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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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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 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].

In this note we investigate the origin of quantum gauge fields and forces in a more general context, by considering the diagonalization of an arbitrary matrix valued quantum Hamiltonian. To be precise, by diagonalization it is meant the derivation of an effective in-band Hamiltonian made of block-diagonal energy subspaces. For that purpose we use the results of a powerful method developed recently [8]. This approach based on a new differential calculus on 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 $\hbar$. Particularly important for our purpose, it is possible to give an explicit effective arbitrary diagonal Hamiltonian to order $\hbar^2$ in terms of non-canonical coordinates and commutators between gauge fields (Eq. (79) in [8]). We will directly apply this result to systems whose Hamiltonian has the simple form $H = T(\mathbf{K}) + V(\mathbf{Q})$ and the components are assumed to fulfill the canonical commutation relations $[Q_i, K_j] = i\hbar\delta_{ij}$. We then discuss how gauge fields arise in physical situations as various as Dirac and Bloch electrons in electric fields or Born-Oppenheimer theory. Note that there exists another totally different method of diagonalization in a formal series expansion in $\hbar$ which uses symbols of operators via Weyl calculus [9]. To our knowledge this method was only applied to a Born-Oppenheimer-type Hamiltonian [9].

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][10], and the other is a new tensor generalizing an additional term found in [9] 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 adiabatic dynamics of the Born-Oppenheimer theory.

Hamiltonian diagonalization. Consider a Hamiltonian of the form

$$H = T(\mathbf{K}) + V(\mathbf{Q}) \tag{1}$$

where we assume that H has a matrix representation with $T(K)$ non-diagonal and $V(Q)$ diagonal. In [8], by considering $\hbar$ as a running parameter, we relate 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. $\varepsilon(\mathbf{X}) = \widehat{O}(\varepsilon_0(\mathbf{X}_0))$ and $U(\mathbf{X}) = \widehat{N}(U_0(\mathbf{X}_0))$, where matrices with the subscribe 0 correspond to operators replaced by classical commuting variables $\mathbf{X}_0 = (\mathbf{Q}_0, \mathbf{K}_0)$. The only requirement of the method is therefore the knowledge of $U_0(\mathbf{X}_0)$ which gives the diagonal form $\varepsilon_0(\mathbf{X}_0)$. 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 Eq. (79) of [8], 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. (1). Indeed, the first order is easily obtain by an unitary transformation $U_0(\mathbf{K})$ diagonalizing $T(\mathbf{K})$ giving $U_0 H U_0^{+} = \varepsilon_0(\mathbf{K}) + V(\mathbf{Q} + \hbar\mathbf{A})$ with $\mathbf{A} \equiv iU_0\nabla_{\mathbf{K}}U_0^{+}$.

Then V is now non-diagonal. The diagonalization at the next order is done by an unitary transformation matrix $U = U_0 + \hbar U_0 U_1$ with the antihermitian matrix $(U_1)_{mn} = \frac{(1-\delta_{mn})}{\varepsilon_m(t)-\varepsilon_n(t)}(\mathbf{A})_{mn}.\nabla V$, which removes the off-diagonal elements of $\mathbf{A}$ and leads to corrections of order $\hbar^2$ such that ε_n in Eq. (79) of [8] becomes

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

where the geometric scalar potential is

$$\Phi_n(\mathbf{Q},\mathbf{K}) = \frac{G_n^{ij}}{2}\partial_i\partial_j V(\mathbf{Q}) + T_n^{ij}\partial_i V(\mathbf{Q})\partial_j V(\mathbf{Q}) \tag{3}$$

with two gauge invariant tensors G_n^{ij} and T_n^{ij} defined as

$$G_n^{ij}(\mathbf{K}) = \frac{1}{2}\sum\nolimits_{m\neq n}\left((A^i)_{nm}(A^j)_{mn} + h.c.\right) \tag{4}$$

and

$$T_n^{ij}(\mathbf{K}) = \frac{1}{2}\sum\nolimits_{m\neq n}\left(\frac{(A^i)_{nm}(A^j)_{mn}}{\varepsilon_{0,m}-\varepsilon_{0,n}} + h.c.\right) \tag{5}$$

