left(\mathbf{X}_\alpha\right)U_\alpha^+-\nabla_{R_i}U_\alpha\nabla_{P_i}H\left(\mathbf{X}_\alpha\right)U_\alpha^+\right)$$
$$-\frac{i}{2}\mathcal{P}_+\left(U_\alpha\nabla_{P_i}H\left(\mathbf{X}_\alpha\right)\nabla_{R_i}U_\alpha^+-U_\alpha\nabla_{R_i}H\left(\mathbf{X}_\alpha\right)\nabla_{P_i}U_\alpha^+\right)$$
$$-\frac{i}{2}\mathcal{P}_+\left(\nabla_{P_i}U_\alpha H\left(\mathbf{X}_\alpha\right)\nabla_{R_i}U_\alpha^+-\nabla_{R_i}U_\alpha H\left(\mathbf{X}_\alpha\right)\nabla_{P_i}U_\alpha^+\right) \quad (39)$$

Now, using our gauge condition which states that the antihermitian part of $\mathcal{P}_+\left(\left(\frac{\partial}{\partial\alpha}+\left\langle.\right\rangle\right)U_\alpha\right)U_\alpha^+$ is null, as well as the fact that $\varepsilon_\alpha\left(\mathbf{X}_\alpha\right)$ is assumed to be an hermitian operator, we are led to the expression :

$$2O_\alpha\varepsilon_\alpha\left(\mathbf{X}_\alpha\right) = \mathcal{P}_+\left[U_\alpha\left(\left(\frac{\partial}{\partial\alpha}+\left\langle.\right\rangle\right)H\left(\mathbf{X}_\alpha\right)\right)U_\alpha^+\right]$$
$$+\frac{i}{2}\varepsilon_\alpha\mathcal{P}_+\left(\nabla_{P_i}U_\alpha\nabla_{R_i}U_\alpha^+-\nabla_{R_i}U_\alpha\nabla_{P_i}U_\alpha^+\right) \quad (40)$$
$$-\frac{i}{2}\mathcal{P}_+\left(\nabla_{P_i}U_\alpha\nabla_{R_i}H\left(\mathbf{X}_\alpha\right)U_\alpha^+-\nabla_{R_i}U_\alpha\nabla_{P_i}H\left(\mathbf{X}_\alpha\right)U_\alpha^+\right)$$
$$-\frac{i}{2}\mathcal{P}_+\left(U_\alpha\nabla_{P_i}H\left(\mathbf{X}_\alpha\right)\nabla_{R_i}U_\alpha^+-U_\alpha\nabla_{R_i}H\left(\mathbf{X}_\alpha\right)\nabla_{P_i}U_\alpha^+\right)$$
$$-\frac{i}{2}\mathcal{P}_+\left(\nabla_{P_i}U_\alpha H\left(\mathbf{X}_\alpha\right)\nabla_{R_i}U_\alpha^+-\nabla_{R_i}U_\alpha H\left(\mathbf{X}_\alpha\right)\nabla_{P_i}U_\alpha^+\right)+H.C. \quad (41)$$

This can be rewritten in terms of physical operators **:**

$$O_\alpha\varepsilon_{\alpha_1}\left(\mathbf{X}_{\alpha_1}\right) = \mathcal{P}_+\left\{\frac{1}{2}\mathcal{A}_{\alpha_1}^{R_l}\nabla_{R_l}\varepsilon_{\alpha_1}+\nabla_{R_l}\varepsilon_{\alpha_1}\mathcal{A}_{\alpha_1}^{R_l}+\mathcal{A}_{\alpha_1}^{P_l}\nabla_{P_l}\varepsilon_{\alpha_1}+\nabla_{P_l}\varepsilon_{\alpha_1}\mathcal{A}_{\alpha_1}^{P_l}\right\}$$
$$+\frac{i}{4}\left\{\mathcal{P}_+\left\{\left[\varepsilon_\alpha,\mathcal{A}_\alpha^{R_l}\right]\mathcal{A}_\alpha^{P_l}-\left[\varepsilon_\alpha,\mathcal{A}_\alpha^{P_l}\right]\mathcal{A}_\alpha^{R_l}\right\}+H.C.\right\}+\mathcal{P}_+\left[U_\alpha\left(\left(\frac{\partial}{\partial\alpha}+\left\langle.\right\rangle\right)H\left(\mathbf{X}_\alpha\right)\right)U_\alpha^+\right] \quad (42)$$

