A Path-Integral Formulation of the Pauli Equation Using Two Real Spin Coordinates

VIKTOR BEZÁK

Electrotechnical Institute, Slovak Academy of Sciences, 809 32 Bratislava, Czechoslovakia

Received: 16 April 1974

Abstract

Feynman's path-integral quantum-mechanical formulation is generalised for particles of spin $\frac{1}{2}$. In the one-particle case, the path-integral formulation uses paths in a Euclidean real five-dimensional space, two coordinates (u, v) being reserved for spin. The path integral is proven to correspond exactly to the Pauli equation. A canonical density-matrix formulation is also dealt with. Basic ideas are to start with differential spin operators instead of the Pauli matrices and apply them to functions $\Psi = \psi_1(\mathbf{r}, t)u + \psi_2(\mathbf{r}, t)v$ where ψ_1, ψ_2 are the Pauli wave functions. Then a 'nilpotent' spin 'kinetic-energy' term is added to the Hamiltonian. This enables us to find a non-matrix spin-dependent Lagrangian which is used as usual in the action of a path integral of the Feynman type. Integral relations are derived from which the path integral can be transformed into components of the Pauli matrix Green's function (propagator) or the canonical density matrix. As an example, a path-integral calculation of the normal Zeeman splitting is carried out.

1. Introduction

The subject of this article is a quantum-mechanical description of a charged particle of spin $\frac{1}{2}$ in an electric field $\mathbf{E}(\mathbf{r}, t)$ and magnetic field $\mathbf{B}(\mathbf{r}, t)$ by means of a continual integral of the Feynman type (Feynman, 1948; Feynman & Hibbs, 1965). Simultaneously, for static fields $\mathbf{E}(\mathbf{r})$, $\mathbf{B}(\mathbf{r})$, we shall also deal with a density matrix formulation, paying attention to a gas of identical non-interacting boltzons (e.g. in a box) at thermodynamic equilibrium.

1.1. Basic Concepts

To introduce the subject, let us consider, at first, a spinless particle or, more generally, a spinless system with d degrees of freedom. The Feynman continual (path) integral represents a compact description of Green's function

Copyright © 1974 Plenum Publishing Company Limited. No part of this publication may be reproduced, stored in a retrieval system, or transmitted, in any form or by any means, electronic, mechanical, photocopying, microfilming, recording or otherwise, without written permission of Plenum Publishing Company Limited.

 $G(Q, Q_0, t)$ for the Schrödinger equation which may be written in the integral form

$$\psi(Q, t) = \int d^d Q_0 G(Q, Q_0, t) \psi(Q_0, 0)$$
(1.1.1)

where Q, Q_0 are positional vectors from a *d*-dimensional coordinate space, S_d , and t > 0 is the time variable. According to Feynman's definition, we may dissect the time interval (0, t) into N equal sub-intervals, define infinitesimal classical actions $S_{j, j+1}$ for each of them (j = 0, 1, ..., N - 1) and write the Green function as the infinitely multiple integral

$$G(Q, Q_0, t) = \lim_{N \to \infty} \tilde{\mathcal{N}}(t) \prod_{j=1}^{N-1} \int_{-\infty}^{\infty} d^d Q_j \exp(iS_{j,j+1})$$
(1.1.2)

 $(Q_N = Q, \hbar = 1)$. The factor $\tilde{\mathcal{N}}(t)$ is independent of the points Q, Q_0 , and is determined by the condition

$$G(Q, Q_0, +0) = \delta^d (Q - Q_0) \tag{1.1.3}$$

If the metric of the space S_d is Euclidean and L(Q, Q, t) denotes the classical Lagrangian corresponding to the Hamiltonian of equation (1.1.1), then the actions $S_{j,j+1}$ used in the continual integral (1.1.2) may be defined by the interpolation formula

$$S_{j,j+1} = L(\frac{1}{2}(Q_j + Q_{j+1}), (Q_{j+1} - \dot{Q}_j)N/t, t/N)t/N$$
(1.1.4)

As long as all the actions $S_{j, j+1}$ mutually commute, we may also write, according to Feynman, the Green function (1.1.2) in the form

$$G(Q, Q_0, t) = \mathcal{N}(t) \int_{Q_0, 0}^{Q, t} \mathcal{D}Q(\tau) \exp\{i \int_{0}^{t} d\tau L(Q(\tau), \dot{Q}(\tau), \tau)\} \quad (1.1.5)$$

(t > 0) so that the name 'path integral' for the functional integral (1.1.5) due to the use of the paths $Q(\tau) (Q(0) = Q_0, Q(t) = Q)$, is doubly emphasised owing to the actual presence of the path integral in the exponent.

1.2. Different Continual-Integral Approaches to the Problem of Spin

Throughout this paper we will confine ourselves to the problem of spin as the proper dynamical variable and will not have in mind any question of statistics, although they are, of course, related to our problem (Klauder, 1960).

There are several ways how spin may be incorporated into continual integrals of the Feynman type. The first was suggested by Feynman himself (Feynman, 1948) and consists, for the case of a particle of spin $\frac{1}{2}$, of completing the classical action $S_{j,j+1}$ by a term involving the Pauli matrices. The exponential expressions $\exp(iS_{j,j+1})$ become 2×2 matrices which cease to commute if the magnetic field is either non-uniform in space or varying in time. The disappearance of the most captivating and useful property of the Feynman continual integral, namely the commutability of all the entities occurring in it, is an uncomfortable defect. Although we may use definition

(1.1.2) in this case, we must keep in mind that the exponential expressions $\exp(iS_{j,j+1})$ must not be mutually exchanged. Of course, the transition to formula (1.1.5) is then not allowed and that is why Feynman considered his own path-integral formulation as inconvenient for particles with spin (Feynman & Hibbs, 1965).

If we do wish to use the path integral in the form (1.1.5), we may do so, but after putting a time-ordering operator in front of it. Moreover, Hamilton & Shulman (1971) have shown that the use of the time-ordering operator is identical to using a rather old mathematical concept of the so-called product integrals.

Furthermore, owing to the analogy between Feynman's continual integrals and the functional integrals introduced by Wiener in his well-known study of the Brownian motion, one could easily foresee that much of the hitherto existing mathematical armament having been developed in the theory of the Wiener processes would also be applicable in quantum mechanics. We can quote, for instance, Garczynski, who elaborated a theory of quantum Markov processes and within its framework has published a paper devoted to spin (Garczynski, 1973). Again, a crucial attribute of his formulation is the use of the time-ordering operator. (We are also aware of another stochastic theory of spin—actually a theory of the Pauli equation—due to de la Peña-Auerbach (1971) whose formalism, however, is not based on Feynman's continual integrals or any similar concepts at all and is, therefore, only indirectly connected with our subject.)

Recently Petráš (private communication) has succeeded in formulating a new, interesting approach to the problem of spin, having dealt with a pathintegral analysis of a charged point particle. He has shown that the Pauli equation results naturally from a path-integral theory where the finite-product approximations of some path integral are due to paths combined from circular (and, in general, even more complicated curvilinear) segments instead of the common straight-line sections used in definition (1.1.2).