The tensor G_n^{ij} is known as the quantum metric tensor [5][10] and T_n^{ij} is a new tensor generalizing an additional term found in [9] for the Born-Oppenheimer theory. In Eq. (2) we introduced 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 $\mathbf{a}_n(\mathbf{K}) \equiv (\mathbf{A})_{nn} = i\langle n|\nabla_{\mathbf{K}} n\rangle$. Here $|n\rangle$ are the eigenstates of the non-diagonal part of H, i.e., $T(\mathbf{K})|n\rangle = \varepsilon_{0,n}(\mathbf{K})|n\rangle$. The introduction of the non-canonical coordinate $\mathbf{q}_n$ essential to maintain the gauge invariance of the Hamiltonian, implies non-canonical commutation relations $\left[q_n^i, q_n^j\right] = i\hbar^2\Theta_n^{ij}$ with $\Theta_n^{ij}(\mathbf{K}) = \frac{\partial a_n^j}{\partial K_i} - \frac{\partial a_n^i}{\partial K_j} + \left[a_n^i, a_n^j\right]$ the Berry gauge curvature in the n-th eigenstate. The Heisenberg equations of motion to the second order in $\hbar$ are

$$\dot{\mathbf{q}}_n = \nabla_{\mathbf{K}}\varepsilon_n - \frac{\hbar}{2}(\dot{\mathbf{K}}\times\mathbf{\Theta}_n - \mathbf{\Theta}_n\times\dot{\mathbf{K}}), \quad \dot{\mathbf{K}} = -\nabla_{\mathbf{q}_n}V \tag{6}$$

where we introduced the "magnetic field" $\Theta_n^i = \varepsilon_{jk}^i\Theta_n^{jk}$. The dynamics of the intraband operators leads directly to a Lorentz-type term. The scalar potential is a consequence of transitions between eigenstates 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 an eigenstate of the full Hamiltonian. This state will evolve in the same energy subspace 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 our diagonalization does not need the adiabatic assumption, because it is an "exact" diagonalization. However, the expansion in $\hbar$ breaks down in regions of mode conversion where $\varepsilon_{0,m} - \varepsilon_{0,n} << \hbar$ or for large values of $(A^i)_{nm} = i\langle m|\partial_i n\rangle$. Now, if in a particular regime the probability transition between different eigenstates is very small, on can neglect with a good approximation the off-diagonal elements. This is usually considered as an adiabatic approximation and we see that it coincides with the semiclassical approximation. In a mode conversion region, one can easily generalize the diagonalization of H to a block-diagonalization allowing transitions between eigenstates inside the block. In this case, we can therefore consider the semiclassical limit without having adiabaticity.

Born-Oppenheimer approximation. Consider the following Hamiltonian describing a fast system in interaction with an external environment

$$H = \frac{1}{2}B_{ij}P^iP^j + \frac{p^2}{2m} + \varphi(\mathbf{R},\mathbf{r}) \tag{7}$$

where the fast system is described by a set of dynamical variables $(\mathbf{r},\mathbf{p})$ and the slow one 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 $\mathbf{Q}\to\mathbf{P}$, $\mathbf{K}\to\mathbf{R}$ (and $i\nabla_{\mathbf{K}}\to -i\nabla_{\mathbf{R}}$) we have $V(\mathbf{Q})\to B_{ij}P_iP_j/2$ and we obtain the following eigenvalues for the slow system (assuming a non-degenerate spectrum for the fast system)

$$\varepsilon_n = \frac{1}{2}B_{ij}p_n^ip_n^j + \hbar^2\Phi_n + E_n(\mathbf{R}) \tag{8}$$

where $\mathbf{p}_n = \mathbf{P} - i\hbar\langle n|\nabla_{\mathbf{R}} n\rangle$ and $|n(\mathbf{R})\rangle$ is the eigenstate of the fast Hamiltonian with energy $E_n(\mathbf{R})$. The scalar potential Eq. (3) then becomes

