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Probabilistic solution of Pauli type equations†

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Abstract. In this paper we extend the Feynman–Kac formula to the case of imaginary time Schrödinger equations (heat equations) for multicomponent wavefunctions. The approach covers in particular the usual Pauli equation for a spin-$\frac{1}{2}$ particle in an arbitrary magnetic field. Our formula contains, besides the expectation with respect to a Wiener process in ordinary space, an expectation with respect to a jump process over the discrete indices describing the internal degrees of freedom. To illustrate the method we evaluate the formula in some special cases and we derive also various inequalities. A detailed comparison is made with a recent work by Gaveau and Vauthier.

1. Motivations

In a previous paper (De Angelis and Jona-Lasinio 1982) we succeeded in giving a stochastic description of a spin-$\frac{1}{2}$ particle in a magnetic field, generalising to this case Nelson stochastic mechanics. This description involves, besides the usual diffusion processes, also generalised Poisson processes over a discrete state space connected with the possible values of a spin component of the particle.

This result naturallly raises the question of whether it is possible to give probabilistic expressions for the solutions of the Pauli equation in terms of appropriate averages over Wiener and Poisson processes. What we have in mind are extensions of the well known Feynman–Kac–Itô (Simon 1979) formula valid for spinless particles in a magnetic field.

In this paper we implement this program for a class of equations that we call 'Pauli type' which includes equations for particles of arbitrary spin or systems of many particles with a given spin.

The main feature of our way of representing solutions consists in treating both continuous variables, like space coordinates, and discrete indices associated with the components of the wavefunction on the same ground.

In other words the wavefunction is considered as a 'scalar' valued function of continuous and discrete variables. This has to be contrasted with the probabilistic representation of the Pauli wavefunctions obtained recently by Gaveau and Vauthier (1981) in terms of averages over the Wiener process alone. In their representation the spin part is not associated with a stochastic process and the solution is expressed in terms of an expectation which contains a matrix valued functional of the Wiener process.

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Of course our representation is not manifestly rotationally invariant as is the one by Gaveau and Vauthier, but it offers from the analytical point of view the greater advantage of working with purely numerical valued quantities. In conclusion we have a complete 'scalarisation' of the problem.

Our technique applies also in a local coordinate system, to heat equations on a space of forms (Malliavin 1978). These arise also in physics in the study of certain supersymmetric models (Witten 1982).

From the point of view of the probabilistic structure and, in particular, for what concerns the Poisson part, our representations are directly inspired by the analogue of Girsanov's formula obtained by Kabanov *et al* (1978) for the Radon–Nikodym derivative connecting two Poisson processes.

We now give an outline of the paper. In § 2 we provide a derivation of our basic formula in the simple case of the Pauli equation in a constant magnetic field. The formula is then extended to arbitrary magnetic field (equation (3.2)) in § 3 where a comparison with Gaveau and Vauthier is also given. In view of the central role of (3.2) an independent discussion is supplied in appendix 2.

Explicit evaluations in simple cases are discussed in § 4. In § 5 various inequalities are derived including one already obtained by Gaveau and Vauthier. In § 6 general Pauli type equations are introduced and the generalisation of our formula to this case is given. Appendix 1 discusses a representation of the solutions of an arbitrary linear ordinary differential equation in p-dimensional space in terms of jump processes over the indices identifying the components of the solutions in a given basis. This representation, which is used in the text to compare our formula with that of Gaveau and Vauthier, has in our opinion an independent interest.

2. The Pauli equation in homogeneous magnetic field

In order to illustrate the type of representations that one can expect for the solution of the Pauli equation, it is very instructive to start from the simple case of a homogeneous magnetic field. In this case spin and space coordinates separate and for the spin part of the wavefunction we obtain (for imaginary time) the equation

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\chi_t(\sigma) &= \tfrac{1}{2}(\boldsymbol{H}\cdot\boldsymbol{\sigma}\chi_t)(\sigma) \\ &= \tfrac{1}{2}H_z\sigma\chi_t(\sigma)+\tfrac{1}{2}(H_x-\mathrm{i}\sigma H_y)\chi_t(-\sigma)\end{aligned} \tag{2.1}$$

where $\sigma=\pm1$ and the usual representation of the Pauli matrices has been used.

As we have discussed in De Angelis and Jona-Lasinio (1982) this evolution equation becomes, via the canonical transformation $\chi\to\Omega^{-1}\chi=f$ where Ω is the ground state wavefunction, the Kolmogorov type equation (after subtracting the ground state energy)

$$\begin{aligned}\mathrm{d}f_t(\sigma)/\mathrm{d}t &= \tfrac{1}{2}(|H|-\sigma H_z)(f_t(-\sigma)-f_t(\sigma)) \\ &= p(\sigma)(f_t(-\sigma)-f_t(\sigma)).\end{aligned} \tag{2.2}$$

It is easily seen that the solution of (2.2) is given by

$$f_t(\sigma)=\mathbb{E}_\sigma[f_0(\sigma(t))] \tag{2.3}$$

where $\sigma(t)$ is the jump process on $\{-1, 1\}$ satisfying the initial condition $\sigma(0)=\sigma$, whose transition probability per unit time is $p(\sigma)$; f_0 is the initial condition. It is now convenient to express $\sigma(t)$ in terms of an auxiliary point process $\bar{N}_t$ which counts the jumps of $\sigma(t)$; clearly $\sigma(t)=\sigma(-1)^{\bar{N}_t}$ with $\bar{N}_0=0$.

