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Semiclassical diagonalization of quantum Hamiltonian and equations of motion with Berry phase corrections

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Abstract. 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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1 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 physics, optics 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 motion of spinning particles, like electrons in electric [3] or magnetic fields [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 have also been the focus of several other works [3, 5,6] and have 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 dynamics 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

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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 [12–14]. However it is only in [15] that the non-canonical Hamiltonian formulation of a semiclassical electron in magnetic Bloch bands has been fully derived. This Hamiltonian approach allows deriving rigorously the semiclassical 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]. 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). In this representation the physical coordinate and momentum become noncommutative operators.

The previous discussion shows that Berry phase terms could be present in semiclassical equations of motion of several physical systems ranging from electrons in vacuum, in solid or in semiconductor to photons in inhomogeneous media, with potential application in the field of spintronics and spinoptics. This in turn called for a general semiclassical Hamiltonian formalism from which semiclassical 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 a Dirac (massive or massless) like-Hamiltonian. Starting with a 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. 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 symmetric static gravitational field (the asymmetric case is studied in Ref. [16]) and compare with the articles [17,18]. As a last application, the reader will find the details of the diagonalization sketched in [15] for the propagation of a Bloch electron (spinless) in an external electromagnetic field. These various physical applications show that our semiclassical Hamiltonian diagonalization approach is potentially promising since it unifies several apparently unrelated problematics in one formalism.

The paper is organized as follows. In Section 2 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 3 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 4 retrieves the equations of motion for an electron in a periodic potential within our general set up. Section 5 is for the conclusion.

2 A general process of semiclassical diagonalization

In this section we present a method to diagonalize at the semiclassical order ($\hbar$) 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 of this system can be written as a matrix $H_0\left(\mathbf{P},\mathbf{R}\right)$ of size $\dim V$ whose elements are operators depending on a couple of canonical variables $\mathbf{P}$ and $\mathbf{R}$. The archetype example is the Dirac Hamiltonian with $V = C^4$, but in Appendix B we show how a spinless electron in a periodic potential fits also in this set up. By diagonalization, we always mean here a unitary transformation setting the Hamiltonian in a diagonal matrix form, the diagonal elements being operators depending on $\mathbf{P}$ and $\mathbf{R}$. That is, we do not aim at finding the eigenvalues, but rather to derive the Band Hamiltonians, that are usually relevant for the semiclassical dynamics.

More precisely, our strategy will be to solve the exact diagonalization for $H_0\left(\mathbf{P},\mathbf{R}\right)$ at order $\hbar$, when the diagonalization of a fictitious Hamiltonian $H_0\left(\mathbf{P},\widetilde{\mathbf{r}}\right)$ is known for a parameter $\widetilde{\mathbf{r}}$ (replacing $\mathbf{R}$) which is supposed to commute with $\mathbf{P}$ (for instance this may be the Foldy-Wouthuysen transformation [19] for a free Dirac particle). We show how to compute the quantum corrections (at leading order in $\hbar$) that were neglected during this formal diagonalization (where position and momenta where considered as commuting quantities). The idea behind this procedure is that it is much easier to solve the diagonalization for $H_0(\mathbf{P},\widetilde{\mathbf{r}})$, as seen in our applications, and only then turn to $H_0(\mathbf{P},\mathbf{R})$.

2.1 Preliminary: products of operators series

To develop our process of diagonalization, the semiclassical expression of products of symmetrized expressions $S\left(\mathbf{P},\mathbf{R}\right)$ 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 $S_1\left(\mathbf{P},\mathbf{R}\right)$ and $S_2\left(\mathbf{P},\mathbf{R}\right)$, 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 $S_1\left(\mathbf{P},\mathbf{R}\right)S_2\left(\mathbf{P},\mathbf{R}\right)$ 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 $S_2\left(\mathbf{P},\mathbf{R}\right)$

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 $\hbar$

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

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

$$Asym\nabla_{R_l}\nabla_{P^l}\left[S_1(\mathbf{P},\mathbf{R})\,S_2(\mathbf{P},\mathbf{R})\right] = \nabla_{R_l}S_1(\mathbf{P},\mathbf{R}) \times \nabla_{P^l}S_2(\mathbf{P},\mathbf{R}) - \nabla_{P^l}S_1(\mathbf{P},\mathbf{R})\,\nabla_{R_l}S_2(\mathbf{P},\mathbf{R}). \quad (2)$$

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

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

where

$$Asym\nabla_{R_l}\nabla_{P^l}\left[S_1(\mathbf{P},\mathbf{R})_{S_2(\mathbf{P},\mathbf{R})}S_3(\mathbf{P},\mathbf{R})\right] = [\nabla_{R_l}S_1(\mathbf{P},\mathbf{R})]\,S_2(\mathbf{P},\mathbf{R})\nabla_{P^l}S_3(\mathbf{P},\mathbf{R}) - [\nabla_{P^l}S_1(\mathbf{P},\mathbf{R})]\,S_2(\mathbf{P},\mathbf{R})\,\nabla_{R_l}S_3(\mathbf{P},\mathbf{R}). \quad (4)$$

Let us stress again that all these identities are valid only at order $\hbar$ and that considering higher order corrections would of course induce more corrections.

2.2 Diagonalization with a parameter $\widetilde{r}$

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 semiclassical diagonalization of this operator, we first consider in this subsection a fictitious Hamiltonian $H_0(\mathbf{P},\widetilde{\mathbf{r}})$ where a parameter $\widetilde{\mathbf{r}}$ commuting with $\mathbf{P}$ has replaced the operator $\mathbf{R}$. We further assume that $H_0(\mathbf{P},\widetilde{\mathbf{r}})$ is known to be exactly diagonalized through a matrix $U(\mathbf{P},\widetilde{\mathbf{r}}) \equiv U$. We assume that U and $U(\mathbf{P},\widetilde{\mathbf{r}})\,H_0(\mathbf{P},\widetilde{\mathbf{r}})\,U^+(\mathbf{P},\widetilde{\mathbf{r}})$ can be expanded in series of P (with positive or negative powers) as it will be the case in our applications, but in fact this assumption which is practical for our proofs could probably be relaxed.

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

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

where $\mathbf{A}(\widetilde{\mathbf{r}})$ mimics a formal magnetic potential. The potential $\mathbf{A}(\widetilde{\mathbf{r}})$ being $\mathbf{R}$ independent, it only shifts the momentum for each value of $\widetilde{\mathbf{r}}$. As a consequence, the usual Foldy Wouthuysen [19] 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 $H_0(\mathbf{P},\widetilde{\mathbf{r}})$ will be written as

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

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

To gain some hints from our initial diagonalization, recall we assumed that the product $\varepsilon(\mathbf{P},\widetilde{\mathbf{r}}) = U(\mathbf{P},\widetilde{\mathbf{r}})\,H_0(\mathbf{P},\widetilde{\mathbf{r}})\,U^+(\mathbf{P},\widetilde{\mathbf{r}})$ can be expanded in series of monomial terms of the form: $\left(\varepsilon_1^{i_1}(\widetilde{\mathbf{r}})P_{i_1}^{k_{i_1}}\right)...\left(\varepsilon_n^{i_n}(\widetilde{\mathbf{r}})P_{i_n}^{k_{i_n}}\right)$ where the $\varepsilon_l^{i_l}(\widetilde{\mathbf{r}})$ are some matrices commuting with $\mathbf{P}$, and $P_{i_l}^{k_{i_l}}$ is the i_lth component of $\mathbf{P}$ $(i_l = 1,2,3)$ at some power k_{i_l} (this power should be written $k_{i_l,l}$ but we will avoid an excess of notation here). As usual, the sums over the i_l are implicit. Rearranging the series in powers of P_1, P_2, P_3 and given that $\widetilde{\mathbf{r}}$ is a parameter, we can write the energy in a symmetrical form:

$$\varepsilon(\mathbf{P},\widetilde{\mathbf{r}}) = \frac{1}{2}\sum_{\mathbf{X}}\left[A_{\mathbf{X}}(\widetilde{\mathbf{r}})\left(\prod_{i=1,2,3}P_i^{X_i}\right) + \left(\prod_{i=1,2,3}P_i^{X_i}\right)A_{\mathbf{X}}(\widetilde{\mathbf{r}})\right] \quad (7)$$

where $\left(\prod_{i=1,2,3}P_i^{X_i}\right)$ is a given momentum power and $A_{\mathbf{X}}(\widetilde{\mathbf{r}})$ is a combination of the $\varepsilon_l^{i_l}(\widetilde{\mathbf{r}})$. The $\mathbf{X}$ labels the multi index $(X_i,\ i=1,2,3)$.

The important consequence here is that the matrix $A_{\mathbf{X}}(\widetilde{\mathbf{r}})$ is diagonal. As an example, think of the Dirac Hamiltonian diagonalization, which involves some products $\alpha\cdot\mathbf{P}\alpha\cdot\mathbf{P}$, rearranged as

$$\frac{1}{2}\left[\alpha_iP_i\alpha_jP_j + \alpha_jP_j\alpha_iP_i\right] = \frac{1}{2}\left[\alpha_i\alpha_j + \alpha_j\alpha_i\right]P_iP_j \quad (8)$$

and $\frac{1}{2}\left[\alpha_i\alpha_j + \alpha_j\alpha_i\right]$ is diagonal, by the usual rules for Dirac matrices.

