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Thomas Precession, Spin-Orbit Interaction, and Berry's Phase

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The spin-orbit interaction is shown to arise as a Berry phase term in the adiabatic effective Hamiltonian for the orbital motion of a Dirac electron. This approach makes explicit the intimate connection of the spin-orbit interaction and Thomas precession.

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The spin-orbit (SO) interaction is of basic importance in atomic and solid-state physics; it is a relativistic effect which arises because in the rest frame of the electron the moving nucleus generates a magnetic field which couples to the electron's spin magnetic moment. It is well known that the correct magnitude of this interaction is obtained semiclassically only after taking into account the relativistic kinematic effect of *Thomas precession* [1]. Alternatively, the effect can be derived rigorously from the Dirac equation in the nonrelativistic limit by the Foldy-Wouthuysen (FW) transformation [2], in which approach the role of Thomas precession is not immediately apparent. In this Letter I show that the SO interaction can be derived by making an adiabatic approximation to the Dirac equation for an electron moving in a smooth external potential, in which the orbital degrees of freedom are treated as slowly varying with respect to the spinor degrees of freedom. It is by now a familiar possibility that the effective Hamiltonian for the slow degrees of freedom may contain a nontrivial gauge potential (Berry phase contribution) [3]. In this case the gauge potential which appears is proportional to the Thomas precession angle, and its dynamical expression is the SO interaction.

The state space of a Dirac particle is spanned by the basis vectors $|o\rangle\otimes|\alpha\rangle\otimes|\mu\rangle$; $|o\rangle$ is a basis for the orbital degrees of freedom (which can be represented in either position or momentum space), $|\alpha\rangle$ for the spin space which is inhabited by Pauli matrices which we denote σ, and $|\mu\rangle$ for another SU(2) space inhabited by Pauli matrices ρ. In what follows we shall span the orbital space by the momentum eigenstates $|\mathbf{p}\rangle$. In this (Dirac) representation, Dirac's Hamiltonian has the form

$$H_D=\rho_1\boldsymbol{\sigma}\cdot\mathbf{p}+\rho_3 m+\hat{V}\,, \tag{1}$$

where $\hat{V}$ is an operator that acts only on the orbital degrees of freedom. Following the usual Born-Oppenheimer method, we identify the orbital degrees of freedom as slow and look for solutions for the fast spinor degrees of freedom determined by the 4×4 matrix Hamiltonian,

$$H_F=\rho_1\boldsymbol{\sigma}\cdot\mathbf{p}+\rho_3 m\,, \tag{2}$$

where $\mathbf{p}$ now appears as a parameter (analogous to nuclear configuration in the adiabatic treatment of molecular problems).

For $\mathbf{p}=0$, we readily obtain $|\alpha,\mu;\mathbf{p}=0\rangle\equiv|\alpha\rangle\otimes|\mu\rangle$, where $\sigma_3|\alpha\rangle=\alpha|\alpha\rangle$ and $\rho_3|\mu\rangle=\mu|\mu\rangle$ with $\alpha,\mu=\pm$, which satisfy

$$H_F|\alpha,\mu;\mathbf{p}=0\rangle=\mu m|\alpha,\mu;\mathbf{p}=0\rangle\,. \tag{3}$$

We obtain finite momentum eigenstates by Lorentz boosting [4] $|\alpha,\mu;\mathbf{p}=0\rangle$. Working to $O(v^2)$ accuracy,

$$\begin{aligned}&\mathbf{p}=mv\hat{\mathbf{n}}\,,\\ &|\alpha,\mu;\mathbf{p}\rangle\equiv N(\mathbf{v})\Lambda(\mathbf{v})|\alpha\rangle\otimes|\mu\rangle\\ &\qquad=\left(1-\frac{v^2}{8}+\frac{\rho_1 v}{2}\boldsymbol{\sigma}\cdot\hat{\mathbf{n}}\rho_3\right)|\alpha\rangle\otimes|\mu\rangle\,,\end{aligned} \tag{4}$$

where $N(\mathbf{v})$ denotes a normalization factor. These states

satisfy

$$H_F|\alpha,\mu;\mathbf{p}\rangle=\mu m(1+\tfrac{1}{2}v^2)|\alpha,\mu;\mathbf{p}\rangle\,,$$
$$\langle\alpha,+;\mathbf{p}|\beta,+;\mathbf{p}\rangle=\delta_{\alpha\beta}\,. \tag{5}$$

