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Appearance of Gauge Fields and Forces beyond the adiabatic approximation

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We investigate the origin of quantum geometric phases, gauge fields and forces beyond the adiabatic regime. In particular, we extend the notions of geometric magnetic and electric forces discovered in studies of the Born-Oppenheimer approximation to arbitrary quantum systems described by matrix valued quantum Hamiltonians. The results are illustrated by several physical relevant examples.

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I. INTRODUCTION

A physical system can never be considered as completely isolated from the rest of the universe. For a slow (adiabatic) cyclic variation of its environment, the wave function of the quantum system gets an additional geometric phase factor, known as the Berry phase [1]. In fact, the driving environment, the 'heavy' or 'slow' system, is also subject to back reaction from the 'light' or 'fast' system. In the context of the Born-Oppenheimer (BO) theory of molecules, the back reaction of the light system leads to the appearance of a gauge field in the effective Hamiltonian for the slow one (the environment) [2][3][4]. The gauge field consists of a vector and a scalar potential and turns out to depend on a quantum geometric tensor [5]. It can both induce interference phenomena and modify the dynamics through geometric Lorentz and electric forces [6][7]. The first measurements of geometric Berry forces were done, on the one hand in the coordinate space for the evolution of trapped particles [8] and on the other hand in the momentum space for the evolution of relativistic particles [9] (see also the comment in [10] which contains related discussion on the geometric forces and fast-slow motion decoupling in physical systems).

Many physical systems, as discussed in this paper, display a separation of scales in terms of slow and fast degrees and thus share a very similar mathematical structure with molecular systems. Actually all these systems have a space-time evolution governed by a multicomponent Schrödinger-like equation, whose Hamiltonian is a matrix valued operator. It is therefore the purpose of the present note to investigate the origin of quantum gauge fields and forces in a more general context than the BO theory, by considering the diagonalization of an arbitrary matrix valued quantum Hamiltonian. To be precise, by diagonalization we mean the derivation of an effective in-band Hamiltonian made of block-diagonal energy subspaces. For that purpose we use the results of a method developed recently [11]. This approach, based on a new differential calculus on a non-commutative space where \hbar plays the role of running parameter, leads to an in-band energy operator that can be obtained systematically up to arbitrary order in \hbar . Note that there exists other totally different methods of diagonalization in a formal series expansion in \hbar which uses symbols of operators via Weyl calculus [12][13]. Particularly important for our purpose, it has been possible, for an arbitrary Hamiltonian $H(\mathbf{K}, \mathbf{Q})$ with the canonical coordinates and momentum $[Q_i, K_j] = i\hbar\delta_{ij}$, to obtain the corresponding diagonal representation $\varepsilon(\mathbf{k}, \mathbf{q})$ to order \hbar^2 , in terms of non-canonical coordinates and momentum (\mathbf{k}, \mathbf{q}) defined later and commutators between gauge fields. The method is quite involved for an arbitrary Hamiltonian, but simplifies greatly for systems whose Hamiltonian has the simple form $H = T(\mathbf{K}) + V(\mathbf{Q})$.

This kind of Hamiltonian that we are considering in this paper allows us to discuss how geometric gauge fields and geometric forces arise at order \hbar^2 in physical situations as various as Dirac and Bloch electrons in electric fields or Born-Oppenheimer theory. Note that first order \hbar corrections (semi-classical) were first treated for Bloch electrons in [14] and for Dirac electrons in [15][16] (see [17] for a review and also [18] which contains an overview of the first-order Berry-phase effects and forces in 4-D space times).

Our approach reveals the appearance at order \hbar^2 of a scalar gauge potential expressed in terms of two tensors. One is the quantum metric tensor [5][19], and the other one is a new tensor generalizing an additional term found in [12] for the Born-Oppenheimer case. Another very important consequence of the Hamiltonian diagonalization is the appearance of gauge invariant intraband coordinates. The advantage of using these coordinates is that the diagonal Hamiltonian is also gauge invariant. Moreover, these coordinates fulfill a non-commutative algebra which strongly affects the dynamics through a Lorentz term and the gradient of a new scalar potential, generalizing thus the dynamics of the Born-Oppenheimer theory.

II. HAMILTONIAN DIAGONALIZATION.

Consider the Schrödinger equation

$$i\hbar \frac{\partial |\Psi\rangle}{\partial t} = H |\Psi\rangle \quad (1)$$

where for the sake of completeness the Hamiltonian is supposed time dependent and of the form

$$H = T(\mathbf{K}, t) + V(\mathbf{Q}, t) \quad (2)$$

where it is assumed that $T(\mathbf{K}, t)$ is a matrix valued operator while $V(\mathbf{Q}, t)$ is a scalar valued one. We aim to diagonalize the full differential operator $D = H - K_0$ where $K_0 \equiv i\hbar\partial/\partial t$ is the conjugate operator of the time $[K_0, t] = i\hbar$.

The mathematical difficulty in performing the diagonalization of D comes from the intricate entanglement of noncommuting operators due to the canonical relation $[Q_i, K_j] = i\hbar\delta_{ij}$. In [11] starting with a very general but time independent $H(\mathbf{K}, \mathbf{Q})$ and by considering \hbar as a running parameter, we related the in-band Hamiltonian $UHU^+ = \varepsilon(\mathbf{X})$ and the unitary transforming matrix $U(\mathbf{X})$ (where $\mathbf{X} \equiv (\mathbf{Q}, \mathbf{K})$) to their classical expressions through integro-differential operators, i.e. $\varepsilon(\mathbf{X}) = \widehat{O}(\varepsilon(\tilde{\mathbf{X}}))$ and $U(\mathbf{X}) = \widehat{N}(U(\tilde{\mathbf{X}}))$, where in the matrices $\varepsilon(\tilde{\mathbf{X}})$ and $U(\tilde{\mathbf{X}})$, the dynamical operators \mathbf{X} are replaced by classical commuting variables $\tilde{\mathbf{X}} = (\tilde{\mathbf{Q}}, \tilde{\mathbf{K}})$.

