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Semiclassical Diagonalization of Quantum Hamiltonian and Equations of Motion with Berry Phase Corrections

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It has been recently found that the equations of motion of several semiclassical systems must take into account terms arising from Berry phases contributions. Those terms are responsible for the spin Hall effect in semiconductor as well as the Magnus effect of light propagating in inhomogeneous media. Intensive ongoing research on this subject seems to indicate that a broad class of quantum systems may be affected by Berry phase terms. It is therefore important to find a general procedure allowing for the determination of semiclassical Hamiltonian with Berry Phase corrections. This article presents a general diagonalization method at order \hbar for a large class of quantum Hamiltonians directly inducing Berry phase corrections. As a consequence, Berry phase terms on both coordinates and momentum operators naturally arise during the diagonalization procedure. This leads to new equations of motion for a wide class of semiclassical system. As physical applications we consider here a Dirac particle in an electromagnetic or static gravitational field, and the propagation of a Bloch electrons in an external electromagnetic field.

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I. INTRODUCTION

Since the seminal work of Berry [1], the notion of Berry phase has found several applications in branches of quantum physics such as atomic and molecular physic, optic and gauge theories. Most studies consider the geometric phase that a wave function acquires when a quantum mechanical system has an adiabatic evolution. Yet, the Berry phase in momentum space has recently found unexpected applications in the topic of spintronics. Such a term may indeed be responsible for a transverse dissipationless spin-current in semiconductors in the presence of electric fields [2]. This effect is a particular case of the Spin-Hall effect which is now predicted and observed in many different physical situations and can be interpreted at the semiclassical level as due to the influence of Berry connections on semiclassical equations of motions of spinning particles, like electrons in electric [3] or magnetic field [4]. In the above cited examples, the semiclassical equations of motion where derived from an approximate semiclassical Hamiltonian in a representation where this latter is diagonal. It was then shown that a noncommutative geometry, originating from the presence of a Berry phase which turns out to be a spin-orbit coupling, underlies the semiclassical dynamics. Spin-orbit contributions on the propagation of light has also been the focus of several other works [3, 5, 6] and has led to a generalization of geometric optics called geometric spinoptics [7].

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 [8]. In a series of papers [9] (see also [10]), a new set of semiclassical equations with a Berry phase correction was proposed to account for the semiclassical dynamic of electrons in magnetic Bloch bands (in the usual one band approximation). These equations were derived by considering a wave packet in a band and using a time-dependent variational principle in a Lagrangian formulation. The derivation of a semiclassical Hamiltonian was shown to lead to difficulties in the presence of Berry phase terms [9]. The apparent non-canonical character of the equations of motion with Berry phase corrections led the authors of [11] to conclude that the naive phase space volume is not conserved in the presence of a Berry phase and a magnetic field. There is nevertheless an invariant measure as found by themselves, so the Liouville theorem is not really violated in the end. This invariant measure is actually a general result of the well-established theory of non-canonical Hamiltonian dynamics, as pointed out by a number of authors [12, 13, 14]. In [15], we presented an alternative approach for the derivation of the equations of motion of an electron in magnetic Bloch bands based on a direct semiclassical diagonalization of the full quantum Hamiltonian. This Hamiltonian approach allows deriving rigorously the semi classical equations of motion, including explicitly the role of the Berry curvature and showed many similarities with the description of a Dirac electron in an electromagnetic field as in [4]. In the present article the reader will find the details of the diagonalization sketched in [15]. The common feature of the Hamiltonian formulations discussed above is that a noncommutative geometry underlies the algebraic structure of both coordinates and momenta. Actually, a Berry phase contribution to the dynamical operators stems from the representation where the kinetic energy is diagonal (for instance Foldy-Wouthuysen or Bloch representation). The components of the coordinate and momentum become

noncommutative when interband transitions are neglected (adiabatic motion).

The previous discussion shows that Berry phase terms could be present in the semiclassical equations of motion of several physical systems ranging from electron in vacuum, in solid or in semiconductor to photon in inhomogeneous media, with potential application in the fields of spintronic and spinoptic. This in turn called for a general semiclassical Hamiltonian formalism from which semi classical dynamics of a quantum system can be derived. This paper presents a general method of diagonalization at order \hbar for a quantum mechanical Hamiltonian presenting bands structure, like for electrons in a periodic potential or for Dirac (massive or massless) like-Hamiltonian. Starting with an Hamiltonian depending only on an invariant momentum \mathbf{P} and whose diagonalization is known, we can introduce a dependence in the variable \mathbf{R} and diagonalize the Hamiltonian in four steps (discussed in the text). During this process of diagonalization, we show that both position and momentum operators acquire a Berry-phase contribution making both the coordinate and momentum algebra noncommutative, in contrast with the approach of [9], where the momentum is always invariant. As physical applications and to check to validity of our method we further consider the case of Dirac particle in an electromagnetic field and compare with the semiclassical diagonalization given in [4]. We also consider the case of a Dirac particle in a static gravitational field where we can compare with the articles [16, 17]. As a last application, we detail the case of the propagation of a Bloch electron (spinless) in an external electromagnetic field already discussed in [15]. This various physical applications show that our semiclassical Hamiltonian diagonalization approach is potentially promising since it unifies several apparently unrelated problematic in one formalism.

The paper is organized as follows. In section II we develop our formalism in the case of a general Hamiltonian which has an energy bands structure. We then derive the very general equations of motion in this case. Section III is devoted to the application of our method to the case of the Dirac Hamiltonian in an electromagnetic field but in a flat space, and to the diagonalization of the Dirac Hamiltonian in a symmetric static gravitational field, allowing us to check the validity of our method. Section IV retrieves the equations of motion for an electron in a periodic potential within our general set up. Section V is for the conclusion.

II. A GENERAL PROCESS OF SEMICLASSICAL DIAGONALIZATION.

In this section we present the method to diagonalize at the semiclassical order (\hbar) a quantum mechanical system with canonical variables \mathbf{P} and \mathbf{R} , where \mathbf{P} is the generator of some translation symmetry, the usual momentum for instance, or the magnetic translation operator in solid state Physics. We assume further that the Hamiltonian can be written as a matrix of a certain size $H_0(\mathbf{P}, \mathbf{R})$. The archetype example is the Dirac Hamiltonian, but in appendix 2 we show how a spinless electron in a periodic potential fits also in this set up. Our purpose is to solve the exact diagonalization for $H_0(\mathbf{P}, \mathbf{R})$ at order \hbar , when the diagonalization of a fictitious Hamiltonian $H_0(\mathbf{P}, \mathbf{r})$ is known for a parameter \mathbf{r} (replacing \mathbf{R}) which is supposed to commute with \mathbf{P} (for instance this may be the Foldy-Wouthuysen transformation [18] for a free Dirac particle). Then we will show how to compute the quantum corrections (at leading order in \hbar) that were neglected during this formal diagonalization (where position and momenta were considered as commuting quantities). The idea behind this procedure is that it is much easier to solve the diagonalization for $H_0(\mathbf{P}, \mathbf{r})$, as seen in our applications, and only then turn to $H_0(\mathbf{P}, \mathbf{R})$.

A. Preliminary : Products of operators series.

To develop our process of diagonalization, the semiclassical expression of products of symmetrized expressions $S(\mathbf{P}, \mathbf{R})$ depending on the canonical couple of variables \mathbf{P} and \mathbf{R} is required. These expressions are also assumed to have series expansions in \mathbf{P} and \mathbf{R} whose coefficients can be of a matrix form (this last assumption allowing to deal with Dirac Hamiltonians). Let us consider two such expressions $S_1(\mathbf{P}, \mathbf{R})$ and $S_2(\mathbf{P}, \mathbf{R})$, supposed to be symmetrized in \mathbf{P} and \mathbf{R} . By symmetrization, we mean that each expression has been written in a form where all the powers of \mathbf{P} have been put half on the left and half on the right of the expression. Our aim is now to write the product $S_1(\mathbf{P}, \mathbf{R}) S_2(\mathbf{P}, \mathbf{R})$ as a symmetric expression in terms of \mathbf{P} and \mathbf{R} . This is easy to realize at order \hbar , since in that case, pushing half of the powers of \mathbf{P} in $S_2(\mathbf{P}, \mathbf{R})$ on the left and half the powers of $S_1(\mathbf{P}, \mathbf{R})$ on the right is equivalent to the computation of some commutators. One can easily see that at order \hbar

$$S_1(\mathbf{P}, \mathbf{R}) S_2(\mathbf{P}, \mathbf{R}) = \text{Sym}(S_1(\mathbf{P}, \mathbf{R}) S_2(\mathbf{P}, \mathbf{R})) + \frac{i}{2} \hbar \text{Asym} \nabla_{R_i} \nabla_{P^i} [S_1(\mathbf{P}, \mathbf{R}) S_2(\mathbf{P}, \mathbf{R})] \quad (1)$$

where $\text{Sym}(S_1(\mathbf{P}, \mathbf{R}) S_2(\mathbf{P}, \mathbf{R}))$ is the symmetrized expression for the product, and Asym is defined through

$$\text{Asym} \nabla_{R_i} \nabla_{P^i} [S_1(\mathbf{P}, \mathbf{R}) S_2(\mathbf{P}, \mathbf{R})] = \nabla_{R_i} S_1(\mathbf{P}, \mathbf{R}) \nabla_{P^i} S_2(\mathbf{P}, \mathbf{R}) - \nabla_{P^i} S_1(\mathbf{P}, \mathbf{R}) \nabla_{R_i} S_2(\mathbf{P}, \mathbf{R}) \quad (2)$$

This formula can be easily generalized to an arbitrary product of n terms, but for the sequel of this paper, only three will be needed

$$\begin{aligned}
S_1(\mathbf{P}, \mathbf{R}) S_2(\mathbf{P}, \mathbf{R}) S_3(\mathbf{P}, \mathbf{R}) &= \text{Sym}(S_1(\mathbf{P}, \mathbf{R}) S_2(\mathbf{P}, \mathbf{R}) S_3(\mathbf{P}, \mathbf{R})) \\
&+ \frac{i}{2} \hbar \text{Asym} \nabla_{R_l} \nabla_{P^l} [S_1(\mathbf{P}, \mathbf{R}) S_2(\mathbf{P}, \mathbf{R})] S_3(\mathbf{P}, \mathbf{R}) \\
&+ \frac{i}{2} \hbar S_1(\mathbf{P}, \mathbf{R}) \text{Asym} \nabla_{R_l} \nabla_{P^l} [S_2(\mathbf{P}, \mathbf{R}) S_3(\mathbf{P}, \mathbf{R})] \\
&+ \frac{i}{2} \hbar S_1(\mathbf{P}, \mathbf{R}) \text{Asym} \nabla_{R_l} \nabla_{P^l} [S_1(\mathbf{P}, \mathbf{R})_{S_2(\mathbf{P}, \mathbf{R})} S_3(\mathbf{P}, \mathbf{R})]
\end{aligned} \tag{3}$$

where

$$\begin{aligned}
&\text{Asym} \nabla_{R_l} \nabla_{P^l} [S_1(\mathbf{P}, \mathbf{R})_{S_2(\mathbf{P}, \mathbf{R})} S_3(\mathbf{P}, \mathbf{R})] \\
&= [\nabla_{R_l} S_1(\mathbf{P}, \mathbf{R})] S_2(\mathbf{P}, \mathbf{R}) \nabla_{P^l} S_3(\mathbf{P}, \mathbf{R}) - [\nabla_{P^l} S_1(\mathbf{P}, \mathbf{R})] S_2(\mathbf{P}, \mathbf{R}) \nabla_{R_l} S_3(\mathbf{P}, \mathbf{R})
\end{aligned} \tag{4}$$

B. Diagonalization with a parameter r

Let us consider a general Hamiltonian $H_0(\mathbf{P}, \mathbf{R})$ which admits a series expansion in \mathbf{P} and \mathbf{R} written here for convenience in a symmetrical form. To perform the semi classical diagonalization of this operator, we first consider in this subsection a fictitious Hamiltonian $H_0(\mathbf{P}, \mathbf{r})$ where a parameter \mathbf{r} commuting with \mathbf{P} has replaced the operator \mathbf{R} . We further assume that $H_0(\mathbf{P}, \mathbf{r})$ is known to be exactly diagonalized through a matrix $U(\mathbf{P}, \mathbf{r}) \equiv U$.