Let us remark, that in most of the physical applications (in particular for Dirac and Bloch electrons) the term $\left(\frac{\partial}{\partial\alpha}+\langle.\rangle\right)H\left(\mathbf{X}_\alpha\right)$ will cancel**.**

C. The full system H and 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

$$\varepsilon\left(\mathbf{X}\right) = \mathcal{E}\left(\left[\exp\left(-\hbar\left\langle.\right\rangle\right)\mathcal{T}\exp\left[\int_{0<\alpha<\hbar}\exp\left(\alpha\left\langle.\right\rangle\right)O_\alpha\exp\left(-\alpha\left\langle.\right\rangle\right)d\alpha\right]\right]\varepsilon_0\left(\mathbf{X}\right)\right) \tag{43}$$

$$U\left(\mathbf{X}\right) = \mathcal{E}\left(\left[\exp\left(-\hbar\left\langle.\right\rangle\right)\mathcal{T}\exp\left[\int_{0<\alpha<\hbar}\exp\left(\alpha\left\langle.\right\rangle\right)N_\alpha\exp\left(-\alpha\left\langle.\right\rangle\right)d\alpha\right]\right]U_0\left(\mathbf{X}\right)\right) \tag{44}$$

where O_α and N_α are given respectively by Eqs.(42) and (36). The only pre-requirement is that the diagonal form at $\alpha=0$, $\varepsilon_0\left(\mathbf{R}_0,\mathbf{P}_0\right)$ is known, i.e., when $\mathbf{R}$ and $\mathbf{P}$ are considered as classical commuting variables (which means that $U_0\left(\mathbf{X}_0\right)$ is known). Of course these equations do not allow to find directly $\varepsilon\left(\mathbf{X}\right)$, $U\left(\mathbf{X}\right)$ since those quantities are involved on the R.H.S. of these relations. However, they allow us to produce the solutions for $\varepsilon\left(\mathbf{X}\right)$ and $U\left(\mathbf{X}\right)$ recursively in a series expansion in $\hbar$. As it will appear clearly later on, having both $\varepsilon\left(\mathbf{X}\right)$ and $U\left(\mathbf{X}\right)$ at order n in $\hbar$, and reinserting in the exponential of Eqs. (43) (44) allows us to find $\varepsilon\left(\mathbf{X}\right)$ and $U\left(\mathbf{X}\right)$ at order $n+1$ in $\hbar$. But before solving recursively the set of equations Eqs.(43) (44), we first compare the present approach with the one developed in article [5]

IV. LINK WITH THE DIFFERENTIAL EQUATION OF REF. [5]

In [5] we developed a different less general approach which led to the differential equation

$$\begin{aligned}\frac{d}{d\alpha}\varepsilon_\alpha\left(\mathbf{X}_\alpha\right) &= \left[\partial_\alpha U_\alpha\left(\mathbf{X}_\alpha\right)U_\alpha^+\left(\mathbf{X}_\alpha\right),\varepsilon_\alpha\left(\mathbf{X}_\alpha\right)\right]+\left\{\frac{1}{2}\mathcal{A}_\alpha^{R_l}\nabla_{R_l}\varepsilon_\alpha+\nabla_{R_l}\varepsilon_\alpha\mathcal{A}_\alpha^{R_l}+\mathcal{A}_\alpha^{P_l}\nabla_{P_l}\varepsilon_\alpha+\nabla_{P_l}\varepsilon_\alpha\mathcal{A}_\alpha^{P_l}\right\}\\ &+\frac{i}{2}\left\{\left[\varepsilon_\alpha,\mathcal{A}_\alpha^{R_l}\right]\mathcal{A}_\alpha^{P_l}-\left[\varepsilon_\alpha,\mathcal{A}_\alpha^{P_l}\right]\mathcal{A}_\alpha^{R_l}-\left[\varepsilon_\alpha,\left[\mathcal{A}_\alpha^{R_l},\mathcal{A}_\alpha^{P_l}\right]\right]\right\}\\ &+\frac{i}{2}\left\{Asym\left\{\nabla_{P_l}\nabla_{R_l}\varepsilon_\alpha\right\}-U_\alpha Asym\left\{\nabla_{P_l}\nabla_{R_l}H\left(\mathbf{X}_\alpha\right)\right\}U_\alpha^+-\left[\mathcal{B}_\alpha\varepsilon_\alpha-\varepsilon_\alpha\mathcal{B}_\alpha^+\right]\right\}\end{aligned} \tag{45}$$