The process $\bar{N}_t$ is not pure Poisson because the transition probability per unit time depends on the parity of $\bar{N}$. The next step consists then in expressing $\bar{N}_t$ in terms of a pure Poisson process N_t of unit parameter i.e. $E(\mathrm{d}N_t)=\mathrm{d}t$. By using the expression for the Radon–Nikodym derivative of $\bar{N}_t$ with respect to N_t as given in Kabanov *et al* (1978), we obtain the following formula for the solution of (2.3):

$$f_t(\sigma)=\mathbb{E}\left[f_0(\sigma(-)^{N_t})\exp\left(\int_0^t \ln\{p(\sigma(-)^{N_\tau})\}\,\mathrm{d}N_\tau+\int_0^t \{1-p(\sigma(-)^{N_\tau})\}\,\mathrm{d}\tau\right)\right] \tag{2.4}$$

where the stochastic integral $\int \mathrm{d}N_t$ with respect to the Poisson process is simply the Stieltjes integral over each trajectory. Performing now, in the backward direction, the canonical transformation, we obtain the solution of (2.1) which can be written as

$$\chi_t(\sigma)=\mathrm{e}^t\mathbb{E}\left[\chi_0(\sigma(-)^{N_t})\exp\left(\int_0^t \ln\{\tfrac{1}{2}[H_x-\mathrm{i}\sigma(-)^{N_\tau}H_y]\}\,\mathrm{d}N_\tau+\int_0^t \tfrac{1}{2}H_z\sigma(-)^{N_\tau}\,\mathrm{d}\tau\right)\right]. \tag{2.5}$$

The structure of (2.5) is very similar to the structure of (2.4), and actually it could have been guessed by generalising formally the basic expression of the Radon–Nikodym derivative to 'complex Kolmogorov equations' like (2.1), i.e. to arbitrary linear systems of two differential equations with constant coefficients. The main point consists in interpreting the off-diagonal part of the coefficient matrix as 'complex' transition probabilities per unit time. The basic strategy of the next subsection will consist in combining, in an appropriate way, (2.5) with the usual Feynman–Kac–Itô formula in order to obtain the solution of the Pauli equation in the general case of an inhomogeneous magnetic field.

3. The Pauli equation in an inhomogeneous magnetic field

We want to solve the equation ($\hbar=m=c=1$)

$$\partial\psi_t/\partial t=-\tfrac{1}{2}(-\mathrm{i}\boldsymbol{\nabla}-\boldsymbol{A})^2\psi_t-V(\boldsymbol{x})\psi_t+\tfrac{1}{2}\boldsymbol{H}(\boldsymbol{x})\cdot\boldsymbol{\sigma}\psi_t. \tag{3.1}$$

We show that the initial value problem for (3.1) is solved by the following formula, if we choose the usual representation for the Pauli matrices:

$$\begin{aligned}\psi_t(\boldsymbol{x},\sigma)=\mathrm{e}^t\mathbb{E}\Big[\psi_0(\boldsymbol{W}_x(t),(-)^{N_t}\sigma)\exp\Big(&-\int_0^t V(\boldsymbol{W}_x(\tau))\,\mathrm{d}\tau-\mathrm{i}\int_0^t \boldsymbol{A}(\boldsymbol{W}_x(\tau))\cdot\mathrm{d}\boldsymbol{W}_x(\tau)\\ &+\int_0^t \tfrac{1}{2}H_z(\boldsymbol{W}_x(\tau))(-)^{N_\tau}\sigma\,\mathrm{d}\tau\\ &+\int_0^t \ln[\tfrac{1}{2}\{H_x(\boldsymbol{W}_x(\tau))-\mathrm{i}\sigma(-)^{N_\tau}H_y(\boldsymbol{W}_x(\tau))\}]\,\mathrm{d}N_\tau\Big)\Big]\end{aligned} \tag{3.2}$$

where $\boldsymbol{W}_x(t)$ is the Wiener process starting from $\boldsymbol{x}$ at $t=0$.

First of all we notice that (3.2) defines a semigroup, as can be verified using the Markov property of the processes involved and their translation invariance in time.

