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1991 Europhys. Lett. 14 95

(http://iopscience.iop.org/0295-5075/14/2/001)

EUROPHYSICS LETTERS 15 January 1991

Europhys. Lett., 14 (2), pp. 95-100 (1991)

Imaginary-Time Path Integral for a Relativistic Spin-(1/2) Particle in a Magnetic Field.

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(received 24 July 1990; accepted in final form 5 November 1990)

PACS. 03.65 – Quantum theory; quantum mechanics.
PACS. 11.10Q – Relativistic wave equations.
PACS. 02.50 – Probability theory, stochastic processes, and statistics.

Abstract. – We construct a Feynman-Kac-Itô formula for positive-energy spin-(1/2) relativistic particles in a purely magnetic external field. We also introduce a new class of quantum Hamiltonians, the «relativistic Pauli operators», along with a path integral representation of their semi-groups. These Hamiltonians differ from the relativistic Schrödinger operators of Carmona, Masters and Simon only when a magnetic field is present.

In this paper we construct a Feynman-Kac-Itô (FKI) type formula for relativistic spin-(1/2) particles in an external magnetic field. Our approach is based upon three facts.

The first one is a generalized Foldy-Wouthuysen (FW) transformation [1] for Dirac Hamiltonians with a purely magnetic external field. The positive part of the transformed Hamiltonian has the form $\sqrt{m^2c^4\boldsymbol{I} + c^2(\boldsymbol{\sigma}\cdot(-i\hbar\nabla - e\boldsymbol{a}))^2}$.

The second fact is the existence of a probabilistic technique which allows us to construct the semi-group $t \mapsto \exp[-(t/\hbar)H]$ of the operator $H = \sqrt{m^2c^4 + 2mc^2\Gamma} - mc^2$ from the semi-group of the operator Γ. Such a procedure extends an old method of Lévy for building up the d-dimensional Cauchy process (with generator $-\sqrt{-\Delta}$) from a $(d+1)$-dimensional Brownian motion [2]. It was first considered by Bakry [3], who generalized the classical Poisson integral [4] which provides harmonic functions in the upper $(d+1)$-dimensional half-space with given boundary values in $\boldsymbol{R}^d$. Carmona, Masters and Simon recognized the usefulness of Bakry's work in their investigations on the asymptotic behaviour of the eigenfunctions of relativistic Schrödinger operators $H = \sqrt{m^2c^4 - c^2\hbar^2\Delta} + V$ via path integral techniques [5, 6]. Two of us, unaware of these papers, rediscovered [7] this same idea in a framework of relativistic stochastic mechanics (which endows it with some physical interpretation) and exploited it by giving a FKI formula for relativistic spinless charged particles in an external magnetic field [8].

The third fact is the existence, for Pauli Hamiltonians, of FKI-type formulae [9, 10] which can be turned, by the method to which we just alluded, into relativistic ones.

The Dirac Hamiltonian, with a purely magnetic external field $\boldsymbol{B} = \text{rot}\boldsymbol{A} = c\,\text{rot}\,\boldsymbol{a}$, is

$$H_D^0(\boldsymbol{a}) = c\rho_1 \otimes (\boldsymbol{\sigma}\cdot(-i\hbar\nabla - e\boldsymbol{a})) + \rho_3 \otimes \boldsymbol{I}mc^2, \tag{1}$$

where the ρ's and σ's are ordinary Pauli matrices acting on different indices of Dirac spinors, namely the σ's matrices act on the «Pauli» (spin) index, while the matrices ρ's act on the «Dirac» index. After the generalized FW transformation of ref. [1], the Dirac Hamiltonian becomes the nonlocal operator (which appears misprinted in the original article):

$$H_D'^0(\boldsymbol{a}) = \rho_3 \otimes \sqrt{m^2c^4\boldsymbol{I} + c^2(\boldsymbol{\sigma}\cdot(-i\hbar\nabla - e\boldsymbol{a}))^2} = \rho_3 \otimes H_{FW}^0(\boldsymbol{a}) + \rho_3 \otimes \boldsymbol{I}mc^2, \tag{2}$$

where $H_{FW}^0(\boldsymbol{a})$, acting on two-component «Pauli» spinors, is given by

$$H_{FW}^0(\boldsymbol{a}) = \sqrt{m^2c^4\boldsymbol{I} + c^2(\boldsymbol{\sigma}\cdot(-i\hbar\nabla - e\boldsymbol{a}))^2} - mc^2\boldsymbol{I}. \tag{3}$$