As an typical example we can consider the following kind of Dirac Hamiltonian

$$H_0 = \alpha \cdot (\mathbf{P} - \mathbf{A}(\mathbf{r})) + \beta m \tag{5}$$

where $\mathbf{A}(\mathbf{r})$ mimics a formal magnetic potential. The potential $\mathbf{A}(\mathbf{r})$ being \mathbf{R} independent, it only shifts the momentum for each value of \mathbf{r} . As a consequence, the usual Foldy Wouthuysen [18] transformation expressed in terms of $\mathbf{P} - \mathbf{A}$ instead of \mathbf{P} , diagonalizes the Dirac Hamiltonian exactly.

Going back to the general case, the diagonalization of $H_0(\mathbf{P}, \mathbf{r})$ will be written as

$$\varepsilon(\mathbf{P}, \mathbf{r}) = U(\mathbf{P}, \mathbf{r}) H_0(\mathbf{P}, \mathbf{r}) U^+(\mathbf{P}, \mathbf{r}) \tag{6}$$

where $\varepsilon(\mathbf{P}, \mathbf{r})$ is a diagonal matrix. For later use, let us notice that we have $U(\mathbf{P}, \mathbf{r}) \mathbf{P} U^+(\mathbf{P}, \mathbf{r}) = \mathbf{P}$.

To gain some hints from our initial diagonalization, let us also remark that if $\varepsilon(\mathbf{P}, \mathbf{r})$ can be expanded in series as

$$\varepsilon(\mathbf{P}, \mathbf{r}) = \sum \prod_i (\mathbf{A}_{k_i}^i(\mathbf{r}) \cdot \mathbf{P}^{k_i}) \tag{7}$$

where the $A_k^i(\mathbf{r})$ are some matrices commuting with \mathbf{P} , it can be written

$$\varepsilon(\mathbf{P}, \mathbf{r}) = \frac{1}{2} \left[\sum \prod_i (\mathbf{A}_{k_i}^i(\mathbf{r})) \prod_i \mathbf{P}^{k_i} + \prod_i \mathbf{P}^{k_i} \prod_i (\mathbf{A}_{k_i}^i(\mathbf{r})) \right]. \tag{8}$$

Note moreover that in general, the diagonalization actually involves a symmetrization process

$$\varepsilon(\mathbf{P}, \mathbf{r}) = \sum \frac{1}{n!} \sum_{\sigma \in \text{permutations}} \prod_i (\mathbf{A}_{\sigma(k_i)}^i(\mathbf{r}) \cdot \mathbf{P}^{\sigma(k_i)}) \tag{9}$$

where $n!$ is a generic notation to denote the number of permutations involved in exchanging the indices k_i . In practice it will never be needed. As an example, think of the Dirac Hamiltonian diagonalization, which involves some products $\alpha \cdot \mathbf{P} \alpha \cdot \mathbf{P}$, rearranged as

$$\frac{1}{2} [\alpha_i P_i \alpha_j P_j + \alpha_j P_j \alpha_i P_i] = [\alpha_i \alpha_j + \alpha_j \alpha_i] P_i P_j \tag{10}$$

Since the $\mathbf{A}_k^i(\mathbf{r})$ do not depend on R , one has also

$$\begin{aligned} \varepsilon(\mathbf{P}, \mathbf{r}) &= \sum_{\sigma \in \text{permutations}} \sum_i \prod_i \left(\mathbf{A}_{\sigma(k_i)}^i(\mathbf{r}) \cdot \mathbf{P}^{k_i} \right) = \frac{1}{2} \sum \frac{1}{n!} \left[\sum_{\sigma \in \text{permutations}} \prod_i \left(\mathbf{A}_{\sigma(k_i)}^i(\mathbf{r}) \right) \right] \prod_i \mathbf{P}^{k_i} \\ &+ \frac{1}{2} \sum \prod_i \mathbf{P}^{k_i} \frac{1}{n!} \left[\sum_{\sigma \in \text{permutations}} \prod_i \left(\mathbf{A}_{\sigma(k_i)}^i(\mathbf{r}) \right) \right] \end{aligned} \quad (11)$$

The important consequence here is that the matrix

$$\left[\sum_{\sigma \in \text{permutations}} \prod_i \left(\mathbf{A}_{\sigma(k_i)}^i(\mathbf{r}) \right) \right] \quad (12)$$

is thus Diagonal. Let us note that these symmetrizations are unnecessary here, but will be of a practical interest when dealing with the exact diagonalization.

C. Introducing the R dependence. The transformation Ansatz.

We are now going to reintroduce \mathbf{R} into H_0 in order to diagonalize exactly $H_0(\mathbf{P}, \mathbf{R})$ at the \hbar order. In the following symmetrization in \mathbf{R} and \mathbf{P} will be assumed in all expressions. To find the diagonalization transformation for $H_0(\mathbf{P}, \mathbf{R})$, we will use the following method. First notice that the Hamiltonian $H_0(\mathbf{P}, \mathbf{R})$ is "almost" diagonalized, that is diagonalized at zeroth order in \hbar , through the transformation $U(\mathbf{P}, \mathbf{R})$ (which is also symmetrized given our convention).

However, through the symmetrization process, the matrix $U(\mathbf{P}, \mathbf{R})$ does not remain unitary. As a consequence, we will rather consider a matrix $U(\mathbf{P}, \mathbf{R}) + X$, where X is a contribution of order \hbar that ensures the unitarity of the transformation at order \hbar .

The matrix X can be explicitly computed. Actually, from the unitary conditions

$$(U(\mathbf{P}, \mathbf{R}) + X)(U^+(\mathbf{P}, \mathbf{R}) + X^+) = 1 \quad (13)$$

and

$$(U^+(\mathbf{P}, \mathbf{R}) + X^+)(U(\mathbf{P}, \mathbf{R}) + X) = 1 \quad (14)$$

or equivalently

$$\begin{aligned} U(\mathbf{P}, \mathbf{R})U^+(\mathbf{P}, \mathbf{R}) + XU^+(\mathbf{P}, \mathbf{R}) + U(\mathbf{P}, \mathbf{R})X^+ &= 1 \\ U^+(\mathbf{P}, \mathbf{R})U(\mathbf{P}, \mathbf{R}) + U^+(\mathbf{P}, \mathbf{R})X + X^+U(\mathbf{P}, \mathbf{R}) &= 1 \end{aligned} \quad (15)$$

one see that X should satisfies the condition

$$U^+(\mathbf{P}, \mathbf{R})U(\mathbf{P}, \mathbf{R}) + U^+(XU^+(\mathbf{P}, \mathbf{R}) + U(\mathbf{P}, \mathbf{R})X^+)U = 1 \quad (16)$$

To solve this equation, let us first notice that $U(\mathbf{P}, \mathbf{R})U^+(\mathbf{P}, \mathbf{R}) \neq 1$ since $U(\mathbf{P}, \mathbf{R})$ is not unitary. The crucial point here and in the sequel of this paper is the computation of a product of expressions in which the \mathbf{R} dependence has been introduced. To do so let us use the initial relation

$$U(\mathbf{P}, \mathbf{r})U^+(\mathbf{P}, \mathbf{r}) = 1 \quad (17)$$

expanded in a symmetric series (as we did for the Hamiltonian)

$$\begin{aligned} U(\mathbf{P}, \mathbf{r})U^+(\mathbf{P}, \mathbf{r}) &= \frac{1}{2} \sum \left[\frac{1}{n!} \sum_{\sigma \in \text{permutations}} \prod_i \left(\mathbf{B}_{\sigma(k_i)}^i(\mathbf{r}) \right) \right] \prod_i \mathbf{P}^{k_i} \\ &+ \frac{1}{2} \sum \prod_i \mathbf{P}^{k_i} \left[\frac{1}{n!} \sum_{\sigma \in \text{permutations}} \prod_i \left(\mathbf{B}_{\sigma(k_i)}^i(\mathbf{r}) \right) \right] = 1. \end{aligned} \quad (18)$$

Therefore the series expansion $\sum \left[\frac{1}{n!} \sum_{\sigma \in \text{permutations}} \prod_i \left(\mathbf{B}_{\sigma(k_i)}^i(\mathbf{r}) \right) \right] \prod_i \mathbf{P}^{k_i}$ reduces to one constant term : the identity matrix.

Now, going back to $U(\mathbf{P}, \mathbf{R})$, we use the symmetrization formula (1)

$$\begin{aligned} U(\mathbf{P}, \mathbf{R})U^+(\mathbf{P}, \mathbf{R}) &= \frac{1}{2} \sum \left[\frac{1}{n!} \sum_{\sigma \in \text{permutations}} \prod_i \left(\mathbf{B}_{\sigma(k_i)}^i(\mathbf{r}) \right) \right] \prod_i \mathbf{P}^{k_i} \\ &+ \frac{1}{2} \sum \prod_i \mathbf{P}^{k_i} \left[\frac{1}{n!} \sum_{\sigma \in \text{permutations}} \prod_i \left(\mathbf{B}_{\sigma(k_i)}^i(\mathbf{R}) \right) \right] \\ &+ \frac{i}{2} \hbar \text{Asym} \nabla_{R_l} \nabla_{P^l} [U^+(\mathbf{P}, \mathbf{R})U(\mathbf{P}, \mathbf{R})] \end{aligned} \quad (19)$$

Since our result about the recombinations of the series expansion of $\left[\sum_{\sigma \in \text{permutations}} \prod_i \left(\mathbf{B}_{\sigma(k_i)}^i(\mathbf{r}) \right) \right]$ applies also to $\left[\sum_{\sigma \in \text{permutations}} \prod_i \left(\mathbf{B}_{\sigma(k_i)}^i(\mathbf{R}) \right) \right]$ after replacing \mathbf{r} by \mathbf{R} , one has :

$$\begin{aligned} U(\mathbf{P}, \mathbf{R})U^+(\mathbf{P}, \mathbf{R}) &= 1 + \frac{i}{2} \hbar \text{Asym} \nabla_{R_l} \nabla_{P^l} [U(\mathbf{P}, \mathbf{R})U^+(\mathbf{P}, \mathbf{R})] \\ &= 1 - \frac{i}{2\hbar} [\mathcal{A}_{P_l}, \mathcal{A}_{R_l}] \end{aligned} \quad (20)$$

where we have defined the Berry phases as

$$\begin{aligned} \mathcal{A}_R &= i\hbar U(\mathbf{P}, \mathbf{R}) \nabla_P U^+(\mathbf{P}, \mathbf{R}) \\ \mathcal{A}_P &= -i\hbar U(\mathbf{P}, \mathbf{R}) \nabla_R U^+(\mathbf{P}, \mathbf{R}). \end{aligned} \quad (21)$$