To check that (3.2) solves (3.1) it is then enough to calculate the derivative at $t=0$. For this we need the extension of Itô calculus to Poisson processes. This exists and the reader may consult Gihman and Skorohod (1972). From this we have (see for example equation (13), p 270 of Gihman and Skorohod (1972)):

$$
\begin{aligned}
\mathrm{d}[f(W,(-)^{N}\sigma)\mathrm{e}^{\xi}]
&= \mathrm{e}^{\xi}\,\mathrm{d}f + f\,\mathrm{d}(\mathrm{e}^{\xi}) + \mathrm{e}^{\xi}\boldsymbol{b}\cdot\nabla f\,\mathrm{d}t + \mathrm{e}^{\xi}(\partial_\sigma f)(\lambda-1)\,\mathrm{d}N \\
&= \mathrm{e}^{\xi}[\tfrac{1}{2}\Delta f\,\mathrm{d}t + \nabla f\cdot\mathrm{d}\boldsymbol{W} + (\partial_\sigma f)\,\mathrm{d}N] + f\,\mathrm{e}^{\xi}[\boldsymbol{b}\cdot\mathrm{d}\boldsymbol{W} \\
&\quad - V\,\mathrm{d}t + \tfrac{1}{2}H_z\sigma(-)^{N}\,\mathrm{d}t + (\lambda-1)\,\mathrm{d}N] + \mathrm{e}^{\xi}[\boldsymbol{b}\cdot\nabla f\,\mathrm{d}t + (\partial_\sigma f)(\lambda-1)\,\mathrm{d}N]
\end{aligned}
\tag{3.3}
$$

where in our case $\boldsymbol{b}=-\mathrm{i}\boldsymbol{A}$, $\lambda=\frac{1}{2}(H_x-\mathrm{i}\sigma(-)^{N_t}H_y)$, $(\partial_\sigma f)(\sigma)=f(-\sigma)-f(\sigma)$.

By taking the expectation at $t=0$ we verify that (3.1) is satisfied.

We now compare our solution with that of Gaveau and Vauthier (1981). It is not difficult to see that (3.2) can be rewritten, by changing the time variable $\tau\to t-\tau$ in the terms containing integrals with respect to the Poisson processes:

$$
\begin{aligned}
\psi_t(\boldsymbol{x},\sigma) = \mathrm{e}^{t}\mathbb{E}\Big[\psi_0(\boldsymbol{W}_x(t),\sigma(-)^{N_t})\exp\Big(&-\int_0^t V(\boldsymbol{W}_x(\tau))\,\mathrm{d}\tau - \mathrm{i}\int_0^t \boldsymbol{A}(\boldsymbol{W}_x(\tau))\cdot\mathrm{d}\boldsymbol{W}_\tau \\
&+\int_0^t \tfrac{1}{2}\sigma H_z(\boldsymbol{W}_x(t-\tau))(-)^{N_{t-\tau}}\,\mathrm{d}\tau \\
&+\int_0^t \ln[\![\tfrac{1}{2}\{H_z(\boldsymbol{W}_x(t-\tau))+\mathrm{i}\sigma(-)^{N_{t-\tau}}H_y(\boldsymbol{W}_x(t-\tau))\}]\!]\,\mathrm{d}N_\tau\Big)\Big].
\end{aligned}
\tag{3.4}
$$

It is important to remark that in the Poisson stochastic integral this change of time variable requires the substitution

$$(-)^{N_\tau}\to(-)^{N_t-N_\tau+1}$$

due to the circumstance that trajectories continuous on the left become continuous on the right.

Using now the results of appendix 1, we recognise that the matrix

$$
\begin{aligned}
N_{\sigma\sigma'} = \mathrm{e}^{t}\mathbb{E}\Big[\frac{1+\sigma\sigma'(-)^{N_t}}{2}\exp\Big(&\int_0^t \tfrac{1}{2}\sigma H_z(\boldsymbol{W}_x(t-\tau))(-)^{N_{t-\tau}}\,\mathrm{d}\tau \\
&+\int_0^t \ln[\![\tfrac{1}{2}\{H_x(\boldsymbol{W}_x(t-\tau))+\mathrm{i}\sigma(-)^{N_{t-\tau}}H_y(\boldsymbol{W}_x(t-\tau))\}]\!]\,\mathrm{d}N_\tau\Big)\Big]
\end{aligned}
\tag{3.5}
$$

for every trajectory of the Wiener process is precisely the matrix given by (9) of lemma 1 of Gaveau and Vauthier (1981).

In conclusion we refer the reader to appendix 2 for a formal derivation of (3.2).

4. Special cases

We now give an example in which the expression (3.2) can be simplified by performing explicitly at least part of Poisson stochastic integration. Suppose that the argument of $H_x - \mathrm{i}H_y$ does not depend on space coordinates. In this case

$$\exp\left(\int_0^t \ln[\![\tfrac{1}{2}\{H_x(\boldsymbol{W}_x(\tau)) - \mathrm{i}\sigma(-)^{N_\tau}H_y(\boldsymbol{W}_x(\tau))\}]\!]\,\mathrm{d}N_\tau\right)$$
$$= \exp\left(\int_0^t \ln[\tfrac{1}{2}(H_x^2 + H_y^2)^{1/2}]\,\mathrm{d}N_\tau + \frac{\mathrm{i}\sigma}{2}\operatorname{Arg}(H_x - \mathrm{i}H_y)[1-(-)^{N_t}]\right). \tag{4.1}$$

