V. THE SEMICLASSICAL FOLDY–WOUTHUYSEN TRANSFORMATION AND THE DERIVATION OF THE BLOCH EQUATION FOR SPIN–1/2 POLARISED BEAMS USING WIGNER FUNCTIONS [a]

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A semiclassical Foldy–Wouthuysen transformation of the Dirac equation is used to obtain the radiationless Bloch equation for the polarisation density.

1 Introduction and Motivation

A complete picture of spin polarisation in accelerators and storage rings, either with or without synchrotron radiation, can only be obtained on the basis of evolution equations for combined spin–orbit distributions. See Article I. Moreover, if we are concerned with the effects of radiation, its simulation by classical white noise and damping does not suffice for all situations. For example we cannot obtain the Sokolov–Ternov effect by that means. In fact to include all the subtleties of radiation, a quantum mechanical approach is needed and then obtaining the 'complete picture' implies that we must begin by finding the equation of motion for the spin–orbit density operator in the presence of radiation. To ensure some level of transparency and trackability one begins by ignoring direct and indirect inter–particle effects so that at the classical level the beam would be described by a single-particle density depending on the six orbital phase space variables, the spin variables and on time as in statistical mechanics in 'μ-space'.

In the single-particle approximation, only positive energy two-component spin-orbit wave functions are needed. The appropriate quantum Hamiltonian is provided by a **Foldy – Wouthuysen** (FW) transform [1] of the Dirac Hamiltonian and in order to get explicit results for time-dependent electromagnetic fields one has to use perturbation theory. Since we are interested in high energy behaviour in storage rings we do **semiclassical** perturbation theory, where the expansion parameter is Planck's constant, not 1/m etc. Before launching into the full blown calculation of the effects of radiation one should first obtain the transformed Hamiltonian for motion due to the Lorentz forces in the fields of the storage ring and then the corresponding equations of motion for the spin and orbital parts of the density operator. The evolution equations for the resulting classical distributions should then be derived. These are the tasks of this paper. Radiation will be considered elsewhere.

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The required Hamiltonian was already stated at first order in $\hbar$ by Derbenev and Kondratenko [2] as the starting point for their radiation calculations, but no construction was given. In this paper we show how to obtain the transformed Hamiltonian to second order in $\hbar$. Owing to space limitations we will be very brief but full details can be found elsewhere [3]; see also [4, 5, 6, 7].

2 The Dirac equation

The underlying Dirac-equation is $i\hbar(\partial\psi/\partial t) = H_{op}\psi$ where:

$$H_{op} := c(\vec{\alpha}_{op}\cdot\vec{\pi}_{op}) + mc^2\gamma_{op,4} + e\phi_{op} \\ \underbrace{-\frac{e(g-2)\hbar}{4mc}(\gamma_{op,4}(\vec{\Sigma}_{op}\cdot\vec{B}_{op}) + (\vec{\gamma}_{op}\cdot\vec{E}_{op}))}_{\text{Pauli term}} \ .$$

We use the matrix representation of [8].

3 The perturbation theory

A unitary operator U_{op} which performs the FW transformation (a 'unitary FW operator') transforms a wave function ψ in the Dirac representation into the corresponding wave function $U_{op}\psi$ in the FW representation. In the FW representation the Dirac equation reads as $i\hbar\frac{\partial\psi}{\partial t} = \tilde{H}_{op}\psi$ where

$$\tilde{H}_{op} := U_{op}H_{op}U_{op}^{-1} + i\hbar\frac{\partial U_{op}}{\partial t}U_{op}^{-1} \tag{1}$$

and the electron wave functions, i.e. the 'positive energy wave functions' have only upper components which we denote by χ_1, χ_2. Then in the Dirac representation the positive energy wave functions read as $\psi = U_{op}^{-1}(\chi_1, \chi_2, 0, 0)$. Thus in this representation the 'positive energy projection operator' $\Lambda_{op}^{(+)}$ reads as

$$\Lambda_{op}^{(+)} := U_{op}^{-1}\frac{1}{2}(1+\gamma_{op,4})U_{op} \ . \tag{2}$$