Similarly, we have also:

$$\begin{aligned} U^+(\mathbf{P}, \mathbf{R})U(\mathbf{P}, \mathbf{R}) &= 1 + \frac{i}{2} \hbar \text{Asym} \nabla_{R_l} \nabla_{P^l} [U^+(\mathbf{P}, \mathbf{R})U(\mathbf{P}, \mathbf{R})] \\ &= 1 - U^+(\mathbf{P}, \mathbf{R}) \frac{i}{2\hbar} [\mathcal{A}_{P_l}, \mathcal{A}_{R_l}] U(\mathbf{P}, \mathbf{R}) \end{aligned} \quad (22)$$

Let us note that, as can be checked easily, the Berry phases are Hermitian. So is $\frac{i}{2\hbar} [\mathcal{A}_{P_l}, \mathcal{A}_{R_l}]$. Therefore we can solve our problem with

$$\begin{aligned} XU^+(\mathbf{P}, \mathbf{R}) &= \frac{i}{4\hbar} [\mathcal{A}_{P_l}, \mathcal{A}_{R_l}] \\ U(\mathbf{P}, \mathbf{R})X^+ &= \frac{i}{4\hbar} [\mathcal{A}_{P_l}, \mathcal{A}_{R_l}] \end{aligned} \quad (23)$$

Let us make an important remark at this point. Our choice for X is obviously not unique. Actually, it has been chosen to ensure the unitarity of the transformation and to obtain a transformation that reduces to the initial one when \mathbf{P} and \mathbf{R} do commute. We could thus add to X an expression like δXU where δX is anti-Hermitian. It is easy to see that the operator $U(\mathbf{P}, \mathbf{R}) + X + \delta XU$ is still unitary. However, we will soon see that this non unicity is irrelevant and that our choice is sufficient to perform the diagonalization at order \hbar .

D. The quasidiagonalization

We will now consider the following quasi-diagonalization transformation

$$[(U(\mathbf{P}, \mathbf{R}) + X)H_0(\mathbf{P}, \mathbf{R})(U^+(\mathbf{P}, \mathbf{R}) + X^+)] \quad (24)$$

To compute this last expression, decompose it at the first order in \hbar as

$$\begin{aligned} &U(\mathbf{P}, \mathbf{R})H_0((\mathbf{P}, \mathbf{R}))U^+(\mathbf{P}, \mathbf{R}) \\ &+ XH_0(\mathbf{P}, \mathbf{R})U^+(\mathbf{P}, \mathbf{R}) + U(\mathbf{P}, \mathbf{R})H_0(\mathbf{P}, \mathbf{R})X^+ \\ \simeq &U((\mathbf{P}, \mathbf{R}))H_0((\mathbf{P}, \mathbf{R}))U^+((\mathbf{P}, \mathbf{R})) + XU^+((\mathbf{P}, \mathbf{R}))\varepsilon((\mathbf{P}, \mathbf{R})) \\ &+ \varepsilon(\mathbf{P}, \mathbf{R})U(\mathbf{P}, \mathbf{R})X^+ \end{aligned} \quad (25)$$

Let us first have a look to $U(\mathbf{P}, \mathbf{R}) H_0(\mathbf{P}, \mathbf{R}) U^+(\mathbf{P}, \mathbf{R})$ and consider it, as before, as a series of products of operators

$$U(\mathbf{P}, \mathbf{R}) H_0(\mathbf{P}, \mathbf{R}) U^+(\mathbf{P}, \mathbf{R}) = \sum \prod_i (\mathbf{A}_{k_i}^i(\mathbf{R}) \cdot \mathbf{P}^{k_i}) \quad (26)$$

We use the same trick as in subsections B and C, and start the symmetrization process by first writing the non symmetrized series expansion

$$U(\mathbf{P}, \mathbf{R}) H_0(\mathbf{P}, \mathbf{R}) U^+(\mathbf{P}, \mathbf{R}) = \sum \frac{1}{n!} \sum_{\sigma \in \text{permutations}} \prod_i (\mathbf{A}_{\sigma(k_i)}^i(\mathbf{R}) \cdot \mathbf{P}^{\sigma(k_i)}) \quad (27)$$

If the matrices $\mathbf{A}_{\sigma(k)}^i(\mathbf{R})$ were commuting with the $\mathbf{P}^{\sigma(k)}$ we would recover the series expansion of $\varepsilon(\mathbf{P}, \mathbf{R})$ given in the subsection B. The variable \mathbf{R} being then seen as a parameter, it would not prevent us from diagonalizing exactly. But now, since, \mathbf{R} do not commute with \mathbf{P} , one has rather

$$\begin{aligned} U(\mathbf{P}, \mathbf{R}) H_0(\mathbf{P}, \mathbf{R}) U^+(\mathbf{P}, \mathbf{R}) &= \sum \frac{1}{n!} \sum_{\sigma \in \text{permutations}} \prod_i (\mathbf{A}_{\sigma(k_i)}^i(\mathbf{R}) \cdot \mathbf{P}^{\sigma(k_i)}) \\ &= \frac{1}{2} \sum \left[\frac{1}{n!} \sum_{\sigma \in \text{permutations}} \prod_i (\mathbf{A}_{\sigma(k_i)}^i(\mathbf{R})) \right] \prod_i \mathbf{P}^{k_i} \\ &\quad \frac{1}{2} \sum \prod_i \mathbf{P}^{k_i} \left[\frac{1}{n!} \sum_{\sigma \in \text{permutations}} \prod_i (\mathbf{A}_{\sigma(k_i)}^i(\mathbf{R})) \right] + [\text{commutators}] \end{aligned} \quad (28)$$

We can compute the first two terms of the right hand side by the same trick as before. Actually, by construction, the coefficients of the series expansion of

$$\left[\sum_{\sigma \in \text{permutations}} \prod_i (\mathbf{A}_{\sigma(k_i)}^i(\mathbf{R})) \right] \quad (29)$$

in the variable \mathbf{R} , are the same as the coefficients (which are diagonal) of the expansion of

$$\left[\sum_{\sigma \in \text{permutations}} \prod_i (\mathbf{A}_{\sigma(k_i)}^i(\mathbf{r})) \right] \quad (30)$$

in the parameter \mathbf{r} . As a consequence,

$$\frac{1}{2} \sum \left[\frac{1}{n!} \sum_{\sigma \in \text{permutations}} \prod_i (\mathbf{A}_{\sigma(k_i)}^i(\mathbf{R})) \right] \prod_i \mathbf{P}^{k_i} + \frac{1}{2} \sum \prod_i \mathbf{P}^{k_i} \left[\frac{1}{n!} \sum_{\sigma \in \text{permutations}} \prod_i (\mathbf{A}_{\sigma(k_i)}^i(\mathbf{R})) \right] \quad (31)$$

is the series expansion of $\varepsilon(\mathbf{P}, \mathbf{R})$, the powers of \mathbf{P} being rejected symmetrically to the left and to the right.

As an example, consider again the case of the Dirac Hamiltonian with an electromagnetic field. The free "Benchmark" case is $\varepsilon^2(\mathbf{P}) = \mathbf{P}^2$, and given our conventions, replacing \mathbf{P} by $\mathbf{P} - \mathbf{A}(\mathbf{R})$ leads us to define $\varepsilon^2(\mathbf{P} - \mathbf{A}(\mathbf{R})) = \mathbf{P}^2 - \mathbf{A}(\mathbf{R}) \cdot \mathbf{P} - \mathbf{P} \cdot \mathbf{A}(\mathbf{R}) + \mathbf{A}^2(\mathbf{R})$, which is simply the usual operator $(\mathbf{P} - \mathbf{A}(\mathbf{R}))^2$. By the same way, we obtain as a series expansion

$$\varepsilon(\mathbf{P} - \mathbf{A}(\mathbf{R})) = \varepsilon(\mathbf{P}) - \frac{1}{2} \left(\mathbf{A}(\mathbf{R}) \cdot \frac{\mathbf{P}}{\mathbf{P}^2} + \frac{\mathbf{P}}{\mathbf{P}^2} \cdot \mathbf{A}(\mathbf{R}) \right) + \frac{1}{4} \left[\frac{1}{\mathbf{P}^2} \mathbf{A}^2(\mathbf{R}) + \mathbf{A}^2(\mathbf{R}) \frac{1}{\mathbf{P}^2} \right] + \dots \quad (32)$$

The last term in the right hand side of (28) involves just half the commutators obtained in pushing the momentum operators to the left or the right. As explained in the subsection A Eq.(3), they are simply given by

$$[\text{commutators}] = \frac{i}{2} \hbar \text{Asym} \nabla_{R_l} \nabla_{P^l} \left[\sum \prod_i \mathbf{A}_{k_i}^i(\mathbf{R}) \cdot \mathbf{P}^{k_i} \right] = \frac{i}{2} \hbar \text{Asym} \nabla_{R_l} \nabla_{P^l} [U(\mathbf{P}, \mathbf{R}) H_0(\mathbf{P}, \mathbf{R}) U^+(\mathbf{P}, \mathbf{R})] \quad (33)$$

As a consequence, we can write

$$U(\mathbf{P}, \mathbf{R}) H_0(\mathbf{P}, \mathbf{R}) U^+(\mathbf{P}, \mathbf{R}) = \varepsilon(\mathbf{P}, \mathbf{R}) + \frac{i}{2} \hbar \text{Asym} \nabla_{R_i} \nabla_{P_i} [U(\mathbf{P}, \mathbf{R}) H_0(\mathbf{P}, \mathbf{R}) U^+(\mathbf{P}, \mathbf{R})] \quad (34)$$

A lengthy but straightforward computation presented in appendix 1 leads to

$$\begin{aligned} U(\mathbf{P}, \mathbf{R}) H_0(\mathbf{P}, \mathbf{R}) U^+(\mathbf{P}, \mathbf{R}) &= \varepsilon(\mathbf{P}, \mathbf{R}) + \frac{1}{2} [\mathcal{A}_{R_i} \nabla_{R_i} \varepsilon(\mathbf{P}, \mathbf{R}) + \nabla_{R_i} \varepsilon(\mathbf{P}, \mathbf{R}) \mathcal{A}_{R_i}] \\ &+ \frac{1}{2} [\mathcal{A}_{P_i} \nabla_{P_i} \varepsilon(\mathbf{P}, \mathbf{R}) + \nabla_{P_i} \varepsilon(\mathbf{P}, \mathbf{R}) \mathcal{A}_{P_i}] \\ &- \frac{i}{2\hbar} [\varepsilon(\mathbf{P}, \mathbf{R}), \mathcal{A}_{P_i}] \mathcal{A}_{R_i} + \frac{i}{2\hbar} [\varepsilon(\mathbf{P}, \mathbf{R}), \mathcal{A}_{R_i}] \mathcal{A}_{P_i} \\ &+ \frac{i}{2\hbar} [\mathcal{A}_{R_i}, \mathcal{A}_{P_i}] \varepsilon(\mathbf{P}, \mathbf{R}), \end{aligned} \quad (35)$$

where we have introduced the transformed variables at order \hbar through the Berry Phases

$$\mathbf{r} = (U(\mathbf{P}, \mathbf{R}) + X) \mathbf{R} (U^+(\mathbf{P}, \mathbf{R}) + X^+) \quad (36)$$

$$\simeq \mathbf{R} + [i\hbar U(\mathbf{R}) \nabla_P U^+(\mathbf{R})]$$

$$= \mathbf{R} + \mathcal{A}_R$$

$$\mathbf{p} = U(\mathbf{P}, \mathbf{R}) \mathbf{P} U^+(\mathbf{P}, \mathbf{R}) \quad (37)$$

$$\simeq \mathbf{P} - [i\hbar U(\mathbf{P}, \mathbf{R}) \nabla_R U^+(\mathbf{P}, \mathbf{R})]$$

$$= \mathbf{P} + \mathcal{A}_P \quad (38)$$

To end up with the quasi-diagonalization, we have to add the expression

$$XU^+(\mathbf{P}, \mathbf{R}) \varepsilon(\mathbf{P}, \mathbf{R}) + \varepsilon(\mathbf{P}, \mathbf{R}) U(\mathbf{P}, \mathbf{R}) X^+ \quad (39)$$