Let us conclude this subsection by noting that the symmetrizations we performed is unnecessary here, but will be of a practical interest when dealing with the exact diagonalization.

2.3 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 $U(\mathbf{P},\mathbf{R}) + XU(\mathbf{P},\mathbf{R})$, where X is a contribution of order $\hbar$ that ensures the unitarity of the transformation at order $\hbar$ (the factor U is a normalization that simplifies the subsequent expressions).

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

$$(U(\mathbf{P},\mathbf{R}) + XU)\left(U^+(\mathbf{P},\mathbf{R}) + U^+X^+\right) = 1 \tag{9}$$

and

$$\left(U^+(\mathbf{P},\mathbf{R}) + U^+X^+\right)(U(\mathbf{P},\mathbf{R}) + XU) = 1 \tag{10}$$

or equivalently

$$\begin{aligned} U(\mathbf{P},\mathbf{R})U^+(\mathbf{P},\mathbf{R}) + X + X^+ &= 1 \\ U^+(\mathbf{P},\mathbf{R})U(\mathbf{P},\mathbf{R}) + U^+\left(X + X^+\right)U &= 1. \end{aligned} \tag{11}$$

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 for the parameter $\widetilde{\mathbf{r}}$

$$U(\mathbf{P},\widetilde{\mathbf{r}})U^+(\mathbf{P},\widetilde{\mathbf{r}}) = 1 \tag{12}$$

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

$$U(\mathbf{P},\widetilde{\mathbf{r}})U^+(\mathbf{P},\widetilde{\mathbf{r}}) = \frac{1}{2}\sum_{\mathbf{X}}\left[B_{\mathbf{X}}(\widetilde{\mathbf{r}})\left(\prod_{i=1,2,3}P_i^{X_i}\right) + \left(\prod_{i=1,2,3}P_i^{X_i}\right)B_{\mathbf{X}}(\widetilde{\mathbf{r}})\right] = 1. \tag{13}$$

Therefore the series expansion $\sum_{\mathbf{X}} B_{\mathbf{X}}(\widetilde{\mathbf{r}})\left(\prod_{i=1,2,3}P_i^{X_i}\right)$ reduces to one constant term: the identity matrix.

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

$$\begin{aligned} &U(\mathbf{P},\mathbf{R})U^+(\mathbf{P},\mathbf{R}) = \\ &\frac{1}{2}\sum_{\mathbf{X}}\left[B_{\mathbf{X}}(\mathbf{R})\left(\prod_{i=1,2,3}P_i^{X_i}\right) + \left(\prod_{i=1,2,3}P_i^{X_i}\right)B_{\mathbf{X}}(\mathbf{R})\right] \\ &\quad + \frac{i}{2}\hbar Asym\nabla_{R_l}\nabla_{P^l}\left[U(\mathbf{P},\mathbf{R})U^+(\mathbf{P},\mathbf{R})\right]. \end{aligned} \tag{14}$$

Since our result about the $B_{\mathbf{X}}(\widetilde{\mathbf{r}})$ applies also to $B_{\mathbf{X}}(\mathbf{R})$ after replacing $\widetilde{\mathbf{r}}$ by $\mathbf{R}$, one has:

$$\begin{aligned} &U(\mathbf{P},\mathbf{R})U^+(\mathbf{P},\mathbf{R}) = \\ &\quad 1 + \frac{i}{2}\hbar Asym\nabla_{R_l}\nabla_{P^l}\left[U(\mathbf{P},\mathbf{R})U^+(\mathbf{P},\mathbf{R})\right] \\ &\quad = 1 - \frac{i}{2\hbar}\left[\mathcal{A}_{P_l},\mathcal{A}_{R_l}\right] \end{aligned} \tag{15}$$

where we have defined the ("non projected", see below) Berry connections (we use the terminology of Ref. [20]) as

$$\begin{aligned} \mathcal{A}_{\mathbf{R}} &= i\hbar U(\mathbf{P},\mathbf{R})\nabla_{\mathbf{P}}U^+(\mathbf{P},\mathbf{R}) \\ \mathcal{A}_{\mathbf{P}} &= -i\hbar U(\mathbf{P},\mathbf{R})\nabla_{\mathbf{R}}U^+(\mathbf{P},\mathbf{R}). \end{aligned} \tag{16}$$

that are non diagonal Hermitian matrices of order $\hbar$. Similarly, we have also:

$$\begin{aligned} &U^+(\mathbf{P},\mathbf{R})U(\mathbf{P},\mathbf{R}) = \\ &\quad 1 + \frac{i}{2}\hbar Asym\nabla_{R_l}\nabla_{P^l}\left[U^+(\mathbf{P},\mathbf{R})U(\mathbf{P},\mathbf{R})\right] \\ &\quad = 1 - U^+(\mathbf{P},\mathbf{R})\frac{i}{2\hbar}\left[\mathcal{A}_{P^l},\mathcal{A}_{R_l}\right]U(\mathbf{P},\mathbf{R}). \end{aligned} \tag{17}$$

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

$$X = \frac{i}{4\hbar}\left[\mathcal{A}_{P^l},\mathcal{A}_{R_l}\right]. \tag{18}$$

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 $U(\mathbf{P},\mathbf{R}) + XU + \delta XU$ 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 $\hbar$.

2.4 The quasidiagonalization

We will now consider the following quasi-diagonalization transformation

$$\left[(U(\mathbf{P},\mathbf{R}) + XU)H_0(\mathbf{P},\mathbf{R})\left(U^+(\mathbf{P},\mathbf{R}) + U^+X^+\right)\right]. \tag{19}$$

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

$$\begin{aligned} &U(\mathbf{P},\mathbf{R})H_0(\mathbf{P},\mathbf{R})U^+(\mathbf{P},\mathbf{R}) + XUH_0(\mathbf{P},\mathbf{R})U^+(\mathbf{P},\mathbf{R}) \\ &\quad + U(\mathbf{P},\mathbf{R})H_0(\mathbf{P},\mathbf{R})U^+X^+ \simeq \\ &U(\mathbf{P},\mathbf{R})H_0(\mathbf{P},\mathbf{R})U^+(\mathbf{P},\mathbf{R}) + X\varepsilon(\mathbf{P},\mathbf{R}) + \varepsilon(\mathbf{P},\mathbf{R})X^+. \end{aligned} \tag{20}$$

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 in $\mathbf{P}$ and $\mathbf{R}$. If this two variables where commuting, we would recover the expansion $\varepsilon(\mathbf{P},\mathbf{R})$ given in Section 1.2. But now, since, $\mathbf{R}$ does not commute with $\mathbf{P}$, one has rather

$$\begin{aligned} &U(\mathbf{P},\mathbf{R})H_0(\mathbf{P},\mathbf{R})U^+(\mathbf{P},\mathbf{R}) = \\ &\frac{1}{2}\sum_{\mathbf{X}}\left[A_{\mathbf{X}}(\mathbf{R})\left(\prod_{i=1,2,3}P_i^{X_i}\right) + \left(\prod_{i=1,2,3}P_i^{X_i}\right)A_{\mathbf{X}}(\mathbf{R})\right] \\ &\quad + [\text{commutators}] \end{aligned} \tag{21}$$

the commutators appearing while pushing the momentum powers on the left or on the right.

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 $A_{\mathbf{X}}(\mathbf{R})$ in the variable $\mathbf{R}$, are the same as the coefficients (which are diagonal) of the expansion of $A_{\mathbf{X}}(\mathbf{r})$ in the parameter $\mathbf{r}$. As a consequence,

$$\frac{1}{2}\sum_{\mathbf{X}}\left[A_{\mathbf{X}}(\mathbf{R})\left(\prod_{i=1,2,3}P_i^{X_i}\right)+\left(\prod_{i=1,2,3}P_i^{X_i}\right)A_{\mathbf{X}}(\mathbf{R})\right] \tag{22}$$

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

$$\varepsilon(\mathbf{P}-\mathbf{A}(\mathbf{R})) = \varepsilon(\mathbf{P}) - \frac{1}{2}\left(\mathbf{A}(\mathbf{R})\cdot\frac{\mathbf{P}}{\mathbf{P}^2}+\frac{\mathbf{P}}{\mathbf{P}^2}\cdot\mathbf{A}(\mathbf{R})\right) + \frac{1}{4}\left[\frac{1}{\mathbf{P}^2}\mathbf{A}^2(\mathbf{R})+\mathbf{A}^2(\mathbf{R})\frac{1}{\mathbf{P}^2}\right]+... \tag{23}$$

The last term in the right hand side of (21) involves just half the commutators obtained in pushing the momentum operators to the left or the right. As explained in Section 2.1 equation (3), they are simply given by

$$[\text{commutators}] = \frac{i}{2}\hbar Asym\nabla_{R_l}\nabla_{P^l}\left[U(\mathbf{P},\mathbf{R})\,H_0(\mathbf{P},\mathbf{R})\,U^+(\mathbf{P},\mathbf{R})\right]. \tag{24}$$

As a consequence, we can write

$$U(\mathbf{P},\mathbf{R})\,H_0(\mathbf{P},\mathbf{R})\,U^+(\mathbf{P},\mathbf{R}) = \varepsilon(\mathbf{P},\mathbf{R}) + \frac{i}{2}\hbar Asym\nabla_{R_l}\nabla_{P^l}\left[U(\mathbf{P},\mathbf{R})\,H_0(\mathbf{P},\mathbf{R})\,U^+(\mathbf{P},\mathbf{R})\right]. \tag{25}$$