By Eq. (2) the FW transformation (and the FW Hamiltonian) is not unique because U_{op} can be replaced by any unitary operator V_{op}, such that $U_{op}V_{op}^{-1}$ is even ('essential uniqueness' of the FW transformation). Our task is now to develop a perturbation theory to construct a U_{op}. Then at k-th order ($k \geq 0$) in $\hbar$, U_{op} is approximated by an operator $U_{op,k}$. Starting with zeroth order, to satisfy Eq. (2), we must choose $U_{op,0}$ such that

$$\Lambda_{op}^{(+)} \stackrel{0}{=} U_{op,0}^{-1}\frac{1}{2}(1+\gamma_{op,4})U_{op,0} \ . \tag{3}$$

Because for semiclassical perturbation theory we have[3]:

$$\Lambda_{op}^{(+)} \stackrel{0}{=} \frac{1}{2}\Big(1 + \frac{c}{J_{op}}(\vec{\alpha}_{op}\cdot\vec{\pi}_{op}) + \frac{mc^2}{J_{op}}\gamma_{op,4}\Big) \ , \tag{4}$$

we can choose [3]:

$$U_{op,0} := \exp\Big(-\frac{1}{2}\gamma_{op,4}\gamma_{op,5}\arctan(\frac{1}{mc}(\vec{\Sigma}_{op}\cdot\vec{\pi}_{op}))\Big)\ .$$

In k-th order Eq. (1) reads as

$$\tilde{H}_{op,k} := U_{op,k}H_{op}U_{op,k}^{-1} + i\hbar\frac{\partial U_{op,k}}{\partial t}U_{op,k}^{-1}\ ,$$

where $\tilde{H}_{op,k}$ denotes the k-th order approximation of the FW Hamiltonian. Having fixed $U_{op,0}$ the remaining task is to choose the $U_{op,k}$ for $k \geq 1$ such that $\tilde{H}_{op,k}$ is even in k-th order. That this procedure leads to a unique energy projection operator can be shown [3] by using a method due to Pursey [9]. For
$k \geq 1$ we compute the $U_{op,k}$ recursively in the form
$U_{op,k} := \tilde{U}_{op,k}\tilde{U}_{op,k-1}\cdots\tilde{U}_{op,1}U_{op,0}$, where:

$$\tilde{U}_{op,j} := \exp\Big(\frac{1}{4}[\frac{1}{J_{op}}\gamma_{op,4}\ ,\ \mathcal{O}_{op,j-1}]\Big)\ , \qquad (j \geq 1)\ ,$$

with $J_{op} := \sqrt{m^2c^4 + c^2(\vec{\pi}_{op}\cdot\vec{\pi}_{op})}$ and where $\mathcal{O}_{op,j}$ is the odd part of the operator $\tilde{H}_{op,j}$, so that $\mathcal{O}_{op,j}$ anticommutes with $\gamma_{op,4}$ and $\tilde{H}_{op,j} - \mathcal{O}_{op,j}$ commutes with $\gamma_{op,4}$. Thus $\mathcal{O}_{op,j}$ is the odd part obtained after the $(j+1)$-th step.

In first order one gets $\tilde{H}_{op,1} \stackrel{1}{=} \tilde{H}_{op}^{dk}$ [3] where:

$$\begin{aligned}\tilde{H}_{op}^{dk} := {} & \frac{1}{2}\gamma_{op,4}J_{op} + \frac{e}{2}\phi_{op} - \frac{e\hbar}{4mc}(\frac{mc^2}{J_{op}} + \frac{g-2}{2})\gamma_{op,4}(\vec{\Sigma}_{op}\cdot\vec{B}_{op}) \\ & + \frac{e\hbar c(g-2)}{8m}\frac{1}{J_{op}(J_{op}+mc^2)}\gamma_{op,4}(\vec{\pi}_{op}\cdot\vec{B}_{op})(\vec{\Sigma}_{op}\cdot\vec{\pi}_{op}) \\ & + \frac{e\hbar}{4m}\Big(\frac{g-2}{2}\frac{1}{J_{op}} + \frac{mc^2}{J_{op}(J_{op}+mc^2)}\Big)\Big(\vec{\Sigma}_{op}\cdot(\vec{\pi}_{op}\wedge\vec{E}_{op})\Big) + \text{h.c.}\ . \end{aligned} \qquad (5)$$