Given the expression obtained previously for $XU^+(\mathbf{P}, \mathbf{R})$, we have thus

$$\begin{aligned} &XU^+(\mathbf{P}, \mathbf{R}) \varepsilon(\mathbf{P}, \mathbf{R}) + \varepsilon(\mathbf{P}, \mathbf{R}) U(\mathbf{P}, \mathbf{R}) X^+ \\ &= -\frac{i}{4\hbar} [\mathcal{A}_{R_i}, \mathcal{A}_{P_i}] \varepsilon(\mathbf{P}, \mathbf{R}) - \frac{i}{4\hbar} \varepsilon(\mathbf{P}, \mathbf{R}) [\mathcal{A}_{R_i}, \mathcal{A}_{P_i}] \end{aligned} \quad (40)$$

We can thus ultimately write the diagonalization process as :

$$\begin{aligned} [(U(\mathbf{P}, \mathbf{R}) + X) H_0(\mathbf{P}, \mathbf{R}) (U^+(\mathbf{P}, \mathbf{R}) + X^+)] &= \varepsilon(\mathbf{P}, \mathbf{R}) + \frac{1}{2} [\mathcal{A}_{R_i} \nabla_{R_i} \varepsilon(\mathbf{P}, \mathbf{R}) + \nabla_{R_i} \varepsilon(\mathbf{P}, \mathbf{R}) \mathcal{A}_{R_i}] \\ &+ \frac{1}{2} [\mathcal{A}_{P_i} \nabla_{P_i} \varepsilon(\mathbf{P}, \mathbf{R}) + \nabla_{P_i} \varepsilon(\mathbf{P}, \mathbf{R}) \mathcal{A}_{P_i}] \\ &- \frac{i}{2\hbar} [\varepsilon(\mathbf{P}, \mathbf{R}), \mathcal{A}_{P_i}] \mathcal{A}_{R_i} + \frac{i}{2\hbar} [\varepsilon(\mathbf{P}, \mathbf{R}), \mathcal{A}_{R_i}] \mathcal{A}_{P_i} \\ &+ \frac{i}{4\hbar} [[\mathcal{A}_{R_i}, \mathcal{A}_{P_i}], \varepsilon(\mathbf{P}, \mathbf{R})] \end{aligned} \quad (41)$$

Let us conclude this section by noting that our transformation is not a diagonalization at order \hbar , since it includes non diagonal contributions of order \hbar through the Berry phases \mathcal{A}_{R_i} and \mathcal{A}_{P_i} , justifying the name quasi-diagonalization. However, the next paragraph will show that these non diagonal terms are only an artifact. Actually, projecting our transformed Hamiltonian on the diagonal will in fact yield the true diagonalization.

E. The "Exact" semiclassical diagonalization

As mentioned in subsection B, our choice of transformation $U(\mathbf{P}, \mathbf{R}) + X$ is somewhat arbitrary, however it is sufficient to perform the exact diagonalization as shown in the present paragraph. Actually, consider the unknown-true Diagonalization unitary operator $U_1(\mathbf{P}, \mathbf{R})$. Given that both $U_1(\mathbf{P}, \mathbf{R})$ and $U(\mathbf{P}, \mathbf{R}) + X$ are equal at the zeroth order in \hbar , that is both reduce to $U(\mathbf{P}, \mathbf{r})$ when $\mathbf{R} \rightarrow \mathbf{r}$, the difference

$$\delta X = U_1(\mathbf{P}, \mathbf{R}) - U(\mathbf{P}, \mathbf{R}) - X \quad (42)$$

is of order \hbar . Moreover $U_1(\mathbf{P}, \mathbf{R})$ and $U(\mathbf{P}, \mathbf{R}) + X$ being both unitary, δX is easily seen to be antihermitian. As a direct consequence, one can check that the difference between the exact diagonalization and our approximate one

$$[(U(\mathbf{P}, \mathbf{R}) + X) H_0(\mathbf{P}, \mathbf{R}) (U^+(\mathbf{P}, \mathbf{R}) + X^+)] - [U_1(\mathbf{P}, \mathbf{R}) H_0(\mathbf{P}, \mathbf{R}) U_1^+(\mathbf{P}, \mathbf{R})] \quad (43)$$

is equal to

$$[\delta X, \varepsilon(\mathbf{P}, \mathbf{R})] \quad (44)$$

Given that $\varepsilon(\mathbf{P}, \mathbf{R})$ is diagonal, this last term is always non diagonal. As a consequence, if we project on the diagonal the difference of our transformations, one gets 0.

$$[(U(\mathbf{P}, \mathbf{R}) + X) H_0(\mathbf{P}, \mathbf{R}) (U^+(\mathbf{P}, \mathbf{R}) + X^+)]^+ - [U_1(\mathbf{P}, \mathbf{R}) H_0(\mathbf{P}, \mathbf{R}) U_1^+(\mathbf{P}, \mathbf{R})]^+ = 0 \quad (45)$$

Here we have denoted the projection on the diagonal by a bracket with the upperscript $+$. This notation must not to be mistaken with the Hermitian conjugate, and has been chosen here to conform with the usual conventions for Berry Phases.

Now, given that $U_1(\mathbf{P}, \mathbf{R}) H_0(\mathbf{P}, \mathbf{R}) U_1^+(\mathbf{P}, \mathbf{R})$ is truly diagonal, one has

$$[U_1(\mathbf{P}, \mathbf{R}) H_0(\mathbf{P}, \mathbf{R}) U_1^+(\mathbf{P}, \mathbf{R})]^+ = U_1(\mathbf{P}, \mathbf{R}) H_0(\mathbf{P}, \mathbf{R}) U_1^+(\mathbf{P}, \mathbf{R}) \quad (46)$$

so that ultimately

$$[(U(\mathbf{P}, \mathbf{R}) + X) H_0(\mathbf{P}, \mathbf{R}) (U^+(\mathbf{P}, \mathbf{R}) + X^+)]^+ = U_1(\mathbf{P}, \mathbf{R}) H_0(\mathbf{P}, \mathbf{R}) U_1^+(\mathbf{P}, \mathbf{R}) \quad (47)$$

We can therefore conclude, that the projection of our quasi-diagonalized Hamiltonian, by eliminating thus the non diagonal parts, is in fact the true diagonalized Hamiltonian at order \hbar . Let us remark that we have just succeeded here to justify the adiabatic approximation.

We can now perform the usual one band projection to get the following Hamiltonian :

$$\begin{aligned} [(U(\mathbf{P}, \mathbf{R}) + X) H_0(\mathbf{P}, \mathbf{R}) (U^+(\mathbf{P}, \mathbf{R}) + X^+)]^+ &= \varepsilon(\mathbf{P}, \mathbf{R}) + \frac{1}{2} [\mathcal{A}_{R_i}^+ \nabla_{R_i} \varepsilon(\mathbf{P}, \mathbf{R}) + \nabla_{R_i} \varepsilon(\mathbf{P}, \mathbf{R}) \mathcal{A}_{R_i}^+] \\ &+ \frac{1}{2} [\mathcal{A}_{P_i}^+ \nabla_{P_i} \varepsilon(\mathbf{P}, \mathbf{R}) + \nabla_{P_i} \varepsilon(\mathbf{P}, \mathbf{R}) \mathcal{A}_{P_i}^+] \\ &+ \left\{ -\frac{i}{2\hbar} [\varepsilon(\mathbf{P}, \mathbf{R}), \mathcal{A}_{P_i}] \mathcal{A}_{R_i} + \frac{i}{2\hbar} [\varepsilon(\mathbf{P}, \mathbf{R}), \mathcal{A}_{R_i}] \mathcal{A}_{P_i} \right\}^+ \end{aligned} \quad (48)$$

which is equal to

$$\begin{aligned} &\varepsilon(\mathbf{P} + \mathcal{A}_P^+, \mathbf{R} + \mathcal{A}_R^+) + \frac{i}{2\hbar} [[\varepsilon(\mathbf{P}, \mathbf{R}), \mathcal{A}_{R_i}] \mathcal{A}_{P_i} - [\varepsilon(\mathbf{P}, \mathbf{R}), \mathcal{A}_{P_i}] \mathcal{A}_{R_i}] \\ &\simeq \varepsilon(\mathbf{p}^+, \mathbf{r}^+) + \frac{i}{2\hbar} [[\varepsilon(\mathbf{p}^+, \mathbf{r}^+), \mathcal{A}_{R_i}] \mathcal{A}_{P_i} - [\varepsilon(\mathbf{p}^+, \mathbf{r}^+), \mathcal{A}_{P_i}] \mathcal{A}_{R_i}]^+ \end{aligned} \quad (49)$$

where we have defined the projected dynamical operators (on the diagonal)

$$\mathbf{r}^+ = \mathbf{R} + \mathcal{A}_R^+ \quad (50)$$

$$\mathbf{p}^+ = \mathbf{P} + \mathcal{A}_P^+ \quad (51)$$

F. The equations of motion

Given the Hamiltonian derived in the previous subsection, the equations of motion can now be easily derived. As usual [3, 15] the dynamics equations have to be considered, not for the usual position and momentum, but rather for the projected variables \mathbf{r}^+ and \mathbf{p}^+ . Actually, these latter naturally appear in our diagonalization process at the \hbar order. Let us remark, as now well known, that their components do not commute any more. Actually

$$[r_i^+, r_j^+] = i\Theta_{ij}^{rr} = i\hbar \left(\nabla_{P_i} \mathcal{A}_{R_j}^+ - \nabla_{P_j} \mathcal{A}_{R_i}^+ \right) + [\mathcal{A}_{R_j}^+, \mathcal{A}_{R_i}^+] \quad (52)$$

$$[p_i^+, p_j^+] = i\Theta_{ij}^{pp} = -i\hbar \left(\nabla_{R_i} \mathcal{A}_{P_j}^+ - \nabla_{R_j} \mathcal{A}_{P_i}^+ \right) + [\mathcal{A}_{P_i}^+, \mathcal{A}_{P_j}^+] \quad (53)$$

$$[p_i^+, r_j^+] = -i\hbar \delta_{ij} + i\Theta_{ij}^{pr} = -i\hbar \delta_{ij} - i\hbar \left(\nabla_{R_i} \mathcal{A}_{R_j}^+ + \nabla_{P_j} \mathcal{A}_{P_i}^+ \right) + [\mathcal{A}_{P_i}^+, \mathcal{A}_{R_j}^+] \quad (54)$$

the Θ_{ij} being the so called Berry curvatures.