A lengthy but straightforward computation presented in Appendix A leads to

$$\begin{aligned}&U(\mathbf{P},\mathbf{R})H_0(\mathbf{P},\mathbf{R})\,U^+(\mathbf{P},\mathbf{R}) = \\ &\varepsilon(\mathbf{P},\mathbf{R}) + \frac{1}{2}\left[\mathcal{A}_{R_l}\nabla_{R^l}\varepsilon(\mathbf{P},\mathbf{R}) + \nabla_{R^l}\varepsilon(\mathbf{P},\mathbf{R})\,\mathcal{A}_{R_l}\right] \\ &+\frac{1}{2}\left[\mathcal{A}_{P^l}\nabla_{P_l}\varepsilon(\mathbf{P},\mathbf{R}) + \nabla_{P_l}\varepsilon(\mathbf{P},\mathbf{R})\,\mathcal{A}_{P^l}\right] \\ &-\frac{i}{2\hbar}\left[\varepsilon(\mathbf{P},\mathbf{R}),\mathcal{A}_{P^l}\right]\mathcal{A}_{R_l} + \frac{i}{2\hbar}\left[\varepsilon(\mathbf{P},\mathbf{R}),\mathcal{A}_{R_l}\right]\mathcal{A}_{P^l} \\ &+\frac{i}{2\hbar}\left[\mathcal{A}_{R_l},\mathcal{A}_{P^l}\right]\varepsilon(\mathbf{P},\mathbf{R}).\end{aligned} \tag{26}$$

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

$$X\varepsilon(\mathbf{P},\mathbf{R}) + \varepsilon(\mathbf{P},\mathbf{R})\,X^+. \tag{27}$$

Given the expression obtained previously for X, we have thus

$$X\varepsilon(\mathbf{P},\mathbf{R}) + \varepsilon(\mathbf{P},\mathbf{R})\,X^+ = -\frac{i}{4\hbar}\left[\mathcal{A}_{R_l},\mathcal{A}_{P^l}\right]\varepsilon(\mathbf{P},\mathbf{R}) - \frac{i}{4\hbar}\varepsilon(\mathbf{P},\mathbf{R})\left[\mathcal{A}_{R_l},\mathcal{A}_{P^l}\right]. \tag{28}$$

We can thus ultimately write the diagonalization process as:

$$\begin{aligned}&\left[\left(U(\mathbf{P},\mathbf{R})+XU\right)H_0(\mathbf{P},\mathbf{R})\left(U^+(\mathbf{P},\mathbf{R})+U^+X^+\right)\right] = \\ &\varepsilon(\mathbf{P},\mathbf{R}) + \frac{1}{2}\left[\mathcal{A}_{R_l}\nabla_{R^l}\varepsilon(\mathbf{P},\mathbf{R}) + \nabla_{R^l}\varepsilon(\mathbf{P},\mathbf{R})\,\mathcal{A}_{R_l}\right] \\ &+\frac{1}{2}\left[\mathcal{A}_{P^l}\nabla_{P_l}\varepsilon(\mathbf{P},\mathbf{R}) + \nabla_{P_l}\varepsilon(\mathbf{P},\mathbf{R})\,\mathcal{A}_{P^l}\right] \\ &-\frac{i}{2\hbar}\left[\varepsilon(\mathbf{P},\mathbf{R}),\mathcal{A}_{P^l}\right]\mathcal{A}_{R_l} + \frac{i}{2\hbar}\left[\varepsilon(\mathbf{P},\mathbf{R}),\mathcal{A}_{R_l}\right]\mathcal{A}_{P^l} \\ &+\frac{i}{4\hbar}\left[\left[\mathcal{A}_{R_l},\mathcal{A}_{P^l}\right],\varepsilon(\mathbf{P},\mathbf{R})\right].\end{aligned} \tag{29}$$

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 connections $\mathcal{A}_{R_l}$ and $\mathcal{A}_{P^l}$, 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 genuine diagonalization.

2.5 The "exact" semiclassical diagonalization

As mentioned in Section 2.2, our choice of transformation $U(\mathbf{P},\mathbf{R}) + XU$ is somewhat arbitrary, however it is sufficient to perform the exact diagonalization as shown in the present paragraph. Actually, since $U(\mathbf{P},\mathbf{R})$ diagonalizes H_0 at zeroth order in $\hbar$, it reasonable to consider an-unknown- true diagonalization unitary operator $U_1(\mathbf{P},\mathbf{R})$ reducing to $U(\mathbf{P},\mathbf{R})$ at zeroth order in $\hbar$ of the following form $U_1(\mathbf{P},\mathbf{R}) = U(\mathbf{P},\mathbf{R}) + \hbar(...)$. As a consequence $U_1(\mathbf{P},\mathbf{R})$ and $U(\mathbf{P},\mathbf{R}) + XU$ are equal at the zeroth order in $\hbar$ and the difference

$$\delta XU \equiv U_1(\mathbf{P},\mathbf{R}) - U(\mathbf{P},\mathbf{R}) - XU \tag{30}$$

is of order $\hbar$. Moreover $U_1(\mathbf{P},\mathbf{R})$ and $U(\mathbf{P},\mathbf{R})+XU$ 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

$$\left[\left(U(\mathbf{P},\mathbf{R})+XU\right)H_0(\mathbf{P},\mathbf{R})\left(U^+(\mathbf{P},\mathbf{R})+U^+X^+\right)\right] - \left[U_1(\mathbf{P},\mathbf{R})\,H_0(\mathbf{P},\mathbf{R})\,U_1^+(\mathbf{P},\mathbf{R})\right] \tag{31}$$

is equal to

$$\left[\delta X,\varepsilon(\mathbf{P},\mathbf{R})\right]. \tag{32}$$

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 between our transformations, one gets 0

$$P\left[\left(U\left(\mathbf{P},\mathbf{R}\right)+XU\right)H_0\left(\mathbf{P},\mathbf{R}\right)\left(U^+\left(\mathbf{P},\mathbf{R}\right)\right.\right.\\ \left.\left.+U^+X^+\right)\right]-P\left[U_1\left(\mathbf{P},\mathbf{R}\right)H_0\left(\mathbf{P},\mathbf{R}\right)U_1^+\left(\mathbf{P},\mathbf{R}\right)\right]=0. \quad (33)$$

Here we have denoted $P[...]$ the projection on the diagonal.

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

$$P\left[U_1\left(\mathbf{P},\mathbf{R}\right)H_0\left(\mathbf{P},\mathbf{R}\right)U_1^+\left(\mathbf{P},\mathbf{R}\right)\right]= \\ U_1\left(\mathbf{P},\mathbf{R}\right)H_0\left(\mathbf{P},\mathbf{R}\right)U_1^+\left(\mathbf{P},\mathbf{R}\right) \quad (34)$$

so that ultimately

$$P\left[\left(U\left(\mathbf{P},\mathbf{R}\right)+XU\right)H_0\left(\mathbf{P},\mathbf{R}\right)\left(U^+\left(\mathbf{P},\mathbf{R}\right)+U^+X^+\right)\right]= \\ U_1\left(\mathbf{P},\mathbf{R}\right)H_0\left(\mathbf{P},\mathbf{R}\right)U_1^+\left(\mathbf{P},\mathbf{R}\right). \quad (35)$$

We can therefore conclude, that the projection of our quasi-diagonalized Hamiltonian, by eliminating thus the non diagonal parts, is in fact the genuine diagonalized Hamiltonian at order $\hbar$.

2.6 The diagonal Hamiltonian

From the previous discussion we understand that the genuine semiclassical diagonal Hamiltonian H_D is simply given by the projection on the diagonal of the Hamiltonian equation (29):

$$\begin{aligned}H_D=&P\left[\left(U\left(\mathbf{P},\mathbf{R}\right)+XU\right)H_0\left(\mathbf{P},\mathbf{R}\right)\left(U^+\left(\mathbf{P},\mathbf{R}\right)+U^+X^+\right)\right]\\ =&\varepsilon\left(\mathbf{P},\mathbf{R}\right)+\frac{1}{2}\left[A_{R_l}\nabla_{R_l}\varepsilon\left(\mathbf{P},\mathbf{R}\right)+\nabla_{R_l}\varepsilon\left(\mathbf{P},\mathbf{R}\right)A_{R_l}\right]\\ &+\frac{1}{2}\left[A_{P_l}\nabla_{P_l}\varepsilon\left(\mathbf{P},\mathbf{R}\right)+\nabla_{P_l}\varepsilon\left(\mathbf{P},\mathbf{R}\right)A_{P_l}\right]\\ &+P\left[-\frac{i}{2\hbar}\left[\varepsilon(\mathbf{P},\mathbf{R}),\mathcal{A}_{P_l}\right]\mathcal{A}_{R_l}+\frac{i}{2\hbar}\left[\varepsilon\left(\mathbf{P},\mathbf{R}\right),\mathcal{A}_{R_l}\right]\mathcal{A}_{P_l}\right]\end{aligned} \quad (36)$$

where we introduced the notation $A=P\left[\mathcal{A}\right]$. This Hamiltonian can be rewritten