which was coupled to the evolution of the transformation matrix $U_\alpha\left(\mathbf{X}_\alpha\right)$ as a function of α [5] :

$$0=\partial_\alpha U_\alpha(\mathbf{X}_\alpha)U_\alpha^+(\mathbf{X}_\alpha)+U_{\boldsymbol{\alpha}}(\mathbf{X}_{\boldsymbol{\alpha}})\partial_\alpha U_{\boldsymbol{\alpha}}^+(\mathbf{X}_{\boldsymbol{\alpha}})-\frac{i}{2}\left(\mathcal{B}_\alpha-\mathcal{B}_\alpha^+\right)-\frac{i}{2}\left[\mathcal{A}_\alpha^{R_l},\mathcal{A}_\alpha^{P_l}\right] \tag{46}$$

where $\mathcal{B}_\alpha=\left(Asym\left[\nabla_{R^l}\nabla_{P_l}U_\alpha\left(\mathbf{X}_\alpha\right)\right]\right)U_\alpha^+\left(\mathbf{X}_\alpha\right)$.With these two equations Eqs. (45) and (46) at hand, the diagonalization process can be performed. Actually, since all quantities are matrix valued and since $\varepsilon_\alpha\left(\mathbf{X}_\alpha\right)$ is by definition a diagonal matrix, we can separate the energy equation Eq. (45) in a diagonal and a off-diagonal part such that we are led to the following two equations

$$\frac{d}{d\alpha}\varepsilon_\alpha\left(\mathbf{X}_\alpha\right) = \mathcal{P}_+[\text{R.H.S. of Eq. 45}] \tag{47}$$

$$0 = \mathcal{P}_-[\text{R.H.S. of Eq. 45}] \tag{48}$$

In [5] it was claimed that those three Eqs. (46) (47) (48) allow us to determine recursively in powers of α the energy of the quantum system in question. Actually, the integration over α of Eq. (47) gives $\varepsilon_\alpha\left(\mathbf{X}_\alpha\right)$ at order n in α when knowing all quantities at order $n-1$. By the same token, Eqs. (48) and (46) (whose meaning is that $U_\alpha\left(\mathbf{X}_\alpha\right)$ is unitary at each order in α) involve $\partial_\alpha U_\alpha\left(\mathbf{X}_\alpha\right)$, and allow to recover $U_\alpha\left(\mathbf{X}_\alpha\right)$ 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 [5] we also provided two physical examples at the order $\hbar^2$.

Now we want to show that our solution Eq. (26) satisfies the differential equation Eq. (45). Indeed, from Eq. (17) we can write