Using now our Hamiltonian yields directly to general equations of motion for \mathbf{r}^+ , \mathbf{p}^+ :

$$\begin{aligned}\dot{\mathbf{r}}^+ &= -\frac{i}{\hbar} [\mathbf{r}^+, \varepsilon(\mathbf{p}^+, \mathbf{r}^+)] - \frac{i}{\hbar} \left[\mathbf{r}^+, \frac{i}{2\hbar} [[\varepsilon(\mathbf{p}^+, \mathbf{r}^+), \mathcal{A}_{R_l}] \mathcal{A}_{P_l} - [\varepsilon(\mathbf{p}^+, \mathbf{r}^+), \mathcal{A}_{P_l}] \mathcal{A}_{R_l}]^+ \right] \\ \dot{\mathbf{p}}^+ &= -\frac{i}{\hbar} [\mathbf{p}^+, \varepsilon(\mathbf{p}^+, \mathbf{r}^+)] - \frac{i}{\hbar} \left[\mathbf{p}^+, \frac{i}{2\hbar} [[\varepsilon(\mathbf{p}^+, \mathbf{r}^+), \mathcal{A}_{R_l}] \mathcal{A}_{P_l} - [\varepsilon(\mathbf{p}^+, \mathbf{r}^+), \mathcal{A}_{P_l}] \mathcal{A}_{R_l}]^+ \right]\end{aligned}\quad (55)$$

where the commutators can be computed through the previous commutation rules between \mathbf{r}^+ and \mathbf{p}^+ . The last term in each equation represents a contribution of "magnetization" type and has the advantage to present this general form whatever the system initially considered. However, to put some flesh on these equations, we now turn to several examples covered by our formalism.

III. APPLICATION 1 : THE DIRAC ELECTRON.

To apply our previous formalism, we will consider two cases of Dirac Hamiltonians : The electromagnetic field and the static symmetrical gravitational field. These two cases have already been treated by different methods ([4] and [16, 17]), but in the second case (gravitational field) no reference to the Berry phases was made previously.

A. The Dirac electron in an electromagnetic field

The diagonalization of the Dirac Hamiltonian in the presence of an electromagnetic field is a difficult problem which was solved only approximately in the non-relativistic limit in an m^{-1} expansion. Another approach consists in diagonalizing the Hamiltonian at the semi-classical order as was done in [4] using an approximate Foldy-Wouthuysen transformation [18]. From the semi-classical Hamiltonian the equations of motion were derived showing a topological spin-transport effect due to the presence of the Berry phases. Here we propose to apply our general formalism for the semi-classical diagonalization of the Dirac Hamiltonian to show the effectiveness of our general method.

We thus start with the following Hamiltonian :

$$H_0(\mathbf{P}, \mathbf{R}) = \alpha \cdot (\mathbf{P} - \mathbf{A}(\mathbf{R})) + \beta m + V(\mathbf{R}) \quad (56)$$

Replacing \mathbf{R} by the parameter \mathbf{r} , $\mathbf{A}(\mathbf{r})$ just shifts the momentum, so that we can diagonalize $H_0(\mathbf{P}, \mathbf{r})$ through the well known Foldy-Wouthuysen transformation

$$U(\mathbf{P}, \mathbf{r}) = \frac{E + m + \beta \alpha \cdot (\mathbf{P} - \mathbf{A}(\mathbf{r}))}{\sqrt{2E(E + m)}} \quad (57)$$

where $E = \sqrt{(\mathbf{P} - \mathbf{A}(\mathbf{r}))^2 + m^2}$. In this context, introducing the dependence in \mathbf{R} we define the Berry phases at first order in \hbar

$$\mathcal{A}_{R_k} = i\hbar U \nabla_{P_j} U^+ = \hbar \frac{i\alpha \cdot (\mathbf{P} - \mathbf{A}(\mathbf{R})) P_j \beta + i\beta E(E + m)\alpha_i - E \boldsymbol{\Sigma} \times (\mathbf{P} - \mathbf{A}(\mathbf{R}))}{2E^2(E + m)} \quad (58)$$

and

$$\mathcal{A}_{P_l} = -i\hbar U \nabla_{R_j} U^+ = \nabla_{R_l} A_k(\mathbf{R}) \mathcal{A}_{R_k} \quad (59)$$

where E will now denote the symmetrized form of $E = \sqrt{(\mathbf{P} - \mathbf{A}(\mathbf{R}))^2 + m^2}$ (here at zeroth order in \hbar we can consider that \mathbf{P} and \mathbf{R} commute). Let us also denote $\varepsilon = \beta E$. Using our general method yields the diagonalized (i.e. proportional to β) energy

$$\varepsilon(\mathbf{p}^+, \mathbf{r}^+) + \frac{i}{2\hbar} [[\varepsilon(\mathbf{p}^+, \mathbf{r}^+), \mathcal{A}_{R_l}] \mathcal{A}_{P_l} - [\varepsilon(\mathbf{p}^+, \mathbf{r}^+), \mathcal{A}_{P_l}] \mathcal{A}_{R_l}]^+ + [V(\mathbf{r})]^+ \quad (60)$$

with $\varepsilon(\mathbf{p}^+, \mathbf{r}^+) = \beta \sqrt{(\mathbf{p}^+ - \mathbf{A}(\mathbf{r}^+))^2 + m^2}$. Using the expressions for the Berry phases, the hamiltonian can be rewritten as:

$$\varepsilon(\mathbf{p}^+, \mathbf{r}^+) + \left[-\frac{i}{2} [\varepsilon(K), U \nabla_{P_i} U^+] \varepsilon^{ijk} U \nabla_{P_j} U^+ \right]^+ \frac{\delta B^k(\hat{\mathbf{r}}^+)}{\hbar} + [V(\mathbf{r})]^+ \quad (61)$$

Moreover, a straightforward computation yields the correction to $\varepsilon(\mathbf{p}^+, \mathbf{r}^+)$:

$$\left[-\frac{i}{2} [\varepsilon(K), U \nabla_{K_i} U^+] \cdot \varepsilon^{ijk} U \nabla_{K_j} U^+ \right]^+ \frac{\delta B^k(\hat{\mathbf{r}}^+)}{\hbar} + [V(\mathbf{r})]^+ = -\frac{\beta}{2E} \boldsymbol{\Sigma} \cdot \mathbf{B} - \frac{\beta}{E} \mathbf{L}^+ \cdot \mathbf{B} + V(\mathbf{r}^+) \quad (62)$$

at the first order in \hbar , where L^+ is defined as :

$$\mathbf{L}^+ = \frac{(\mathbf{P} \times \boldsymbol{\Sigma})}{2E(E+m)} = \mathbf{P} \times [iU \nabla_K U^+]^+ = \mathbf{P} \times \mathcal{A}^+ \quad (63)$$

and $\mathcal{A}_{\mathbf{R}}^+$ is the Berry Connection

$$\mathcal{A}_{\mathbf{R}}^+ = \hbar \frac{(\mathbf{P} - \mathbf{A}(\mathbf{R})) \times \boldsymbol{\Sigma}}{2E(E+m)} \quad (64)$$

As a consequence, the diagonal Hamiltonian to be considered is

$$\varepsilon(\mathbf{p}^+, \mathbf{r}^+) + \frac{\beta}{2E} \boldsymbol{\Sigma} \cdot \mathbf{B} - \frac{\beta}{E} \mathbf{L}^+ \cdot \mathbf{B} + V(\mathbf{r}^+) \quad (65)$$

which is the Hamiltonian considered in [4] which leads of course to the dynamics described in that paper.

B. The electron in a static gravitational field

The behaviour of Dirac particles in static gravitational field is an important issue. Different approaches for the diagonalization of the Hamiltonian leads to contradictory results in particular with regard to the existence of a dipole spin-gravity coupling [16, 17]. It is not our goal to discuss this specific point but we study the semiclassical diagonalization of the Hamiltonian to get the velocity and momentum evolution. We can in particular compare our results with the article [17] who uses a Foldy-Wouthuysen transformation.

The interaction of a Dirac particle with a symmetric static gravitational field ($g_{00} = V(\mathbf{R})$, $g_{i0} = 0$, $g_{ij} = \delta_{ij} F(\mathbf{R})$) is described by the Hamiltonian

$$H_0 = \frac{1}{2} (\alpha \cdot \mathbf{P} F(\mathbf{R}) + F(\mathbf{R}) \alpha \cdot \mathbf{P}) + \beta m V(\mathbf{r}) \quad (66)$$

The Foldy Whouthuysen transformation when \mathbf{R} is replaced by a parameter \mathbf{r} is given by

$$U(\mathbf{P}, \mathbf{r}) = \frac{E + mV(\mathbf{r}) + \beta F(\mathbf{r}) \alpha \cdot \mathbf{P}}{\sqrt{2E(E + mV^2(\mathbf{r}))}} \quad (67)$$

with $E = \sqrt{F^2(\mathbf{r}) \mathbf{P}^2 + m^2 V^2(\mathbf{r})}$. This is quite the same as the free particle transformation. As a consequence introducing again the \mathbf{R} dependence yields the non projected Berry phases for the position and the momentum operators :

$$\mathcal{A}_{R_k} = i\hbar U \nabla_{P_j} U^+ = \hbar \frac{iF^3(\mathbf{R}) \alpha \cdot \mathbf{P} P_i \beta + i\beta F(\mathbf{R}) E(E + mV(\mathbf{r})) \alpha_i - EF^2(\mathbf{R}) \boldsymbol{\Sigma} \times \mathbf{P}}{2E^2(E + mV(\mathbf{r}))} \quad (68)$$

$$\mathcal{A}_{P_k} = -i\hbar U \nabla_{P_j} U^+ = -\hbar i \frac{m \nabla \phi \beta F^2(\mathbf{R}) \alpha \cdot \mathbf{P}}{E^2} \quad (69)$$

with $\phi = \frac{V}{F}$, and $\boldsymbol{\Sigma}$ the spin of the electron.