The best known path-integral approach to the problem of spin to which our path-integral approach particularly refers is due to Shulman (1968). The Green function of his symmetric spinning top is a direct analogy to the probability distribution function investigated in the theory of the rotational Brownian motion (Valiev & Ivanov, 1973) and represents a sum of contributions due to all the quantum numbers of the angular momentum. It is clear then that Shulman's Green function necessarily bears a high redundancy of information in the case of a particle with a concrete prescribed spin since it involves terms due to all other spins allowed for a classical top $(\frac{1}{2}, 1, \frac{3}{2}, 2, ...)$. The basic idea of Shulman's conception is the use of paths in a composite space $R^3 \times SO(3)$. where R^3 is the common real three-dimensional space and SO(3) the quotient space induced by the three-dimensional irreducible representation of the group of rotations. In consequence of such a choice of the coordinate space, Shulman's theory bears two features which make it so sophisticated: the space $R^3 \times SO(3)$ is both multiply connected and curved so that the simple definition (1.1.4) of the actions $S_{i,i+1}$ is insufficient.

None of these features will occur in our formulation described in the present paper. Our expression is tailored right to particles of spin $\frac{1}{2}$ and does not carry information about other spins. In our formulation we use a real Euclidean space (whose metric is trivial) instead of $R^3 \times SO(3)$. Our coordinate space is five-dimensional in the one-particle case, two dimensions being reserved for spin. (A generalisation—whose discussion, however, will not be treated in this paper—is also possible where the coordinates due to the spin subspace are not real, as in the present formulation, but complex, so that four dimensions may be reserved for spin.) For our expression it is sufficient to use definition (1.1.2) with the actions $S_{j,j+1}$ given by formula (1.1.4). Thus, in the case of multiple-integral approximations of Green's function, we have in mind broken paths rectified by straight-line sections. Finally, as there are only commuting entities in our Green's function, we need not use any time-ordering operation.

To develop our formulation, we commence with a purely differential representation of the Pauli equation which is defined in Section 2. Instead of directly using the Pauli spinor functions, we combine their components $\psi_1(\mathbf{r}, t), \psi_2(\mathbf{r}, t)$ into bilinear forms $\psi_1 u + \psi_2 v$ where u, v are formal coordinates reserved for spin in our five-dimensional space. Our basic idea is to add a 'nilpotent' kinetic-energy term $-\frac{\partial^2}{\partial u^2} - \frac{\partial^2}{\partial v^2}$ into the Hamiltonian.

Although the addition of such a nilpotent operator is the same as adding zero to the Hamiltonian (hence the prefix 'nil'), a vital kinetic-energy term corresponds to it in the Lagrangian. The Green function derived as a path integral with respect to paths in the space $\{\mathbf{r}, u, v\}$ can be transformed by simple integral formulae into the matrix components of Green's function in the usual Pauli matrix representation.

In order to verify the direct use of our conception on a simple example, we shall also present, in an appendix, a path integral calculation of the Zeeman splitting in a uniform time-independent magnetic field.

2. Basic Analysis

2.1. The Purely Differential Representation of the Pauli Equation

The standard Pauli equation for a particle of spin $\frac{1}{2}$, charge e and mass m, with using units when $\hbar = c = 1$, reads

$$i\frac{\partial\Psi^{P}(\mathbf{r},t)}{\partial t} = H^{P}\Psi^{P}(\mathbf{r},t)$$
(2.1.1)

where

$$H^{P} = \frac{1}{2m} \left(\hat{\mathbf{p}} - e \mathbf{A}(\mathbf{r}, t) \right)^{2} \mathbf{I} + e \varphi(\mathbf{r}, t) \mathbf{I} - \frac{e}{2m} \mathbf{B}(\mathbf{r}, t) \cdot \sigma \qquad (2.1.2)$$

Beside the differential operator $\hat{\mathbf{p}} = -i\nabla$, the Hamiltonian H^P involves the matrix spin operator σ whose components are

$$\sigma_{\mathbf{x}} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_{\mathbf{y}} = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \sigma_{z} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$
(2.1.3)

and the unit matrix I. We have written on purpose the suffix P with the Hamiltonian and the two-component wave function

$$\Psi^{P}(\mathbf{r},t) = \begin{pmatrix} \Psi_{1}(\mathbf{r},t) \\ \Psi_{2}(\mathbf{r},t) \end{pmatrix}$$
(2.1.4)

in order to emphasise that they are defined in the Pauli matrix representation. The functions $\varphi(\mathbf{r}, t)$, $\mathbf{A}(\mathbf{r}, t)$ are the scalar and vector potential, respectively, related to the electric and magnetic field,

$$\mathbf{E}(\mathbf{r},t) = -\nabla \varphi(\mathbf{r},t) - \frac{\partial \mathbf{A}(\mathbf{r},t)}{\partial t}, \qquad \mathbf{B}(\mathbf{r},t) = \nabla \mathbf{x} \mathbf{A}(\mathbf{r},t) \quad (2.1.5)$$

In analogy to equation (1.1.1), we can rewrite the Pauli equation in the integral form

$$\Psi^{P}(\mathbf{r},t) = \int d^{3}r_{0}G^{P}(\mathbf{r},\mathbf{r}_{0},t)\Psi^{P}(\mathbf{r}_{0},0)$$
(2.1.6)

whose kernel $G^{P}(\mathbf{r}, \mathbf{r}_{0}, t)$ is a 2 x 2 matrix,

$$G^{P}(\mathbf{r}, \mathbf{r}_{0}, t) = \begin{pmatrix} G_{11}(\mathbf{r}, \mathbf{r}_{0}, t) & G_{12}(\mathbf{r}, \mathbf{r}_{0}, t) \\ G_{21}(\mathbf{r}, \mathbf{r}_{0}, t) & G_{22}(\mathbf{r}, \mathbf{r}_{0}, t) \end{pmatrix}$$
(2.1.7)

In the special case when the potentials φ , **A** are time-independent, we may also write the stationary-state equation

$$H^{P}\Psi^{P}(\mathbf{r}) = E_{n}\Psi_{n}^{P}(\mathbf{r})$$
(2.1.8)

where

$$\Psi_n^P(\mathbf{r}) = \begin{pmatrix} \Psi_{1n}(\mathbf{r}) \\ \Psi_{2n}(\mathbf{r}) \end{pmatrix}$$
(2.1.9)

Assuming, for simplicity, that all the states Ψ_n^P are discrete (situating the particle in a box, say), we may consider the normalisation

$$\int d^3 r[|\psi_{1n}(\mathbf{r})|^2 + |\psi_{2n}(\mathbf{r})|^2] = 1$$
 (2.1.10)

and write Green's function (2.1.7) as the sum

$$G^{P}(\mathbf{r}, \mathbf{r}_{0}, t) = \sum_{n} \Psi_{n}^{P}(\mathbf{r}) \Psi_{n}^{P+}(\mathbf{r}_{0}) \exp(-iE_{n}t) \qquad (t > 0) \quad (2.1.11)$$

over the complete set of the eigenstates $\Psi_n^{P}(\mathbf{r})$. For the components of Green's function (2.1.7), we have the relations

$$G_{\mu\nu}(\mathbf{r}, \mathbf{r}_0, t) = \sum_n \psi_{\mu n}(\mathbf{r}) \psi_{\nu n}^*(\mathbf{r}_0) \exp(-iE_n t); \qquad \mu, \nu = 1, 2$$
(2.1.11a)

Obviously, Green's function (2.1.7) fulfils the initial condition

$$G^{P}(\mathbf{r}, \mathbf{r}_{0} + 0) = \delta^{3}(\mathbf{r} - \mathbf{r}_{0})\mathbf{I}$$
 (2.1.12)