The semi-group $t \mapsto \exp[-(t/\hbar)H_D^0(\boldsymbol{a})]$ has very bad properties, since the full Dirac Hamiltonian is not bounded from below. The important point to be noticed is that the physical electron is described precisely by the FW Hamiltonian $H_{FW}^0(\boldsymbol{a})$ and not by $H_D^0(\boldsymbol{a})$, as negative-energy states are related to the states of the positron in a standard manner (by the way, the Hamiltonian of the physical positron is $H_{FW}^0(-\boldsymbol{a})$, not $-(H_{FW}^0(\boldsymbol{a}) + mc^2\boldsymbol{I})$). Therefore our task is to give a path integral representation of the semi-group $t \mapsto \exp[-(t/\hbar)H_{FW}^0(\boldsymbol{a})]$. Now we turn to the Pauli Hamiltonians, namely

$$H_P^0(\boldsymbol{a}) = (1/2m)(-i\hbar\nabla - e\boldsymbol{a})^2 - (e\hbar/2m)\,\boldsymbol{\sigma}\cdot\boldsymbol{b} = (1/2m)(\boldsymbol{\sigma}\cdot(-i\hbar\nabla - e\boldsymbol{a}))^2, \tag{4}$$

where $\boldsymbol{b} = \text{rot}\,\boldsymbol{a}$. The associated semi-group $t \mapsto \exp[-(t/\hbar)H_P^0(\boldsymbol{a})]$ admits a path integral representation which we introduce now in the form given in ref. [10]. Henceforth we shall consider the three parameters i) $\varepsilon = \hbar/m$ (which gives the scale of quantum fluctuations), ii) $\mu = e/m$ (the charge/mass ratio, related to the magnetic moment of the particle), iii) $\lambda = me^4/\hbar^3$ (with dimensions of an inverse time) and the following stochastic processes: $s \mapsto \boldsymbol{w}_s = (w_s^1, w_s^2, w_s^3)$, a three-dimensional Brownian motion starting of the origin at $\boldsymbol{R}^3$, with generator $1/2\Delta$, $s \mapsto \boldsymbol{B}_s^x = \boldsymbol{x} + \sqrt{\varepsilon}\,\boldsymbol{w}_s$, a related three-dimensional Brownian motion, starting at the point $\boldsymbol{x}$, with generator $\varepsilon/2\Delta$, $s \mapsto N_s$ an independent Poisson process with probability rate λ ($\boldsymbol{E}(\text{d}N_s) = \lambda\,\text{d}s$) and, finally, $s \mapsto S_s^\sigma = \sigma(-1)^{N_s}$, where $\sigma \in \boldsymbol{Z}_2 = \{-1, 1\}$.

Let us consider Pauli spinors as complex-valued functions of the space coordinates $\boldsymbol{x}$ and of a dichotomic variable $\sigma \in \boldsymbol{Z}_2$ (spin variable) then

$$\left(\exp\left[-\frac{t}{\hbar}H_P^0(\boldsymbol{a})\right]\psi\right)(\boldsymbol{x}, \sigma) = \boldsymbol{E}\left(\psi(\boldsymbol{B}_t^x, S_t^\sigma)\exp\left[-\frac{1}{\hbar}\{\mathscr{F}_e(t, \boldsymbol{a}, \boldsymbol{B}^x) + \mathscr{G}_\mu(t, \boldsymbol{b}, \boldsymbol{B}^x, S^\sigma)\}\right]\right), \tag{5}$$

where

$$\mathscr{F}_e(t, \boldsymbol{a}, \boldsymbol{B}^x) = ie\left(\sqrt{\varepsilon}\int_0^t \boldsymbol{a}(\boldsymbol{B}_s^x)\cdot\text{d}\boldsymbol{w}_s + (\varepsilon/2)\int_0^t (\text{div}\,\boldsymbol{a})(\boldsymbol{B}_s^x)\,\text{d}s\right) \tag{6}$$

and

$$\mathscr{G}_\mu(t, \boldsymbol{b}, \boldsymbol{B}^x, S^\sigma) =$$
$$= -m\varepsilon\int_{[0,t)} \log\left[\left(\frac{\mu}{2\lambda}\right)(b_1(\boldsymbol{B}_s^x) - iS_s^\sigma b_2(\boldsymbol{B}_s^x))\right]\text{d}N_s - m\mu(\varepsilon/2)\int_0^t b^3(\boldsymbol{B}_s^x)S_s^\sigma\,\text{d}s - mt\varepsilon\lambda. \tag{7}$$