The expressions for \mathcal{A}_{R_k} and \mathcal{A}_{P_k} allow us ultimately to define the semi classical transformation : $U(\mathbf{P}, \mathbf{R}) + \frac{i}{4\hbar} [\mathcal{A}_{P_i}, \mathcal{A}_{R_i}] U(\mathbf{P}, \mathbf{R})$ and to compute the diagonalized Hamiltonian

$$\varepsilon(\mathbf{p}^+, \mathbf{r}^+) = \sqrt{F^2(\mathbf{r}^+) \mathbf{P}^2 + \mathbf{P}^2 F^2(\mathbf{r}^+) + mV^2(\mathbf{r}^+)} - \frac{F^3(\mathbf{r}^+)}{2E^2} m \hbar \nabla \phi(\mathbf{r}^+) \cdot (\mathbf{P} \times \boldsymbol{\Sigma}) \quad (70)$$

where the dynamical variables are obtained through the projection

$$\mathbf{r}^+ = \mathbf{R} + \mathcal{A}_R^+ = \mathbf{R} - \hbar \frac{F^2(\mathbf{R}) \boldsymbol{\Sigma} \times \mathbf{P}}{2E(E + mV(\mathbf{R}))} \quad (71)$$

$$\mathbf{p}^+ = \mathbf{P} + \mathcal{A}_P^+ = \mathbf{P} \quad (72)$$

The commutators of these variables are thus

$$[r_i^+, r_j^+] = i\Theta_{ij}^{rr} \quad (73)$$

$$[p_i^+, r_j^+] = -i\hbar\delta_{ij} + i\Theta_{ij}^{pr} \quad (74)$$

$$[p_i^+, P_j] = 0 \quad (75)$$

with

$$\Theta_{ij}^{rr} = -\frac{\hbar^2 F^3(\mathbf{r}^+) \varepsilon^{ijk}}{2\varepsilon^3(\mathbf{p}^+, \mathbf{r}^+)} \left(m\phi(\mathbf{r}^+) \Sigma_k + \frac{F(\mathbf{r}^+) (\boldsymbol{\Sigma} \cdot \mathbf{p}^+) \mathbf{p}_k^+}{\varepsilon(\mathbf{p}^+, \mathbf{r}^+) + mV(\mathbf{r}^+)} \right) \quad (76)$$

$$\Theta_{ij}^{pr} = -\frac{\hbar^2 F^3(\mathbf{r}^+)}{2\varepsilon^3(\mathbf{p}^+, \mathbf{r}^+)} m \nabla_i \phi(\mathbf{r}^+) (\boldsymbol{\Sigma} \times \mathbf{p}^+)_j \quad (77)$$

$$\Theta_{ij}^{pp} = 0 \quad (78)$$

One can check, after developing \mathbf{r}^+ as a function of \mathbf{R} and the Berry phase, that our Hamiltonian coincides with the one given in [17] at order \hbar . This confirms also the validity of the Foldy Wouthuysen approach asserted in [17] in opposition with the transformation proposed in [16]. However our approach is more general since our computation does not require an expansion in V and F as done in [17]. Of course, we retrieve the result of [17] if we expand expression 78 at the leading order in F and V . Note also that when $m = 0$ one recovers the Hamiltonian for the Neutrino or the photon proposed in [3].

To conclude this paragraph, we can derive the equations of motion with the help of:

$$\Theta_{ij}^{r\Sigma} = [r_i^+, \Sigma_j] = i\hbar c^2 \frac{-p_j^+ \Sigma_i + \mathbf{p}^+ \cdot \boldsymbol{\Sigma} \delta_{ij}}{\varepsilon(\mathbf{p}^+, \mathbf{r}^+) (\varepsilon(\mathbf{p}^+, \mathbf{r}^+) + mV(\mathbf{r}^+))} + o(\hbar^2) \quad (79)$$

$$\Theta_{ij}^{p\Sigma} = [p_i^+, \Sigma_j] = 0 \quad (80)$$

leading to

$$\begin{aligned} \dot{\mathbf{r}}^+ &= \nabla_{\mathbf{p}} \varepsilon - \frac{1}{\hbar} \dot{\mathbf{p}}^+ \times \Theta^{rr} + \frac{i}{\hbar} \nabla_{\boldsymbol{\Sigma}} \tilde{\varepsilon} \cdot \Theta^{r\Sigma} \\ \dot{\mathbf{p}}^+ &= \nabla_{\mathbf{r}^+} \varepsilon - \frac{1}{\hbar} \nabla_{\mathbf{r}^+} \varepsilon \cdot \Theta^{rp} \end{aligned} \quad (81)$$

where we have defined the vectors Θ^{rr} and Θ^{rp} through

$$\Theta_{ij}^{rr} = \varepsilon^{ijk} \Theta_k^{rr} \quad (82)$$

$$\Theta_{ij}^{rp} = \varepsilon^{ijk} \Theta_k^{rp} \quad (83)$$

An explicit computation gives (we drop the suffix +)

$$\begin{aligned} \dot{\mathbf{r}} &= \frac{F\mathbf{p}}{\varepsilon(\mathbf{p}, \mathbf{r})} + \frac{\hbar F^2(\mathbf{r}) m \phi(\mathbf{r})}{2\varepsilon^2(\mathbf{p}, \mathbf{r})} \frac{\nabla F}{F} \times \boldsymbol{\Sigma} + \hbar \left(\frac{F^2(\mathbf{r}) m}{2\varepsilon(\mathbf{p}, \mathbf{r})^2} + \frac{F^4(\mathbf{r}) m^3 \phi^2(\mathbf{r})}{2\varepsilon^4(\mathbf{p}, \mathbf{r})} \right) \nabla \phi(\mathbf{r}) \times \boldsymbol{\Sigma} \\ &\quad + \frac{\hbar F^4(\mathbf{r}) (\boldsymbol{\Sigma} \cdot \mathbf{p}) \left(\frac{\nabla F}{F} + \frac{m(Fm\phi(\mathbf{r}) - \varepsilon(\mathbf{p}, \mathbf{r})) \nabla \phi(\mathbf{r})}{\varepsilon(\mathbf{p}, \mathbf{r})} \right) \times \mathbf{p}}{2\varepsilon^3(\mathbf{p}, \mathbf{r}) (\varepsilon(\mathbf{p}, \mathbf{r}) + mV(\mathbf{r}))} \end{aligned} \quad (84)$$

$$\begin{aligned} \dot{\mathbf{p}} &= -\left(\frac{\nabla F}{F} \varepsilon(\mathbf{p}, \mathbf{r}) + \frac{Fm^2 \phi(\mathbf{r}) \nabla \phi(\mathbf{r})}{\varepsilon(\mathbf{p}, \mathbf{r})} \right) + \hbar \nabla \left(\frac{F^2(\mathbf{r})}{2\varepsilon^2} m \nabla \phi(\mathbf{r}) \cdot (\mathbf{p} \times \boldsymbol{\Sigma}) \right) \\ &\quad - \frac{\hbar F^3(\mathbf{r}) m \nabla \phi(\mathbf{r})}{2\varepsilon^3(\mathbf{p}, \mathbf{r})} (\boldsymbol{\Sigma} \times \mathbf{p}) \cdot \left(\frac{\nabla F}{F} \varepsilon(\mathbf{p}, \mathbf{r}) + \frac{Fm^2 \phi(\mathbf{r}) \nabla \phi(\mathbf{r})}{\varepsilon(\mathbf{p}, \mathbf{r})} \right) \end{aligned} \quad (85)$$

$$\hbar \dot{\boldsymbol{\Sigma}} = -\left(\left(\frac{-\hbar F^2(\mathbf{r}) \frac{\nabla F}{F}}{(\varepsilon(\mathbf{p}, \mathbf{r}) + mV(\mathbf{r}))} + \frac{\hbar F^2(\mathbf{r}) m \nabla \phi(\mathbf{r})}{\varepsilon(\mathbf{p}, \mathbf{r}) (\varepsilon(\mathbf{p}, \mathbf{r}) + mV(\mathbf{r}))} \right) \times \mathbf{p} \right) \times \boldsymbol{\Sigma} \quad (86)$$

IV. APPLICATION 2 : THE ELECTRON IN A PERIODIC POTENTIAL

This application has already been independently studied in [15], and is easily recovered by the present general setup. The purpose is to find the Hamiltonian for an electron in a periodic potential facing an electromagnetic field. This topic was also already dealt with in [9] in the context of wave packets dynamics. We will show that the semiclassical equations of motions which are very essential in the solid state physics context must be corrected by Berry phases terms. To apply our formalism, we start with the following unperturbed Hamiltonian including a periodic potential

$$H_0 = \frac{1}{2m} (\mathbf{P} - A(\mathbf{R}))^2 + V(\mathbf{R}) \quad (87)$$

whose symmetries are a lattice translation group. The Diagonalization is performed to diagonalize simultaneously H_0 and the magnetic translation operators. These ones are

$$T(R_i) = \exp\left(-\frac{i}{\hbar} \int_0^{R_i} A_i(\mathbf{R} + \mathbf{r}) d\mathbf{r}\right) \exp\left(\frac{i}{\hbar} \mathbf{R}_i \cdot \mathbf{P}\right) \quad (88)$$

whose generator are

$$\mathbf{K}_i = -\frac{i}{R_i} \log(T(R_i)) \quad (89)$$

There is of course an ambiguity in the definition of the log which is dealt with in appendix 2, by a particular choice. The diagonalization is performed as follows : Start with an arbitrary basis of eigenvectors of the $T(R_i)$. As explained in detail in Appendix 3, in this basis H_0 can be seen as a square matrix with operators entries. H_0 is diagonalized through a unitary matrix U which should depend only on $\hat{\mathbf{K}}$ (since U should leave $\hat{\mathbf{K}}$ invariant). We will thus consider $U = U(\mathbf{K})$. Now, to add a perturbation $\delta A(\mathbf{R})$ as in ([15]), that breaks the translational symmetry, we have to replace \mathbf{K} in the Hamiltonian by

$$\tilde{\mathbf{K}} = \mathbf{K} - \frac{\delta A(\mathbf{R})}{\hbar} \quad (90)$$

and $U = U(\tilde{\mathbf{K}})$ so that the non projected Berry phases are

$$\mathcal{A}_{R_k} = iU \nabla_{K_i} U^\dagger \quad (91)$$

and

$$\mathcal{A}_{P_l} = \nabla_{R_l} A_k(\mathbf{R}) \mathcal{A}_{R_k} \quad (92)$$

Using our results of section 2, the Hamiltonian

$$H = \frac{1}{2m} (\mathbf{P} - A(\mathbf{R}) - \delta A(\mathbf{R}))^2 + V(\mathbf{R}) \quad (93)$$

can thus be diagonalized through the transformation $U(\tilde{\mathbf{K}}) + \frac{i}{4\hbar} [\mathcal{A}_{R_k}, \mathcal{A}_{P_l}] U(\tilde{\mathbf{K}})$ plus a projection on the chosen n -th Band (denoted \mathcal{P}_n in the context of the Solid state Physics)

$$\begin{aligned} [U(\tilde{\mathbf{K}}) H U^\dagger(\tilde{\mathbf{K}})]^+ &= \mathcal{P}_n \left[\varepsilon(\tilde{\mathbf{k}}) - \frac{i}{4} [\varepsilon(K), U \nabla_{K_i} U^\dagger] \varepsilon^{ijk} \frac{\delta B^k(\mathbf{r})}{\hbar} U \nabla_{K_j} U^\dagger - \frac{i}{4} U \nabla_{K_j} U^\dagger [\varepsilon(K), U \nabla_{K_i} U^\dagger] \varepsilon^{ijk} \frac{\delta B^k(\mathbf{r})}{\hbar} \right] \\ &= \varepsilon_n(\tilde{\mathbf{k}}^+) - \mathcal{P}_n \left[\frac{i}{2} [\varepsilon(K), U \nabla_{K_i} U^\dagger] \varepsilon^{ijk} U \nabla_{K_j} U^\dagger \right] \frac{\delta B^k(\hat{\mathbf{r}}^+)}{\hbar}, \end{aligned} \quad (94)$$

where

$$\tilde{\mathbf{k}} = U(\tilde{\mathbf{K}}) \tilde{\mathbf{K}} U^\dagger(\tilde{\mathbf{K}}) \quad (95)$$

therefore

$$\tilde{\mathbf{k}}^+ = \mathcal{P}_n(U(\tilde{\mathbf{K}}) \tilde{\mathbf{K}} U^\dagger(\tilde{\mathbf{K}})) \quad (96)$$

This is the expression obtained in [15] and leading to the semiclassical equations of motion in the Magnetic Bloch bands. The term proportional to the magnetic field is nothing else but the magnetization defined by the n -th band projection

$$\begin{aligned} - \left[\frac{i}{2} [\varepsilon(K), U \nabla_{K_i} U^+] \cdot \varepsilon^{ijk} U \nabla_{K_j} U^+ \right]^+ \frac{\delta B^k(\hat{\mathbf{r}}^+)}{\hbar} &= \mathbf{M}(\tilde{\mathbf{K}}) \\ &= \mathcal{P}_n \left(\frac{i}{2\hbar} [\varepsilon(\tilde{\mathbf{K}}), \mathbf{A}(\tilde{\mathbf{K}})] \times \mathbf{A}(\tilde{\mathbf{K}}) \right) \end{aligned} \quad (97)$$

This magnetization can also be written under the usual form [19] in the (\mathbf{K}, n) representation

$$\mathcal{M}_i(\tilde{\mathbf{K}}) = e/2m \sum_{n'} (\mathcal{A}_k)_{nn'} (\mathcal{A}_j)_{n'n} - (\mathcal{A}_j)_{nn'} (\mathcal{A}_k)_{n'n} \quad (98)$$

We sum up here the results we obtained (with the upperscript + omitted)

$$\begin{aligned} \dot{\mathbf{r}} &= \partial E(\tilde{\mathbf{k}})/\hbar \partial \tilde{\mathbf{k}} - \dot{\tilde{\mathbf{k}}} \times \Theta(\tilde{\mathbf{k}}) \\ \hbar \dot{\tilde{\mathbf{k}}} &= -e\mathbf{E} - e\dot{\mathbf{r}} \times \delta \mathbf{B}(\mathbf{r}) - \mathbf{M} \partial \delta \mathbf{B} / \partial \mathbf{r} \end{aligned} \quad (99)$$

As explained in [15] these equations are formally the same as the one derived in [9], with the exception of a contribution depending on the gradient of the magnetic field.