$$
\begin{aligned}
\frac{\partial}{\partial\hbar}\varepsilon\left(\mathbf{X}_\hbar\right) &= \mathcal{E}\left(\left[\exp\left(-\hbar\left\langle .\right\rangle\right)\mathcal{T}\exp\left[\int_{0<\alpha_1<\hbar}\exp\left(\alpha_1\left\langle .\right\rangle\right)O_{\alpha_1}\exp\left(-\alpha_1\left\langle .\right\rangle\right)d\alpha_1\right]\right]\varepsilon_0\left(\mathbf{X}_\hbar\right)\right)\\
&= \left\langle .\right\rangle\varepsilon_\hbar\left(\mathbf{X}_\hbar\right)\\
&\quad+\mathcal{E}\left(e^{-\hbar\left\langle .\right\rangle}\sum_n\left[\int_{0<\alpha_n<...<\alpha_2<\hbar}e^{\hbar\left\langle .\right\rangle}O_\hbar...e^{-(\alpha_{n-2}-\alpha_{n-1})\left\langle .\right\rangle}O_{\alpha_{n-1}}e^{-(\alpha_{n-1}-\alpha_n)\left\langle .\right\rangle}O_{\alpha_n}e^{-\alpha_n\left\langle .\right\rangle}\right]\varepsilon_0\left(\mathbf{X}_\hbar\right)\right)\\
&= -\left\langle .\right\rangle\varepsilon_\hbar\left(\mathbf{X}_\hbar\right)\\
&\quad+O_\hbar\mathcal{E}\left(\sum_n\left[\int_{0<\alpha_n<...<\alpha_2<\hbar}e^{-(\hbar-\alpha_2)\left\langle .\right\rangle}O_{\alpha_2}...e^{-(\alpha_{n-2}-\alpha_{n-1})\left\langle .\right\rangle}O_{\alpha_{n-1}}e^{-(\alpha_{n-1}-\alpha_n)\left\langle .\right\rangle}O_{\alpha_n}e^{-\alpha_n\left\langle .\right\rangle}\right]\varepsilon_0\left(\mathbf{X}_\hbar\right)\right)\\
&= -\left\langle .\right\rangle\varepsilon_\hbar\left(\mathbf{X}_\hbar\right)\\
&\quad+O_\hbar\mathcal{E}e^{-\hbar\left\langle .\right\rangle}\left(\sum_n\left[\int_{0<\alpha_n<...<\alpha_2<\hbar}e^{\alpha_2\left\langle .\right\rangle}O_{\alpha_2}...e^{-(\alpha_{n-2}-\alpha_{n-1})\left\langle .\right\rangle}O_{\alpha_{n-1}}e^{-(\alpha_{n-1}-\alpha_n)\left\langle .\right\rangle}O_{\alpha_n}e^{-\alpha_n\left\langle .\right\rangle}\right]\varepsilon_0\left(\mathbf{X}_\hbar\right)\right)\\
&= -\left\langle .\right\rangle\varepsilon_\hbar\left(\mathbf{X}_\hbar\right)+O_\hbar\varepsilon_\hbar\left(\mathbf{X}_\hbar\right) \qquad (49)
\end{aligned}
$$

We have given previously the expression for $O_\hbar\varepsilon_\hbar\left(\mathbf{Y}_\hbar\right)$. Using that $\left\langle .\right\rangle\varepsilon_\hbar\left(\mathbf{X}_\hbar\right)=-\frac{i}{2}Asym\left\{\nabla_{P_l}\nabla_{R_l}\varepsilon_\alpha\left(\mathbf{X}_\alpha\right)\right\}$ and Eq. (46) one gets directly that $\left(\varepsilon\left(\mathbf{R},\mathbf{P}\right)-\varepsilon_0\left(\mathbf{R},\mathbf{P}\right)\right)$ is a solution of the differential (45).

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 naturally during the diagonalization and are more suitably to correspond to physical operators (for the physical discussion of this point see [8][6][5][9]).

From Eq.(18) one sees that the operator $O_\alpha=\left(\partial_\alpha+\left\langle .\right\rangle\right)$ acting on $\varepsilon_0\left(\mathbf{X}_\alpha\right)$ can be decomposed as a sum of a "translation" operator T and a "magnetisation" M operator (this terminology is explained in [5])

$$O_\alpha\varepsilon_0\left(\mathbf{X}_\alpha\right)=\left(T_\alpha+M_\alpha\right)\varepsilon_0\left(\mathbf{X}_\alpha\right). \qquad (50)$$

where the "magnetisation" operator acts as

$$M\varepsilon_0\left(\mathbf{X}_\alpha\right)=\frac{i}{2}\mathcal{P}_+\left\{\left[\varepsilon_\alpha,\mathcal{A}_\alpha^{R_l}\right]\mathcal{A}_\alpha^{P_l}-\left[\varepsilon_\alpha,\mathcal{A}_\alpha^{P_l}\right]\mathcal{A}_\alpha^{R_l}\right\}+\mathcal{P}_+\left[U_\alpha\left(\left(\frac{\partial}{\partial\alpha}+\left\langle .\right\rangle\right)H\left(\mathbf{X}_\alpha\right)\right)U_\alpha^+\right] \qquad (51)$$