We observe that (5) generalizes the ordinary FKI formula for Schrödinger particles in a magnetic field [11], namely

$$\left(\exp\left[-\frac{t}{\hbar}H_S^0(\boldsymbol{a})\right]\psi\right)(\boldsymbol{x})=\boldsymbol{E}\left(\psi(\boldsymbol{B}_t^x)\exp\left[-\frac{1}{\hbar}\mathscr{F}_e(t,\boldsymbol{a},\boldsymbol{B}^x)\right]\right), \tag{8}$$

where $H_S^0(\boldsymbol{a})=(1/2m)(-i\hbar\nabla-e\boldsymbol{a})^2$. The extra factor $\mathscr{G}_\mu(t,\boldsymbol{b},\boldsymbol{B}^x,S^\sigma)$ in (5) accounts for the coupling $-\mu\hbar/2\boldsymbol{\sigma}\cdot\boldsymbol{b}$ between the spin and the magnetic field $c\boldsymbol{b}$ in the Pauli Hamiltonian (see ref. [10] for more details, some inequalities and the connection with the different and less explicit approach by Gaveau and Vauthier [9]).

In order to obtain an analogous path integral representation for the relativistic semigroup $t\mapsto\exp[-(t/\hbar)H_{FW}^0(\boldsymbol{a})]$, we trivially observe that

$$H_{FW}^0(\boldsymbol{a})=\sqrt{m^2c^4+2mc^2H_P^0(\boldsymbol{a})}-mc^2. \tag{9}$$

Despite the troublesome square root in (9) there is a simple way of turning the nonrelativistic formula (5) into the relativistic one.

Let $s\mapsto w_s^0$ be an additional one-dimensional Brownian motion (starting at 0 and with unit diffusion coefficient) independent of the space process $s\mapsto\boldsymbol{B}_s^x$ and the Poisson process $s\mapsto N_s$ appearing in (5). For all $\alpha,\beta\geqslant 0$, let $\tau_{\alpha,\beta}$ be the smallest s such that $\beta s+w_s^0=\alpha$:

$$\tau_{\alpha,\beta}=\inf\{s\geqslant 0:\beta s+w_s^0=\alpha\}. \tag{10}$$

The random variable $\tau_{\alpha,\beta}$ is an optional time finite a.s. and it is easy to see that $\alpha\mapsto\tau_{\alpha,\beta}$ is a nondecreasing jump stochastic process with independent and stationary increments. The case without drift ($\beta=0$) is well known [11, 12]:

$$\boldsymbol{E}(\exp[-\gamma\tau_{\alpha,0}])=\exp[-\alpha\sqrt{2\gamma}] \tag{11}$$

for any $\gamma\geqslant 0$. It follows, by the spectral theorem, that for any nonnegative self-adjoint operator Γ, $\exp[-t\sqrt{2\Gamma}]=\boldsymbol{E}(\exp[-\tau_{t,0}\Gamma])$. In particular, if $\Gamma=-1/2\Delta$, $\exp[-t\sqrt{-\Delta}]=\boldsymbol{E}(\exp[\tau_{t,0}/2\Delta])$ a formula which is related to the construction of the d-dimensional Cauchy process $t\mapsto\xi_t$ as $\xi_t=\boldsymbol{w}_{\tau_{t,0}}$, where $s\mapsto\boldsymbol{w}_s$ is a d-dimensional Brownian motion independent of $s\mapsto w_s^0$. The Cauchy process is subordinated to the d-dimensional Brownian motion in the sense of Bochner [13].