$$\Phi_n(\mathbf{R},\mathbf{P}) = \frac{G_n^{ij}(\mathbf{R})}{2}B_{ij} + T_n^{ij}(\mathbf{R})B_{il}B_{jk}P^lP^k \tag{9}$$

with the quantum metric tensor $G_n^{ij}(\mathbf{R}) = \mathrm{Re}\sum_{m\neq n}\langle\partial_i n|m\rangle\langle m|\partial_j n\rangle$ and $T_n^{ij}(\mathbf{R}) = \mathrm{Re}\sum_{m\neq n}\frac{\langle\partial_i n|m\rangle\langle m|\partial_j n\rangle}{\varepsilon_{0,m}-\varepsilon_{0,n}}$. 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 $T_n^{ij}(\mathbf{R})B_{il}B_{jk}P^lP^k$ was found in [9]. 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.(6) we immediately get the Born-Oppenheimer equations of motion $\dot{\mathbf{p}}_n = -\nabla_{\mathbf{R}}E_n - \frac{\hbar}{2}(\dot{\mathbf{R}}\times\mathbf{\Theta}_n - \mathbf{\Theta}_n\times\dot{\mathbf{R}}) - \hbar^2\nabla_{\mathbf{R}}\Phi_n$ with $\dot{R}_i = B_{ij}p_n^j$. 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.

Particle in a linear potential. Another interesting relevant situation concerns a particle in a linear potential exemplified here by a Bloch electron in an constant external electric field (see also ref. [11]). Consider $H = H_0(\mathbf{P},\mathbf{R}) + \varphi(\mathbf{R})$ with H_0 the energy of a particle in a periodic potential and $\varphi(\mathbf{R}) = -e\mathbf{E}.\mathbf{R}$ the external electric perturbation (and $e<0$ the charge). Using the mapping $\mathbf{Q}\to\mathbf{R}$, the scalar gauge potential reduces to $\Phi_n(\mathbf{k}) = e^2 T_n^{ij} E_i E_j$, and the energy eigenvalues are

$$\varepsilon_n = \varepsilon_{0,n}(\mathbf{k}) - e\mathbf{E}.\mathbf{r_n} + e^2\hbar^2 T_n^{ij}(\mathbf{k}) E_i E_j \qquad (10)$$

with $\varepsilon_{0,n}(\mathbf{k})$ is the n-th energy band and $\mathbf{k}$ the pseudo-momentum. The intraband position operator is $\mathbf{r}_n = \mathbf{R} + i\hbar\langle u_n|\nabla_{\mathbf{k}}u_n\rangle$ with $|u_n(\mathbf{k})\rangle$ the periodic part of the Bloch wave function and $T_n^{ij}(\mathbf{k}) = \mathrm{Re}\sum_{m\neq n}\frac{\langle\partial_i u_n|u_m\rangle\langle u_m|\partial_j u_n\rangle}{\varepsilon_{0,m}-\varepsilon_{0,n}}$. Introducing the "magnetic field" $\boldsymbol{\omega}_n = \frac{\hbar}{eE^2}\mathbf{E}\times\nabla_{\mathbf{k}}\Phi_n$ and $\boldsymbol{\chi}_n = \frac{1}{eE^2}\mathbf{E}.\nabla_{\mathbf{k}}\Phi_n$ the equations of motion are

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

where $\Omega_n = \boldsymbol{\Theta}_n + \hbar\boldsymbol{\omega}_n$. 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. Φ_n contributes also to the velocity in the direction of $\mathbf{E}$, through the term $\hbar^2\boldsymbol{\chi}_n\dot{\mathbf{k}}$.