V. CONCLUSION

Some recent applications of semi classical methods to several branches of Physics, such as spintronics or solid state physics have shown the relevance of Berry Phases contributions to the dynamics of a system. However, these progresses called for a rigorous Hamiltonian treatment that would allow for deriving naturally the role of the Berry phase.

This paper has been devoted to derive a semi classical diagonalization method for a broad class of quantum systems, including the electron in a periodic potential and the Dirac Hamiltonian. Doing so, we have exhibited a general pattern for this class of systems implying the role of the Berry phases both for the position and the momentum. In such a context, the coordinates and momenta algebra are no longer commutative, and the dynamical equations for these variables directly include the influence of Berry phases through the parameters of noncommutativity (Berry curvatures) and through an abstract magnetization term. Applications of our formalism consider the Dirac electron in an electromagnetic field, or in a particular case of static gravitational field, as well as the electron in a periodic potential. Our results are promising and indicate that our method will probably apply to several other systems.

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A. Appendix 1

To start our computation, we will use the formula given in the preliminary :

$$\begin{aligned}
& \frac{i}{2} \hbar \text{Asym} \nabla_{R_l} \nabla_{P^l} [U(\mathbf{P}, \mathbf{R}) H_0(\mathbf{P}, \mathbf{R}) U^+(\mathbf{P}, \mathbf{R})] \\
= & \frac{i}{2} \hbar \text{Asym} \nabla_{R_l} \nabla_{P^l} [U(\mathbf{P}, \mathbf{R})] H_0(\mathbf{P}, \mathbf{R}) U^+(\mathbf{P}, \mathbf{R}) \\
& + \frac{i}{2} \hbar U(\mathbf{P}, \mathbf{R}) \text{Asym} \nabla_{R_l} \nabla_{P^l} [H_0(\mathbf{P}, \mathbf{R})] U^+(\mathbf{P}, \mathbf{R}) \\
& + \frac{i}{2} \hbar U(\mathbf{P}, \mathbf{R}) H_0(\mathbf{P}, \mathbf{R}) \text{Asym} \nabla_{R_l} \nabla_{P^l} [U^+(\mathbf{P}, \mathbf{R})] \\
& + \frac{i}{2} \hbar \nabla_{R_l} U(\mathbf{P}, \mathbf{R}) \nabla_{P^l} H_0(\mathbf{P}, \mathbf{R}) U^+(\mathbf{P}, \mathbf{R}) \\
& - \frac{i}{2} \hbar \nabla_{P^l} U(\mathbf{P}, \mathbf{R}) \nabla_{R_l} H_0(\mathbf{P}, \mathbf{R}) U^+(\mathbf{P}, \mathbf{R}) \\
& - \frac{i}{2} \hbar U(\mathbf{P}, \mathbf{R}) \nabla_{P^l} H_0(\mathbf{P}, \mathbf{R}) \nabla_{R_l} U^+(\mathbf{P}, \mathbf{R}) \\
& + \frac{i}{2} \hbar \nabla_{P^l} U(\mathbf{P}, \mathbf{R}) \nabla_{R_l} H_0(\mathbf{P}, \mathbf{R}) \nabla_{P^l} U^+(\mathbf{P}, \mathbf{R}) \\
& + \frac{i}{2} \hbar \nabla_{R_l} U(\mathbf{P}, \mathbf{R}) H_0(\mathbf{P}, \mathbf{R}) \nabla_{P^l} U^+(\mathbf{P}, \mathbf{R}) \\
& - \frac{i}{2} \hbar \nabla_{P^l} U(\mathbf{P}, \mathbf{R}) H_0(\mathbf{P}, \mathbf{R}) \nabla_{R_l} U^+(\mathbf{P}, \mathbf{R})
\end{aligned} \tag{100}$$

Let us first remark that $H_0(\mathbf{P}, \mathbf{R})$ is already symmetrized in \mathbf{R} and \mathbf{P} . As a consequence $\text{Asym} \nabla_{R_l} \nabla_{P^l} [H_0(\mathbf{P}, \mathbf{R})] = 0$. Actually, remember that the asymmetrisation term was the sum of commutators obtained by pushing the momentum half on the left and half on the right. For the same reason

$$\text{Asym} \nabla_{R_l} \nabla_{P^l} [U(\mathbf{P}, \mathbf{R})] = \text{Asym} \nabla_{R_l} \nabla_{P^l} [U^+(\mathbf{P}, \mathbf{R})] = 0 \tag{101}$$

Now, we introduce the transformed variables and the non projected Berry Phases at order \hbar :

$$\begin{aligned}
\mathbf{r} &= (U(\mathbf{P}, \mathbf{R}) + X) \mathbf{R} (U^+(\mathbf{P}, \mathbf{R}) + X^+) \\
&\simeq \mathbf{R} + [i\hbar U(\mathbf{P}, \mathbf{R}) \nabla_P U^+(\mathbf{P}, \mathbf{R})] \\
&= \mathbf{R} + \mathcal{A}_R \\
\mathbf{p} &= U(\mathbf{P}, \mathbf{R}) \mathbf{P} U^+(\mathbf{P}, \mathbf{R}) \\
&\simeq \mathbf{P} - [i\hbar U(\mathbf{P}, \mathbf{R}) \nabla_R U^+(\mathbf{P}, \mathbf{R})] \\
&= \mathbf{P} + \mathcal{A}_P
\end{aligned} \tag{102}$$

Before going further, we can find some relations on the Berry Phases. Given that :

$$U(\mathbf{P}, \mathbf{R}) U^+(\mathbf{P}, \mathbf{R}) = 1 \tag{103}$$

at the zeroth order in \hbar we have the following relations at the first order in \hbar :

$$\begin{aligned}
\mathcal{A}_R &= i\hbar U(\mathbf{P}, \mathbf{R}) \nabla_P U^+(\mathbf{P}, \mathbf{R}) = -i \nabla_P U(\mathbf{P}, \mathbf{R}) U^+(\mathbf{P}, \mathbf{R}) \\
\mathcal{A}_P &= -i\hbar U(\mathbf{P}, \mathbf{R}) \nabla_R U^+(\mathbf{P}, \mathbf{R}) = i \nabla_R U(\mathbf{P}, \mathbf{R}) U^+(\mathbf{P}, \mathbf{R})
\end{aligned} \tag{104}$$

Using these results as well as $\nabla_{P^l} = \frac{-i}{\hbar} [R_l, \cdot]$, $\nabla_{R_l} = \frac{i}{\hbar} [P^l, \cdot]$ and inserting the operators $U(\mathbf{P}, \mathbf{R})$ and $U^+(\mathbf{P}, \mathbf{R})$

when needed, we get :

$$\begin{aligned}
& \frac{i}{2}\hbar \text{Asym} \nabla_{R_l} \nabla_{P_l} [U(\mathbf{P}, \mathbf{R}) H_0(\mathbf{P}, \mathbf{R}) U^+(\mathbf{P}, \mathbf{R})] \\
= & \frac{-i}{2\hbar} \mathcal{A}_{P_l} U(\mathbf{P}, \mathbf{R}) [R_l, H_0(\mathbf{P}, \mathbf{R})] U^+(\mathbf{P}, \mathbf{R}) \\
& + \frac{i}{2\hbar} \mathcal{A}_{R_l} U(\mathbf{P}, \mathbf{R}) [P_l, H_0(\mathbf{P}, \mathbf{R})] U^+(\mathbf{P}, \mathbf{R}) \\
& - \frac{i}{2\hbar} U(\mathbf{P}, \mathbf{R}) [R_l, H_0(\mathbf{P}, \mathbf{R})] U^+(\mathbf{P}, \mathbf{R}) \mathcal{A}_{P_l} \\
& + \frac{i}{2\hbar} U(\mathbf{P}, \mathbf{R}) [P_l, H_0(\mathbf{P}, \mathbf{R})] U^+(\mathbf{P}, \mathbf{R}) \mathcal{A}_{R_l} \\
& - \frac{i}{2\hbar} \mathcal{A}_{P_l} \varepsilon(\mathbf{P}, \mathbf{R}) \mathcal{A}_{R_l} + \frac{i}{2\hbar} \mathcal{A}_{R_l} \varepsilon(\mathbf{P}, \mathbf{R}) \mathcal{A}_{P_l} \\
= & \frac{-i}{2\hbar} \mathcal{A}_{P_l} [r_l, \varepsilon(\mathbf{P}, \mathbf{R})] + \frac{i}{2\hbar} \mathcal{A}_{R_l} [p_l, \varepsilon(\mathbf{P}, \mathbf{R})] \\
& - \frac{i}{2\hbar} [r_l, \varepsilon(\mathbf{P}, \mathbf{R})] \mathcal{A}_{P_l} + \frac{i}{2\hbar} [p_l, \varepsilon(\mathbf{P}, \mathbf{R})] \mathcal{A}_{R_l} \\
& - \frac{i}{2\hbar} \mathcal{A}_{P_l} \varepsilon(\mathbf{P}, \mathbf{R}) \mathcal{A}_{R_l} + \frac{i}{2\hbar} \mathcal{A}_{R_l} \varepsilon(\mathbf{P}, \mathbf{R}) \mathcal{A}_{P_l} \\
= & \frac{1}{2} [\mathcal{A}_{R_l} \nabla_{R_l} \varepsilon(\mathbf{P}, \mathbf{R}) + \nabla_{R_l} \varepsilon(\mathbf{P}, \mathbf{R}) \mathcal{A}_{R_l}] \\
& + \frac{1}{2} [\mathcal{A}_{P_l} \nabla_{P_l} \varepsilon(\mathbf{P}, \mathbf{R}) + \nabla_{P_l} \varepsilon(\mathbf{P}, \mathbf{R}) \mathcal{A}_{P_l}] \\
& - \frac{i}{2\hbar} \mathcal{A}_{P_l} [\mathcal{A}_{R_l}, \varepsilon(\mathbf{P}, \mathbf{R})] - \frac{i}{2\hbar} [\mathcal{A}_{R_l}, \varepsilon(\mathbf{P}, \mathbf{R})] \mathcal{A}_{P_l} \\
& + \frac{i}{2\hbar} \mathcal{A}_{R_l} [\mathcal{A}_{P_l}, \varepsilon(\mathbf{P}, \mathbf{R})] + \frac{i}{2\hbar} [\mathcal{A}_{P_l}, \varepsilon(\mathbf{P}, \mathbf{R})] \mathcal{A}_{R_l} \\
& - \frac{i}{2\hbar} \mathcal{A}_{P_l} \varepsilon(\mathbf{P}, \mathbf{R}) \mathcal{A}_{R_l} + \frac{i}{2\hbar} \mathcal{A}_{R_l} \varepsilon(\mathbf{P}, \mathbf{R}) \mathcal{A}_{P_l} \tag{105}
\end{aligned}$$