The only requirement of the method is therefore the knowledge of $U(\tilde{\mathbf{X}})$ which gives the diagonal form $\varepsilon(\tilde{\mathbf{X}})$. Generally, these equations do not allow to find directly $\varepsilon(\mathbf{X})$, $U(\mathbf{X})$, however, they allow us to produce the solution recursively in a series expansion in \hbar . With this assumption that both ε and U can be expanded in power series of \hbar , we determined in [11], the explicit diagonalization of an arbitrary Hamiltonian to order \hbar^2 . The expression of the effective n -th in-band energy ε_n greatly simplifies for Hamiltonian given by Eq. (2) and the result is given by Eq. (3). But, for this simplified problem, it is interesting to give the principal steps leading to this result. In the first step, assuming that the unitary matrix $U_0(\tilde{\mathbf{K}}, t)$ diagonalizing $T(\tilde{\mathbf{K}}, t)$ only, that is $U_0 T U_0^+ = \varepsilon_0(\tilde{\mathbf{K}}, t)$, is known ($\varepsilon_0(\tilde{\mathbf{K}}, t)$ is the matrix of the eigenvalues of $T(\tilde{\mathbf{K}}, t)$), we obtain the semiclassical expression

$$U_0 D U_0^+ = \varepsilon_0(\mathbf{K}, t) + V(\mathbf{Q} + \hbar\mathbf{A}, t) - K_0 + \hbar A^0$$

with $\mathbf{A}(\mathbf{K}, t) = iU_0 \nabla_{\mathbf{K}} U_0^+$ and $A^0(\mathbf{K}, t) = -iU_0 \frac{\partial}{\partial t} U_0^+$ two non diagonal matrices. The diagonalization at the next order (\hbar^2) is done by an unitary transformation matrix $U = U_0 + \hbar U_1 U_0$. The general method of [11] gives an explicit procedure to determine the antihermitian matrix $(U_1)_{mn} = \frac{(1-\delta_{mn})}{\varepsilon_m(t) - \varepsilon_n(t)} (\mathbf{A})_{mn} \cdot \nabla V$, which removes the off-diagonal elements of \mathbf{A} and A^0 , so that Eq. (1) becomes $i\hbar \frac{\partial |\Psi'\rangle}{\partial t} = \varepsilon |\Psi'\rangle$ with $|\Psi'\rangle = U |\Psi\rangle$ with the diagonal energy matrix ε whose elements ε_n to order \hbar^2 are

$$\varepsilon_n(\mathbf{K}, \mathbf{q}_n, t) = \varepsilon_{0,n}(\mathbf{K}, t) + V(\mathbf{q}_n, t) + \hbar A_n^0 + \hbar^2 \Phi_n \quad (3)$$

where the geometric scalar potential is

$$\Phi_n(\mathbf{Q}, \mathbf{K}, t) = \frac{G_n^{ij}}{2} \partial_i \partial_j V + M_n^{ij} \partial_i V \partial_j V + (M_n^{0i} + M_n^{i0}) \partial_i V + M_n^{00} \quad (4)$$

with two gauge invariant tensors G_n^{ij} and $M_n^{\mu\nu}$ defined as

$$G_n^{ij}(\mathbf{K}, t) = \frac{1}{2} \sum_{m \neq n} ((A^i)_{nm}(A^j)_{mn} + h.c.) \quad (5)$$

and

$$M_n^{\mu\nu}(\mathbf{K}, t) = \frac{1}{2} \sum_{m \neq n} \left(\frac{(A^\mu)_{nm}(A^\nu)_{mn}}{\varepsilon_{0,m} - \varepsilon_{0,n}} + h.c. \right) \quad (6)$$

Indices μ corresponding to $\mu = 0, 1, 2, 3$, such that $\mu = 0$ is the temporal variable and $\mu = i = 1, 2, 3$ the spatial ones. The tensor G_n^{ij} is known as the quantum metric tensor [5][19] and $M_n^{\mu\nu}$ is a new tensor generalizing an additional term found in [12] for the Born-Oppenheimer theory.

In Eq. (3) the operator $\mathbf{q} \equiv \mathbf{Q} + \hbar \mathbf{A}$ which is non diagonal has been replaced after application of U by the intraband coordinate $\mathbf{q}_n = \mathbf{Q} + \hbar \mathbf{a}_n$ where \mathbf{a}_n is a gauge connection usually called the Berry connection defined as the projection of $\mathbf{A} \equiv iU_0 \nabla_{\mathbf{K}} U_0^+$ on the n -th eigenstate $\mathbf{a}_n(\mathbf{K}, t) \equiv (\mathbf{A})_{nn} = i \langle n | \nabla_{\mathbf{K}} n \rangle$. Here $|n\rangle$ are the eigenstates of the non-diagonal part of H , i.e., $T(\mathbf{K}, t)|n\rangle = \varepsilon_{0,n}(\mathbf{K}, t)|n\rangle$. In the same manner $a_n^0 \equiv (A^0)_{nn} = -i \langle n | \dot{n} \rangle$ is the scalar gauge potential. Note that even though it is formally indifferent to express Φ_n in terms of \mathbf{Q} or \mathbf{q}_n the difference being of higher order in \hbar , the introduction of the non-canonical coordinate \mathbf{q}_n is essential to maintain the gauge invariance of the Hamiltonian. The formal similarity with gauge theories is evident as we can define a Berry curvature the n -th eigenstate (which can be degenerate)