Formula (11) admits a generalization. By the optional stopping theorem applied to the continuous exponential martingale $s\mapsto\exp[\theta w_s^0-s\theta^2/2]$ with $\theta>0$, one can check that (ref. [2], page 27, see also ref. [7] for a different demonstration):

$$\boldsymbol{E}(\exp[-\gamma\tau_{\alpha,\beta}])=\exp[-\alpha\{\sqrt{\beta^2+2\gamma}-\beta\}]. \tag{12}$$

It is expedient [7] to choose $\alpha=t\sqrt{mc^2/\hbar}$ and $\beta=\sqrt{mc^2/\hbar}$. Let $\tau_c(t)=\inf\{s\geqslant 0: cs+\sqrt{\varepsilon}w_s^0=ct\}$, then, from (12), we get

$$\boldsymbol{E}\left(\exp\left[-\frac{\gamma}{\hbar}\tau_c(t)\right]\right)=\exp\left[-\frac{t}{\hbar}\{\sqrt{m^2c^4+2mc^2\gamma}-mc^2\}\right] \tag{13}$$

for all $\gamma\geqslant 0$. Therefore, if Γ is any nonnegative self-adjoint operator,

$$\exp\left[-\frac{t}{\hbar}\{\sqrt{m^2c^4+2mc^2\Gamma}-mc^2\}\right]=\boldsymbol{E}\left(\exp\left[-\frac{\tau_c(t)}{\hbar}\Gamma\right]\right). \tag{14}$$

In other words the semi-group $t \mapsto \exp[-(t/\hbar)H]$ for $H = \sqrt{m^2c^4 + 2mc^2\Gamma} - mc^2$ can be constructed as the averaged semi-group of Γ after replacing [5, 8] the deterministic time t by the random one $\tau_c(t)$.

It may be interesting to observe that, when the speed of light c goes to the infinity, the random process $t \mapsto \tau_c(t)$ converges in probability to the deterministic time t uniformly on bounded intervals [7]. By this remark one can easily grasp the probabilistic mechanism behind the nonrelativistic limit for the semi-group $t \mapsto \exp[-(t/\hbar)H] = \boldsymbol{E}(\exp[-(\tau_c(t)/\hbar)\Gamma])$. Now, by choosing the operator Γ as the Pauli Hamiltonian $H_P^0(\boldsymbol{a})$ we obtain, from (5) and (14), our FKI formula

$$\left(\exp\left[-\frac{t}{\hbar}H_{\mathrm{FW}}^0(\boldsymbol{a})\right]\psi\right)(\boldsymbol{x},\sigma) =$$
$$= \boldsymbol{E}\left(\psi(\xi_t^x,\eta_t^\sigma)\exp\left[-\frac{1}{\hbar}\{\mathscr{F}_e(\tau_c(t),\boldsymbol{a},\boldsymbol{B}^x) + \mathscr{G}_\mu(\tau_c(t),\boldsymbol{b},\boldsymbol{B}^x,S^\sigma)\}\right]\right), \qquad (15)$$

where $\xi_t^x = \boldsymbol{B}_{\tau_c(t)}^x$ and $\eta_t^\sigma = S_{\tau_c(t)}^\sigma$. In this formula the expectation is taken with respect to the Poisson process $s \mapsto N_s$ and the four-dimensional Brownian motions $s \mapsto (w_s^0, \boldsymbol{w}_s)$. The stochastic process $t \mapsto \xi_t^x$ (the «relativistic space process») is a jump Markov process with independent and stationary increments already considered by Ichinose and Tamura [14] in their construction of a path integral for relativistic spinless particles in an electromagnetic field. We remark, however, that the starting Hamiltonian in ref. [14] is not gauge invariant up to a unitary transformation when a magnetic field is present (see also ref. [8]). The above-mentioned construction of the process $t \mapsto \xi_t^x$ lends itself to a physical interpretation in a frame of relativistic stochastic mechanics.

We claim that the random variable ξ_t^x describes the position in space, at the time t, of a free relativistic particle, with rest mass $m > 0$, which, at the time $t = 0$, has been created still (*i.e.* with the initial energy mc^2) at the point $\boldsymbol{x}$.