If, in addition, $H_x^2 + H_y^2$ does not depend on space coordinates, the Poisson integral can be performed completely and one obtains:

$$\exp\left(\int_0^t \ln[\![\tfrac{1}{2}\{H_x(\boldsymbol{W}_x(\tau)) - \mathrm{i}\sigma(-)^{N_\tau}H_y(\boldsymbol{W}_x(\tau))\}]\!]\,\mathrm{d}N_\tau\right)$$
$$= \exp\left(N_t \ln[\tfrac{1}{2}(H_x^2 + H_y^2)^{1/2}] + \frac{\mathrm{i}\sigma}{2}\operatorname{Arg}(H_x - \mathrm{i}H_y)[1-(-)^{N_t}]\right). \tag{4.2}$$

Therefore in this case and for neutral particles, (3.2) takes a form very close to the usual Feynman–Kac formula as all stochastic integrations have disappeared:

$$\psi_t(\boldsymbol{x},\sigma) = \mathrm{e}^t\mathbb{E}\left[\psi_0(\boldsymbol{W}_x(t), (-)^{N_t}\sigma)\exp\left(-\int_0^t V(\boldsymbol{W}_x(\tau))\,\mathrm{d}\tau + \tfrac{1}{2}\int_0^t H_z(\boldsymbol{W}_x(\tau))(-)^{N_\tau}\sigma\,\mathrm{d}\tau\right.\right.$$
$$\left.\left. + N_t \ln[\tfrac{1}{2}(H_x^2 + H_y^2)^{1/2}] + \frac{\mathrm{i}\sigma}{2}\operatorname{Arg}(H_x - \mathrm{i}H_y)[1-(-)^{N_t}]\right)\right]. \tag{4.3}$$

Let us mention also the following special case which will be used in the next section. When there is no magnetic field in the z and y directions and when the initial condition does not depend on σ, one can explicitly perform the Poisson average with the aid of the formula

$$\mathbb{E}\left[\exp\left(\int_0^t \ln[C(\tau)]\,\mathrm{d}N_\tau\right)\right] = \exp\left(\int_0^t C(\tau)\,\mathrm{d}\tau - t\right). \tag{4.4}$$

5. Some inequalities

A general inequality which follows immediately from (3.2) is

$$|\psi_t(\boldsymbol{x},\sigma)| \leqslant \mathrm{e}^t\mathbb{E}\left[|\psi_0(\boldsymbol{W}_x(t), (-)^{N_t}\sigma)|\exp\left(-\int_0^t V(\boldsymbol{W}_x(\tau))\,\mathrm{d}\tau + \int_0^t \frac{\sigma}{2}H_z(\boldsymbol{W}_x(\tau))(-)^{N_\tau}\,\mathrm{d}\tau\right.\right.$$
$$\left.\left. + \int_0^t \ln[\![\tfrac{1}{2}\{H_x^2(\boldsymbol{W}_x(\tau)) + H_y^2(\boldsymbol{W}_x(\tau))\}^{1/2}]\!]\,\mathrm{d}N_\tau\right)\right]. \tag{5.1}$$

The right-hand side of this inequality can be interpreted as the evolution of a neutral particle in a magnetic field which has only two components $\boldsymbol{H}' = ((H_x^2 + H_y^2)^{1/2}, 0, H_z)$ and with the initial condition $\psi_0'(\boldsymbol{x},\sigma) = |\psi_0(\boldsymbol{x},\sigma)|$. Equation (5.1) can be rewritten slightly differently as

$$|[\exp(-t\mathscr{H})\psi_0](\boldsymbol{x},\sigma)| \leqslant [\exp(-t\mathscr{H}')|\psi_0|](\boldsymbol{x},\sigma) \tag{5.2}$$

where $\mathscr{H}$ and $\mathscr{H}'$ are the corresponding Hamiltonian operators which implies, for instance, the inequality $E_0 \geqslant E_0'$ for the corresponding ground state energies. This inequality is a generalisation of the well known diamagnetic inequality (Simon 1979).

From (5.1) the rougher estimate follows

$$\begin{aligned}
|\psi_t(\boldsymbol{x},\sigma)| &\leqslant \mathbb{E}\bigg[\sup_\sigma|\psi_0(\boldsymbol{W}_x(t),\sigma)| \\
&\quad\times\exp\bigg(-\int_0^t V(\boldsymbol{W}_x(\tau))\,\mathrm{d}\tau \int_0^t \tfrac{1}{2}|H_z(\boldsymbol{W}_x(\ \ )|\,\mathrm{d}\tau \\
&\quad+\int_0^t \tfrac{1}{2}(H_x^2+H_y^2)^{1/2}(\boldsymbol{W}_x(\tau))\,\mathrm{d}\tau\bigg)\bigg] \\
&= \mathbb{E}\bigg[\sup_\sigma|\psi_0(\boldsymbol{W}_x(t),\sigma)|\exp\bigg(-\int_0^t \bar{V}(\boldsymbol{W}_x(\tau))\,\mathrm{d}\tau\bigg)\bigg]
\end{aligned} \tag{5.3}$$

in which only the Wiener process appears and which can be used as the starting point for pointwise estimates in the spirit of Carmona (1978) or qualitative analysis of bound states.