For time-independent potentials φ , **A**, we may also define the one-particle canonical density matrix for a temperature T:

$$C^{P}(\mathbf{r}, \mathbf{r}_{0}, \beta) = \sum_{n} \Psi_{n}^{P}(\mathbf{r}) \Psi_{n}^{P+}(\mathbf{r}_{0}) \exp\left(-\beta E_{n}\right), \qquad \beta = 1/k_{B}T$$
(2.1.13)

or

$$C_{\mu\nu}(\mathbf{r}, \mathbf{r}_0, \beta) = \sum_n \psi_{\mu n}(\mathbf{r}) \psi_{\nu n}^*(\mathbf{r}_0) \exp\left(-\beta E_n\right), \qquad \mu, \nu = 1, 2$$
(2.1.13a)

The canonical density matrix is the finite solution of the equation

$$-\frac{\partial C^{P}(\mathbf{r}, \mathbf{r}_{0}, \beta)}{\partial \beta} = \left[\frac{1}{2m} \left(\mathbf{p} - e\mathbf{A}(\mathbf{r})\right)^{2} + e\varphi(\mathbf{r}) - \frac{e}{2m} \mathbf{B}(\mathbf{r}) \cdot \sigma\right] C^{P}(\mathbf{r}, \mathbf{r}_{0}, \beta)$$
(2.1.14)

for $\beta > 0$, satisfying the 'initial' condition

$$C^{P}(\mathbf{r}, \mathbf{r}_{0}, +0) = \delta^{3}(\mathbf{r} - \mathbf{r}_{0})\mathbf{I}$$
 (2.1.15)

Comparing formulae (2.1.11) and (2.1.13), we state the validity of the relations

$$G^{P}(\mathbf{r}, \mathbf{r}_{0}, t) = C^{P}(\mathbf{r}, \mathbf{r}_{0}, it), \qquad C^{P}(\mathbf{r}, \mathbf{r}_{0}, \beta) = G^{P}(\mathbf{r}, \mathbf{r}_{0}, -i\beta) \quad (2.1.16)$$

The trace of the canonical density matrix (2.1.13) represents the partition sum for a gas of identical particles of charge e and mass m, provided that one may neglect any interaction between the particles:

$$Z(\beta) = \operatorname{Tr} C^{P}(\mathbf{r}, \mathbf{r}_{0}, \beta) = \int d^{3} \mathbf{r} [C_{11}(\mathbf{r}, \mathbf{r}, \beta) + C_{22}(\mathbf{r}, \mathbf{r}, \beta)]$$
$$= \sum_{n} \exp(-\beta E_{n}) \qquad (2.1.17)$$

If we know the function $Z(\beta)$ we can, in principle, calculate any thermodynamic quantity of the gas, as well as the energy-level density.

Now, our first step is to exclude the 2×2 matrices from the theory. To achieve this, let us introduce a functional space L_2 spanned by the functions

$$\Psi(Q, t) = \psi_1(\mathbf{r}, t)u + \psi_2(r, t)v$$
(2.1.18)

where $\psi_1(\mathbf{r}, t)$, $\psi_2(\mathbf{r}, t)$ are components of the Pauli spinor functions (2.1.4) and u, v are two formal real variables. The only property which we require of the variables u, v is that they are mutually independent, as well as independent of \mathbf{r} and t, and span the whole real axis. We may then define a five-dimensional space S_5 of vectors $Q = (\mathbf{r}, u, v)$. Of course, the functions $\Psi(Q, t) \in L_2$ are no proper quantum-mechanical wave functions (since they are not quadratically integrable in S_5) but are uniquely related to them by the Pauli functions

 $\psi_1(\mathbf{r}, t), \psi_2(\mathbf{r}, t)$. As far as we consider functions from the space L_2 , we can introduce the following differential equivalents to the matrices $\sigma_x, \sigma_y, \sigma_z$:

$$\hat{\sigma}_{\mathbf{x}} = v \frac{\partial}{\partial u} + u \frac{\partial}{\partial v}, \qquad \hat{\sigma}_{\mathbf{y}} = i \left(v \frac{\partial}{\partial u} - u \frac{\partial}{\partial v} \right), \qquad \hat{\sigma}_{\mathbf{z}} = u \frac{\partial}{\partial u} - v \frac{\partial}{\partial v}$$
(2.1.19)

Instead of the unit matrix $\hat{\mathbf{I}}$ we may use the operator $\hat{I} = u \partial/\partial u + v \partial/\partial v$ or simply unity. Here it is pertinent to recollect that similar operators occur in the theory of spinor invariants (Brinkman, 1956) due to Kramers where, however, u, v are complex components of spinors. No such meaning may be ascribed to our variables u, v (in the present paper at least) which we let represent two auxiliary real parameters without giving them physical meaning. They are merely taken as corresponding to the indices 1 and 2, nothing else. Thus, to avoid any misunderstanding, it should be pointed out that if any rotation is applied the real variables u, v are, by definition, intact whilst both the spatial coordinates x, y, z are subject to some transformation and the complex values ψ_1, ψ_2 are transformed like spinor components, $\psi'_1 = a\psi_1 + b\psi_2, \psi'_2 =$ $-b^*\psi_1 + a^*\psi_2$. (Of course, if the variables *u*, *v* themselves were considered as components of some spinor, we could then consider a transformation $u, v \rightarrow v$ u', v'; then, however, necessarily the variables u, v should be, in general, complex-a property from which we wish to refrain in the present paper.) The actual physical meaning is obviously hidden in the Pauli wave functions $\psi_1(\mathbf{r},t), \psi_2(\mathbf{r},t).$

The space L_2 is invariant with respect to the algebra of operators $\hat{\sigma}_x$, $\hat{\sigma}_y$, σ_z , \hat{I} , i.e. if any linear combination of any product of these operators is applied to any function from L_2 the result is again a function from L_2 . Let us take, for instance, the product

$$\hat{\sigma}_{x}\hat{\sigma}_{y} = i\left(v^{2}\frac{\partial^{2}}{\partial u^{2}} - u^{2}\frac{\partial^{2}}{\partial v^{2}} + u\frac{\partial}{\partial u} - v\frac{\partial}{\partial v}\right)$$

Operators like $v^2(\partial^2/\partial u^2) - u^2(\partial^2/\partial v^2)$, which give zero when applied to any function from L_2 , may be called 'additionally nilpotent' with respect to the space L_2 . If we delete additionally nilpotent operators, we can write the relations

 $\hat{\sigma}_x \hat{\sigma}_y = -\hat{\sigma}_y \hat{\sigma}_x = i\sigma_z, \dots$ (cyclic permutations of x, y, z) (2.1.20)

which mean, in fact, that the algebra of the differential operators $\hat{\sigma}_x$, $\hat{\sigma}_y$, $\hat{\sigma}_z$ and \hat{I} is isomorphic to the algebra of the matrices σ_x , σ_y , σ_z , I. Therefore, for functions (2.1.18), i.e. $\Psi(Q, t) \in L_2$, we may rewrite the Pauli equation (2.1.1) into the purely differential form

$$i\frac{\partial\Psi(Q,t)}{\partial t} = \hat{H}\Psi(Q,t) \qquad (2.1.21)$$

with the Hamiltonian

$$\hat{H} = \frac{1}{2m} \left(\hat{\mathbf{p}} - e \mathbf{A}(\mathbf{r}, t) \right)^2 + e \varphi(\mathbf{r}, t) - \frac{e}{2m} \mathbf{B}(\mathbf{r}, t) \cdot \hat{\sigma} \qquad (2.1.22)$$

where $\hat{\sigma}$ is the vector operator with components $\hat{\sigma}_x$, $\hat{\sigma}_y$, $\hat{\sigma}_z$ given by formulae (2.1.19). Physically, of course, equation (2.1.21) does not give anything new and is only another compact formulation of the same two differential equations (given after equalising, respectively, the coefficients at u and v on both sides of equation (2.1.21)) for the Pauli functions $\psi_1(\mathbf{r}, t), \psi_2(\mathbf{r}, t)$ which are also given by equation (2.1.1).