Classically, the worldline of such a motionless particle would be $x_s^0 = cs$, $\boldsymbol{x}_s = \boldsymbol{x}$ (where $s \geq 0$ is the proper time) but, owing to the quantum fluctuations, the actual worldline is the intricate space-time path $x_s^0 = cs + \sqrt{\varepsilon}\,w_s^0$, $\boldsymbol{x}_s = \boldsymbol{x} + \sqrt{\varepsilon}\,\boldsymbol{w}_s$ (see ref. [7]). The operational procedure for localizing the particle in space rests upon a vicious minefield in the space-time. At the time $t > 0$, synchronized timers trigger a space filling net of previously dormant booby traps. Each of them is engineered in order to annihilate incoming particles and, meanwhile, to record the annihilation. The position in space of the particle is precisely the «serial number» of the device which made the score. In this way, our quantum vagabond gets killed as soon as he hits the hypersurface $x^0 = ct$ and the resulting position is exactly ξ_t^x. Formula (15) gives a complete answer to the problem of finding a path integral representation of the semi-group $t \mapsto \exp[-(t/\hbar)H_{\mathrm{FW}}^0(\boldsymbol{a})]$ associate to the Dirac Hamiltonian (1) with a purely magnetic external field. We consider now the case in which also an electrostatic field $E = -e^{-1}\nabla V$ acts on our particle that carries an electric charge e. Generally speaking, due to the possibility of spontaneous pair creation in an external electric field, the Dirac equation is no longer a single-particle theory and must be treated as the equation for a quantized Fermi field. However, if the external electric field is sufficiently weak, a single-particle interpretation of the Dirac equation is still tenable [15, 16]. Indeed in such sufficiently weak external electric field, it is possible to separate, in a consistent way, «positive frequencies» from «negative frequencies» in the energy spectrum and to define, at least in some abstract sense, a FW transformation [16] which isolates the true single-particle Hamiltonian. This Hamiltonian $H_{\mathrm{FW}}(\boldsymbol{a}, V)$, which is not explicitly known, will be different from $H_{\mathrm{FW}}^0(\boldsymbol{a}) + V$. Nevertheless, to the first order of perturbation theory, if the electric field is not too inhomogeneous, the true Hamiltonian $H_{\mathrm{FW}}(\boldsymbol{a}, V)$ is approximated [17] by the operator

$$H_{\mathrm{RP}}(\boldsymbol{a}, V) = H^0_{\mathrm{FW}}(\boldsymbol{a}) + V, \tag{16}$$

which we propose to call a «relativistic Pauli operator». Without magnetic field these relativistic Pauli operators coincide with the extensively studied relativistic Schrödinger operators considered by Weder, Herbst, Lieb and Daubechies in their papers on the stability of relativistic matter (see for instance, ref. [18] and reference to be found therein) but, when a magnetic field is also present, the relativistic Pauli operator (16) will differ from $\sqrt{m^2c^4 + c^2(-i\hbar\nabla - e\boldsymbol{a})^2} - mc^2 + V$ which obeys diamagnetic inequalities [8].

We remark that in the nonrelativistic case the inclusion of the coupling between the spin and the magnetic field has important effects on the stability of matter and there are deep differences between Schrödinger particles and Pauli particles in a magnetic field [19], presumably the same differences will hold also in the relativistic context. A FKI formula for the relativistic Pauli operator (16) can be easily constructed. Indeed, by using the Trotter product formula, it follows from (15) that

$$\left(\exp\left[-\frac{t}{\hbar}H_{\mathrm{RP}}(\boldsymbol{a}, V)\right]\psi\right)(\boldsymbol{x}, \sigma) =$$
$$= \boldsymbol{E}\left(\psi(\xi^x_t, \eta^\sigma_t)\exp\left[-\frac{1}{\hbar}\left\{\mathcal{F}_e(\tau_c(t), \boldsymbol{a}, \boldsymbol{B}^x) + \mathcal{G}_\mu(\tau_c(t), \boldsymbol{b}, \boldsymbol{B}^x, S^\sigma) + \int_0^t V(\xi^x_s)\,\mathrm{d}s\right\}\right]\right), \tag{17}$$

which, when the magnetic field is absent, becomes

$$\left(\exp\left[-\frac{t}{\hbar}H_{\mathrm{RP}}(0, V)\right]\psi\right)(\boldsymbol{x}, \sigma) = \boldsymbol{E}\left(\psi(\xi^x_t, \sigma)\exp\left[-\frac{1}{\hbar}\int_0^t V(\xi^x_s)\,\mathrm{d}s\right]\right), \tag{18}$$

namely the relativistic Feynman-Kac formula considered in [5, 6] to which we refer for the description of a large class of acceptable potentials V.

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