More detailed estimates can be obtained if we assume for example, following Gaveau and Vauthier, that the magnetic field has axial symmetry. We now derive in a very simple way from our representation of the solution an improved version of the Gaveau and Vauthier inequality.

By using a vector potential of the form

$$\boldsymbol{A} = (-yf+xg,\ xf+yg,\ h) \tag{5.4}$$

where f, g and h are functions of $\rho=(x^2+y^2)^{1/2}$ and z, the corresponding magnetic field is

$$\boldsymbol{H} = (-xf_z - y[g_z - h_\rho/\rho],\ -yf_z + x[g_z - h_\rho/\rho],\ 2f+\rho f_\rho), \qquad f_z = \partial f/\partial z\ \ldots . \tag{5.5}$$

This represents the most general axially symmetric field. The whole discussion which follows can be carried through for such fields; however, for simplicity we give the formula in the special case considered by Gaveau and Vauthier which corresponds to $g=h=0$.

We consider a spinor of the form

$$\psi_n(\rho,\theta,z,\sigma) = \exp[\tfrac{1}{2}\mathrm{i}(2n+1-\sigma)\theta]\varphi_n(\rho,z,\sigma) \tag{5.6}$$

which is the most general eigenvector of the z component of the total angular momentum. Next we decompose the three-dimensional Wiener process into its components in cylindrical coordinates $W_t=(\rho_t,\theta_t,z_t)$. In particular θ_t can be written as

$$\theta_t = \theta_0 + \int_0^t \frac{\mathrm{d}b_s}{\rho_s} \tag{5.7}$$

where b_t is an auxiliary one-dimensional Brownian motion independent of ρ_t and z_t. ρ_t is the usual Bessel process on the half line. We now insert (5.6) and (5.7) in (3.2) and calculate explicitly the expectation over the angular part. We obtain

$$\begin{aligned}
&\psi_n(t,\rho,\theta,z,\sigma) \\
&\quad= \exp[\tfrac{1}{2}\mathrm{i}(2n+1-\sigma)\theta + t]\mathbb{E}\bigg\{(-)^{N_t}\varphi_n(\rho_t,z_t,\sigma(-)^{N_t}) \\
&\quad\quad\times\exp\bigg[\int_0^t \ln(\rho f_z)\,\mathrm{d}N_\tau + \int_0^t\bigg(\frac{H_z\sigma}{2}(-)^{N_\tau} - V\bigg)\mathrm{d}\tau \\
&\quad\quad-\tfrac{1}{2}\int_0^t\bigg(\frac{n}{\rho_\tau}+\frac{1}{2\rho_\tau}[1-\sigma(-)^{N_\tau}]-\rho_\tau f\bigg)^2\mathrm{d}\tau\bigg]\bigg\}.
\end{aligned} \tag{5.8}$$

In arriving at (5.8) the following formula (of integration by parts) has been useful:

$$\int_0^t (-)^{N_\tau}\,\mathrm{d}N_\tau \int_0^\tau f(s)\,\mathrm{d}X_s = \int_0^t \tfrac{1}{2}[(-)^{N_\tau} - (-)^{N_t}] f(\tau)\,\mathrm{d}X_\tau \tag{5.9}$$

where $\int \mathrm{d}X_s$ in our case is a stochastic integral with respect to a Wiener process.

To establish (5.9) consider a trajectory of the Poisson process satisfying $N_t = n$ and having jumps at the times $0 < t_1 < t_2 \ldots < t_n \leq t$. The left-hand side of (5.9) can be written

$$\begin{aligned}\sum_{i=1}^{n} (-)^{i-1} \sum_{j=1}^{i} \int_{t_{j-1}}^{t_j} f(\tau)\,\mathrm{d}X_\tau &= \sum_{j=1}^{n} \int_{t_{j-1}}^{t_j} f(\tau)\,\mathrm{d}X_\tau \sum_{i=j}^{n} (-)^{i-1} \\ &= \sum_{j=1}^{n} \int_{t_{j-1}}^{t_j} f(\tau)\,\mathrm{d}X_\tau \tfrac{1}{2}[(-)^{j-1} - (-)^n] \\ &= \int_0^t f(\tau) \tfrac{1}{2}[(-)^{N_\tau} - (-)^{N_t}]\,\mathrm{d}X_\tau.\end{aligned}$$