Rearranging the commutators leads to :

$$\begin{aligned}
& \frac{i}{2}\hbar \text{Asym} \nabla_{R_l} \nabla_{P_l} [U(\mathbf{P}, \mathbf{R}) H_0(\mathbf{P}, \mathbf{R}) U^+(\mathbf{P}, \mathbf{R})] \\
= & \frac{1}{2} [\mathcal{A}_{R_l} \nabla_{R_l} \varepsilon(\mathbf{P}, \mathbf{R}) + \nabla_{R_l} \varepsilon(\mathbf{P}, \mathbf{R}) \mathcal{A}_{R_l}] \\
& + \frac{1}{2} [\mathcal{A}_{P_l} \nabla_{P_l} \varepsilon(\mathbf{P}, \mathbf{R}) + \nabla_{P_l} \varepsilon(\mathbf{P}, \mathbf{R}) \mathcal{A}_{P_l}] \\
& - \frac{i}{2\hbar} \mathcal{A}_{R_l} [\varepsilon(\mathbf{P}, \mathbf{R}), \mathcal{A}_{P_l}] - \frac{i}{2\hbar} [\varepsilon(\mathbf{P}, \mathbf{R}), \mathcal{A}_{P_l}] \mathcal{A}_{R_l} \\
& + \frac{i}{2\hbar} \mathcal{A}_{P_l} [\varepsilon(\mathbf{P}, \mathbf{R}), \mathcal{A}_{R_l}] + \frac{i}{2\hbar} [\varepsilon(\mathbf{P}, \mathbf{R}), \mathcal{A}_{R_l}] \mathcal{A}_{P_l} \\
& - \frac{i}{2\hbar} \mathcal{A}_{P_l} \varepsilon(\mathbf{P}, \mathbf{R}) \mathcal{A}_{R_l} + \frac{i}{2\hbar} \mathcal{A}_{R_l} \varepsilon(\mathbf{P}, \mathbf{R}) \mathcal{A}_{P_l} \tag{106}
\end{aligned}$$

rewrite

$$\begin{aligned}
& \frac{-i}{2\hbar} \mathcal{A}_{P_l} \varepsilon(\mathbf{P}, \mathbf{R}) \mathcal{A}_{R_l} + \frac{i}{2\hbar} \mathcal{A}_{R_l} \varepsilon(\mathbf{P}, \mathbf{R}) \mathcal{A}_{P_l} \\
= & -\frac{i}{2\hbar} \mathcal{A}_{P_l} [\varepsilon(\mathbf{P}, \mathbf{R}), \mathcal{A}_{R_l}] + \frac{i}{2\hbar} \mathcal{A}_{R_l} [\varepsilon(\mathbf{P}, \mathbf{R}), \mathcal{A}_{P_l}] \\
& + \frac{i}{2\hbar} [\mathcal{A}_{R_l}, \mathcal{A}_{P_l}] \varepsilon(\mathbf{P}, \mathbf{R}) \tag{107}
\end{aligned}$$

so that :

$$\begin{aligned}
& \frac{i}{2}\hbar A_{sym} \nabla_{R_l} \nabla_{P_l} [U(\mathbf{P}, \mathbf{R}) H_0(\mathbf{P}, \mathbf{R}) U^+(\mathbf{P}, \mathbf{R})] \\
= & \frac{1}{2} [\mathcal{A}_{R_l} \nabla_{R_l} \varepsilon(\mathbf{P}, \mathbf{R}) + \nabla_{R_l} \varepsilon(\mathbf{P}, \mathbf{R}) \mathcal{A}_{R_l}] \\
& + \frac{1}{2} [\mathcal{A}_{P_l} \nabla_{P_l} \varepsilon(\mathbf{P}, \mathbf{R}) + \nabla_{P_l} \varepsilon(\mathbf{P}, \mathbf{R}) \mathcal{A}_{P_l}] \\
& - \frac{i}{2\hbar} [\varepsilon(\mathbf{P}, \mathbf{R}), \mathcal{A}_{P_l}] \mathcal{A}_{R_l} + \frac{i}{2\hbar} [\varepsilon(\mathbf{P}, \mathbf{R}), \mathcal{A}_{R_l}] \mathcal{A}_{P_l} \\
& + \frac{i}{2\hbar} [\mathcal{A}_{R_l}, \mathcal{A}_{P_l}] \varepsilon(\mathbf{P}, \mathbf{R})
\end{aligned} \tag{108}$$

And we thus have :

$$\begin{aligned}
U(\mathbf{P}, \mathbf{R}) H_0(\mathbf{P}, \mathbf{R}) U^+(\mathbf{P}, \mathbf{R}) = & \varepsilon(\mathbf{P}, \mathbf{R}) + \frac{1}{2} [\mathcal{A}_{R_l} \nabla_{R_l} \varepsilon(\mathbf{P}, \mathbf{R}) + \nabla_{R_l} \varepsilon(\mathbf{P}, \mathbf{R}) \mathcal{A}_{R_l}] \\
& + \frac{1}{2} [\mathcal{A}_{P_l} \nabla_{P_l} \varepsilon(\mathbf{P}, \mathbf{R}) + \nabla_{P_l} \varepsilon(\mathbf{P}, \mathbf{R}) \mathcal{A}_{P_l}] \\
& - \frac{i}{2\hbar} [\varepsilon(\mathbf{P}, \mathbf{R}), \mathcal{A}_{P_l}] \mathcal{A}_{R_l} + \frac{i}{2\hbar} [\varepsilon(\mathbf{P}, \mathbf{R}), \mathcal{A}_{R_l}] \mathcal{A}_{P_l} \\
& + \frac{i}{2\hbar} [\mathcal{A}_{R_l}, \mathcal{A}_{P_l}] \varepsilon(\mathbf{P}, \mathbf{R})
\end{aligned} \tag{109}$$

as claimed in the text.

VI. APPENDIX 2. HOW SOLID STATES PHYSICS FITS IN OUR FRAMEWORK.

In solid state Physics, we assume that the hamiltonian is invariant through a discrete group of translations, for example a group of lattice translations, whose elements have the form

$$T(\mathbf{b}) = \exp\left(-\frac{i}{\hbar} \int_0^{\mathbf{b}} A_i(\mathbf{R} + \mathbf{r}) d\mathbf{r}\right) \exp\left(\frac{i}{\hbar} \mathbf{P} \cdot \mathbf{b}\right) \tag{110}$$

where \mathbf{b} is an arbitrary lattice vector. The eigenvalues of this operator are degenerated and have the form

$$\exp(i\mathbf{k} \cdot \mathbf{b}) \tag{111}$$

where \mathbf{k} belongs to some reduced dual lattice (a fraction of the dual lattice, i.e. a plaquette in solid state physics). We aim at defining the generators \mathbf{K} of these transformations as

$$\mathbf{K} \cdot \mathbf{b} = \log(T(\mathbf{b})) \tag{112}$$

so that we can define

$$K_i = \partial_{b_i} \mathbf{K} \cdot \mathbf{b} \tag{113}$$

However, this logarithm cannot be defined uniquely, and we will build an explicit choice in the sequel.

To do so, we work with the extended representation, so that the considered state space is defined, similarly to the Dirac case, by : $L^2(R^3) \otimes E$, where $L^2(R^3)$ is seen as the set of functions of the variable \mathbf{k} , running on R^3 . E is a vector space of infinite size representing the Brillouin zones. For each value of \mathbf{k} , $T(\mathbf{b})$ is diagonal in E , with eigenvalues $\exp(i\mathbf{k} \cdot \mathbf{b})$. We define K_i as acting diagonally as the multiplication by k_i . In other words, we have defined the momentum through an extension : $K \equiv K \otimes Id_E$.

Now, define the position operator \mathbf{R} as acting as $i\nabla_{\mathbf{K}}$. Turning now to the diagonalization process for the Hamiltonian, this last one can be performed independently for each value of \mathbf{k} , since the Hamiltonian commutes with the translations. We can thus see the Hamiltonian as a set of square matrices indexed by \mathbf{k} , each of them acting on each copy of E . As a consequence the diagonalization matrix is a Block acting on E for each value of \mathbf{k} .

Note that this diagonalization matrix can of course be seen as an operator $U(\mathbf{K}, \mathbf{R})$ or, and this is the point of view we adopt here, as a matrix acting on each copy of E , that is, a matrix $U(\mathbf{K})$, whose entries depend on \mathbf{K} only.

Actually, the dependence in \mathbf{R} appears in the non diagonal elements, and we can discard them if we consider this "half matrix, half operator" version. This mixed representation has the advantage to do the connection with the Dirac Hamiltonian.

In this set up, \mathbf{K} being diagonal and proportional to the identity, it commutes with every matrix $U(\mathbf{K}, \mathbf{R})$ preserving the Blocks. When considering the diagonalized Hamiltonian $\varepsilon(\mathbf{R}, \mathbf{K})$, it can also be seen as a diagonal matrix (implicitly denoted $\varepsilon(\mathbf{K})$) whose components are diagonal and denoted $\varepsilon_n(\mathbf{K})$, the n th band energy. The commutator

$$[\mathbf{R}, \varepsilon(\mathbf{K})] = \nabla \varepsilon(\mathbf{K}) \quad (114)$$

is again a diagonal matrix whose entries are $\nabla \varepsilon_n(\mathbf{K})$ (sketch of proof : $\varepsilon(\mathbf{K})$ is a series whose elements are products of powers of \mathbf{K} and \mathbf{R} . For each power of \mathbf{K} , the fact that $\varepsilon(\mathbf{K})$ is diagonal implies that the dependence in \mathbf{R} is a diagonal matrix. The gradient in \mathbf{K} acting only on the power of \mathbf{K} , this diagonality is preserved.) Turning now to the perturbation $\delta A(\mathbf{R})$, let us remark that if the operator $\delta A(\mathbf{R})$ preserves the bands, all operators $\varepsilon(\mathbf{K})\delta A(\mathbf{R})$, $[\varepsilon(\mathbf{K}), \delta A(\mathbf{R})]$ are diagonal, and given our previous remarks, the same is true for $\nabla \varepsilon(\mathbf{K})\delta A(\mathbf{R})$, $[\nabla \varepsilon(\mathbf{K}), \delta A(\mathbf{R})]$.

All this remarks that are obviously true for the Dirac case, appear to be useful in the solid state physics case (application 2), since it shows that the electron in an periodic potential fits in our framework. Actually, we can formally consider the Hamiltonian of such a problem as given by a matrix depending on the momenta and the coordinates.

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