$$\begin{aligned}H_D=&\varepsilon\left(\mathbf{P}+A_P,\mathbf{R}+A_R\right)+\frac{i}{2\hbar}P\left[\left[\varepsilon\left(\mathbf{P},\mathbf{R}\right),\mathcal{A}_{R_l}\right]\mathcal{A}_{P_l}\right.\\ &\left.-\left[\varepsilon\left(\mathbf{P},\mathbf{R}\right),\mathcal{A}_{P_l}\right]\mathcal{A}_{R_l}\right]\\ \simeq&\varepsilon\left(\mathbf{p},\mathbf{r}\right)+\frac{i}{2\hbar}P\left[\left[\varepsilon\left(\mathbf{p},\mathbf{r}\right),\mathcal{A}_{R_l}\right]\mathcal{A}_{P_l}-\left[\varepsilon\left(\mathbf{p},\mathbf{r}\right),\mathcal{A}_{P_l}\right]\mathcal{A}_{R_l}\right]\end{aligned} \quad (37)$$

where we have defined the projected dynamical operators

$$\begin{aligned}\mathbf{r}&=P\left[\left(U\left(\mathbf{P},\mathbf{R}\right)\right)\mathbf{R}U^+(\mathbf{P},\mathbf{R})\right]=\mathbf{R}+A_{\mathbf{R}}\\ \mathbf{p}&=P\left[U\left(\mathbf{P},\mathbf{R}\right)\mathbf{P}U^+(\mathbf{P},\mathbf{R})\right]=\mathbf{P}+A_{\mathbf{P}}.\end{aligned} \quad (38)$$

The non-canonical dynamical variables $(\mathbf{p},\mathbf{r})$ have corrections of order $\hbar$ through the presence of the Berry connections.

2.7 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 has to be considered, not for the usual position $\mathbf{R}$ and momentum $\mathbf{P}$, but rather for the projected variables $\mathbf{r}$ and $\mathbf{p}$. These new dynamical operators which naturally appear in our diagonalization process at the $\hbar$ order have components which do not commute any more. Actually

$$\begin{aligned}\left[r_i,r_j\right]&=i\Theta_{ij}^{rr}=i\hbar\left(\nabla_{P_i}A_{R_j}-\nabla_{P_j}A_{R_i}\right)+\left[A_{R_j},A_{R_i}\right]\\ \left[p_i,p_j\right]&=i\Theta_{ij}^{pp}=-i\hbar\left(\nabla_{R_i}A_{P_j}-\nabla_{R_j}A_{P_i}\right)+\left[A_{P_i},A_{P_j}\right]\\ \left[r_i,p_j\right]&=i\hbar\delta_{ij}+i\Theta_{ij}^{rp}=i\hbar\delta_{ij}+i\hbar\left(\nabla_{R_j}A_{R_i}+\nabla_{P_i}A_{P_j}\right)\\ &\quad+\left[A_{R_i},A_{P_j}\right]\end{aligned} \quad (39)$$

the Θ_{ij} being the so called non-Abelian Berry curvatures. They are of order $\hbar^2$ as lowest order corrections to the commutators, but will actually induce semiclassical corrections of order $\hbar$ to the equations of motion. Indeed the one band-Hamiltonian equation (37) yields directly to general equations of motion for $\mathbf{r}$, $\mathbf{p}$:

$$\begin{aligned}\dot{\mathbf{r}}=&\frac{i}{\hbar}\left[\mathbf{r},\varepsilon\left(\mathbf{p},\mathbf{r}\right)\right]+\frac{i}{\hbar}\left[\mathbf{r},\frac{i}{2\hbar}P\left[\left[\varepsilon\left(\mathbf{p},\mathbf{r}\right),\mathcal{A}_{R_l}\right]\mathcal{A}_{P^l}\right.\right.\\ &\left.\left.-\left[\varepsilon\left(\mathbf{p},\mathbf{r}\right),\mathcal{A}_{P^l}\right]\mathcal{A}_{R_l}\right]\right]\\ \dot{\mathbf{p}}=&\frac{i}{\hbar}\left[\mathbf{P},\varepsilon\left(\mathbf{p},\mathbf{r}\right)\right]+\frac{i}{\hbar}\left[\mathbf{p},\frac{i}{2\hbar}P\left[\left[\varepsilon\left(\mathbf{p},\mathbf{r}\right),\mathcal{A}_{R_l}\right]\mathcal{A}_{P^l}\right.\right.\\ &\left.\left.-\left[\varepsilon\left(\mathbf{p},\mathbf{r}\right),\mathcal{A}_{P^l}\right]\mathcal{A}_{R_l}\right]\right]\end{aligned} \quad (40)$$

where the commutators can be computed through the previous commutation rules equation (39). The last term in each equation represents a contribution of "magnetization" type (see the following applications) 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.

3 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 ([4,17, 18]), but in the second case (gravitational field) references to Berry phases was made for the first time in [16].

3.1 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 semiclassical order as was done in [4] using an approximate Foldy-Wouthuysen transformation [19]. From the semiclassical

$$\mathcal{A}_{R_i} = i\hbar U \nabla_{P_i} U^+ = \hbar \frac{i\alpha\cdot(\mathbf{P}-\mathbf{A}(\mathbf{R}))\,P_i\beta + i\beta E(E+m)\alpha_i - E\,(\mathbf{\Sigma}\times(\mathbf{P}-\mathbf{A}(\mathbf{R})))_i}{2E^2(E+m)} \tag{45}$$

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 semiclassical diagonalization of the Dirac Hamiltonian to show the effectiveness of our general method. It is worth noticing that the method developed above has now to be adapted as we will transform the Dirac Hamiltonian into a (2×2) block-diagonal matrix (due to the spin degree of freedom). However, it is easy to check that, since the non diagonal components for the energy blocks are of order $\hbar$, these corrections do not impair our general formulas for the Berry phases contributions.

We thus start with the following Dirac Hamiltonian:

$$H_0(\mathbf{P},\mathbf{R}) = \alpha\cdot(\mathbf{P}-\mathbf{A}(\mathbf{R})) + \beta m + V(\mathbf{R}) \tag{41}$$

where the matrix α and β are the usual (4×4) Dirac matrices:

$$\alpha_i = \begin{pmatrix} 0\,0 & \sigma_i \\ 0\,0 & \\ & 0\,0 \\ \sigma_i & 0\,0 \end{pmatrix} \tag{42}$$

with σ_i the usual (2×2) Pauli matrices $(i=1,2,3)$ and

$$\beta = \begin{pmatrix} 1\,0 & 0 & 0 \\ 0\,1 & 0 & 0 \\ 0\,0 & -1 & 0 \\ 0\,0 & 0 & -1 \end{pmatrix}. \tag{43}$$

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

$$U(\mathbf{P},\widetilde{\mathbf{r}}) = \frac{E+m+\beta\alpha\cdot(\mathbf{P}-\mathbf{A}(\widetilde{\mathbf{r}}))}{\sqrt{2E(E+m)}} \tag{44}$$

where $E=\sqrt{(\mathbf{P}-\mathbf{A}(\widetilde{\mathbf{r}}))^2+m^2}$. In this context, introducing the dependence in $\mathbf{R}$ we define the (non projected) Berry connections at first order in $\hbar$ as a (4×4) matrix

see equation (45) above

and

$$\mathcal{A}_{P_l} = -i\hbar U\nabla_{R_l}U^+ = \nabla_{R_l}A_k(\mathbf{R})\mathcal{A}_{R_k} \tag{46}$$

where E will now denote the symmetrized form of $E=\sqrt{(\mathbf{P}-A(\mathbf{R}))^2+m^2}$ (here at zeroth order in $\hbar$ we can consider that $\mathbf{P}$ and $\mathbf{R}$ commute). The spin matrices Σ_i $(i=1,2,3)$ are given by

$$\mathbf{\Sigma}_i = \begin{pmatrix} 0\,0 & \\ \sigma_i & 0\,0 \\ & 0\,0 \\ 0\,0 & \sigma_i \end{pmatrix}.$$

The general method developed in the previous section allows us to write the diagonal Hamiltonian H_D as a matrix generalization of equation (37)

$$\begin{aligned} H_D =& P\left[UH_0U^+\right] = \varepsilon(\mathbf{p},\mathbf{r}) + \frac{i}{2\hbar}P[[\varepsilon(\mathbf{p},\mathbf{r}),\mathcal{A}_{R_l}]\,\mathcal{A}_{P^l} \\ &- [\varepsilon(\mathbf{p},\mathbf{r}),\mathcal{A}_{P^l}]\,\mathcal{A}_{R_l}] + V(\mathbf{r}) \end{aligned} \tag{47}$$

where $\varepsilon(\mathbf{p},\mathbf{r})$ is the matrix $\beta\sqrt{(\mathbf{p}-\mathbf{A}(\mathbf{r}))^2+m^2}$ and $P[...]$ now projects on the diagonal blocks.