The integral form of equation (2.1.21) reads

$$\Psi(Q, t) = \int d^5 Q_0 G(Q, Q_0, t) \Psi(Q_0, 0)$$
 (2.1.23)

where $G(Q, Q_0, t)$ is a function defined for t > 0 which must satisfy the condition

$$G(Q, Q_0, +0) = \delta^3 (\mathbf{r} - \mathbf{r}_0) \delta(u - u_0) \delta(v - v_0)$$
(2.1.24)

Analogically to relations (2.1.16), we may also define the function $C(Q, Q_0, \beta)$ for $\beta > 0$:

$$G(Q, Q_0, t) = C(Q, Q_0, it), \quad C(Q, Q_0, \beta) = G(Q, Q_0, -\beta) \quad (2.1.25)$$

For $\beta \rightarrow +0$ we have the condition

$$C(Q, Q_0, +0) = \delta^3(\mathbf{r} - \mathbf{r}_0)\delta(u - u_0)\delta(v - v_0)$$
(2.1.26)

It should be pointed out that the functions $G(Q, Q_0, t)$, $C(Q, Q_0, \beta)$ cannot more be represented by sums of the form (2.1.11), (2.1.13), respectively, since the functions $\psi_{1n}(\mathbf{r})u + \psi_{2n}(\mathbf{r})v$ do not form an orthonormal set. Moreover, the function $C(Q, Q_0, \beta)$ does not mean any density matrix at all. Nevertheless, after comparing equations (2.1.23) and (2.1.25) with equations (2.1.6) and (2.1.16), we obtain the following relations:

$$G_{11}(\mathbf{r}, \mathbf{r}_{0}, t) = \int_{-\infty}^{\infty} du_{0} dv_{0} \frac{\partial}{\partial u} G(Q, Q_{0}, t)u^{0}$$

$$G_{12}(\mathbf{r}, \mathbf{r}_{0}, t) = \int_{-\infty}^{\infty} du_{0} dv_{0} \frac{\partial}{\partial u} G(Q, Q_{0}, t)v_{0}$$

$$G_{21}(\mathbf{r}, \mathbf{r}_{0}, t) = \int_{-\infty}^{\infty} du_{0} dv_{0} \frac{\partial}{\partial v} G(Q, Q_{0}, t)u_{0}$$

$$G_{22}(\mathbf{r}, \mathbf{r}_{0}, t) = \int_{-\infty}^{\infty} du_{0} dv_{0} \frac{\partial}{\partial v} G(Q, Q_{0}, t)v_{0}$$
(2.1.27)

$$C_{11}(\mathbf{r}, \mathbf{r}_{0}, \beta) = \int_{-\infty}^{\infty} du_{0} dv_{0} \frac{\partial}{\partial u} C(Q, Q_{0}, \beta)u_{0}$$

$$C_{12}(\mathbf{r}, \mathbf{r}_{0}, \beta) = \int_{-\infty}^{\infty} du_{0} dv_{0} \frac{\partial}{\partial u} C(Q, Q_{0}, \beta)v_{0}$$

$$C_{21}(\mathbf{r}, \mathbf{r}_{0}, \beta) = \int_{-\infty}^{\infty} du_{0} dv_{0} \frac{\partial}{\partial v} C(Q, Q_{0}, \beta)u_{0}$$

$$C_{22}(\mathbf{r}, \mathbf{r}_{0}, \beta) = \int_{-\infty}^{\infty} du_{0} dv_{0} \frac{\partial}{\partial v} C(Q, Q_{0}, \beta)v_{0}$$
(2.1.28)

Thus, if we know the function $G(Q, Q_0, t)$ or $C(Q, Q_0, \beta)$ we can calculate the components $G_{\mu\nu}(\mathbf{r}, \mathbf{r}_0, t)$, $C_{\mu\nu}(\mathbf{r}, \mathbf{r}_0, \beta)$ of Green's function or the canonical density matrix in the Pauli matrix representation. In particular, according to formula (2.1.17), the partition sum $Z(\beta)$ is given by the integral formula

$$Z(\beta) = \int d^3 r \int_{-\infty}^{\infty} du_0 \, dv_0 \cdot \left(u_0 \frac{\partial}{\partial u} + v_0 \frac{\partial}{\partial v} \right) C(Q, Q_0, \beta) / _{\mathbf{r}_0 = \mathbf{r}}$$
(2.1.29)

Let us finally note that the functions $G(Q, Q_0, t)$, $C(Q, Q_0, \beta)$ do not belongas conditions (2.1.24) and (2.1.26) must be satisfied, respectively-to the space L_2 , although, by definition, $\Psi(Q, t) \in L_2$.

In the next section we shall show that the functions $G(Q, Q_0, t), C(Q, Q_0, \beta)$ can be calculated as path integrals of the Feynman type.

2.2. The Spin-Dependent Path Integral

To derive a path integral corresponding to the function $G(Q, Q_0, t)$, let us add the nilpotent operator

$$\hat{T}_{\rm nil} = -\frac{1}{2m^0} \left(\frac{\partial^2}{\partial u^2} + \frac{\partial^2}{\partial v^2} \right), \qquad m^0 > 0$$
(2.2.1)

to the Hamiltonian (2.1.22). The operator (2.2.1) provokes some association with a kinetic-energy operator of a symmetric top although it means actually 'nothing' (nil) physically when applied, together with the operator (2.1.22), to any function $\Psi(Q, t) \in L_2$. (Of course, we could also use a more general operator, $-1/(2m_1) \partial^2/\partial u^2 - 1/(2m_2) \partial^2/\partial v^2$, instead of (2.2.1) but it would be, as it seems at least from the viewpoint of simplicity, superfluous, similarly as in Shulman's formulation there was no evident advantage to consider an asymmetric top (Shulman, 1968).)

One can easily see, by consulting equations (2.1.23) and (2.1.25), that the

functions $G(Q, Q_0, t)$, $C(Q, Q_0, \beta)$ may be defined, for any value $m^0 > 0$, as the finite solutions for t > 0, $\beta > 0$, of the equations

$$i\frac{\partial G(Q,Q_0,t)}{\partial t} = (\hat{T}_{nil} + \hat{H})G(Q,Q_0,t)$$
(2.2.2)

$$-\frac{\partial C(Q, Q_0, \beta)}{\partial \beta} = (\hat{T}_{nil} + \hat{H})C(Q, Q_0, \beta)$$
(2.2.3)

with the initial conditions (2.1.24) and (2.1.26), respectively.

The real parameter m^0 may be arbitrary but must necessarily be positive since otherwise the function $C(Q, Q_0, \beta)$ would not be finite for $Q \neq Q_0$, $\beta \rightarrow +0$. As the parameter m^0 is only occurring with a nilpotent, i.e. nonphysical operator, the functions $G_{\mu\nu}$, $C_{\mu\nu}$ (cf. (2.1.27) and (2.1.28) that bear the proper physical information are independent of m^0 despite the m^{0} dependence of the functions $G(Q, Q_0, t)$, $C(Q, Q_0, \beta)$ induced by equations (2.2.2) and (2.2.3). (This is also in agreement with Shulman's formulation where the projection of his multispin Green function into the subspace of states corresponding to a given spin is independent of the momentum of inertia of his classical top (Shulman, 1968).)