and

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

It is very interesting to observe that the quantity $\mathcal{T}\exp\left[\int_{0<\alpha<\hbar}T_\alpha d\alpha\right]\varepsilon_0\left(\mathbf{X}\right)$ can be written in a compact form. Indeed let $A_\alpha^{\mathbf{R}}=\mathcal{P}_+\left[\mathcal{A}_\alpha^{\mathbf{R}}\right]$ and $A_\alpha^{\mathbf{P}}=\mathcal{P}_+\left[\mathcal{A}_\alpha^{\mathbf{P}}\right]$, with the following definitions for the "non-projected" Berry connections $\mathcal{A}_\alpha^{\mathbf{R}}=i\left[U_\alpha\boldsymbol{\nabla}_{\mathbf{P}}U_\alpha^+\right]$ and $\mathcal{A}_\alpha^{\mathbf{P}}=-i\left[U_\alpha\boldsymbol{\nabla}_{\mathbf{R}}U_\alpha^+\right]$, we can introduce the following transformation

$$\mathcal{T}\exp\left[\int_{0<\alpha<\hbar}T_\alpha d\alpha\right]\varepsilon_0\left(\mathbf{X}\right)=\varepsilon_0\left(\mathbf{x}\right) \qquad (52)$$

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

$$
\begin{aligned}
\mathbf{r} &= \mathbf{R}+\int_{0<\alpha<\hbar}A_\alpha^{\mathbf{R}}d\alpha\equiv\mathbf{R}+A_{\mathbf{R}}\\
\mathbf{p} &= \mathbf{P}+\int_{0<\alpha<\hbar}A_\alpha^{\mathbf{P}}d\alpha\equiv\mathbf{P}+A_{\mathbf{P}} \qquad (53)
\end{aligned}
$$

justifying the name translation operator (the identity can be checked by noting that both quantity satisfy the same differential equation $\frac{\partial}{\partial\hbar}X=T_\hbar X$).

Note that at the lowest order we have :

$$\begin{aligned} \mathbf{r} &= \mathbf{R} + \hbar A_0^{\mathbf{R}} \\ \mathbf{p} &= \mathbf{P} + \hbar A_0^{\mathbf{P}} \end{aligned} \tag{54}$$

where $A_0^{\mathbf{R}}$ and $A_0^{\mathbf{P}}$ are the usual "semiclassical Berry connections" defined previously [5].

From equations Eq. (53) we readily deduce the following non trivial algebra

$$\begin{aligned} [r_i, r_j] &= i\hbar^2 \Theta_{ij}^{rr} = i\hbar^2 \left(\nabla_{P_i} A_{R_j} - \nabla_{P_j} A_{R_i} \right) + \hbar^2 \left[A_{R_j}, A_{R_i} \right] \\ [p_i, p_j] &= i\hbar^2 \Theta_{ij}^{pp} = -i\hbar^2 \left(\nabla_{R_i} A_{P_j} - \nabla_{R_j} A_{P_i} \right) + \hbar^2 \left[A_{P_i}, A_{P_j} \right] \\ [p_i, r_j] &= -i\hbar\delta_{ij} + i\hbar^2 \Theta_{ij}^{pr} = -i\hbar\delta_{ij} - i\hbar^2 \left(\nabla_{R_i} A_{R_j} + \nabla_{P_j} A_{P_i} \right) + \hbar^2 \left[A_{P_i}, A_{R_j} \right] \end{aligned} \tag{55}$$

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 [5][6][8]. 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. (51) (52) will be very 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. (26), 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 $\varepsilon(\mathbf{R}, \mathbf{P})$.

A. First order in $\hbar$

At the first order we obviously get the following expression :

$$\begin{aligned} \varepsilon(\mathbf{X}) &= \varepsilon_0(\mathbf{X}) + \int_0^\hbar O_\alpha d\alpha \varepsilon_0(\mathbf{X}) \\ &= \varepsilon_0(\mathbf{X}) + \hbar \left(\frac{\partial}{\partial \alpha} + \langle . \rangle \right) \varepsilon_0(\mathbf{X}) \\ &= \varepsilon_0(\mathbf{x}) + \frac{i}{2} \mathcal{P}_+ \left\{ \left[\varepsilon_0(\mathbf{X}), \mathcal{A}_0^{R_l} \right] \mathcal{A}_0^{P_l} - \left[\varepsilon_0(\mathbf{X}), \mathcal{A}_0^{P_l} \right] \mathcal{A}_0^{R_l} \right\} \end{aligned} \tag{56}$$

One then recover the formula first derived in ref. [5] where $x = (\mathbf{r}, \mathbf{p})$ are given by the expression Eq. (53).