In equation (47) the operators $(\mathbf{p},\mathbf{r})$ are the physical dynamical variables satisfying the non-canonical commutations relations equation (39). Using the expressions for the Berry connections, H_D can be rewritten as:

$$\begin{aligned} H_D = \varepsilon(\mathbf{p},\mathbf{r}) + P\left[-\frac{i}{2}\left[\varepsilon(\mathbf{p},\mathbf{r}),U\nabla_{P^i}U^+\right]\varepsilon^{ijk}U\nabla_{P^j}U^+\right] \\ \times\frac{B^k(\mathbf{r})}{\hbar} + V(\mathbf{r}). \end{aligned} \tag{48}$$

Moreover, a straightforward computation shows that one can write
$P\left[-\frac{i}{2}\left[\varepsilon(\mathbf{p},\mathbf{r}),U\nabla_{P^i}U^+\right]\cdot\varepsilon^{ijk}U\nabla_{P_j}U^+\right]\frac{B^k(\mathbf{r})}{\hbar} = \beta\frac{\hbar\mathbf{\Sigma}\cdot\mathbf{B}}{2E} - \beta\frac{\mathbf{L}\cdot\mathbf{B}}{E}$
at the first order in $\hbar$, where we have introduced the intrinsic angular momentum of semiclassical particles $\mathbf{L}=\mathbf{P}\times A_{\mathbf{R}}$ with $A_{\mathbf{R}}=P[\mathcal{A}_R]=\hbar\frac{(\mathbf{P}-\mathbf{A}(\mathbf{R}))\times\mathbf{\Sigma}}{2E(E+m)}$ the projection of the Berry connection on the diagonal. As a consequence, the Hamiltonian to be considered is given by

$$H_D = \varepsilon(\mathbf{p},\mathbf{r}) + \beta\frac{\hbar\mathbf{\Sigma}\cdot\mathbf{B}}{2E} - \beta\frac{\mathbf{L}\cdot\mathbf{B}}{E} + V(\mathbf{r}) \tag{49}$$

which is the Hamiltonian deduced in [4] from a different approach and which leads of course to the dynamics described in that paper.

3.2 The electron in a static gravitational field

The behavior of Dirac particles in static gravitational field is an important issue, at the crossroad of particle physics and cosmology. Different approaches for the diagonalization of the Hamiltonian lead to contradictory results in particular with regard to the existence of a dipole spin-gravity coupling [17,18]. 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 [18] where a Foldy-Wouthuysen transformation instead of a semiclassical approximation is used.

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 [18]

$$H_0 = \frac{1}{2}(\alpha\cdot\mathbf{P}F(\mathbf{R}) + F(\mathbf{R})\alpha\cdot\mathbf{P}) + \beta m V(\mathbf{r}). \tag{50}$$

$$\mathcal{A}_{R_i} = i\hbar U\nabla_{P_i}U^+ = \hbar\frac{iF^3(\mathbf{R})\alpha\cdot\mathbf{P}P_i\beta + i\beta F(\mathbf{R})E(E+mV(\mathbf{R}))\alpha_i - EF^2(\mathbf{R})\left(\mathbf{\Sigma}\times\mathbf{P}\right)_i}{2E^2\left(E+mV(\mathbf{R})\right)}$$
$$\mathcal{A}_{P_i} = -i\hbar U\nabla_{R_i}U^+ = -\hbar i\frac{m\left(\nabla_{R_i}\phi\right)\beta F^2(\mathbf{R})\alpha\cdot\mathbf{P}}{2E^2} \tag{52}$$

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

$$U\left(\mathbf{P},\widetilde{\mathbf{r}}\right) = \frac{E+mV(\widetilde{\mathbf{r}})+\beta F(\widetilde{\mathbf{r}})\alpha\cdot\mathbf{P}}{\sqrt{2E(E+mV(\widetilde{\mathbf{r}}))}} \tag{51}$$

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

see equation (52) above

with $\phi = V/F$, $\mathbf{\Sigma}$ the spin of the electron and the energy E is now given by $E\left(\mathbf{P},\mathbf{R}\right) = \sqrt{\left(F^2(\mathbf{R})\mathbf{P}^2+\mathbf{P}^2F^2(\mathbf{R})\right)/2+m^2V^2(\mathbf{R})}$.

The expressions for $\mathcal{A}_{R_i}$ and $\mathcal{A}_{P_i}$ allow us ultimately to define the semiclassical transformation: $U\left(\mathbf{P},\mathbf{R}\right) + \frac{i}{4\hbar}\left[\mathcal{A}_{P^l},\mathcal{A}_{R_l}\right]U\left(\mathbf{P},\mathbf{R}\right)$ and to compute the diagonal Hamiltonian

$$H_D = P\left[UH_0U^+\right] = \varepsilon\left(\mathbf{p},\mathbf{r}\right) - \beta\frac{F^3(\mathbf{r})}{2E^2}m\hbar\nabla\phi(\mathbf{r})\cdot\left(\mathbf{p}\times\mathbf{\Sigma}\right) \tag{53}$$

with $\varepsilon\left(\mathbf{p},\mathbf{r}\right) = \beta\sqrt{\left(F^2(\mathbf{r})\mathbf{p}^2+\mathbf{p}^2F^2(\mathbf{r})\right)/2+m^2V^2(\mathbf{r})}$ where the dynamical variables which are deduced from the projections $A_{\mathbf{R}} = P[\mathcal{A}_{\mathbf{R}}] = \hbar\frac{F^2\mathbf{\Sigma}\times\mathbf{P}}{2E(E+mV)}$ and $A_{\mathbf{P}} = P[\mathcal{A}_{\mathbf{P}}] = 0$ are given by

$$\mathbf{r} = \mathbf{R}+A_{\mathbf{R}} = \mathbf{R}-\hbar\frac{F^2(\mathbf{R})\mathbf{\Sigma}\times\mathbf{P}}{2E(E+mV(\mathbf{R}))}$$
$$\mathbf{p} = \mathbf{P}+A_{\mathbf{P}} = \mathbf{P}. \tag{54}$$

The commutators between these variables are thus

$$[r_i,r_j] = i\Theta^{rr}_{ij}$$
$$[r_i,p_j] = i\hbar\delta_{ij}+i\Theta^{rp}_{ij}$$
$$[p_i,p_j] = 0 \tag{55}$$

where the Berry curvatures expressed in terms of the operators $(\mathbf{p},\mathbf{r})$ are

$$\Theta^{rr}_{ij} = -\frac{\hbar^2F^3(\mathbf{r})\varepsilon^{ijk}}{2E^3\left(\mathbf{p},\mathbf{r}\right)}\left(m\phi(\mathbf{r})\mathbf{\Sigma}_k+\frac{F(\mathbf{r})\left(\mathbf{\Sigma}\cdot\mathbf{p}\right)\mathbf{p}_k}{E\left(\mathbf{p},\mathbf{r}\right)+mV(\mathbf{r})}\right)$$
$$\Theta^{rp}_{ij} = \frac{\hbar^2F^3(\mathbf{r})}{2E^3\left(\mathbf{p},\mathbf{r}\right)}m\nabla_i\phi(\mathbf{r})\left(\mathbf{\Sigma}\times\mathbf{p}\right)_j$$
$$\Theta^{pp}_{ij} = 0. \tag{56}$$

One can check, after developing $\mathbf{r}$ as a function of $\mathbf{R}$ and the Berry connection, that the Hamiltonian equation (53) coincides with the one given in [18] at order $\hbar$. This confirms also the validity of the Foldy Wouthuysen approach asserted in [18] in opposition with the transformation proposed in [17]. However our approach is more general since it does not require an expansion in V and F as done in [18]. Of course, we retrieve the result of [18] if we expand expression (56) 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 [3,16].

To conclude this paragraph, we can derive the equations of motion with the help the noncanonical commutators between the coordinates and the spin

$$\Theta^{r\Sigma}_{ij} = [r_i,\Sigma_j] = i\hbar c^2\frac{-p_j\mathbf{\Sigma}_i+\mathbf{p}\cdot\mathbf{\Sigma}\delta_{ij}}{E\left(\mathbf{p},\mathbf{r}\right)\left(E\left(\mathbf{p},\mathbf{r}\right)+mV(\mathbf{r})\right)}$$
$$\Theta^{p\Sigma}_{ij} = [p_i,\Sigma_j] = 0. \tag{57}$$

We then can deduce the semiclassical equations of motion for the electron in a symmetric static gravitational field (by projecting on the positive energy subspace)

$$\dot{\mathbf{r}} = \left(1-\frac{\Theta^{rp}}{\hbar}\right)\nabla_{\mathbf{p}}E-\frac{1}{\hbar}\dot{\mathbf{p}}\times\Theta^{rr}+\frac{i}{\hbar}\Theta^{r\Sigma}\cdot\nabla_{\mathbf{\Sigma}}E$$
$$\dot{\mathbf{p}} = -\left(1-\frac{\Theta^{rp}}{\hbar}\right)\nabla_{\mathbf{r}}E \tag{58}$$

where we have defined the vectors Θ^{rr} through $\Theta^{rr}_{ij} = \varepsilon^{ijk}\Theta^{rr}_k$. We defined also in equation (58) the vector components $\left(\Theta^{rp}\nabla_{\mathbf{p}}E\right)_i = \Theta^{rp}_{ij}\nabla_{p^j}E$ and $\left(\Theta^{r\Sigma}\cdot\nabla_{\mathbf{\Sigma}}E\right)_i = \Theta^{r\Sigma}_{ij}\nabla_{\Sigma^j}E$. The velocity equation in equation (58) contains in particular an anomalous velocity term $\dot{\mathbf{p}}\times\Theta^{rr}/\hbar$ of order $\hbar$ which causes an additional displacement of the electrons orthogonally to the momentum $\mathbf{p}$. The dynamics of the system must be completed by the spin dynamics which is

$$\hbar\dot{\mathbf{\Sigma}} = \frac{mV(\mathbf{r})\hbar}{\varepsilon(\varepsilon+mV(\mathbf{r}))}\mathbf{\Sigma}\times\left(\nabla V(\mathbf{r})\times\mathbf{P}\right)-\frac{\hbar}{\varepsilon}\mathbf{\Sigma}\times\left(\nabla F(\mathbf{r})\times\mathbf{P}\right). \tag{59}$$

Although the position dynamics differs from the one of obtained in [18], due to our choice for the physical position operator ($\mathbf{r}$ instead of $\mathbf{R}$), one can show that the equations for $\dot{\mathbf{p}}$ and $\hbar\dot{\mathbf{\Sigma}}$ reduce to [18] in the case of weak fields.