In second order, i.e. in $\tilde{H}_{op,2}$, terms quadratic in $\vec{E}_{op}$ and $\vec{B}_{op}$ and gradient terms in $\vec{E}_{op}$ and $\vec{B}_{op}$ (e.g. the 'Darwin term') appear but no spin terms.

4 The two-component formalism

The two-component Hamiltonian h_{op}^{dk}, the 'DK-Hamiltonian', is obtained from $\tilde{H}_{op}^{dk}$ by the replacements $\gamma_{op,4} \to 1$ and $\vec{\Sigma}_{op} \to \vec{\sigma}_{op}$ so that:

$$h_{op}^{dk} := h_{op,orb}^{dk} + \frac{\hbar}{2}\cdot(\vec{\sigma}_{op}\cdot\vec{\Omega}_{op})\ , \qquad (6)$$

where $h_{op,orb}^{dk} := J_{op} + e\phi_{op}$ and:

$$\begin{aligned}\vec{\Omega}_{op} := {} & -\frac{e}{2mc}(\frac{mc^2}{J_{op}} + \frac{g-2}{2})\vec{B}_{op} + \frac{ec(g-2)}{4m}\frac{1}{J_{op}(J_{op}+mc^2)}(\vec{\pi}_{op}\cdot\vec{B}_{op})\vec{\pi}_{op} \\ & + \frac{e}{2m}\Big(\frac{g-2}{2J_{op}} + \frac{mc^2}{J_{op}(J_{op}+mc^2)}\Big)(\vec{\pi}_{op}\wedge\vec{E}_{op}) + \text{h.c.}\ . \end{aligned} \qquad (7)$$

5 Nonrelativistic approximation

Expanding h_{op}^{dk} w.r.t. $1/m$ one gets in first order in $1/m$ ('nonrelativistic limit'): $mc^2 + (1/2m)(\vec{\pi}_{op} \cdot \vec{\pi}_{op}) + e\phi_{op} - (e\hbar g/4mc)(\vec{\sigma}_{op} \cdot \vec{B}_{op})$ which for $g = 2$ is the Pauli-Schroedinger Hamiltonian.

6 The density operator in the two-component formalism

The density operator ρ_{op} reads as:

$$\rho_{op} = \frac{1}{2} \left(\rho_{op,orb} + \vec{\sigma}_{op} \cdot \vec{\xi}_{op}\right) , \tag{8}$$

where $\rho_{op,orb}$ and $\vec{\xi}_{op}$ do not contain spin degrees of freedom. The normalisation of the density operator reads as $1 = Tr[\rho_{op}] = Tr[\rho_{op,orb}]$. Expanding the Hamiltonian and the density operator to second order, the evolution equation for the density operator, the 'von-Neumann equation', reads in first order as:

$$0 \stackrel{1}{=} -\frac{\partial \rho_{op}}{\partial t} + \frac{i}{\hbar}[\rho_{op} \, , \, h_{op}^{dk}] \, .$$

Note that the second order parts of the Hamiltonian drop out of this von-Neumann equation because they are independent of spin. By Eq. (8) the von-Neumann equation is in first order equivalent to:

$$0 \stackrel{1}{=} -\frac{\partial \rho_{op,orb}}{\partial t} + \frac{i}{\hbar}[\rho_{op,orb} \, , \, h_{op,orb}^{dk}] + \frac{i}{2}\Big((\vec{\xi}_{op} \cdot \vec{\Omega}_{op}) - (\vec{\Omega}_{op} \cdot \vec{\xi}_{op})\Big) \, , \tag{9}$$

$$0 \stackrel{1}{=} -\frac{\partial \vec{\xi}_{op}}{\partial t} + \frac{1}{2}(\vec{\Omega}_{op} \wedge \vec{\xi}_{op}) - \frac{1}{2}(\vec{\xi}_{op} \wedge \vec{\Omega}_{op}) + \frac{i}{\hbar}[\vec{\xi}_{op} \, , \, h_{op,orb}^{dk}] + \frac{i}{2}[\rho_{op,orb} \, , \, \vec{\Omega}_{op}] \, . \tag{10}$$