As previously mentioned we only need to have $U_0(\mathbf{Y})$ and thus the zeroth order Berry phases to get the energy expansion at the first order. Now with the first order expansion for the diagonalization matrix :

$$\begin{aligned} U(\mathbf{X}) &= U_0(\mathbf{X}) + \int_0^\hbar N_\alpha d\alpha U_0(\mathbf{X}) \equiv U_0(\mathbf{X}) + \hbar U_1(\mathbf{X}) \\ &= \left(1 - \hbar \left[., \varepsilon_0 \right]^{-1} . \left[\mathcal{P}_- \left\{ \frac{1}{2} \mathcal{A}_0^{R_l} \nabla_{R_l} \varepsilon_0(\mathbf{X}) + \nabla_{R_l} \varepsilon_0(\mathbf{X}) \mathcal{A}_0^{R_l} + \mathcal{A}_0^{P_l} \nabla_{P_l} \varepsilon_0(\mathbf{X}) + \nabla_{P_l} \varepsilon_0(\mathbf{X}) \mathcal{A}_0^{P_l} \right\} \right. \right. \\ &\quad \left. \left. - \frac{i}{2} \left\{ \left[\varepsilon_0(\mathbf{X}), \mathcal{A}_0^{R_l} \right] \mathcal{A}_0^{P_l} - \left[\varepsilon_0(\mathbf{X}), \mathcal{A}_0^{P_l} \right] \mathcal{A}_0^{R_l} \right\} \right] - \frac{i}{4} \left[\mathcal{A}_0^{R_l}, \mathcal{A}_0^{P_l} \right] \right) U_0(\mathbf{X}) \end{aligned} \tag{57}$$

the (non-diagonal) Berry connections at this approximation are given by :

$$\begin{aligned} \mathcal{A}^{\mathbf{R}} &= i \left[U_\hbar \nabla_{\mathbf{P}} U_\hbar^+ \right] = \mathcal{A}_0^{\mathbf{R}} + i\hbar \left[U_0 \nabla_{\mathbf{P}} U_1^+ \right] + \hbar U_1(\mathbf{X}) U_0^+(\mathbf{X}) \mathcal{A}_0^{\mathbf{R}} \equiv \mathcal{A}_0^{\mathbf{R}} + \hbar \mathcal{A}_1^{\mathbf{R}} \\ \mathcal{A}^{\mathbf{P}} &= -i \left[U_\hbar \nabla_{\mathbf{R}} U_\hbar^+ \right] = \mathcal{A}_0^{\mathbf{P}} + i\hbar \left[U_0 \nabla_{\mathbf{R}} U_1^+ \right] + \hbar U_1(\mathbf{X}) U_0^+(\mathbf{X}) \mathcal{A}_0^{\mathbf{P}} \equiv \mathcal{A}_0^{\mathbf{P}} + \hbar \mathcal{A}_1^{\mathbf{P}} \end{aligned} \tag{58}$$

B. Second order

To the second order, expanding the compact form of the energy operator leads to :

$$\varepsilon(\mathbf{X}) = \varepsilon_0(\mathbf{x}) + \int_0^\hbar O_\alpha d\alpha \varepsilon_0(\mathbf{X}) + \int_0^\hbar O_{\alpha_1} \int_0^{\alpha_1} O_{\alpha_2} d\alpha_2 d\alpha_1 \varepsilon_0(\mathbf{X}) + \hbar \langle \varepsilon_0(\mathbf{X}) \rangle$$

The last contribution is simply

$$\hbar \langle \varepsilon_0(\mathbf{X}) \rangle = \frac{i}{2} \hbar Asym \{ \nabla_{P_l} \nabla_{R_l} \varepsilon_0(\mathbf{X}) \}$$

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

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

where the Berry connections have to be expanded to the first order, whereas the second order contribution

$$\int_0^\hbar O_{\alpha_1} \int_0^{\alpha_1} O_{\alpha_2} d\alpha_2 d\alpha_1 \varepsilon_0(\mathbf{X}) - \hbar \langle \varepsilon_0(\mathbf{X}) \rangle$$

has to be expanded to the zeroth order in the Berry connections.