$$\Theta_n^{ij}(\mathbf{K}) = \frac{\partial a_n^j}{\partial K_i} - \frac{\partial a_n^i}{\partial K_j} + [a_n^i, a_n^j] \quad (7)$$

leading to the following non-canonical commutation relations

$$[q_n^i, q_n^j] = i\hbar^2 \Theta_n^{ij} \quad (8)$$

As usual, the curvature leads to introduce a magnetic-type vector field $\Theta_n(\mathbf{K}, t)$ whose components are defined as $\Theta_n^i = \varepsilon_{jk}^i \Theta_n^{jk}/2$ and in the same manner from the temporal component $a_n^0(\mathbf{K}, t)$ an electric-type field is defined as

$$\mathbf{E}_n(\mathbf{K}, t) = -\frac{\partial \mathbf{a}_n}{\partial t} - \nabla a_n^0 \quad (9)$$

Note that extension of the first-order (\hbar) Berry adiabatic formalism to the 4D space-time evolution with the ‘‘magnetic’’ and ‘‘electric’’ geometric fields and the corresponding Hamiltonian approach has been made in [16][18].

For certain systems, like spinning particles in ferromagnets, the electric-type field leads to spin motive forces (Faraday law of spin) [20]. Here the motive force is given by

$$\xi = -\oint_C \mathbf{E}_n \cdot d\mathbf{K} = \frac{\partial}{\partial t} \int_S \Theta_n \cdot d\mathbf{S}_K = \frac{\partial \phi}{\partial t}$$

where C is a closed curve in \mathbf{K} space, and S the surface delimited by C ($d\mathbf{S}_K$ being the infinitesimal surface vector orthogonal to S), and ϕ the magnetic type flux through S . The motive force is independent of the charge of the particle and requires only a time dependent Berry curvature.

The Heisenberg equations of motion $\dot{\mathbf{q}}_n = -i\hbar [\mathbf{q}_n, \varepsilon_n] + \frac{\partial \mathbf{q}_n}{\partial t}$ et $\dot{\mathbf{K}} = -i\hbar [\mathbf{K}, \varepsilon_n]$ to the second order in \hbar are

$$\dot{\mathbf{q}}_n = \nabla_{\mathbf{K}} \varepsilon_{0,n} - \hbar \mathbf{E}_n - \frac{\hbar}{2} (\dot{\mathbf{K}} \times \Theta_n - \Theta_n \times \dot{\mathbf{K}}) + \hbar^2 \nabla_{\mathbf{K}} \Phi_n, \quad \dot{\mathbf{K}} = -\nabla_{\mathbf{q}_n} V \quad (10)$$

The dynamics of the intraband operators leads directly to a Lorentz-type term. The scalar potential is a consequence of transitions between eigenstates $|n\rangle$ of T and impacts the dynamics through its gradient. Working with the non-canonical coordinates is a short-cut to determine the dynamics of a system prepared in a second order in \hbar eigenstate of the diagonalized Hamiltonian Eq. (3). This state will evolve in the same energy subspace n , as there are no transitions between these eigenlevels as far as we can neglect higher contributions in the expansion in \hbar . In comparison, the

equations of motion derived from the Hamiltonian H do not seem to include a Lorentz force, and the determination of the "eigendynamics" can be a very difficult to achieve. An appealing example is given in [6][7] where the "exact" slow motion of a massive neutral particle coupled to a spin is compared with the Born-Oppenheimer theory.

We underline that the expansion in \hbar breaks down in regions of mode conversion where $\varepsilon_{0,m} - \varepsilon_{0,n} \ll \hbar$ or for large values of $\langle m | \partial_\mu n \rangle$. In a mode conversion region, one can easily generalize the diagonalization of H to a block-diagonalization where transitions between states inside the block are allowed (off-diagonal elements), but there are no transitions between different blocks. The expansion in \hbar is consistent with the adiabatic approximation (see [13] and related discussion in [18]). Indeed, the semiclassical order (\hbar) where the potential Φ_n is absent corresponds to a situation of no-transitions between the states $|n\rangle$ (or between states in different blocks) whereas the expansion to second order in \hbar corresponds to post-adiabatic corrections [21] where there is no transition of higher order between eigenlevels and eigenstates of the diagonalized Hamiltonian Eq. (3).

The virtue of our approach is its full generality which sheds a new light and provides an unified description of several phenomena which were considered case by case. We are now going to illustrate the results by several physical examples.

III. BORN-OPPENHEIMER APPROXIMATION.

Consider the following Hamiltonian describing a fast system in interaction with an external environment

$$H = \frac{1}{2} B_{ij} P^i P^j + \frac{p^2}{2m} + \varphi(\mathbf{R}, \mathbf{r}) \quad (11)$$