The terms proportional to $\vec{\Omega}_{op}$ in Eq. (9) account for the effect of the SG force on the orbital motion and the second and third terms on the rhs of Eq. (10) have the same structure as the Thomas-BMT equation.

The terms $h_{op,orb}^{dk}$ and $\vec{\Omega}_{op}$ in the von-Neumann equation are not unique because the FW Hamiltonian depends on the chosen FW transformation. However, essential uniqueness allows the forms in Eqs. (6) and (7).

7 The Weyl transform in the two-component formalism

The 'Weyl transform' allows q-numbers to be represented by c-numbers. In the two-component formalism an operator K_{op} is represented by its Weyl transform K_{wt} via:

$$K_{wt,\nu\lambda}(\vec{r},\vec{p};t) := Tr[K_{op}\mathcal{M}_{op,\nu\lambda}\Delta_{op}(\vec{r},\vec{p})] \, , \qquad (\nu,\lambda = 1,2) \, , \tag{11}$$

where the operator Δ_{op} is defined by:

$$\Delta_{op}(\vec{r},\vec{p}) := \frac{1}{8\pi^3\hbar^3} \int d^3x \, d^3u \exp\Big(\frac{i}{\hbar}[\vec{x} \cdot (\vec{r} - \vec{r}_{op}) + \vec{u} \cdot (\vec{p} - \vec{p}_{op})]\Big) \, ,$$

and where the operators $\mathcal{M}_{op,11}, ...$ are defined by:

$$(\mathcal{M}_{op,\nu\lambda}\ \chi)_\mu = \delta_{\mu\nu}\chi_\lambda\ , \qquad (\mu,\nu,\lambda = 1,2)\ .$$

Conversely one has:

$$K_{op} = \frac{1}{8\pi^3\hbar^3}\sum_{\nu,\lambda=1}^{2}\ \mathcal{M}_{op,\nu\lambda}\int\ d^3r\ d^3p\ K_{wt,\nu\lambda}\Delta_{op}\ . \tag{12}$$

Thus the Weyl transform is a 2×2 matrix valued phase space function; the t-dependence in K_{wt} only occurs for time-dependent operators. In terms of its Weyl transform the trace of an operator K_{op} reads as:

$$Tr[K_{op}] = \frac{1}{8\pi^3\hbar^3}tr[\int\ d^3r\ d^3p\ K_{wt}]\ , \tag{13}$$

where tr denotes the matrix trace.

8 The Wigner function

The chosen normalisation of the density operator ρ_{op} leads to:

$$1 = \frac{1}{8\pi^3\hbar^3}tr[\int\ d^3r\ d^3p\ \rho_{wt}]\ , \tag{14}$$

for its Weyl transform ρ_{wt} (see Eq. (13)) and one calls $(1/8\pi^3\hbar^3)\rho_{wt}$ the 'Wigner function' of that state. In terms of Weyl transforms the expectation value of an operator K_{op} reads as:

$$< K_{op} >= \frac{1}{8\pi^3\hbar^3}tr[\int\ d^3r\ d^3p\ \rho_{wt}K_{wt}]\ . \tag{15}$$

9 The Wigner-Kirkwood expansion

Since we are dealing with a beam, which in a high energy accelerator occupies a phase space volume many orders of magnitude greater then $\hbar^3$, we are very far from dealing with a pure state. Then, applying semi-classical perturbation theory to the density operator, its Weyl transform has the 'Wigner-Kirkwood' form:

$$\rho_{wt} = \underbrace{\rho_0}_{Classical\ part} + \underbrace{\hbar\cdot\rho_1 + \hbar^2\cdot\rho_2 + ...}_{Quantum\ corrections}\ , \tag{16}$$

where $\rho_0, \rho_1, \rho_2, ...$ are of zeroth order in $\hbar$ [b]. In reality, 'classical distributions' ρ_0 do not exist so that one has to deal with Eq. (16).