From (5.8) we have then the obvious estimate

$$\begin{aligned}&|\psi_n(t, \rho, \theta, z, \sigma)| \\ &\quad\leq \mathrm{e}^t \mathbb{E}\bigg\{ |\psi_n(\rho_t, 0, z_t, \sigma(-)^{N_t})| \exp\bigg[\int_0^t \ln(\tfrac{1}{2}\rho |f_z|)\,\mathrm{d}N_\tau \\ &\qquad + \int_0^t \left(\frac{H_z}{2}\sigma(-)^{N_\tau} - V\right) \mathrm{d}\tau - \tfrac{1}{2}\int_0^t \left(\frac{n}{\rho_\tau} + \frac{1}{2\rho_\tau}[1 - \sigma(-)^{N_\tau}] - \rho_\tau f\right)^2 \mathrm{d}\tau\bigg]\bigg\}.\end{aligned} \tag{5.10}$$

From (5.10), using (4.4), we derive the simpler inequality

$$\begin{aligned}&|\psi_n(t, \rho, \theta, z, \sigma)| \\ &\quad\leq \mathbb{E}\bigg(\sup_\sigma |\psi_n(\rho_t, 0, z_t, \sigma)| \\ &\qquad \times \exp\bigg[\!\!\bigg[\int_0^t \left\{\frac{\rho |f_z|}{2} + \frac{|H_z|}{2} - V - \tfrac{1}{2}\min\left[\left(\frac{n}{\rho_\tau} - \rho_\tau f\right)^2, \left(\frac{n+1}{\rho_\tau} - \rho_\tau f\right)^2\right]\right\} \mathrm{d}\tau\bigg]\!\!\bigg]\bigg).\end{aligned} \tag{5.11}$$

This coincides with the inequality derived in Gaveau and Vauthier (1981).

6. General Pauli type equations

The general type of equation that we consider is

$$\begin{aligned}&\partial\psi_t(\boldsymbol{x}, \alpha)/\partial t \\ &\quad= \tfrac{1}{2}(\Delta_x \psi_t)(\boldsymbol{x}, \alpha) + \boldsymbol{b}(\boldsymbol{x}) \cdot (\boldsymbol{\nabla}_x \psi_t)(\boldsymbol{x}, \alpha) \\ &\qquad + \sum_{\beta=1}^{p-1} \lambda_\beta(\boldsymbol{x}, \alpha)\psi_t(\boldsymbol{x}, \alpha \oplus \beta) + V(\boldsymbol{x}, \alpha)\psi_t(\boldsymbol{x}, \alpha)\end{aligned} \tag{6.1}$$

where $x \in R^d$, the index α takes p values, $\alpha = 1, \ldots, p$, and $\oplus$ means addition modulo p. This way of writing (6.1) does not imply any restriction on the matrix acting on the discrete indices of ψ_t. If $N_t^1, \ldots, N_t^{p-1}$ are $p-1$ independent Poisson processes with parameter 1, we define

$$N_t = \sum_{\beta=1}^{p-1} \beta N_t^\beta \tag{6.2}$$

and using the same technique of § 3 one can verify that the expression

$$\psi_t(\boldsymbol{x}, \alpha) = \mathrm{e}^{(p-1)t} \mathbb{E}\bigg[\psi_0(\boldsymbol{W}_x(t), \alpha \oplus N_t) \times \exp\bigg(-\int_0^t V(\boldsymbol{W}_x(\tau), \alpha \oplus N_\tau)\,\mathrm{d}\tau - \tfrac{1}{2}\int_0^t \boldsymbol{b}(\boldsymbol{W}_x(\tau))^2\,\mathrm{d}\tau + \int_0^t \boldsymbol{b}(\boldsymbol{W}_x(\tau)) \cdot \mathrm{d}\boldsymbol{W}_\tau + \sum_{\beta=1}^{p-1} \int_0^t \ln[\lambda_\beta(\boldsymbol{W}_x(\tau), \alpha \oplus N_\tau)]\,\mathrm{d}N_\tau^\beta\bigg)\bigg] \tag{6.3}$$

is the solution of (6.1) satisfying the initial condition $\psi_{t=0}(\boldsymbol{x}, \alpha) = \psi_0(\boldsymbol{x}, \alpha)$.

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Appendix 1. Probabilistic expression for the solution of a linear system of ordinary differential equations

The purpose of this appendix is to give a probabilistic expression for the solution of a system of ordinary linear differential equations

$$\mathrm{d}\psi_\alpha(t)/\mathrm{d}t = \sum_{\beta=1}^{p} A_{\alpha\beta}(t)\psi_\beta(t) \tag{A1.1}$$

subjected to the initial condition

$$\psi_\alpha(t=0) = \psi_\alpha. \tag{A1.2}$$

As indicated before, it is convenient to consider $\psi_\alpha(t)$ as a function of both the time t and the discrete variable α, $\alpha = 1, \ldots, p$. Since we are mainly interested in the Pauli equation (i.e. $p=2$) we shall concentrate on this case and give later the formulae corresponding to the general case. In this case we introduce the spin variable $\sigma = 2\alpha - 3$ and $\psi(t, \sigma) = \psi_\alpha(t)$.

With an obvious definition of C and V, equation (A1.1) can be rewritten

$$\mathrm{d}\psi(t, \sigma)/\mathrm{d}t = V(t, \sigma)\psi(t, \sigma) + \exp[C(t, \sigma)]\psi(t, -\sigma). \tag{A1.3}$$

C may be complex valued.