Desiring to have our space S_5 Euclidean, we define two operators of 'spin momenta':

$$\hat{p}_u = -i\frac{\partial}{\partial u}, \qquad \hat{p}_v = -i\frac{\partial}{\partial v}$$
 (2.2.4)

Then, with respect to formulae (2.1.19), we may write the Hamiltonian of equations (2.2.2) and (2.2.3) in the form

$$\hat{T}_{\text{nil}} + \hat{H} = \frac{\hat{\mathbf{p}}^2}{2m} + \frac{\hat{p}_u^2 + \hat{p}_v^2}{2m^0} + e\varphi(\mathbf{r}, t) - e[\hat{\mathbf{p}} \cdot \mathbf{A}(\mathbf{r}, t) + \mathbf{A}(\mathbf{r}, t) \cdot \hat{\mathbf{p}}] + \frac{e^2}{2m^2} \mathbf{A}^2(\mathbf{r}, t) - \frac{ie}{2m} \{ ([B_x(\mathbf{r}, t) + iB_y(\mathbf{r}, t)]v + B_z(\mathbf{r}, t)u)\hat{p}_u + ([B_x(\mathbf{r}, t) - iB_y(\mathbf{r}, t)]u - B_z(\mathbf{r}, t)v)\hat{p}_v \}$$
(2.2.5)

We may ascribe a 'classical' Hamiltonian to it by the correspondence principle $\hat{\mathbf{p}} \rightarrow \mathbf{p}, \hat{p}_u \rightarrow p_u, \hat{p}_v \rightarrow p_v$ and introduce the velocities $\dot{\mathbf{r}}, \dot{u}, \dot{v}$ by the formula

$$\dot{q}_i = \frac{\partial}{\partial p_i} \left(T_{\text{nil}} + H \right)$$

PATH-INTEGRAL FORMULATION OF THE PAULI EQUATION 331

borrowed from classical analytical mechanics. In this way we obtain the expressions

$$\mathbf{p} = m\dot{\mathbf{r}} + e\mathbf{A}$$

$$p_u = m^0 \left\{ \dot{u} + \frac{ie}{2m} \left[(B_x + iB_y)v + B_z u \right] \right\}$$

$$p_v = m^0 \left\{ \dot{v} + \frac{ie}{2m} \left[(B_x - iB_y)u - B_z v \right] \right\}$$

After substituting them into the formula

$$L(Q, \dot{Q}, t) = \sum_{i} p_{i}q_{i} - (T_{\text{nil}} + H)$$

for the Lagrangian $(Q = (\mathbf{r}, u, v))$, we obtain the result

$$L(\underline{Q}, \dot{\underline{Q}}, t) = L_{\text{non}\,\sigma}(\mathbf{r}, \dot{\mathbf{r}}, t) + L_{\sigma}(\underline{Q}, \dot{\underline{Q}}, t)$$
(2.2.6)

where

$$L_{\operatorname{non}\sigma}(\mathbf{r},\dot{\mathbf{r}},t) = \frac{1}{2}m\dot{\mathbf{r}}^{2} + e\mathbf{A}(\mathbf{r},t)\cdot\dot{\mathbf{r}} - e\varphi(\mathbf{r},t)$$
(2.2.7)

and

$$L_{\sigma}(Q, \dot{Q}, t) = m^{0} \Biggl\{ \frac{1}{2} \dot{u}^{2} + \frac{1}{2} \dot{v}^{2} + \frac{ie}{2m} \left(\left[(B_{x} + iB_{y})v + B_{z}u \right] \dot{u} + \left[(B_{x} - iB_{y})u - B_{z}v \right] \dot{v} \right] - \frac{e^{2}}{8m^{2}} \left(\left[(B_{x} + iB_{y})v + B_{z}u \right]^{2} + \left[(B_{x} - iB_{y})u - B_{z}v \right]^{2} \right) \Biggr\}$$

$$(2.2.8)$$

 $(\mathbf{B} = \mathbf{B}(\mathbf{r}, t)).$

Taking into account paths $Q(\tau)$ ($Q(0) = Q_0$, Q(t) = Q, t > 0) from our fivedimensional space S_5 , we may use formula (1.1.5) to obtain the function $G(Q, Q_0, t)$ or, provided that A, B, φ do not depend explicitly on time, the formula

$$C(Q, Q_0, \beta) = \mathcal{N}(\beta) \int_{Q_0, 0}^{Q, \beta} \mathscr{D}Q(\tau) \exp\{\int_0^\beta d\tau L(Q(\tau), iQ(\tau))\},$$
$$Q(0) = Q_0, \qquad Q(\beta) = Q, \qquad \beta > 0 \qquad (2.2.9)$$

Let us assume that $\tau = t/N > 0$ is an infinitesimal quantity and Q_j , Q_{j+1} are two points from S_5 ; j = 0, 1, ..., N-1. Then, for any time interval $(j\tau, (j+1)\tau)$, we define the following approximate expression for the function $G(Q_{j+1}, Q_j, \tau)$:

$$G(Q_{j+1}, Q_j, \tau) = \frac{m^{3/2}m^0}{(2\pi\tau i)^{5/2}}$$

$$\exp\left[i \cdot \left(\frac{1}{2}m \frac{(\mathbf{r}_{j+1} - \mathbf{r}_j)^2}{\tau} + e\mathbf{A}(\frac{1}{2}(\mathbf{r}_{j+1} + \mathbf{r}_j)) \cdot (\mathbf{r}_{j+1} - \mathbf{r}_j)\right) - e \cdot \varphi(\mathbf{r}_j)\tau\right)\right] \exp\left[im^0 \left(\frac{1}{2} \frac{(u_{j+1} - u_j)^2}{\tau} + \frac{1}{2} \frac{(v_{j+1} - v_j)^2}{\tau} + \frac{ie}{2m} \left(\left[(B_x(\mathbf{r}_j) + iB_y(\mathbf{r}_j))v_j + B_z(\mathbf{r}_j)u_j\right](u_{j+1} - u_j)\right) + \left[(B_x(\mathbf{r}_j) - iB_y(\mathbf{r}_j))u_j - B_z(\mathbf{r}_j)v_j\right](v_{j+1} - v_j)\right) - \frac{e^2}{8m^2} \left(\left[(B_x(\mathbf{r}_j) + iB_y(\mathbf{r}_j))v_j + B_z(\mathbf{r}_j)u_j\right]^2 + \left[(B_x(\mathbf{r}_j) - iB_y(\mathbf{r}_j))u_j - B_z(\mathbf{r}_j)v_j\right]^2\right) \right] - \frac{m^{3/2}m^0}{(2\pi\tau i)^{5/2}} \exp(iS_{j,j+1})$$
(2.2.10)

(cf. formulae (1.1.2) and (1.1.4). In writing the action $S_{j,j+1}$ in formula (2.2.10), we have not strictly adhered to the interpolation scheme (1.1.4) (although we might use it!) and have replaced $\frac{1}{2}(q_{j+1} + q_j)$ by q_j where possible; only the replacement of $\mathbf{A}(\frac{1}{2}(\mathbf{r}_{j+1} + \mathbf{r}_j))$ by $\mathbf{A}(\mathbf{r}_j)$ would be erroneous, as was shown by Feynman (1948). For brevity, we have not written explicitly the time argument (which may be taken as $j\tau$) in the quantities $\mathbf{A}, \mathbf{B}, \varphi$ occurring in formula (2.2.10). (Moreover, to write $j\tau$ in $\mathbf{A}, \mathbf{B}, \varphi$ might be somewhat confusing since $j\tau$ is not an infinitesimal quantity for most values of j(0 < j < N)despite that τ is!)