where the fast system is described by a set of dynamical variables (\mathbf{r}, \mathbf{p}) (not to be confused with the non-canonical coordinate and momentum operators) and the slow one (the environment) by coordinates (\mathbf{R}, \mathbf{P}) . As in [5] we consider a general kinetic energy with B , a positive definite inverse mass tensor. Applying the previous results with the mapping $\mathbf{Q} \rightarrow \mathbf{P}$, $\mathbf{K} \rightarrow \mathbf{R}$ (and $i\nabla_{\mathbf{K}} \rightarrow -i\nabla_{\mathbf{R}}$) we have $V(\mathbf{Q}) \rightarrow B_{ij} P_i P_j / 2$ and we can check that the operator $T(\mathbf{R})$ corresponds to $T(\mathbf{R}) = \frac{p^2}{2m} + \varphi(\mathbf{R}, \mathbf{r})$. We assume that its eigenvalues $E_n(\mathbf{R})$ are known (or equivalently the matrix U_0 diagonalizing T). This eigenvalues are the energy levels of the fast system for given position \mathbf{R} of the slow one, such that the matrix elements in this representation reads $\langle m | T(\mathbf{R}) | n \rangle = \delta_{m,n} E_n(\mathbf{R})$. In this representation the Hamiltonian of the slow part is non-diagonal but we can now directly apply formula Eq. (3) to obtain the following eigenvalues of H to order \hbar^2 in terms of the slow variables (assuming a non-degenerate spectrum for the fast system) :

$$\varepsilon_n(\mathbf{p}_n, \mathbf{R}) = \frac{1}{2} B_{ij} p_n^i p_n^j + \hbar^2 \Phi_n + E_n(\mathbf{R}) \quad (12)$$

where $\mathbf{p}_n = \mathbf{P} - i\hbar \langle n | \nabla_{\mathbf{R}} n \rangle$ is the gauge invariant momentum of the slow system. The scalar potential Eq. (4) then becomes

$$\Phi_n(\mathbf{R}, \mathbf{P}) = \frac{G_n^{ij}(\mathbf{R})}{2} B_{ij} + M_n^{ij}(\mathbf{R}) B_{il} B_{jk} P^l P^k \quad (13)$$

with the quantum metric tensor $G_n^{ij}(\mathbf{R}) = \text{Re} \sum_{m \neq n} \langle \partial_i n | m \rangle \langle m | \partial_j n \rangle$ and $M_n^{ij}(\mathbf{R}) = \text{Re} \sum_{m \neq n} \frac{\langle \partial_i n | m \rangle \langle m | \partial_j n \rangle}{\varepsilon_{0,m} - \varepsilon_{0,n}}$. The term $G_n^{ij}(\mathbf{R}) B_{ij}$ is the usual part of the scalar potential discussed in several circumstances [5][6][7], whereas the term $M_n^{ij}(\mathbf{R}) B_{il} B_{jk} P^l P^k$ was found in [12]. Here we see that the Born-Oppenheimer theory can be obtained straightforwardly from our Hamiltonian diagonalization to order \hbar^2 . In the same manner from Eq.(10) we immediately get the Born-Oppenheimer equations of motion $\dot{\mathbf{p}}_n = -\nabla_{\mathbf{R}} E_n - \frac{\hbar}{2} (\dot{\mathbf{R}} \times \boldsymbol{\Theta}_n - \boldsymbol{\Theta}_n \times \dot{\mathbf{R}}) - \hbar^2 \nabla_{\mathbf{R}} \Phi_n$ with $\dot{R}_i = B_{ij} \dot{p}_n^j$. Similar equations of motion for a classical system consisting of a classical magnetic moment interacting with an inhomogeneous magnetic field [6][7] were studied in details. It was found that the Lorentz force results from a slight misalignment of the magnetic moment relative to the magnetic field. This corresponds to the semi-classical approximation. The electric force is a time average of a strong oscillatory force induced by the precession of the magnetic moment. This is a kind of zitterbewegung effect.

IV. PARTICLE IN A LINEAR EXTERNAL POTENTIAL.

Another interesting relevant situation concerns a particle in a linear potential exemplified here by a Bloch electron in a constant external electric field (see also [22] and for the first semi-classical treatment see [14]). Consider $H = H_0(\mathbf{P}, \mathbf{R}) + \varphi(\mathbf{R})$ with H_0 the energy of a particle in a periodic potential and $\varphi(\mathbf{R}) = -e\mathbf{E}\cdot\mathbf{R}$ the external electric perturbation (and $e < 0$ the charge). Again assuming that one knows U_0 diagonalizing H_0 we then have $U_0 H_0 U_0^\dagger = \varepsilon_{0,n}(\mathbf{k})$ with $\varepsilon_{0,n}(\mathbf{k})$ the n -th energy band and \mathbf{k} the pseudo-momentum in the absence of the external field. Or, we can also write $\langle u_m(\mathbf{k}) | H_0(\mathbf{P}, \mathbf{R}) | u_n(\mathbf{k}) \rangle = \delta_{m,n} \varepsilon_{0,n}(\mathbf{k})$ with $|u_n(\mathbf{k})\rangle$ the periodic part of the Bloch wave function (for a more detailed discussion see also [23]).

Then, for the determination of the full eigenvalues of H we use formula (3) with the mapping $\mathbf{Q} \rightarrow \mathbf{R}$, so that the scalar gauge potential reduces to $\Phi_n(\mathbf{k}) = e^2 T_n^{ij} E_i E_j$, and the energy eigenvalues are

$$\varepsilon_n = \varepsilon_{0,n}(\mathbf{k}) - e\mathbf{E}\cdot\mathbf{r}_n + e^2 \hbar^2 M_n^{ij}(\mathbf{k}) E_i E_j \quad (14)$$