4 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 set-up. The purpose is to find the semiclassical 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, consider an electron in an crystal lattice perturbated by the presence of an external electromagnetic field. As is usual, we express the total magnetic field as the sum of a constant field $\mathbf{B}$ and small nonuniform part $\delta\mathbf{B}(\mathbf{R})$. The Schrödinger equation reads $(H_0 - e\phi(\mathbf{R}))\Psi(\mathbf{R}) = E\Psi(\mathbf{R})$ with H_0 the magnetic contribution (ϕ being the electric potential) which reads

$$H_0 = \left(\frac{\mathbf{P}}{2m} + e\mathbf{A}(\mathbf{R}) + e\delta\mathbf{A}(\mathbf{R})\right)^2 + V(\mathbf{R}),\ \mathbf{P} = -i\hbar\nabla \tag{60}$$

where $\mathbf{A}(\mathbf{R})$ and $\delta\mathbf{A}(\mathbf{R})$ are the vectors potential of the homogeneous and inhomogeneous magnetic field, respectively, and $V(\mathbf{R})$ the periodic potential. The large constant part $\mathbf{B}$ is chosen such that the magnetic flux through a unit cell is a rational fraction of the flux quantum h/e. The advantage of such a decomposition is that for $\delta\mathbf{A}(\mathbf{R}) = 0$ the magnetic translation operators $\mathbf{T}(\mathbf{b}) = \exp(i\mathbf{K}\cdot\mathbf{b})$ defined in Appendix B, with $\mathbf{K}$ the generator of translation, are commuting quantities allowing to exactly diagonalize the Hamiltonian and to treat $\delta\mathbf{A}(\mathbf{R})$ as a small perturbation. The state space of the Bloch electron in the periodic zone scheme [21] is spanned by the basis vectors of plane waves $|n,\mathbf{k}\rangle = |\mathbf{k}\rangle\otimes|n\rangle$ with n corresponding to a band index and $\mathbf{k}$ vary in R^3. The state $|n\rangle$ can be seen as a canonical base vector $|n\rangle = (0...010...0...)$ (with 1 at the nth position) such that $U^+(\mathbf{k})|n\rangle = |u_n(\mathbf{k})\rangle$ with $|u_n(\mathbf{k})\rangle$ the periodic part (in space) of the magnetic Bloch waves [9,22]. In this representation $\mathbf{K}|n,\mathbf{k}\rangle = \mathbf{k}|n,\mathbf{k}\rangle$ and consequently the position operator is $\mathbf{R} = i\partial/\partial\mathbf{k}$, implying the canonical commutation relations $\left[\mathbf{R}_i, \mathbf{K}_j\right] = i\delta_{ij}$.

We first perform the diagonalization of the Hamiltonian in equation (60) for $\delta\mathbf{A} = 0$ by diagonalizing simultaneously H_0 and the magnetic translation operators $\mathbf{T}$. The diagonalization is performed as follows: start with an arbitrary basis of eigenvectors of $\mathbf{T}$. As explained in Appendix B, in this basis H_0 can be seen as a square matrix with operators entries. H_0 is diagonalized through a unitary matrix $U(\mathbf{K})$ which should depend only on $\mathbf{K}$ (since U should leave $\mathbf{K}$ invariant, i.e., $U\mathbf{K}U^+ = \mathbf{K}$) and whose precise expression is not necessary for the derivation of the equations of motion, such that $UHU^+ = \mathcal{E}(\mathbf{K}) - e\phi(U\mathbf{R}U^+)$, where $\mathcal{E}(\mathbf{K})$ is the diagonal energy matrix made of elements $\mathcal{E}_n(\mathbf{K})$ with n the band index (i.e. the diagonal representation of H_0).

Now, to add a perturbation $\delta A(\mathbf{R})$ as in [15], that breaks the translational symmetry, we have to replace $\mathbf{K}$ in all expressions by

$$\tilde{\mathbf{K}} = \mathbf{K} + e\frac{\delta A(\mathbf{R})}{\hbar} \tag{61}$$

and as the flux $\delta\mathbf{B}$ on a plaquette is not a rational multiple of the flux quantum, we cannot diagonalize simultaneously its components $\tilde{K}_i$ since they do not commute anymore. Actually

$$\hbar[\tilde{K}^i, \tilde{K}^j] = -ie\varepsilon^{ijk}\delta B_k(\mathbf{R}). \tag{62}$$

As a consequence of this non-commutativity, we just aim at quasi-diagonalizing our Hamiltonian at the semiclassical order (with accuracy $\hbar$). To do that we replace $U(\mathbf{K})$ by $U\left(\tilde{\mathbf{K}}\right)$, so that the non projected Berry connections are $\mathcal{A}_{R_i} = iU\nabla_{\tilde{K}_i}U^+$ and $\mathcal{A}_{K_l} = \nabla_{R_l}\delta A_k(\mathbf{R})\mathcal{A}_{R_k}$. From these we can define the nth intraband position and momentum operators $\mathbf{r}_n = \mathbf{R} + A_n$ and $\tilde{\mathbf{k}}_n \simeq \tilde{\mathbf{K}} - eA_n(\tilde{\mathbf{k}}_n) \times \delta\mathbf{B}(\mathbf{r}_n)/\hbar + O(\hbar)$ with $A_n = P_n(U\nabla_{\tilde{\mathbf{K}}}U^+)$ the projection of the Berry connection on the chosen nth Band [15]. It can be readily seen that the matrix elements of A_n can be written $A_n(\mathbf{k}) = i\langle u_n(\mathbf{k})|\nabla_{\mathbf{k}}|u_n(\mathbf{k})\rangle$ (see also Ref. [22] for the derivation of the position operator in the diagonal representation). What is totally new here is the transformation on the momentum operator $\tilde{k}_n$ which get also a Berry connection correction.

Using our results of Section 2, the full Hamiltonian equation (60) can thus be diagonalized through the transformation $U(\tilde{\mathbf{K}}) + \frac{i}{4\hbar}[\mathcal{A}_{R_l}, \mathcal{A}_{P^l}]U(\tilde{\mathbf{K}})$ plus a projection on the chosen nth Band as it is usual in solid state physics (the so-called one band approximation)

$$\begin{aligned} P_n\left[U\left(\tilde{\mathbf{K}}\right)HU^+\left(\tilde{\mathbf{K}}\right)\right] = \\ P_n\Bigg[\mathcal{E}\left(\tilde{\mathbf{k}}\right) - \frac{i}{4}\left[\mathcal{E}(\mathbf{K}), U\nabla_{K_i}U^+\right]\varepsilon^{ijk}\frac{\delta B^k(\mathbf{r})}{\hbar}U\nabla_{K_j}U^+ \\ -\frac{i}{4}U\nabla_{K_j}U^+\left[\mathcal{E}(\mathbf{K}), U\nabla_{K_i}U^+\right]\varepsilon^{ijk}\frac{\delta B^k(\mathbf{r})}{\hbar}\Bigg] \\ = \mathcal{E}_n\left(\tilde{\mathbf{k}}_n\right) - \mathcal{M}(\tilde{\mathbf{K}}).\delta\mathbf{B}(\mathbf{r}_n) + O(\hbar^2). \end{aligned} \tag{63}$$

where the energy levels $\mathcal{E}_n\left(\tilde{\mathbf{k}}_n\right)$ are the same as $\mathcal{E}_n(\mathbf{K})$ with $\tilde{\mathbf{k}}_n$ replacing $\mathbf{K}$. The magnetization $\mathcal{M}(\tilde{\mathbf{K}}) = P_n(\frac{ie}{2\hbar}\left[\mathcal{E}(\tilde{\mathbf{K}}), \mathcal{A}(\tilde{\mathbf{K}})\right] \times \mathcal{A}(\tilde{\mathbf{K}}))$ can be written under the usual form [22] in the $(\mathbf{k}, n)$ representation

$$\mathcal{M}^i_{nn} = \frac{ie}{2\hbar}\varepsilon^{ijk}\sum_{n'\neq n}(\mathcal{E}_n - \mathcal{E}_{n'})(\mathcal{A}_j)_{nn'}(\mathcal{A}_k)_{n'n}.$$

We mention that this magnetization (the orbital magnetic moment of Bloch electrons), has been obtained previously in the context of electron wave packets dynamics [9].