[b] Note that ρ_{op} has a related expansion and that this was used in Eqs. (9) and (10).

10 The Weyl transform of the Hamiltonian

The Weyl transform of the Hamiltonian is $h^{dk}_{wt} \stackrel{1}{=} h^{dk}_{orb} + \frac{\hbar}{2}(\vec{\sigma}\cdot\vec{\Omega}_{dk})$ where:

$$
\begin{aligned}
h^{dk}_{orb} &:= J + e\phi \ , \\
\vec{\Omega}_{dk} &:= -\frac{e}{mc}\Big(\frac{mc^2}{J} + \frac{g-2}{2}\Big)\vec{B} + \frac{ce(g-2)}{2m}\frac{1}{J(J+mc^2)}(\vec{\pi}\cdot\vec{B})\vec{\pi} \\
&\quad + \frac{e}{m}\Big(\frac{g-2}{2}\frac{1}{J} + \frac{mc^2}{J(J+mc^2)}\Big)(\vec{\pi}\wedge\vec{E}) \ ,
\end{aligned}
$$

and where $\vec{\pi} := \vec{p} - \frac{e}{c}\vec{A}$ and $J := \sqrt{m^2c^4 + c^2(\vec{\pi}\cdot\vec{\pi})}$.

11 The Weyl transform of the von-Neumann equation

The Weyl transform of the von-Neumann equation is an evolution equation for ρ_{wt}. In particular from Eqs. (9) and (10) and in first order using section 7, one gets:

$$
0 \stackrel{1}{=} \underbrace{-\frac{\partial \rho_{wt,orb}}{\partial t} + \{h^{dk}_{orb}\ ,\ \rho_{wt,orb}\}}_{\text{classical Liouville terms}} + \underbrace{\frac{\hbar}{2}\{\Omega_{dk,j}\ ,\ \xi_{wt,j}\}}_{\text{SG term}} \ , \tag{17}
$$

$$
0 \stackrel{1}{=} \underbrace{-\frac{\partial \vec{\xi}_{wt}}{\partial t} + \{h^{dk}_{orb}\ ,\ \vec{\xi}_{wt}\} + \vec{\Omega}_{dk}\wedge\vec{\xi}_{wt}}_{\text{Thomas-BMT terms}} + \underbrace{\frac{\hbar}{2}\{\vec{\Omega}_{dk}\ ,\ \rho_{wt,orb}\}}_{\text{SG backreaction term}} \ , \tag{18}
$$

where $\{\ ,\ \}$ is the usual Poisson bracket w.r.t. $\vec{r}$ and $\vec{p}$ and where repeated indices are summed over. As in Eqs. (9) and (10) the second order parts of the Hamiltonian drop out. The vector $\vec{\xi}_{wt}$ is the **polarisation density** and Eq. (18) is its **Bloch equation** in first order [3]. Note that these equations are not restricted to dipole and quadrupole magnetic fields. It is the ρ_{wt} and $\vec{\xi}_{wt}$ which serve as the 'classical distribution functions' which we have been seeking.

These equations are easily transformed from cartesian coordinates to 'machine coordinates' since with the Weyl transform one only has to deal with c-numbers instead of q-numbers [10]. After transforming to machine coordinates the zeroth order limits of the transformed Eqs. (17) and (18) correspond to the classical Eqs. (17) and (40) in Article I.

For FW transformations of the Dirac equation where time has been replaced by the longitudinal coordinate in a paraxial approximation see [11].

12 Radiation

Now that the radiationless case is on a firm basis, one can include radiation. In a classical treatment of radiation effects one gets the Fokker-Planck and Bloch equations of Eqs. (24) and (39) in Article I. To include the Sokolov-Ternov effect one needs a full quantum treatment [12].

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