with the covariant coordinate $\mathbf{r}_n = \mathbf{R} + i\hbar \langle u_n | \nabla_{\mathbf{k}} u_n \rangle$ and $M_n^{ij}(\mathbf{k}) = \text{Re} \sum_{m \neq n} \frac{\langle \partial_i u_n | u_m \rangle \langle u_m | \partial_j u_n \rangle}{\varepsilon_{0,m} - \varepsilon_{0,n}}$. Introducing the "magnetic field" $\omega_n(\mathbf{k}) = \frac{\hbar}{eE^2} \mathbf{E} \times \nabla_{\mathbf{k}} \Phi_n$ and $\chi_n(\mathbf{k}) = \frac{1}{eE^2} \mathbf{E} \cdot \nabla_{\mathbf{k}} \Phi_n$ the equations of motion are

$$\dot{\mathbf{r}}_n = \nabla_{\mathbf{k}} \varepsilon_{0,n} - \frac{\hbar}{2} (\dot{\mathbf{k}} \times \Omega_n - \Omega_n \times \dot{\mathbf{k}}) + \hbar^2 \chi_n \dot{\mathbf{k}}, \quad \dot{\mathbf{k}} = e\mathbf{E}$$

where $\Omega_n(\mathbf{k}) = \Theta_n(\mathbf{k}) + \hbar \omega_n(\mathbf{k})$. This shows that Φ_n contributes to the Lorentz term $\hbar \dot{\mathbf{k}} \times \Omega_n$ known as the anomalous velocity which is orthogonal to the applied electric field. This anomalous velocity is at the center of many recent experimental and theoretical works and led to the discovery the magnetic-type monopole in solids [24]. The scalar potential Φ_n contributes also to the velocity in the direction of \mathbf{E} , through the term $\hbar^2 \chi_n \dot{\mathbf{k}}$.

V. BEYOND THE BERRY PHASE.

The linear potential case has another interest. It allows us to also consider the fast system to derive the Berry phase in a different way and to get a correction term to the phase of the wave function.

A. General results

Indeed, consider a time dependent Hamiltonian $H(t)$ and introduce the differential operator $D = H(t) - P_0$ where $P_0 \equiv i\hbar \partial / \partial t$ is the conjugate of time which is treated formally as an operator such that $[P_0, t] = i\hbar$. The time dependence is due to the time evolution of some parameters $x(t)$ describing the environment. Assuming that we know $\varepsilon_n(t)$ and $|n(t)\rangle$ the instantaneous eigenvalues and eigenstates of H , i.e., $H(t)|n(t)\rangle = \varepsilon_n(t)|n(t)\rangle$, then D is a non-diagonal matrix in this representation because of the presence of the time derivative operator P_0 . To transform the system of differential equations (Schrödinger equation) $D|\Psi(t)\rangle = 0$, which couples all components of $|\Psi(t)\rangle$ into a decoupled set of differential equations, we introduce a unitary transformation $|\Psi'(t)\rangle = U(t)|\Psi(t)\rangle$ such that $U(t)D(t, P_0)U^\dagger(t) = \tilde{\Lambda}(t, P_0)$ is a diagonal differential operator and $\tilde{\Lambda}(t, P_0)|\Psi'(t)\rangle = 0$. Therefore the time evolution is given by $|\Psi'(t)\rangle = e^{-\frac{i}{\hbar} \int_0^t \Lambda(t) dt} |\Psi'(0)\rangle$. Since $\Lambda(t) = \tilde{\Lambda}(t) + P_0$ is diagonal, no time ordered product is required. Returning back to the initial state we have

$$|\Psi(t)\rangle = U^\dagger(t) e^{-\frac{i}{\hbar} \int_0^t \Lambda(t) dt} U(0) |\Psi(0)\rangle \quad (15)$$

A system prepared in a state $|\Lambda_n(0)\rangle$ which is an eigenstate of D , i.e., $D(0)|\Lambda_n(0)\rangle = \tilde{\Lambda}_n(0)|\Lambda_n(0)\rangle$ will evolve with $\Lambda(t)$ and thus stays in the instantaneous eigenstates $|\Lambda_n(t)\rangle$ of $D(t)$ (for simplicity we assume non degenerate eigenvalues). In this case the wave function becomes $|\Psi(t)\rangle = e^{-\frac{i}{\hbar} \int_0^t \Lambda_n(t) dt} |\Lambda_n(t)\rangle$. Since eigenstates of D instead of H are considered, the time evolution Eq. (15) is exact and thus valid for adiabatic as well as for nonadiabatic

evolution. Therefore for a periodic motion of period T , such that $|\Lambda_n(T)\rangle = |\Lambda_n(0)\rangle$ (single valued eigenstates), we have, if $|\Psi(0)\rangle = |\Lambda_n(0)\rangle$

$$|\Psi(T)\rangle = e^{\frac{-i}{\hbar} \int_0^T \varepsilon_n(t) dt} e^{-i\beta_n} |\Psi(0)\rangle \quad (16)$$

with $\beta_n = \frac{1}{\hbar} \int_0^t \Lambda_n(t) dt - \frac{1}{\hbar} \int_0^T \varepsilon_n(t) dt$ the exact geometric phase of the system without any approximation which corresponds to the Aharonov-Anandan phase [25]. Indeed, these authors extended the notion of Berry geometric phase for cyclic adiabatic evolutions to nonadiabatic cyclic evolutions (see also [26] and references therein).