As is seen from expression (2.2.10), the integrals (2.1.27) (where we take $u_j, v_j \rightarrow u_0, v_0, u_{j+1}, v_{j+1} \rightarrow u, v$) are not dependent on m^0 . Neither will the infinitely multiple integral

$$G(Q, Q_0, t) = \lim_{N \to \infty} \int_{-\infty}^{\infty} \dots \int d^5 Q_1 \dots d^5 Q_{N-1}$$

$$G(Q, Q_{N-1}, t/N) \dots G(Q_1, Q_0, t/N)$$
(2.2.11)

inserted in formulae (2.1.27) give a dependence on m^0 . Expression (2.2.11) is representing the desired path integral (1.1.5) with paths $Q(\tau) = (\mathbf{r}(\tau), u(\tau), v(\tau))$ starting from $Q_0 = (\mathbf{r}_0, u_0, v_0)$ at $\tau = 0$ and ending in $Q = (\mathbf{r}, u, v)$ at $\tau = t$. The integration with respect to the spatial and spin coordinates on the righthand side of formula (2.2.11) may be performed in arbitrary order. The fulfilment of the initial condition (2.1.24) has been guaranteed by the choice of the factor in front of the exponential in expression (2.2.10).

The proof that formulae (2.2.10) and (2.2.11) give the correct function

 $G(Q, Q_0, t)$ which, when inserted into the integral equation (2.1.23), must give the Pauli equation, is straightforward and repeats Feynman's proof for his spinless Green function (i.e. propagator, Feynman, 1948).

Let us write equation (2.1.23) for an infinitesimal time τ as follows.

$$\Psi(Q, t+\tau) = \int d^5 \delta Q G(Q, Q-\delta Q, \tau) \cdot \Psi(Q-\delta Q, t) \qquad (2.2.12)$$

where $\Psi \in L_2$ (cf. (2.1.18)) and G is taken in the form (2.2.10) with $Q_i \rightarrow Q$ – $\delta Q, Q_{i+1} \rightarrow Q$. As is seen from expression (2.2.10), only those points $\dot{Q}_0 =$ $Q - \delta Q$ give a substantial contribution to the value of the integral on the righthand side of equation (2.2.12) while lie at an infinitesimally small distance from the point Q, i.e. $||Q - Q_0|| = ||\delta Q|| \to 0$ if $\tau \to 0$. In the kernel $G(Q, Q - Q_0)$ $\delta Q, \tau$) of equation (2.2.12), therefore, it is sufficient to leave over the terms $|\delta q_i|^2/\tau$ in the exponent and carry out the MacLaurin development of the remaining exponential with respect to $|\delta q_i|$ and τ . Similarly, we may also develop the function $\Psi(Q, Q - \delta Q, t)$ with respect to δQ . As follows from definition (2.1.18), the development of the function $\Psi(Q, Q - \delta Q, t)$ will not yield operators $\partial^2/\partial u^2$, $\partial^2/\partial v^2$, etc. (a result which is only a confirmation of the fact that the operator T_{nil} added deliberately to the Hamiltonian (2.1.22) has indeed been nilpotent). The left-hand side of equation (2.2.12) gives a development $\Psi(Q, t) + \partial \Psi(Q, t)/\partial t \cdot \tau + \dots$ and on the right-hand side there are Gaussian integrals which are easy to calculate. After comparing the proportionality coefficients at τ obtained in this way on both the sides of equation (2.2.12), one can directly persuade oneself that equation (2.2.12)has given the differential equation (2.1.21) with the purely differential Hamiltonian (2.1.22) and without any nilpotent operator. (Of course, we may add a nilpotent operator to H if we wish to and such a formal addition has actually made our path-integral formulation possible.)

Thus, we have proven that if the initial function $\Psi(Q, 0)$ is of the form $\psi_1(\mathbf{r}, 0)u + \psi_2(\mathbf{r}, 0)v$, then the function $\Psi(Q, t)$ given by the transformation (2.1.23) with the function $G(Q, Q_0, t)$ calculated as the path integral (2.2.11) is also of the form $\psi_1(\mathbf{r}, t)u + \psi_2(\mathbf{r}, t)v$ (i.e. $\Psi(Q, t) \in L_2$) for all the time instants t > 0.

The spin-dependent portion of the action $S_{j, j+1}$, i.e. the expression $\{ \}$ in formula (2.2.10), is dependent quadratically on the variables u, v. If the action is quadratic, then, as is well-known (Feynman & Hibbs, 1965), it is possible to transform the path integral into a product of factors which can be evaluated separately. Occasionally, as in the case of the harmonic oscillator, one may even succeed in finding a suitable replacement of the product by a simple function. Therefore, for a given magnetic field $\mathbf{B}(\mathbf{r}, t)$ and a given spatial path $\mathbf{r}(\tau)$ ($\mathbf{r}(0) = \mathbf{r}_0, \mathbf{r}(t) = \mathbf{r}$), one may expect the solvability of the condition spindependent path integral

$$G_{\sigma} \{ \mathbf{B}(\mathbf{r}(\tau), \tau), Q, Q_{0}, t \} = \mathcal{N}_{\sigma} \{ \mathbf{B}(\mathbf{r}(\tau), \tau), \mathbf{r}, \mathbf{r}_{0}, t \}$$
$$\int_{u_{0}}^{u} \int_{v_{0}, 0}^{v, t} \mathscr{D}u(\tau) \mathscr{D}v(\tau) \exp[i \int_{0}^{t} d\tau L_{\sigma}(Q(\tau), \dot{Q}(\tau), \tau)]$$
(2.2.13)

subjected to the condition

$$G_{\sigma}\{\mathbf{B}(\mathbf{r}(\tau),\tau), Q, Q_0, +0\} = \delta(u - u_0)\delta(v - v_0)$$
(2.2.14)

Unfortunately, the path integral (2.2.13) in general, surely cannot be transformed into a simple function since, for a general field $\mathbf{B}(\mathbf{r}, t) \neq \text{const.}$, the standard method of calculating path integrals with quadratic actions, when used for the path integral (2.2.13), leads to a linear second-order differential equation with non-constant coefficients and, as is well known, solutions of such equations cannot always be written down in an analytical form. Moreover, one must be very careful with the standard method since it leads to 'classical paths' $(u_c(\tau), v_c(\tau))$ which do not lie in the space S_5 , as the intermediate values of the variables $u_c(\tau), v_c(\tau)$ are, in general, complex although the terminal values u_0, v_0, u, v , according to our definition, are real.

Therefore, within the framework of the present formulation, we must be content with the final result in the form

3. Concluding Remarks

In principle, there are no obstacles to generalise our path-integral formulation to a more complicated case of n particles with spin. We may define a space $L_2 \times \ldots \times L_2$ (an *n*-fold direct product of L_2) spanned by the functions

$$(\psi_1^{(1)}u_1 + \psi_2^{(1)}v_1)(\psi_1^{(2)}u_2 + \psi_2^{(2)}v_2)\dots(\psi_1^{(n)}u_n + \psi_2^{(n)}v_n)$$

and use a nilpotent operator as a sum of operators (2.2.1), etc.