Since the solutions of Eq. (5) are independent of the index α for a given $\mathbf{p}$ we obtain two levels, each twofold degenerate, the well-known positive and negative energy states of the Dirac particle, with an enormous level spacing (of the order of an electron's mass), much greater than the typical orbital energy in a nonrelativistic problem. Whenever such a situation occurs, in which the fast degrees of freedom have widely spaced energy levels compared to the slow ones, e.g., in molecular physics where the electronic level spacing is much greater than the nuclear rotational-vibrational energies, an adiabatic approximation should give the dominant behavior. As in the molecular case, we are motivated to look for approximate eigenstates of the full Hamiltonian of the type

$$|\psi\rangle=\int d\mathbf{p}\sum_\alpha \psi_\alpha(\mathbf{p})|\mathbf{p}\rangle\otimes|\alpha,+;\mathbf{p}\rangle\,. \tag{6}$$

Our task now is to project H_D onto the space of the two-component wave functions of Eq. (6) and obtain an effective Hamiltonian for the orbital degrees of freedom. Before we do so, we note that $|\alpha,+;\mathbf{p}\rangle$ for $\mathbf{p}\neq0$ are not eigenstates of σ_3, which is the relativistic spin-z operator. It is crucial in what follows that they are, in fact, eigenstates of the appropriate nonrelativistic spin operator; we shall return to this point below. Hence the two-component function $\psi_\alpha(\mathbf{p})$ of Eq. (6) may be viewed as a nonrelativistic momentum-space wave function for a spin-$\frac{1}{2}$ particle. Its real-space counterpart is obtained as usual by Fourier transformation.

We now express the eigenvalue problem $H_D|\psi\rangle=E|\psi\rangle$ in terms of the wave functions of Eq. (6) by applying $\langle\mathbf{p}'|\otimes\langle\beta,+;\mathbf{p}'|$ to its left. In doing so we neglect the matrix elements of $\hat{V}$ between positive and negative energy states, as is appropriate for a Born-Oppenheimer approximation. We find the following:

$$\left(m+\frac{p'^2}{2m}\right)\psi_\beta(\mathbf{p}')+\int d\mathbf{p}\sum_\alpha\langle\beta,+;\mathbf{p}'|\alpha,+;\mathbf{p}\rangle\langle\mathbf{p}'|\hat{V}|\mathbf{p}\rangle\psi_\alpha(\mathbf{p})=E\psi_\beta(\mathbf{p}')\,. \tag{7}$$

Now since $V(\mathbf{r})$ is slowly varying in a sense to be made precise below, $\langle\mathbf{p}'|\hat{V}|\mathbf{p}\rangle$ is sharply peaked about $\mathbf{p}'\simeq\mathbf{p}$ and vanishes otherwise. We may therefore expand

$$\langle\beta,+;\mathbf{p}'|\alpha,+;\mathbf{p}\rangle\simeq\delta_{\beta\alpha}-\mathbf{A}_{\beta\alpha}(\mathbf{p})\cdot(\mathbf{p}'-\mathbf{p})+\cdots\,,$$
$$\mathbf{A}_{\beta\alpha}(\mathbf{p})\equiv\langle\beta,+;\mathbf{p}|\nabla_{\mathbf{p}}|\alpha,+;\mathbf{p}\rangle\,. \tag{8}$$

$\mathbf{A}_{\beta\alpha}(\mathbf{p})$, as we have defined it, is the usual non-Abelian generalization of Berry's gauge potential [5,6]. Straightforward calculation reveals

$$\mathbf{A}_{\beta\alpha}(\mathbf{p})=-\frac{i}{4m^2}\mathbf{p}\times\boldsymbol{\sigma}_{\beta\alpha}\,, \tag{9}$$

where $\boldsymbol{\sigma}_{\beta\alpha}\equiv\langle\beta|\boldsymbol{\sigma}|\alpha\rangle$. Inserting (8) in (7) we obtain

$$\left(m+\frac{p'^2}{2m}\right)\psi_\beta(\mathbf{p}')+\int d\mathbf{p}\langle\mathbf{p}'|\hat{V}|\mathbf{p}\rangle\psi_\beta(\mathbf{p})-\int d\mathbf{p}\sum_\alpha\mathbf{A}_{\beta\alpha}(\mathbf{p})\cdot(\mathbf{p}'-\mathbf{p})\langle\mathbf{p}'|\hat{V}|\mathbf{p}\rangle\psi_\alpha(\mathbf{p})=E\psi_\beta(\mathbf{p}')\,. \tag{10}$$