Notice that due to the integration process, the squared terms in $\mathcal{A}_0^{\mathbf{R}}$, $\mathcal{A}_0^{\mathbf{P}}$ as well as the first order terms in the Berry phase $\mathcal{A}_1^{\mathbf{R}}$ and$\mathcal{A}_1^{\mathbf{P}}$ get a $\frac{1}{2}$ factor. The consequence is that these contribution can be recombined to yield :

$$\begin{aligned}
\varepsilon(\mathbf{X}) &= \varepsilon_0(\mathbf{x}) + \frac{i}{2} \mathcal{P}_+ \left\{ \left[\varepsilon_0(\mathbf{x}), \mathcal{A}^{R_l} \right] \mathcal{A}^{P_l} - \left[\varepsilon_0(\mathbf{x}), \mathcal{A}^{P_l} \right] \mathcal{A}^{R_l} - \left[\varepsilon_0(\mathbf{x}), \left[\mathcal{A}^{R_l}, \mathcal{A}^{P_l} \right] \right] \right\} \\
&- \frac{1}{8} \mathcal{P}_+ \left\{ \left[\left[\varepsilon_0(\mathbf{x}), \mathcal{A}^{R_l} \right] \mathcal{A}^{P_l} - \left[\varepsilon_0(\mathbf{x}), \mathcal{A}^{P_l} \right] \mathcal{A}^{R_l}, \mathcal{A}^{R_l} \right] \mathcal{A}^{P_l} - \left[\left[\varepsilon_0(\mathbf{x}), \mathcal{A}^{R_l} \right] \mathcal{A}^{P_l} - \left[\varepsilon_0(\mathbf{x}), \mathcal{A}^{P_l} \right] \mathcal{A}^{R_l}, \mathcal{A}^{P_l} \right] \mathcal{A}^{R_l} \right\} \\
&+ \frac{i}{2} Asym \{ \nabla_{P_l} \nabla_{R_l} \varepsilon_0(\mathbf{x}) \}
\end{aligned} \tag{59}$$

where now :

$$\begin{aligned}
\mathbf{r} &= \mathbf{R} + \mathcal{A}^{\mathbf{R}} = \mathbf{R} + \int_0^\hbar \mathcal{P}_+ \mathcal{A}_{\alpha_1}^{\mathbf{R}} d\alpha_1 = \mathbf{R} + \hbar \mathcal{P}_+ \mathcal{A}_0^{\mathbf{R}} + \frac{\hbar}{2}^2 \mathcal{P}_+ \mathcal{A}_1^{\mathbf{R}} \equiv \mathbf{R} + \hbar A_0^{\mathbf{R}} + \frac{\hbar}{2}^2 A_1^{\mathbf{R}} \\
\mathbf{p} &= \mathbf{P} + \mathcal{A}^{\mathbf{P}} = \mathbf{P} + \int_0^\hbar \mathcal{P}_+ \mathcal{A}_{\alpha_1}^{\mathbf{P}} d\alpha_1 = \mathbf{P} + \hbar \mathcal{P}_+ \mathcal{A}_0^{\mathbf{P}} + \frac{\hbar}{2}^2 \mathcal{P}_+ \mathcal{A}_1^{\mathbf{P}} \equiv \mathbf{P} + \hbar A_0^{\mathbf{P}} + \frac{\hbar}{2}^2 A_1^{\mathbf{P}}
\end{aligned} \tag{60}$$

which of course satisfy the algebra Eq. (55).

Note that in the Berry connections A^{R_l}, and A^{P_l} one can safely replace the operators $(\mathbf{R}, \mathbf{P})$ by $(\mathbf{r}, \mathbf{p})$ at each order of the expansion.

VII. PHYSICAL APPLICATION: 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. Note that contrary to the FW which is not an expansion in $\hbar$, the method is valid for strong external fields (actually a FW transformation expanded into a power series in $\hbar$ was also recently proposed [7]).