Berry phase. The linear potential case has another interest. It allows us to also consider the fast system and derive the Berry phase in a different way. 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. 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 an unitary transformation $|\Psi'(t)\rangle = U(t)|\Psi(t)\rangle$ such that $U(t)D(t,P_0)U^+(t) = \widetilde{\Lambda}(t,P_0)$ is a diagonal differential operator and $\widetilde{\Lambda}(t,P_0)|\Psi'(t)\rangle = 0$. Therefore the time evolution is given by $|\Psi'(t)\rangle = e^{\frac{-i}{\hbar}\int_0^t\Lambda(t)dt}|\Psi'(0)\rangle$. Since $\Lambda(t) = \widetilde{\Lambda}(t) + P_0$ is diagonal, no time ordered product is required. Returning back to the initial state we have

$$|\Psi(t)\rangle = U^+(t)e^{\frac{-i}{\hbar}\int_0^t\Lambda(t)dt}U(0)|\Psi(0)\rangle \qquad (11)$$

A system prepared in a state $|\Lambda_n(0)\rangle$ which is an eigenstate of D, i.e., $D(0)|\Lambda_n(0)\rangle = \widetilde{\Lambda}_n(0)|\Lambda_n(0)\rangle$ 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. (11) is non-adiabatic. 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 $\Lambda_n = \widetilde{\Lambda}_n(t) + P_0$ is formally equivalent to the Bloch electron example discussed above with $K\to t$, $Q\equiv R\to P_0$ and $eE = 1$. We obtain from Eq.(10)

$$\Lambda_n = \varepsilon_n(t) - i\hbar\left\langle n\middle|\dot{n}\right\rangle + \hbar^2 T_n(t) \qquad (12)$$

where $\varepsilon_n(t)$ and $n(t)$ are instantaneous eigenvalues and eigenstates of H, i.e., $H(t)|n(t)\rangle = \varepsilon_n(t)|n(t)\rangle$, and $T_n(t) = \mathrm{Re}\sum_{m\neq n}\frac{\left\langle\dot{n}\middle|m\right\rangle\left\langle m\middle|\dot{n}\right\rangle}{\varepsilon_m-\varepsilon_n}$. Therefore for a periodic motion of period T, not necessarily adiabatic, such that $|\Lambda_n(T)\rangle = |\Lambda_n(0)\rangle$ (single valued eigenstates), we have

$$|\Psi(T)\rangle = e^{-i\gamma_n}|\Psi(0)\rangle \qquad (13)$$

with

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

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 $\hbar\int_0^T T_n(t)\,dt$ of order $\hbar$ is non-geometric as it depends on $\dot{x}$. It cancels in the infinitely slow $\dot{x}\to 0$ adiabatic regime, which thus coincides with the semiclassical approximation. Diagonalization at order $\hbar^2$ thus goes beyond the adiabatic approximation and takes into account transitions between eigenstates. Quantitatively, if the system is prepared in an eigenstate $|n(0)\rangle$ of $H(0)$, then $|\Psi(t)\rangle$ is given by Eq. (11) with $U = U_0 + \hbar U_1 U_0$ where $U_1(t)_{mn} = i\frac{(1-\delta_{mn})\left\langle m\middle|\dot{n}\right\rangle}{\varepsilon_m(t)-\varepsilon_n(t)}$, so that we have the following expansion up to order $\hbar$:

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

The magnitude of transitions is then controlled by the term $A_{mn} = \frac{i\left\langle m(t)\middle|\dot{n}(t)\right\rangle}{\varepsilon_n(t)-\varepsilon_m(t)}$ which is neglected in the adiabatic limit $\left\langle m(t)\middle|\dot{n}(t)\right\rangle \to 0$. Note that $|\Psi(t)\rangle$ is normalized to unity at order $\hbar$ only. A normalization at a

higher order needs an expansion of U to the same order [8].