The third (Berry phase) term in (10) is the SO interaction as may be seen more clearly by Fourier transforming. We find the real-space adiabatic effective Hamiltonian to be

$$\left(m-\frac{\nabla^2}{2m}+V(\mathbf{r})\right)\delta_{\beta\alpha}-\boldsymbol{\sigma}_{\beta\alpha}\cdot\frac{i}{4m^2}\nabla V(\mathbf{r})\times\nabla\,. \tag{11}$$

We now briefly discuss corrections to this expression. The neglect of the off-diagonal matrix elements $\langle\beta,-;\mathbf{p}'|\alpha,+;\mathbf{p}\rangle$ in Eq. (7) may be shown to produce corrections λ/L smaller than SO effects where λ is the typical de Broglie wavelength of the electron and L is the length scale over which the potential $V(x)$ varies. Replacing the approximation in Eq. (8) with the exact expression produces corrections smaller by an additional factor. SO effects are, in turn, smaller than the kinetic and potential terms by a factor of $\lambda_C^2/\lambda L$, where λ_C is the Compton wavelength of the electron. So long as $L\gg\lambda$, a condition which is frequently satisfied, e.g., in the Thomas-Fermi treatment of atoms, SO effects will dominate the off-diagonal terms and are hence a legitimate ingredient of the nonrelativistic Hamiltonian in the adiabatic approximation, even though they are higher order in powers of $1/m$ than the off-diagonal terms. The same considerations apply to the standard FW approach, although the SO effects are frequently excluded from the

first-order Hamiltonian on the basis of a naive estimation of terms simply by counting powers of $1/m$. In fact the normalized Lorentz boost equation (4) corresponds to the first-order FW transformation and the adiabatic Hamiltonian agrees exactly with the first-order FW Hamiltonian. What is new in this approach is its interpretation as an adiabatic approximation where the SO interaction arises from a nontrivial Berry phase.

We now show that the Berry connection $\mathbf{A}_{\beta\alpha}(\mathbf{p})$ is directly related to the relativistic kinematic effect of Thomas precession. Thomas precession [up to $O(v^2)$ accuracy] is the following property of the Lorentz transformations:

$$\Lambda(\mathbf{v}+\delta\mathbf{v})=R(\delta\boldsymbol{\theta})\Lambda(\delta\mathbf{v})\Lambda(\mathbf{v}),\quad \delta\boldsymbol{\theta}=\tfrac{1}{2}(\delta\mathbf{v}\times\mathbf{v}). \tag{12}$$

Here $\Lambda(\mathbf{v})$ denotes a boost to a velocity $\mathbf{v}$ and $R(\delta\boldsymbol{\theta})$ a rotation of $|\delta\boldsymbol{\theta}|$ about $\delta\boldsymbol{\theta}$. The physical effect of the rotation R in Eq. (12) is that an accelerating particle moving at relativistic speed appears to precess in orientation: This precession was shown by Thomas to add to the Larmor precession to give the correct value to the SO interaction. Equation (12) as we have written it is a Lorentz-group property valid in all representations. In context of the Dirac particle we use Eq. (12) to go from $|\alpha,+;\mathbf{p}\rangle$ to $|\alpha,+;\mathbf{p}+\delta\mathbf{p}\rangle$:

$$|\alpha,+;\mathbf{p}+\delta\mathbf{p}\rangle=N(\mathbf{v},\delta\mathbf{v})\left(1-i\frac{\delta\boldsymbol{\theta}}{2}\cdot\boldsymbol{\sigma}\right)\left(1+\frac{\boldsymbol{\sigma}\cdot\delta\mathbf{p}}{2m}\rho_1\right)|\alpha,+;\mathbf{p}\rangle, \tag{13}$$