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

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

At the first order in $\hbar$ we just need the zero order transformation

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

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

$$\begin{aligned} \mathcal{A}_0^R &= U_0 \mathbf{R} U_0^{-1} = i\hbar \frac{-\beta \boldsymbol{\alpha}.\mathbf{P}\mathbf{P} + E\left(E+m\right)\beta\boldsymbol{\alpha} - iE\mathbf{P}\times\boldsymbol{\Sigma}}{2E^2\left(E+m\right)} \\ \mathcal{A}_0^P &= U_0^i \mathbf{P} U_0^{-1} = 0 \end{aligned}$$

which leads to the Berry connections (we use the block diagonal projector $\mathcal{P}_+$):

$$\begin{aligned} A_0^{\mathbf{R}} &= \frac{\mathbf{P}\times\boldsymbol{\Sigma}}{2E\left(E+m\right)} \\ A_0^{\mathbf{P}} &= 0 \end{aligned}$$

For the second order we need the first order unitary matrix we can be deduce directly from Eq. 57

$$U_1 = \left[\left(1 + \frac{\beta}{2E}\mathcal{P}_-\left(\mathcal{A}_0^R\right).\boldsymbol{\nabla}_R V\right)\right] U_0$$

From U_1 and using Eqs. 58 we can compute the projected Berry connections to the second order in powers of $\hbar$ and thus write the dynamical operators as

$$\begin{aligned} \mathbf{r} &= \mathbf{R} + \hbar A_0^{\mathbf{R}} + \frac{\hbar}{2}^2 A_1^{\mathbf{R}} = \hbar \frac{\mathbf{P}\times\boldsymbol{\Sigma}}{2E\left(E+m\right)} + \frac{\hbar^2}{2}\beta \frac{E^2\boldsymbol{\nabla}_R V - \left[\mathbf{P}.\boldsymbol{\nabla}_R V\right]\mathbf{P}}{4E^5} \\ \mathbf{p} &= \mathbf{P} \end{aligned}$$

Now using expression Eq. 59 we arrive at the following expression for the diagonal representation of the energy operator

$$\begin{aligned} \varepsilon &= \beta E\left(\mathbf{r},\mathbf{p}\right) - \beta E\left(\mathbf{r},\mathbf{p}\right)\Theta_{ij}^{pr}\left(\mathbf{r},\mathbf{p}\right) + V\left(\mathbf{r}\right) \\ &= \beta\sqrt{\mathbf{p}^2+m^2} + \frac{\hbar^2}{2}\beta\boldsymbol{\nabla}_{\mathbf{r}}.\frac{E^2\boldsymbol{\nabla}_{\mathbf{r}}V - \left[\mathbf{p}.\boldsymbol{\nabla}_{\mathbf{r}}V\right]\mathbf{p}}{4E^5} + V\left(\mathbf{r}\right) \end{aligned} \tag{61}$$

This expression being fully relativistic, to compare with the usual FW [1] approach we consider the non-relativistic limit and expand our results 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) [1] :

$$\varepsilon = \frac{\mathbf{P}^2}{2m} - \frac{\mathbf{P}^4}{8m^3c^2} + \frac{1}{2m^2c^2}\frac{1}{R}\left(\frac{d}{dR}V\right)\mathbf{L}.\mathbf{S} + \frac{\hbar^2}{8m^2c^2}\boldsymbol{\nabla}^2 V$$

with $\mathbf{L} = \mathbf{R}\wedge\mathbf{P}$ the angular momentum and $\mathbf{S} = \hbar\boldsymbol{\sigma}/\mathbf{2}$ the spin. Note that it is the term order $\hbar^2$ in Eq. 61 which, in the non relativistic limit, leads to the Darwin term.

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 very compact form. This approach reveals a very rich mathematical structure very reminiscent of the stochastic calculus, and show once more the very important role played by Berry phases in these systems. It was also found that the diagonal representation of the energy is solution of a differential equation in $\hbar$ presented previously in [5] and which could only be solved recursively in a series expansion in $\hbar$. Actually the solution presented here can also be written explicitly in 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 to the simple case of a Dirac electron in an external electric field and recover the usual Pauli-Hamiltonian in the non relativistic limit. This approach is general and very promising. We leave for subsequent work its application to more complicated systems in condensed matter or relativistic particle physics.

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