In principle deviation from adiabaticity could be measured by interferometry. Consider a periodic two states system, and write the initial state in the eigenbase $|n(0)\rangle = |\Lambda_n(0)\rangle + \hbar A_{nm}(0)\,|\Lambda_m(0)\rangle$. Then, after one cycle $|\Psi(T)\rangle = e^{-i\gamma_n}\,|\Lambda_n(0)\rangle + \hbar e^{-i\gamma_m} A_{nm}(T)\,|\Lambda_m(0)\rangle$. 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 $2\hbar\,\mathrm{Re}\left(A_{nm}(T)\,\langle\Lambda_n(0)|\,O\,|\Lambda_m(0)\rangle\,e^{-i(\gamma_n-\gamma_m)}\right)$ which would signal deviation from adiabaticity. As discussed below, this interference effect is formally equivalent to the zitterbewegung of Dirac particles.

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 [12]. The Hamiltonian is (with $c = 1$)

$$H = \boldsymbol{\alpha}.\mathbf{p} + \beta m + V(\mathbf{R}) \tag{14}$$

where $\boldsymbol{\alpha}$ 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 $U_0\,(\boldsymbol{\alpha}.\mathbf{p} + \beta m)\,U_0^+ = \beta E$ with $E = \sqrt{\mathbf{p}^2 + m^2}$ is the usual Foldy Wouthuysen unitary transformation $U_0 = \frac{E+m+\beta\boldsymbol{\alpha}\mathbf{P}}{(2E(E+m))^{1/2}}$. For the Dirac particles we have two energy subspaces $\varepsilon_\pm$ of dimension 2 corresponding to the positive and negative energy. Now with the correspondence $\mathbf{Q}\to\mathbf{R}$, $\mathbf{K}\to\mathbf{p}$ and formula Eq. (2), one easily sees that the diagonal matrix can be written

$$\varepsilon(\mathbf{p},\mathbf{r}) = \beta E(\mathbf{p}) + V(\mathbf{r}) + \beta\Phi \tag{15}$$

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 $T^{ij} = \frac{1}{8E^3}g^{ij}$ with the notation $g^{ij} = \delta^{ij} - \frac{p^i p^j}{E^2}$, so that finally we can write

$$\Phi = \frac{\hbar^2}{8E^2}g^{ij}(\partial_i\partial_j V + \frac{1}{E}\partial_i V\partial_j V) \tag{16}$$

If for central potential one can neglect the contribution $\frac{1}{E}\partial_i V\partial_j V$, this is not always true and for some potentials both terms in Eq. (16) can be of the same magnitude. In fact for constant electric field $V = -e\mathcal{E}.\mathbf{R}$, 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 $\mathbf{p} << m$, Φ becomes $\Phi \approx \frac{\hbar^2}{8m^2}\left(\boldsymbol{\Delta}V + \frac{1}{m}(\boldsymbol{\nabla}V)^2\right) + O(\hbar^2 p^2/m^4)$ which gives two contributions. The first one is the usual Darwin term $\frac{\hbar^2}{8m^2}\boldsymbol{\Delta}V$ traditionally obtained as the result of the Foldy Wouthuysen transformation expanded in power of $1/m$. The second term $\frac{\hbar^2}{8m^3}(\boldsymbol{\nabla}V)^2$ 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 $V(\mathbf{r}) \approx V(\mathbf{R}) + \frac{\hbar}{4m^2}\boldsymbol{\Sigma}.(\boldsymbol{\nabla}V\times\mathbf{p}) + O(\hbar^2 p^2/m^4)$ where $\frac{\hbar}{4m^2}\boldsymbol{\Sigma}.(\boldsymbol{\nabla}V\times\mathbf{p})$ is the spin-orbit coupling term. Therefore the Hamiltonian can be approximated as

$$\begin{aligned}\varepsilon \;\approx\; & \beta\left(m + \frac{\mathbf{P}^2}{2m} - \frac{\mathbf{P}^4}{8m^3}\right) + V(\mathbf{R}) + \frac{\hbar}{4m^2}\boldsymbol{\Sigma}.(\boldsymbol{\nabla}V\times\mathbf{p}) \\ & + \frac{\hbar^2}{8m^2}\beta\left(\boldsymbol{\Delta}V + \frac{1}{m}(\boldsymbol{\nabla}V)^2\right)\end{aligned} \tag{17}$$

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. (17) but without the scalar potential [13]. 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.

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