where the factor $N(\mathbf{v},\delta\mathbf{v})=1-\mathbf{v}\cdot\delta\mathbf{v}/2$ is to keep the new states orthonormalized. Recalling the definition of the non-Abelian potential and using Eq. (13),

$$\mathbf{A}_{\beta\alpha}\cdot\delta\mathbf{p}=\langle\beta,+;\mathbf{p}|\alpha,+;\mathbf{p}+\delta\mathbf{p}\rangle-\langle\beta,+;\mathbf{p}|\alpha,+;\mathbf{p}\rangle=-\tfrac{1}{2}i\delta\boldsymbol{\theta}\cdot\langle\beta|\boldsymbol{\sigma}|\alpha\rangle. \tag{14}$$

Inserting the value of the Thomas rotation from Eq. (12) gives us back our previous expression for $\mathbf{A}_{\beta\alpha}(\mathbf{p})$, Eq. (9).

Finally, we return to the interpretation of the states $|\alpha,+;\mathbf{p}\rangle$ as nonrelativistic spin-z eigenstates. The distinction between relativistic and nonrelativistic spin has previously been discussed by Foldy and Wouthuysen [2]. We consider how an infinitesimal rotation ϵ about an axis $\hat{\boldsymbol{\Omega}}$ shuffles the components of the two-component wave function $\psi_\alpha(\mathbf{p})$:

$$(1-i\epsilon\mathbf{J}\cdot\hat{\boldsymbol{\Omega}})|\mathbf{p}\rangle=|\mathbf{p}+\epsilon\hat{\boldsymbol{\Omega}}\times\mathbf{p}\rangle,$$

$$\left(1-i\epsilon\frac{\boldsymbol{\sigma}\cdot\hat{\boldsymbol{\Omega}}}{2}\right)|\alpha,+;\mathbf{p}\rangle=N(\mathbf{v})\Lambda(\mathbf{v})\left(1-i\epsilon\frac{\boldsymbol{\sigma}\cdot\hat{\boldsymbol{\Omega}}}{2}\right)|\alpha\rangle\otimes|+\rangle-i\frac{\epsilon}{4}\rho_1 v[\boldsymbol{\sigma}\cdot\hat{\boldsymbol{\Omega}},\boldsymbol{\sigma}\cdot\hat{\mathbf{n}}]|\alpha\rangle\otimes|+\rangle$$

$$=|\alpha,+;\mathbf{p}+\epsilon\hat{\boldsymbol{\Omega}}\times\mathbf{p}\rangle-\sum_\beta i\frac{\epsilon}{2}(\boldsymbol{\sigma}\cdot\hat{\boldsymbol{\Omega}})_{\beta\alpha}|\beta,+;\mathbf{p}\rangle\simeq\sum_\beta\left(\delta_{\beta\alpha}-i\frac{\epsilon}{2}(\boldsymbol{\sigma}\cdot\hat{\boldsymbol{\Omega}})_{\beta\alpha}\right)|\beta,+;\mathbf{p}+\epsilon\hat{\boldsymbol{\Omega}}\times\mathbf{p}\rangle. \tag{15}$$

$\mathbf{J}\equiv$the generator of rotations in orbital space, $(\boldsymbol{\sigma}\cdot\hat{\boldsymbol{\Omega}})_{\beta\alpha}\equiv\langle\beta|\boldsymbol{\sigma}\cdot\hat{\boldsymbol{\Omega}}|\alpha\rangle$. And so, e.g., a rotation about $\hat{\boldsymbol{\Omega}}=\hat{\mathbf{e}}_z$, $R(\hat{\mathbf{e}}_z,\epsilon)$, looks like

$$R(\hat{\mathbf{e}}_z,\epsilon)|\psi\rangle=\int d\mathbf{p}\sum_{\beta\alpha}\left(1-\epsilon\frac{\partial}{\partial\phi}-i\frac{\epsilon}{2}(\sigma_z)_{\beta\alpha}\right)\psi_\alpha(\mathbf{p})|\mathbf{p}\rangle\otimes|\beta,+;\mathbf{p}\rangle, \tag{16}$$

which supports our identification. [We have used a polar representation (p,θ,ϕ) for $\mathbf{p}$.] This completes our derivation of the SO interaction from the adiabatic limit of the Dirac equation.

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