But, in general we need an approximation scheme for the diagonalization of D and we will use the expansion to order \hbar^2 . The problem of finding $\Lambda_n = \tilde{\Lambda}_n(t) + P_0$ is formally equivalent to the Bloch electron example discussed above with $K \rightarrow t$, $Q \equiv R \rightarrow P_0$ and $eE = 1$. We obtain from Eq.(14)

$$\Lambda_n = \varepsilon_n(t) - i\hbar \langle n | \dot{n} \rangle + \hbar^2 M_n(t) \quad (17)$$

with $M_n(t) = \text{Re} \sum_{m \neq n} \frac{\langle \dot{n} | m \rangle \langle m | \dot{n} \rangle}{\varepsilon_m - \varepsilon_n}$. Therefore for a periodic motion of period T , Eq. (16) becomes

$$|\Psi(T)\rangle = e^{-i\gamma_n} |\Psi(0)\rangle \quad (18)$$

with

$$\gamma_n = \frac{1}{\hbar} \int_0^T \varepsilon_n(t) dt + i \int_0^T \langle n | \dot{n} \rangle dt + \hbar \int_0^T M_n(t) dt$$

The phase γ_n appears as an expansion in power of \hbar . The first term is the usual dynamical phase and the second one the geometric Berry phase independent of \hbar and of the velocity of parameters $\dot{x}(t)$. The additional phase $\hbar \int_0^T M_n(t) dt$ of order \hbar is apparently non-geometric as it depends on \dot{x} . It cancels in the infinitely slow $\dot{x} \rightarrow 0$ adiabatic regime, which thus coincides with the semiclassical approximation. Nevertheless, it is worth noticing that the higher order phase corrections can also be seen as geometric in the Aharonov-Anandan meaning [27][28], since $\int_0^T M_n(t) dt$ can also be presented as a contour integral in a generalized parameter space [27].

Quantitatively, if the system is prepared in an eigenstate $|n(0)\rangle$ of $H(0)$, then $|\Psi(t)\rangle$ is given by Eq. (15) with $U = U_0 + \hbar U_1 U_0$ where $U_1(t)_{mn} = i \frac{(1-\delta_{mn}) \langle m | \dot{n} \rangle}{\varepsilon_m(t) - \varepsilon_n(t)}$, so that we have the following expansion up to order \hbar :

$$\begin{aligned} |\Psi(t)\rangle &= e^{\frac{-i}{\hbar} \int_0^t \Lambda_n(t) dt} |n(t)\rangle + \hbar \sum_{m \neq n} \left(e^{\frac{-i}{\hbar} \int_0^t \Lambda_n(t) dt} A_{mn}(t) \right. \\ &\quad \left. - e^{\frac{-i}{\hbar} \int_0^t \Lambda_m(t) dt} A_{mn}(0) \right) |m(t)\rangle + O(\hbar^2) \end{aligned}$$

The magnitude of transitions is then controlled by the term $A_{mn} = \frac{i \langle m(t) | \dot{n}(t) \rangle}{\varepsilon_n(t) - \varepsilon_m(t)}$ which is neglected in the strict adiabatic limit $\langle m(t) | \dot{n}(t) \rangle \rightarrow 0$.

In principle deviation from adiabaticity at the semi-classical level could be measured by interferometry. Consider a periodic two states system, and write the initial state in the eigenbase $|n(0)\rangle = |\Lambda_n(0)\rangle + \hbar A_{mn}(0) |\Lambda_m(0)\rangle$. Then, after one cycle $|\Psi(T)\rangle = e^{-i\gamma_n} |\Lambda_n(0)\rangle + \hbar e^{-i\gamma_m} A_{mn}(0) |\Lambda_m(0)\rangle$. For an observable O which does not commute with H one will find in the average $\langle \Psi(T) | O | \Psi(T) \rangle$ an interference term $2\hbar \text{Re} (A_{mn}(0) \langle \Lambda_n(0) | O | \Lambda_m(0) \rangle e^{-i(\gamma_n - \gamma_m)})$ which is formally equivalent to the zitterbewegung of Dirac particles.

Note that $|\Psi(t)\rangle$ is normalized to unity at order \hbar only; i.e. $\langle \Psi(t) | \Psi(t) \rangle = 1 + O(\hbar^2)$ so that a normalization at a higher order needs an expansion of U to the same order. To second order, the diagonalizing matrix $U_2(t)$ is given by the procedure described in [11] leading to $U_2(t)_{mn} = - \sum_{k \neq n, m} \frac{\langle m | \dot{k} \rangle \langle k | \dot{n} \rangle}{(\varepsilon_m(t) - \varepsilon_k(t))(\varepsilon_k(t) - \varepsilon_n(t))}$ so that the wave function

reads

$$\begin{aligned}
|\Psi(t)\rangle = & \left(e^{-\frac{i}{\hbar} \int_0^t \Lambda_n(t) dt} - \hbar^2 \sum_{m \neq n} e^{-\frac{i}{\hbar} \int_0^t \Lambda_m(t) dt} A_{nm}(t) A_{mn}(0) + \hbar^2 e^{-\frac{i}{\hbar} \int_0^t \Lambda_n(t) dt} (U_2^+(t)_{nn} + U_2(0)_{nn}) \right) |n(t)\rangle \\
& \left(\hbar \sum_{m \neq n} \left(e^{-\frac{i}{\hbar} \int_0^t \Lambda_n(t) dt} A_{mn}(t) - e^{-\frac{i}{\hbar} \int_0^t \Lambda_m(t) dt} A_{mn}(0) \right) + \hbar^2 \sum_{m \neq n} \left(e^{-\frac{i}{\hbar} \int_0^t \Lambda_n(t) dt} U_2^+(t)_{mn} + e^{-\frac{i}{\hbar} \int_0^t \Lambda_m(t) dt} U_2(0)_{mn} \right) \right. \\
& \left. - \hbar^2 \sum_{p, m \neq n} e^{-\frac{i}{\hbar} \int_0^t \Lambda_p(t) dt} A_{mp}(t) A_{pn}(0) \right) |m(t)\rangle
\end{aligned} \tag{19}$$