From the expression of the energy equation (63) we can deduce the equations of motion (with the band index n now omitted)

$$\begin{aligned} \dot{\mathbf{r}} &= \partial E(\tilde{\mathbf{k}})/\hbar\partial\tilde{\mathbf{k}} - \dot{\tilde{\mathbf{k}}} \times \Theta(\tilde{\mathbf{k}}) \\ \hbar\dot{\tilde{\mathbf{k}}} &= -e\mathbf{E} - e\dot{\mathbf{r}} \times \delta\mathbf{B}(\mathbf{r}) - \mathbf{M}\partial\delta\mathbf{B}/\partial\mathbf{r} \end{aligned} \tag{64}$$

where $\left[r^i, r^j\right] = i\Theta^{ij}(\tilde{\mathbf{k}})$ with $\Theta^{ij}(\tilde{\mathbf{k}}) = \partial^i\mathcal{A}^j(\tilde{\mathbf{k}}) - \partial^j\mathcal{A}^i(\tilde{\mathbf{k}})$ the Berry curvature.

As explained in [15] these equations are the same as the one derived in [9] from a completely different formalism.

$$\begin{aligned}\frac{i}{2}\hbar Asym\nabla_{R_l}\nabla_{P^l}\left[U\left(\mathbf{P},\mathbf{R}\right)H_0\left(\mathbf{P},\mathbf{R}\right)U^+\left(\mathbf{P},\mathbf{R}\right)\right] &= \frac{i}{2}\hbar Asym\nabla_{R_l}\nabla_{P^l}\left[U\left(\mathbf{P},\mathbf{R}\right)\right]H_0\left(\mathbf{P},\mathbf{R}\right)U^+\left(\mathbf{P},\mathbf{R}\right)\\ &+\frac{i}{2}\hbar U\left(\mathbf{P},\mathbf{R}\right)Asym\nabla_{R_l}\nabla_{P^l}\left[H_0\left(\mathbf{P},\mathbf{R}\right)\right]U^+\left(\mathbf{P},\mathbf{R}\right)\\ &+\frac{i}{2}\hbar U\left(\mathbf{P},\mathbf{R}\right)H_0\left(\mathbf{P},\mathbf{R}\right)Asym\nabla_{R_l}\nabla_{P^l}\left[U^+\left(\mathbf{P},\mathbf{R}\right)\right]\\ &+\frac{i}{2}\hbar\nabla_{R_l}U\left(\mathbf{P},\mathbf{R}\right)\nabla_{P^l}H_0\left(\mathbf{P},\mathbf{R}\right)U^+\left(\mathbf{P},\mathbf{R}\right)\\ &-\frac{i}{2}\hbar\nabla_{P^l}U\left(\mathbf{P},\mathbf{R}\right)\nabla_{R_l}H_0\left(\mathbf{P},\mathbf{R}\right)U^+\left(\mathbf{P},\mathbf{R}\right)\\ &-\frac{i}{2}\hbar U\left(\mathbf{P},\mathbf{R}\right)\nabla_{P^l}H_0\left(\mathbf{P},\mathbf{R}\right)\nabla_{R_l}U^+\left(\mathbf{P},\mathbf{R}\right)\\ &+\frac{i}{2}\hbar\nabla_{P^l}U\left(\mathbf{P},\mathbf{R}\right)\nabla_{R_l}H_0\left(\mathbf{P},\mathbf{R}\right)\nabla_{P^l}U^+\left(\mathbf{P},\mathbf{R}\right)\\ &+\frac{i}{2}\hbar\nabla_{R_l}U\left(\mathbf{P},\mathbf{R}\right)H_0\left(\mathbf{P},\mathbf{R}\right)\nabla_{P^l}U^+\left(\mathbf{P},\mathbf{R}\right)\\ &-\frac{i}{2}\hbar\nabla_{P^l}U\left(\mathbf{P},\mathbf{R}\right)H_0\left(\mathbf{P},\mathbf{R}\right)\nabla_{R_l}U^+\left(\mathbf{P},\mathbf{R}\right)\end{aligned}\tag{A.1}$$

5 Conclusion

Some recent applications of semiclassical 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 semiclassical 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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Appendix A

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

see equation (A.1) above

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

$$\begin{aligned}Asym\nabla_{R_l}\nabla_{P^l}[U(\mathbf{P},\mathbf{R})] &= Asym\nabla_{R_l}\nabla_{P^l}\left[U^+(\mathbf{P},\mathbf{R})\right]\\ &= 0.\end{aligned}\tag{A.2}$$

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

$$\begin{aligned}\mathbf{r} &= \left(U\left(\mathbf{P},\mathbf{R}\right)+X\right)\mathbf{R}\left(U^+(\mathbf{P},\mathbf{R})+X^+\right)\\ &\simeq \mathbf{R}+\left[i\hbar U\left(\mathbf{P},\mathbf{R}\right)\nabla_P U^+\left(\mathbf{P},\mathbf{R}\right)\right]=\mathbf{R}+\mathcal{A}_R\\ \mathbf{p} &= U\left(\mathbf{P},\mathbf{R}\right)\mathbf{P}U^+(\mathbf{P},\mathbf{R})\\ &\simeq \mathbf{P}-\left[i\hbar U\left(\mathbf{P},\mathbf{R}\right)\nabla_R U^+\left(\mathbf{P},\mathbf{R}\right)\right]=\mathbf{P}+\mathcal{A}_P.\end{aligned}\tag{A.3}$$

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

$$U\left(\mathbf{P},\mathbf{R}\right)U^+(\mathbf{P},\mathbf{R})=1\tag{A.4}$$

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

$$\begin{aligned}\mathcal{A}_R &= i\hbar U\left(\mathbf{P},\mathbf{R}\right)\nabla_P U^+\left(\mathbf{P},\mathbf{R}\right)\\ &= -i\nabla_P U\left(\mathbf{P},\mathbf{R}\right)U^+\left(\mathbf{P},\mathbf{R}\right)\\ \mathcal{A}_P &= -i\hbar U\left(\mathbf{P},\mathbf{R}\right)\nabla_R U^+\left(\mathbf{P},\mathbf{R}\right)\\ &= i\nabla_R U\left(\mathbf{P},\mathbf{R}\right)U^+\left(\mathbf{P},\mathbf{R}\right).\end{aligned}\tag{A.5}$$

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

$$\begin{aligned}
\frac{i}{2}\hbar Asym\nabla_{R_l}\nabla_{P^l}\left[U\left(\mathbf{P},\mathbf{R}\right)H_0\left(\mathbf{P},\mathbf{R}\right)U^+\left(\mathbf{P},\mathbf{R}\right)\right] &= \frac{-i}{2\hbar}\mathcal{A}_{P^l}U\left(\mathbf{P},\mathbf{R}\right)\left[R_l,H_0\left(\mathbf{P},\mathbf{R}\right)\right]U^+\left(\mathbf{P},\mathbf{R}\right)\\
&+\frac{i}{2\hbar}\mathcal{A}_{R_l}U\left(\mathbf{P},\mathbf{R}\right)\left[P_l,H_0\left(\mathbf{P},\mathbf{R}\right)\right]U^+\left(\mathbf{P},\mathbf{R}\right)\\
&-\frac{i}{2\hbar}U\left(\mathbf{P},\mathbf{R}\right)\left[R_l,H_0\left(\mathbf{P},\mathbf{R}\right)\right]U^+\left(\mathbf{P},\mathbf{R}\right)\mathcal{A}_{P^l}\\
&+\frac{i}{2\hbar}U\left(\mathbf{P},\mathbf{R}\right)\left[P^l,H_0\left(\mathbf{P},\mathbf{R}\right)\right]U^+\left(\mathbf{P},\mathbf{R}\right)\mathcal{A}_{R_l}\\
&-\frac{i}{2\hbar}\mathcal{A}_{P^l}\varepsilon\left(\mathbf{P},\mathbf{R}\right)\mathcal{A}_{R_l}+\frac{i}{2\hbar}\mathcal{A}_{R_l}\varepsilon\left(\mathbf{P},\mathbf{R}\right)\mathcal{A}_{P^l}\\
&=\frac{-i}{2\hbar}\mathcal{A}_{P^l}\left[r_l,\varepsilon\left(\mathbf{P},\mathbf{R}\right)\right]+\frac{i}{2\hbar}\mathcal{A}_{R_l}\left[p^l,\varepsilon\left(\mathbf{P},\mathbf{R}\right)\right]-\frac{i}{2\hbar}\left[r_l,\varepsilon\left(\mathbf{P},\mathbf{R}\right)\right]\mathcal{A}_{P^l}\\
&+\frac{i}{2\hbar}\left[p^l,\varepsilon\left(\mathbf{P},\mathbf{R}\right)\right]\mathcal{A}_{R_l}-\frac{i}{2\hbar}\mathcal{A}_{P^l}\varepsilon\left(\mathbf{P},\mathbf{R}\right)\mathcal{A}_{R_l}+\frac{i}{2\hbar}\mathcal{A}_{R_l}\varepsilon\left(\mathbf{P},\mathbf{R}\right)\mathcal{A}_{P^l}\\
&=\frac{1}{2}\left[\mathcal{A}_{R_l}\nabla_{R^l}\varepsilon\left(\mathbf{P},\mathbf{R}\right)+\nabla_{R^l}\varepsilon\left(\mathbf{P},\mathbf{R}\right)\mathcal{A}_{R_l}\right]\\
&+\frac{1}{2}\left[\mathcal{A}_{P^l}\nabla_{P_l}\varepsilon\left(\mathbf{P},\mathbf{R}\right)+\nabla_{P_l}\varepsilon\left(\mathbf{P},\mathbf{R}\right)\mathcal{A}_{P^l}\right]-\frac{i}{2\hbar}\mathcal{A}_{P^l}\left[\mathcal{A}_{R_l},\varepsilon\left(\mathbf{P},\mathbf{R}\right)\right]\\
&-\frac{i}{2\hbar}\left[\mathcal{A}_{R_l},\varepsilon\left(\mathbf{P},\mathbf{R}\right)\right]\mathcal{A}_{P^l}+\frac{i}{2\hbar}\mathcal{A}_{R_l}\left[\mathcal{A}_{P^l},\varepsilon\left(\mathbf{P},\mathbf{R}\right)\right]+\frac{i}{2\hbar}\left[\mathcal{A}_{P^l},\varepsilon\left(\mathbf{P},\mathbf{R}\right)\right]\mathcal{A}_{R_l}\\
&-\frac{i}{2\hbar}\mathcal{A}_{P^l}\varepsilon\left(\mathbf{P},\mathbf{R}\right)\mathcal{A}_{R_l}+\frac{i}{2\hbar}\mathcal{A}_{R_l}\varepsilon\left(\mathbf{P},\mathbf{R}\right)\mathcal{A}_{P^l}. \qquad \text{(A.6)}
\end{aligned}$$