The main result of this appendix is given in the following.

Proposition A1.1. The solution of (A1.3) is given by

$$\psi(t,\sigma)=\mathrm{e}^{t}\mathbb{E}\left[\psi((-)^{N_t}\sigma)\exp\left(\int_0^t V(\tau,(-)^{N_t-N_\tau}\sigma)\,\mathrm{d}\tau+\int_0^t C(\tau,(-)^{N_t-N_\tau+1}\sigma)\,\mathrm{d}N_\tau\right)\right]$$

where N_t is the ordinary Poisson process of unit intensity starting at zero at time zero.

To prove that the previous expression satisfies the differential equations we shall use standard techniques of the Itô calculus. The general theory is developed in Gihman and Skorohod (1972); however, for the sake of completeness we recall a lemma which is of central importance in what follows.

Lemma. Let ϕ and ψ be sufficiently smooth functions and N_t be the ordinary Poisson process of intensity one and starting at zero at time zero; then

$$\begin{aligned}\mathrm{d}\left[\exp\left(\int_0^t \phi(\tau,N_\tau)\,\mathrm{d}\tau+\int_0^t \psi(\tau,N_\tau)\,\mathrm{d}N_\tau\right)\right]\\ &=\exp\left(\int_0^t \phi(\tau,N_\tau)\,\mathrm{d}\tau+\int_0^t \psi(\tau,N_\tau)\,\mathrm{d}N_\tau\right)\\ &\quad\times[\![\phi(t,N_t)\,\mathrm{d}t+\{\exp[\psi(t,N_t)]-1\}\,\mathrm{d}N_t]\!].\end{aligned}\tag{A1.4}$$

The previous formula has an intuitive content. Consider the obvious formula

$$\begin{aligned}\exp\left(\int_0^{t+\Delta t}\psi(\tau,N_\tau)\,\mathrm{d}N_\tau\right)-\exp\left(\int_0^{t}\psi(\tau,N_\tau)\,\mathrm{d}N_\tau\right)\\ =\exp\left(\int_0^{t}\psi(\tau,N_\tau)\,\mathrm{d}N_\tau\right)\left[\exp\left(\int_t^{t+\Delta t}\psi(\tau,N_\tau)\,\mathrm{d}N_\tau\right)-1\right].\end{aligned}$$

If within the time interval Δt there is just one jump, the right-hand side is different from zero and equal to the second term in (A1.4) (when $\phi=0$). We are justified in considering only one jump since for a Poisson process the probability of n jumps in the time interval Δt is proportional to $(\Delta t)^n$. Then up to terms of order $(\Delta t)^2$ our formula is correct.

Now the proof of proposition (A1.1) follows through elementary observations.

(i) Since the system is linear we can restrict ourselves to initial conditions of the form

$$\psi_\varepsilon(\sigma)=\sigma^\varepsilon,\qquad \varepsilon=0,1.$$

(ii) One has the following identity:

$$\begin{aligned}(-)^{\varepsilon N_t}\exp\left(\int_0^t V(\tau,(-)^{N_t-N_\tau}\sigma)\,\mathrm{d}\tau+\int_0^t C(\tau,(-)^{N_t-N_\tau+1}\sigma)\,\mathrm{d}N_\tau\right)\\ =\tfrac{1}{2}\exp\left(\int_0^t V(\tau,(-)^{N_\tau}\sigma)\,\mathrm{d}\tau+\int_0^t C(\tau,(-)^{N_\tau+1}\sigma)\,\mathrm{d}N_\tau\right)\\ +\tfrac{1}{2}(-)^\varepsilon\exp\left(\int_0^t V(\tau,(-)^{N_\tau+1}\sigma)\,\mathrm{d}\tau+\int_0^t C(\tau,(-)^{N_\tau}\sigma)\,\mathrm{d}N_\tau\right)\end{aligned}$$

$$+\tfrac{1}{2}(-)^{N_t}\exp\left(\int_0^t V(\tau,(-)^{N_\tau}\sigma)\,\mathrm{d}\tau+\int_0^t C(\tau,(-)^{N_\tau+1}\sigma)\,\mathrm{d}N_\tau\right)$$

$$-\tfrac{1}{2}(-)^{\varepsilon}(-)^{N_t}\exp\left(\int_0^t V(\tau,(-)^{N_\tau+1}\sigma)\,\mathrm{d}\tau+\int_0^t C(\tau,(-)^{N_\tau}\sigma)\,\mathrm{d}N_\tau\right).$$