From this result we can compute the so called fidelity defined as $|\langle \Psi_{ad}(t) | \Psi(t) \rangle|^2$ where $|\Psi_{ad}(t)\rangle$ correspond to the wave function in the adiabatic limit. Using Eq. (19) we obtain

$$\begin{aligned}
|\langle \Psi_{ad}(t) | \Psi(t) \rangle|^2 = & 1 - \hbar^2 \sum_{k \neq n} \left(\frac{|\langle n | \dot{k} \rangle|^2}{(\varepsilon_n(t) - \varepsilon_k(t))^2} + \frac{|\langle n | \dot{k} \rangle_0^2}{(\varepsilon_n(0) - \varepsilon_k(0))^2} \right) \\
& - \hbar^2 \sum_{k \neq n} \frac{e^{-i(\gamma_k - \gamma_n)} \langle n | \dot{k} \rangle \langle k | \dot{n} \rangle + e^{i(\gamma_k - \gamma_n)} \left(\langle n | \dot{k} \rangle \langle k | \dot{n} \rangle \right)^*}{(\varepsilon_n(t) - \varepsilon_k(t)) (\varepsilon_n(0) - \varepsilon_k(0))}
\end{aligned} \tag{20}$$

with $e^{-i(\gamma_k - \gamma_n)} = e^{-i \int \left[\frac{\varepsilon_k - \varepsilon_n}{\hbar} + (\phi_k - \phi_n) + \hbar(M_k - M_n) \right] dt}$ with $\phi_n = \langle n | \dot{n} \rangle$.

B. Example

As a physical illustration let consider the Hamiltonian

$$H = \mathbf{B}(t) \cdot \boldsymbol{\sigma}$$

corresponding to the paradigmatic example of a spin coupled to a magnetic field. The eigenvalues of $D = H(t) - i\hbar \partial / \partial t$ at order \hbar^2 are given by Eq. (17)

$$\Lambda_l = \varepsilon_l(t) + \hbar a_l^0 + \hbar^2 M_l(t) \tag{21}$$

The Hamiltonian being diagonalized by the matrix $U_0 = \frac{(\mathbf{n} \cdot \boldsymbol{\sigma} + \sigma_z)}{\sqrt{2(1+n_z)}}$ with $\mathbf{n} = \mathbf{B}/B$, we have the two level eigenvalues $\varepsilon_l(t) = B(t) (\sigma_z)_{ll}$ with $l = 1, 2$, and the matrix $A^0 = -i\hbar U_0 \frac{\partial}{\partial t} U_0^+$ is thus given

$$A^0 = -\hbar \left(\frac{((\mathbf{n} + \mathbf{k}) \times \dot{\mathbf{n}}) \cdot \boldsymbol{\sigma}}{2(1+n_z)} \right)$$

As a consequence the scalar gauge potential $a_l^0 = -i \langle l | \dot{l} \rangle = -i\hbar (U_0 \frac{\partial}{\partial t} U_0^+)_{ll}$ reads $a_l^0 = -\frac{\hbar((\mathbf{n} + \mathbf{k}) \times \dot{\mathbf{n}}) \cdot \mathbf{k}}{2(1+n_z)} (\sigma_z)_{ll}$ and $M_l(t) = M_l^{00} = \frac{1}{2} \sum_{m \neq l} \left(\frac{(A^0)_{lm} (A^0)_{ml}}{\varepsilon_{m-} - \varepsilon_{0,l}} + h.c. \right)$ can therefore be written

$$M_l = -\frac{2(1+n_z) \dot{n}^2 - \dot{n}_z^2 - \left((\mathbf{n} \times \dot{\mathbf{n}}) \cdot \mathbf{k} \right)^2}{8(1+n_z)^2 \varepsilon_l(t)} \tag{22}$$

The Berry phase can thus be cast in the form

$$\phi_{l,B} = -(\sigma_z)_l \int_0^T dt \frac{(\mathbf{n} \times \dot{\mathbf{n}}) \cdot \mathbf{k}}{2(1+n_z)} \quad (23)$$

It is interesting to introduce the Euler angles $\mathbf{n} = (\sin \theta \cos \varphi, \sin \theta \sin \varphi, \cos \theta)$, so that the Berry phase reads $\phi_{l,B} = (\sigma_z)_l \frac{1}{2} \int_L (1 - \cos \theta) d\varphi$ and the correction of higher order to the phase γ_l is thus

$$\hbar \int_0^T M_l(t) dt = \frac{\hbar}{8B} \int_0^T (\sin^2 \theta \dot{\varphi}^2 + \dot{\theta}^2) dt. \quad (24)$$

We retrieve the result of [27] for $\varphi = 0$. Note that, it was shown in [27], this higher order contribution to the geometric phase is a part of the non-adiabatic Aharonov-Anandan geometric phase.

Let compute the fidelity in the simple case $\theta = \text{const}$ and $\varphi = \omega t$. A direct application of Eq. (20) gives

$$|\langle \Psi_{ad}(t) | \Psi(t) \rangle|^2 = 1 - \frac{\omega^2 \sin^2 \theta}{4\omega_0^2} \sin^2(\omega_0 - \omega)t + \dots \quad (25)$$

where we introduced the notation $B = \hbar\omega_0$. The usual criteria for adiabaticity is given by the condition $\frac{\sin^2 \theta \omega^2}{4\omega_0^2} \ll 1$. At the resonance $\frac{\omega_0}{\omega} = 1$ fidelity is always one at this order of the expansion.