As was mentioned in the Introduction, it is also possible to do a minor complication of our formulation consisting of using complex-valued variables $u = u_1 + iu_2$, $v = v_1 + iv_2$ instead of the real ones. Then we may assume that if rotations are applied, then the variables u, v are subject to transformations like components of a spinor. (Of course, we must not require the fulfilment of the normalisation condition $|u^2| + |v^2| = 1$ since u_1, u_2, v_1, v_2 must be allowed to

represent arbitrary real numbers.) Such a formulation (whose description in more detail is intended to be presented in a further paper) has the advantage that the positively defined nilpotent operator

$$T_{\text{nil}}^{c} = -\frac{1}{2m^{0}} \left(\frac{\partial^{2}}{\partial u_{1}^{2}} + \frac{\partial^{2}}{\partial u_{2}^{2}} + \frac{\partial^{2}}{\partial v_{1}^{2}} + \frac{\partial^{2}}{\partial v_{2}^{2}} \right)$$
(3.1)

 $(m^0 > 0)$ is invariant with respect to the group of rotations.

Furthermore, the idea of using a second-order positively-defined nilpotent operator (say, of the type of the Laplace operator) can be applied even to other equations which need not be related just to spin. In this manner, for instance, first-order equations can be completed by such an operator (after defining a space L_2 , with respect to which this operator must be nilpotent) and thus even solutions of first-order equations (or of their systems) can be represented by path integrals. (The relativistic quantum-mechanical Dirac equation seems to be the most honorific case in this regard.) Therefore, the idea of nilpotent operators, as the author believes, can invoke the spirit of stochastic theory in a novel manner in a new class of problem besides the hitherto developed stochastic theories of the Brownian motion or potential.

Much is dependent on improving the numerical methods (of a Monte-Carlo type, say) for calculating path integrals like our integral (2.2.15). In the Appendix we present an analytical solution of this integral but in such a case when only the magnetic field **B** is both uniform in space and constant in time. Such a calculation serves, of course, merely as a verification of our general path-integral formulation. Otherwise, for a constant uniform magnetic field, one could use a much simpler path integral than ours. Namely, one could orientate the z-axis, as usual, into the direction of the magnetic field **B** and use the two-component Lagrangian

$$L(\mathbf{r}(\tau), \dot{\mathbf{r}}(\tau)) = \left[\frac{1}{2}m\dot{\mathbf{r}}^2(\tau) + e\mathbf{A}(\mathbf{r}(\tau)) \cdot \dot{\mathbf{r}}(\tau)\right]\mathbf{I} - \frac{e|\mathbf{B}|}{2m}\sigma_z \qquad (3.2)$$

in the Feynman path integral (1.1.5). No problems would arise in this case due to the presence of spin since the unit matrix I and the Pauli matrix σ_z are commuting. The matrix Green function would simply be separated into two independent scalar Green functions.

Therefore, one might raise an objection whether it is at all useful to calculate the normal Zeeman effect in such a way, as is shown in the Appendix. The author hopes that it is, since the experience gained from such a path-integral calculation gives a springboard for a more ambitious task which might be difficult to solve within the framework of the traditional operator formulation of quantum mechanics. The author has in mind one particular kind of task which may occur, say, in the theory of magnetically disordered semiconductors: where electrons move in a randomly distributed magnetic field, i.e. in a random vector potential. For this case, the very non-operator nature of the path integral (2.2.15) is a substantial advantage which, as in the case of a scalar random potential (cf. e.g. Bezák, 1970, 1971; Papadopoulos, 1974), might eventually allow us to derive new results.

Appendix

Our aim is to present a path-integral calculation of the spin-dependent part

$$Z_{\sigma}(\beta) = \int_{-\infty}^{\infty} du_0 \, dv_0 \left(u_0 \, \frac{\partial}{\partial u} + v_0 \, \frac{\partial}{\partial v} \right) C_{\sigma}(u, \, v, \, u_0, \, v_0, \, \beta) \tag{A.1}$$

(cf. (2.1.29)) of the partition sum (2.1.17) ($\beta = 1/k_BT > 0$) provided that the magnetic field **B** is uniform in space and constant in time. The basic problem is to calculate the path integral

$$C_{\sigma}(u, v, u_{0}, v_{0}, \beta) = \mathcal{N}_{\sigma}(\beta) \int_{u_{0}v_{0}, 0}^{u, v, \beta} \mathcal{D}u(\tau) \mathcal{D}v(\tau) \exp\left[\int_{0}^{\beta} d\tau \mathcal{L}_{\sigma}\right] \quad (A.2)$$

where the function \mathscr{L}_{σ} is defined (cf. (2.2.9) and (2.2.13)) by the expression

$$\begin{aligned} \mathscr{L}_{\sigma} &= L_{\sigma}(u(\tau), v(\tau), i\dot{u}(\tau), i\dot{v}(\tau)) \\ &= -\frac{1}{2} \{ \dot{u}^{2}(\tau) + \dot{v}^{2}(\tau) + 2\omega([(b_{x} + ib_{y})v(\tau) + b_{z}u(\tau)]\dot{u}(\tau) \\ &+ [(b_{x} - ib_{y})u(\tau) - b_{z}v(\tau)]\dot{v}(\tau)) \\ &+ \omega^{2}([(b_{x} + ib_{y})v(\tau) + b_{z}u(\tau)]^{2} + [(b_{x} - ib_{y})u(\tau) - b_{z}v(\tau)]^{2}) \} \end{aligned}$$
(A.3)

For elegance, we have introduced the quantity $\omega = eB/2m$ (sign $\omega = \text{sign } e$, $|\omega_i|$ being the Larmor frequency in units when $\hbar = c = 1$) and the directional cosines b_x , b_y , b_z of the vector **B** ($|\mathbf{b}| = 1$, **B** = B**b**). Obviously, the spindependent part of the function $G(Q, Q_0, t)$, i.e. function (2.2.13), is related to (A.2), $G_{\sigma}(u, v, u_0, v_0, t) = C_{\sigma}(u, v, u_0, v_0, it)$, t > 0 (cf. (2.1.25)). The paths $u(\tau), v(\tau)$ are continuous and $u(0) = u_0, v(0) = v_0, u(\beta) = u, v(\beta) = v$. In agreement with condition (2.1.26), we must required the fulfilment of the condition

$$C_{\sigma}(u, v, u_0, v_0, +0) = \delta(u - u_0)\delta(v - v_0)$$
 (A.4)

Then the function (A.2) is the finite solution of the equation

$$\frac{\partial C_{\sigma}(u, v, u_{0}, v_{0}, \beta)}{\partial \beta} = \frac{1}{2} \left(\frac{\partial^{2}}{\partial u^{2}} + \frac{\partial^{2}}{\partial v^{2}} \right) C_{\sigma}(u, v, u_{0}, v_{0}, \beta)$$
$$+ \omega \left\{ \left[(b_{x} + ib_{y})v + b_{z}u \right] \frac{\partial}{\partial u} + \left[(b_{x} - ib_{y})u - b_{z}v \right] \frac{\partial}{\partial v} \right\}$$
(A.5)

 $\times C_{\sigma}(u, v, u_0, v_0, \beta)$

for $\beta > 0$ (cf. (2.1.22), (2.2.1) and (2.2.3); we have used $m^0 = 1$ here).