$U^+\left(\mathbf{P},\mathbf{R}\right)$ when needed, we get:

see equation (A.6) above

Rearranging the commutators leads to:

$$\begin{aligned}
&\frac{i}{2}\hbar Asym\nabla_{R_l}\nabla_{P^l}\left[U\left(\mathbf{P},\mathbf{R}\right)H_0\left(\mathbf{P},\mathbf{R}\right)U^+\left(\mathbf{P},\mathbf{R}\right)\right]=\\
&\frac{1}{2}\left[\mathcal{A}_{R_l}\nabla_{R_l}\varepsilon\left(\mathbf{P},\mathbf{R}\right)+\nabla_{R_l}\varepsilon\left(\mathbf{P},\mathbf{R}\right)\mathcal{A}_{R_l}\right]\\
&+\frac{1}{2}\left[\mathcal{A}_{P_l}\nabla_{P_l}\varepsilon\left(\mathbf{P},\mathbf{R}\right)+\nabla_{P_l}\varepsilon\left(\mathbf{P},\mathbf{R}\right)\mathcal{A}_{P_l}\right]\\
&-\frac{i}{2\hbar}\mathcal{A}_{R_l}\left[\varepsilon\left(\mathbf{P},\mathbf{R}\right),\mathcal{A}_{P_l}\right]-\frac{i}{2\hbar}\left[\varepsilon\left(\mathbf{P},\mathbf{R}\right),\mathcal{A}_{P_l}\right]\mathcal{A}_{R_l}\\
&+\frac{i}{2\hbar}\mathcal{A}_{P^l}\left[\varepsilon\left(\mathbf{P},\mathbf{R}\right),\mathcal{A}_{R_l}\right]+\frac{i}{2\hbar}\left[\varepsilon\left(\mathbf{P},\mathbf{R}\right),\mathcal{A}_{R_l}\right]\mathcal{A}_{P^l}\\
&-\frac{i}{2\hbar}\mathcal{A}_{P^l}\varepsilon\left(\mathbf{P},\mathbf{R}\right)\mathcal{A}_{R_l}+\frac{i}{2\hbar}\mathcal{A}_{R_l}\varepsilon\left(\mathbf{P},\mathbf{R}\right)\mathcal{A}_{P^l} \qquad \text{(A.7)}
\end{aligned}$$

rewrite $\frac{-i}{2\hbar}\mathcal{A}_{P^l}\varepsilon\left(\mathbf{P},\mathbf{R}\right)\mathcal{A}_{R_l}+\frac{i}{2\hbar}\mathcal{A}_{R_l}\varepsilon\left(\mathbf{P},\mathbf{R}\right)\mathcal{A}_{P^l}$ as $-\frac{i}{2\hbar}\mathcal{A}_{P^l}\left[\varepsilon\left(\mathbf{P},\mathbf{R}\right),\mathcal{A}_{R_l}\right]+\frac{i}{2\hbar}\mathcal{A}_{R_l}\left[\varepsilon\left(\mathbf{P},\mathbf{R}\right),\mathcal{A}_{P^l}\right]+\frac{i}{2\hbar}\left[\mathcal{A}_{R_l},\mathcal{A}_{P^l}\right]\varepsilon\left(\mathbf{P},\mathbf{R}\right)$ so that:

$$\begin{aligned}
&\frac{i}{2}\hbar Asym\nabla_{R_l}\nabla_{P^l}\left[U\left(\mathbf{P},\mathbf{R}\right)H_0\left(\mathbf{P},\mathbf{R}\right)U^+\left(\mathbf{P},\mathbf{R}\right)\right]=\\
&\frac{1}{2}\left[\mathcal{A}_{R_l}\nabla_{R^l}\varepsilon\left(\mathbf{P},\mathbf{R}\right)+\nabla_{R^l}\varepsilon\left(\mathbf{P},\mathbf{R}\right)\mathcal{A}_{R_l}\right]\\
&+\frac{1}{2}\left[\mathcal{A}_{P^l}\nabla_{P_l}\varepsilon\left(\mathbf{P},\mathbf{R}\right)+\nabla_{P_l}\varepsilon\left(\mathbf{P},\mathbf{R}\right)\mathcal{A}_{P^l}\right]\\
&-\frac{i}{2\hbar}\left[\varepsilon\left(\mathbf{P},\mathbf{R}\right),\mathcal{A}_{P^l}\right]\mathcal{A}_{R_l}\\
&+\frac{i}{2\hbar}\left[\varepsilon\left(\mathbf{P},\mathbf{R}\right),\mathcal{A}_{R_l}\right]\mathcal{A}_{P^l}+\frac{i}{2\hbar}\left[\mathcal{A}_{R_l},\mathcal{A}_{P^l}\right]\varepsilon\left(\mathbf{P},\mathbf{R}\right). \qquad \text{(A.8)}
\end{aligned}$$

And we thus have:

$$\begin{aligned}
&U\left(\mathbf{P},\mathbf{R}\right)H_0\left(\mathbf{P},\mathbf{R}\right)U^+\left(\mathbf{P},\mathbf{R}\right)=\\
&\varepsilon\left(\mathbf{P},\mathbf{R}\right)+\frac{1}{2}\left[\mathcal{A}_{R_l}\nabla_{R^l}\varepsilon\left(\mathbf{P},\mathbf{R}\right)+\nabla_{R^l}\varepsilon\left(\mathbf{P},\mathbf{R}\right)\mathcal{A}_{R_l}\right]\\
&+\frac{1}{2}\left[\mathcal{A}_{P^l}\nabla_{P_l}\varepsilon\left(\mathbf{P},\mathbf{R}\right)+\nabla_{P_l}\varepsilon\left(\mathbf{P},\mathbf{R}\right)\mathcal{A}_{P^l}\right]\\
&-\frac{i}{2\hbar}\left[\varepsilon\left(\mathbf{P},\mathbf{R}\right),\mathcal{A}_{P^l}\right]\mathcal{A}_{R_l}\\
&+\frac{i}{2\hbar}\left[\varepsilon\left(\mathbf{P},\mathbf{R}\right),\mathcal{A}_{R_l}\right]\mathcal{A}_{P^l}+\frac{i}{2\hbar}\left[\mathcal{A}_{R_l},\mathcal{A}_{P^l}\right]\varepsilon\left(\mathbf{P},\mathbf{R}\right) \qquad \text{(A.9)}
\end{aligned}$$

as claimed in the text.

Appendix B: 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

$$T(\mathbf{b})=\exp\left(-\frac{i}{\hbar}\int_0^{\mathbf{b}}A_i(\mathbf{R}+\mathbf{r})\mathbf{dr}\right)\exp\left(\frac{i}{\hbar}\mathbf{P}\cdot\mathbf{b}\right) \qquad \text{(B.1)}$$

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

$$\exp\left(i\mathbf{k}\cdot\mathbf{b}\right) \qquad \text{(B.2)}$$

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

$$\mathbf{K} \cdot \mathbf{b} = \log\left(T(\mathbf{b})\right) \tag{B.3}$$

so that we can define

$$K_i = \partial_{b_i} \mathbf{K} \cdot \mathbf{b} \tag{B.4}$$

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 bands. 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: $K \equiv K \otimes Id_E$. Consequently the position operator $\mathbf{R}$ is acting as $i\nabla_{\mathbf{k}}$. Therefore the state space of the Bloch electron is spanned by the basis vector of plane waves $|n, \mathbf{k}\rangle = |\mathbf{k}\rangle \otimes |n\rangle$ with n corresponding to a band index. The state $|n\rangle$ can be seen as a canonical base vector $|n\rangle = (0...010...0...)$ (with 1 at the nth position).

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

$$[\mathbf{R}, \varepsilon(\mathbf{K})] = \nabla\varepsilon(\mathbf{K}) \tag{B.5}$$

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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