VI. DIRAC PARTICLE IN AN EXTERNAL POTENTIAL.

We will now show that our formalism can also be used for relativistic Dirac particles, which are usually treated with the Foldy Wouthuysen approach [29]. The semiclassical treatment of the problem was first considered in [15] and [16]. The direct second order in \hbar diagonalization being done in [11], we can now fully appreciate how simple and straightforward is the application of the formalism presented here.

The Hamiltonian is (with $c = 1$)

$$H = \alpha \cdot \mathbf{p} + \beta m + V(\mathbf{R}) \quad (26)$$

where α and β are the usual (4×4) Dirac matrices and $V(\mathbf{R})$ is the external potential. The matrix diagonalizing the free part of the Hamiltonian $U_0 (\alpha \cdot \mathbf{p} + \beta m) U_0^\dagger = \beta E$ with $E = \sqrt{\mathbf{p}^2 + m^2}$ is the usual Foldy Wouthuysen unitary transformation $U_0 = \frac{E+m+\beta \alpha \cdot \mathbf{p}}{(2E(E+m))^{1/2}}$. For the Dirac particles we have two energy subspaces ε_\pm of dimension 2 corresponding to the positive and negative energy. Now with the correspondence $\mathbf{Q} \rightarrow \mathbf{R}$, $\mathbf{K} \rightarrow \mathbf{p}$ and formula Eq. (3), one easily sees that the diagonal matrix can be written

$$\varepsilon(\mathbf{p}, \mathbf{r}) = \beta E(\mathbf{p}) + V(\mathbf{r}) + \beta \Phi \quad (27)$$

The position operator is given by the (4×4) matrix $\mathbf{r} = \mathbf{R} + \frac{\hbar \mathbf{p} \times \boldsymbol{\Sigma}}{2E(E+m)}$ with $\boldsymbol{\Sigma} = \mathbf{1} \otimes \boldsymbol{\sigma}$ where $\boldsymbol{\sigma}$ are the Pauli matrices. The band index of the scalar potential has been transferred to the matrix β , and we have $G^{ij} = \frac{1}{4E^2} g^{ij}$ and $M^{ij} = \frac{1}{8E^3} g^{ij}$ with the notation $g^{ij} = \delta^{ij} - \frac{p^i p^j}{E^2}$, so that finally we can write

$$\Phi = \frac{\hbar^2}{8E^2} g^{ij} (\partial_i \partial_j V + \frac{1}{E} \partial_i V \partial_j V) \quad (28)$$

Note the presence of a new term not presented in other considerations of the Dirac equation (see for instance [30]), which is nonlinear in scalar potential and which stems from the new tensor M^{ij} . If for central potential one can neglect this new contribution $\frac{1}{E} \partial_i V \partial_j V$, this is not always true and for some potentials both terms in Eq. (28) can be of the same magnitude. In fact for constant electric field $V = -e\mathcal{E} \cdot \mathbf{R}$, the first term vanishes and $\Phi = \frac{e^2 \hbar^2}{8E^2} g^{ij} \mathcal{E}_i \mathcal{E}_j$.

In the non-relativistic limit $\mathbf{p} \ll m$, Φ becomes $\Phi \approx \frac{\hbar^2}{8m^2} (\Delta V + \frac{1}{m} (\nabla V)^2) + O(\hbar^2 p^2 / m^4)$ which gives two contributions. The first one is the usual Darwin term $\frac{\hbar^2}{8m^2} \Delta V$ traditionally obtained as the result of the Foldy Wouthuysen

transformation expanded in power of $1/m$. The second term $\frac{\hbar^2}{8m^3} (\nabla V)^2$ of higher order in $1/m$ is usually not considered in the Foldy Wouthuysen approach. It is also interesting to note that the external potential in the non relativistic limit can be expanded as $V(\mathbf{r}) \approx V(\mathbf{R}) + \frac{\hbar}{4m^2} \boldsymbol{\Sigma} \cdot (\nabla V \times \mathbf{p}) + O(\hbar^2 p^2/m^4)$ where $\frac{\hbar}{4m^2} \boldsymbol{\Sigma} \cdot (\nabla V \times \mathbf{p})$ is the spin-orbit coupling term. Therefore the Hamiltonian can be approximated as

$$\begin{aligned} \varepsilon \approx & \beta \left(m + \frac{\mathbf{P}^2}{2m} - \frac{\mathbf{P}^4}{8m^3} \right) + V(\mathbf{R}) + \frac{\hbar}{4m^2} \boldsymbol{\Sigma} \cdot (\nabla V \times \mathbf{p}) \\ & + \frac{\hbar^2}{8m^2} \beta \left(\Delta V + \frac{1}{m} (\nabla V)^2 \right) \end{aligned} \quad (29)$$

A Born-Oppenheimer treatment of the Dirac equation where the spin is the fast variable and the momentum the slow one has led to the same Hamiltonian Eq. (29) but without the scalar potential [31]. This corresponds to the semiclassical approximation. The additional electric-type potential Φ is a consequence of transitions between energy levels. This is in agreement with the usual interpretation of the physical origin of the Darwin term, the zitterbewegung phenomenon, whereby the electron does not move smoothly but instead undergoes extremely rapid small-scale fluctuations due to an interference between positive and negative energy states.

VII. CONCLUSION.

In this paper we investigated the origin of quantum geometric phases, gauge fields and forces beyond the adiabatic approximation for physical systems displaying a separation of scales in terms of slow and fast degrees. In particular we extended the notions of geometric magnetic and electric forces discovered in studies of the Born-Oppenheimer approximation. Our approach is very general and results found here have been straightforwardly applied to several physical systems.

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