The partition sum $Z_{\sigma}(\beta)$ must not depend on the orientation of the magnetic field **B**. Therefore, we may choose an orientation of **B** for which the path-integration of C_{σ} is simple. If we choose $|b_z| = 1$ (i.e. $b_x = b_y = 0$), then the integrations with respect to $u(\tau)$ and $v(\tau)$ are independent; such a case, however, is not so interesting to the verification of our path-integral formulation. A more elegant path integration concerns the choice $b_y = 1$ ($b_x = b_z = 0$), we will only confine ourselves to this case. The Lagrangian \mathscr{L}_{σ} is reduced to the form

$$\mathcal{L}_{\sigma} = -\frac{1}{2} [\dot{u}^{2}(\tau) + \dot{v}^{2}(\tau)] + i\omega [u(\tau)\dot{v}(\tau) - v(\tau)\dot{u}(\tau)] + \frac{1}{2} \omega^{2} [u^{2}(\tau) + v^{2}(\tau)]$$
(A.6)

and the function C_{σ} satisfies the equation

$$\frac{\partial C_{\sigma}(u, v, u_{0}, v_{0}, \beta)}{\partial \beta} = \frac{1}{2} \left(\frac{\partial^{2}}{\partial u^{2}} + \frac{\partial^{2}}{\partial v^{2}} \right) C_{\sigma}(u, v, u_{0}, v_{0}, \beta)$$
$$+ i\omega \left(v \frac{\partial}{\partial u} - u \frac{\partial}{\partial v} \right) C_{\sigma}(u, v, u_{0}, v_{0}, \beta)$$
(A.7)

As will be seen, it is advantageous to introduce the complex-valued paths

$$\chi(\tau) = u(\tau) + iv(\tau) \tag{A.8}$$

 $\chi_0 = u_0 + iv_0, \chi = u + iv$. In accordance with the general scheme of calculating path integrals with quadratic Lagrangians (Feynman & Hibbs, 1965), we define the 'classical path' $\chi_c(\tau)$ by the condition that the contribution in the action $\int_0^\beta d\tau \, \mathscr{L}_\sigma$ involving products $\chi_c^* \cdot \delta \chi_c \cdot \delta \chi_c^*$ has to vanish if one inserts

$$\chi(\tau) = \chi_c(\tau) + \delta\chi(\tau) \tag{A.9}$$

into \mathscr{L}_{σ} . Such a condition implies the equation

$$\ddot{\chi}_c(\tau) + 2\omega\dot{\chi}_c(\tau) + \omega^2\chi_c(\tau) = 0$$
(A.10)

$$\chi_c(0) = u_0 + iv_0, \qquad \chi_c(\beta) = u + iv$$
 (A.11)

and the 'classical action' is then

$$S_{\sigma,c} = \int_{0}^{\beta} d\tau \,\mathscr{L}_{\sigma,c} = -\frac{1}{2} \chi_{c}^{*}(\tau) \chi_{c}^{'}(\tau) |_{0}^{\beta} - \frac{\omega}{2} |\chi_{c}(\tau)|^{2} |_{0}^{\beta} \qquad (A.12)$$

which gives the (u, v)-dependence of the function $C_{\sigma}(u, v, u_0, v_0, \beta)$. To calculate the full β -dependence of $C_{\sigma}(u, v, u_0, v_0, \beta)$, we must still perform the path integration with respect to the closed paths $\delta\chi(\tau)$,

$$\delta\chi(0) = \delta\chi(\beta) = 0 \tag{A.13}$$

In this case, we can write the 'action', after integrating its 'kinetic-energy' term by parts, in the form

$$\delta S_{\sigma} = \int_{0}^{\beta} d\tau \delta \chi^{*}(\tau) \left[\frac{1}{2} \frac{d^{2}}{d\tau^{2}} + \omega \frac{d}{d\tau} + \frac{1}{2} \omega^{2} \right] \delta \chi(\tau)$$

which suggests that it is natural to use the eigenfunctions $\chi_n(\tau)$ of the equation

$$\ddot{\chi}_n(\tau) + 2\omega\dot{\chi}_n(\tau) + \omega^2\chi_n(\tau) = -\lambda_n^2\chi_n(\tau)$$
(A.14)

defined with respect to the conditions $\chi_n(0) = \chi_n(\beta) = 0$, and develop the closed paths $\delta\chi(\tau)$ in the series

$$\delta\chi(\tau) = \sum_{n} a_n \chi(\tau) \tag{A.15}$$

It is nice to state here that the eigenvalues $-\lambda_n^2$ of equation (A.14) are independent of ω ,

$$\lambda_n = \pi n / \beta \tag{A.16}$$

Therefore, we must obtain the same value of $C_{\sigma}(0, 0, 0, 0, \beta)$ as in the case when the magnetic field is absent, i.e.

$$C_{\sigma}(0, 0, 0, 0, \beta) = (2\pi\beta)^{-1}$$

Thus, after inserting the solution

$$\chi_{c}(\tau) = (u_{0} + iv_{0})(1 - \tau/\beta) \exp(-\omega\tau) + (u + iv)(\tau/\beta) \exp[\omega(\beta - \tau)]$$
(A.17)

of equation (A.10) into the action (A.12), we are obtaining the final result

$$C_{\sigma}(u, v, u_{0}, v_{0}, \beta) = (2\pi\beta)^{-1} \exp \left[S_{\sigma,c}(u, v, u_{0}, v_{0}, \beta)\right]$$

= $(2\pi\beta)^{-1} \exp \left\{-(1/2\beta)\left[(u_{0} - u \cosh \omega\beta - iv \sinh \omega\beta)^{2}\right] + (v_{0} - v \cosh \omega\beta + iu \sinh \omega\beta)^{2}\right] \right\}$
= $(2\pi\beta)^{-1} \exp \left\{-(1/2\beta)\left[(u - u_{0} \cosh \omega\beta + iv_{0} \sinh \omega\beta)^{2}\right] + (v - v_{0} \cosh \omega\beta - iv_{0} \sinh \omega\beta)^{2}\right] \right\}$ (A.18)

which is the correct solution of equation (A.7) satisfying condition (A.4).

The direct substitution of this function into formula (A.1) gives the result

$$Z_{\sigma}(\beta) = 2 \cosh \omega\beta = \exp(\omega\beta) + \exp(-\omega\beta) \qquad (A.19)$$

which means nothing but the partition sum over the two energies $E_1 = |\omega| = |e|B/2m$, $E_2 = -|\omega| = -|e|B/2m$ representing the normal Zeeman splitting in the magnetic field **B** provided that no spin-orbital interaction is present. In conclusion, it should be stressed that our Lagrangian has not been due to

PATH-INTEGRAL FORMULATION OF THE PAULI EQUATION 339

something spinning classically (like a top). On the contrary we have accepted the validity of the Pauli equation at the very outset and have only elaborated a new path-integral grammary for it.

Acknowledgement

The author would like to express his gratitude to M. Petráš of the Comenius University, Bratislava, for critical comments.

References

Bezák, V. (1970). Proceedings of the Royal Society, A, 315, 339.

- Bezák, V. (1971). Journal of Physics, A, 4, 324.
- Brinkman, H. C. (1956). Applications of Spinor Invariants in Atomic Physics. Amsterdam. Russian translation, Moscow 1959.

Feynman, R. P. (1948). Review of Modern Physics, 20, 367.

Feynman, R. P. and Hibbs, A. R. (1965). Quantum Mechanics and Path Integrals. New York.

Garczynski, W. (1973). Bulletin de l'Académie polonaise des sciences. Série des sciences mathematiques, astronomiques et physiques, 21, 359.

Hamilton, J. F. and Shulman, L. S. (1971). Journal of Mathematical Physics, 12, 160.

Klauder, J. R. (1960). Annals of Physics, 11, 123.

Papadopoulos, G. J. (1974). Journal of Physics, A: Mathematical, Nuclear, General, 7, 183.

de la Peña-Auerbach, L. (1971). Journal of Mathematical Physics, 12, 453.

Shulman, L. S. (1968). Physical Review, 176, 1558.

Valiev, K. A. and Ivanov, E. M. (1973). Uspekhi Fizicheskikh Nauk, 109, 31.