(iii) Direct application of the lemma shows that

$$\mathrm{d}\left[(-)^{\varepsilon N_t}\exp\left(\int_0^t V(\tau,(-)^{N_t-N_\tau}\sigma)\,\mathrm{d}\tau+\int_0^t C(\tau,(-)^{N_t-N_\tau+1}\sigma)\,\mathrm{d}N_\tau\right)\right]$$

$$=V(t,\sigma)\exp\left(\int_0^t V(\tau,(-)^{N_t-N_\tau}\sigma)\,\mathrm{d}\tau+\int_0^t C(\tau,(-)^{N_t-N_\tau+1}\sigma)\,\mathrm{d}N_\tau\right)(-)^{\varepsilon N_t}\,\mathrm{d}t$$

$$+\left[\mathrm{e}^{C(t,\sigma)}\exp\left(\int_0^t V(\tau,(-)^{N_t-N_\tau+1}\sigma)\,\mathrm{d}\tau\right.\right.$$

$$\left.+\int_0^t C(\tau,(-)^{N_t-N_\tau}\sigma)\,\mathrm{d}N_\tau\right)(-)^{\varepsilon(N_t+1)}$$

$$\left.-\exp\left(\int_0^t V(\tau,(-)^{N_t-N_\tau}\sigma)\,\mathrm{d}\tau+\int_0^t C(\tau,(-)^{N_t-N_\tau+1}\sigma)\,\mathrm{d}N_\tau\right)(-)^{\varepsilon N_t}\right]\mathrm{d}N_t.$$

The independence of $\mathrm{d}N_t$ on what is on its left and $E(\mathrm{d}N_t)=\mathrm{d}t$ achieve the proof.

One can guess the formula solving the general case ($p>2$) and it can be verified using the same techniques as before.

The solution of the linear system of ordinary differential equations

$$\frac{\mathrm{d}\psi}{\mathrm{d}t}(t,\alpha)=\sum_{\beta=1}^{p-1}\exp[C(t,\alpha,\beta)]\psi(t,\alpha\oplus\beta)+V(t,\alpha)\psi(t,\alpha)$$

with the initial condition

$$\psi(t=0,\alpha)=\psi(\alpha)$$

is given by

$$\psi(t,\alpha)=\mathrm{e}^{(p-1)t}\mathbb{E}\left[\psi(\alpha\oplus N_t)\exp\left(\int_0^t V(\tau,\alpha\oplus N_t\ominus N_\tau)\,\mathrm{d}\tau\right.\right.$$

$$\left.\left.+\sum_{\beta=1}^{p-1}\int_0^t C(\tau,\alpha\oplus N_t\ominus N_\tau\ominus\beta,\beta)\,\mathrm{d}N_\tau^\beta\right)\right]$$

where $N_t=\Sigma_{\beta=1}^{p-1}\beta N_t^\beta$ is the sum of $p-1$ independent usual Poisson processes and the sums $\alpha\oplus N_t$, $\alpha\oplus N_t\ominus N_t$ and $\alpha\oplus N_t\ominus N_t\ominus\beta$ stand for the same sums modulo p.

A special case of this formula has been already obtained by Ginibre (1968) in the case where the matrix elements of the linear system do not depend on time and the matrix is symmetric.

Appendix 2. A formal derivation of equation (3.2)

Since the coefficients of the Pauli equation are time independent one can identify this equation with a backward 'Kolmogorov equation' (BKE). After a reflection of time, the Pauli equation can be rewritten

$$\frac{\partial\psi}{\partial t}(t,\boldsymbol{x},\sigma)+\tfrac{1}{2}\Delta_x\psi(t,\boldsymbol{x},\sigma)+\mathrm{i}\boldsymbol{A}(\boldsymbol{x})\cdot\boldsymbol{\nabla}_x\psi(t,\boldsymbol{x},\sigma)-\tfrac{1}{2}|\boldsymbol{A}(\boldsymbol{x})|^2\psi(t,\boldsymbol{x},\sigma)$$

$$+V_1(\boldsymbol{x},\sigma)\psi(t,\boldsymbol{x},\sigma)+V_2(\boldsymbol{x},\sigma)\psi(t,\boldsymbol{x},-\sigma)=0, \tag{A2.1}$$

$$V_1(\boldsymbol{x},\sigma)=-V(\boldsymbol{x})+\tfrac{1}{2}H_z(\boldsymbol{x})\sigma, \tag{A2.2}$$

$$V_2(\boldsymbol{x},\sigma)=\tfrac{1}{2}H_x(\boldsymbol{x})-\tfrac{1}{2}\mathrm{i}H_y(\boldsymbol{x})\sigma. \tag{A2.3}$$

We assume that $V_2(\boldsymbol{x},\sigma)$ is non zero, and define

$$V_2(\boldsymbol{x},\sigma)=\exp[C(\boldsymbol{x},\sigma)]. \tag{A2.4}$$

Furthermore let

$$\Psi(t,\boldsymbol{x},\boldsymbol{y},z,\sigma)=\exp\Big(z\sqrt{2}+\mathrm{i}\sum_{i=1}^{3}y_i\Big)\psi(t,\boldsymbol{x},\sigma) \tag{A2.5}$$

which due to (A2.1) satisfies the equation

$$\frac{\partial\Psi}{\partial t}(t,\boldsymbol{x},\boldsymbol{y},z,\sigma)+\tfrac{1}{2}\Delta_x\Psi(t,\boldsymbol{x},\boldsymbol{y},z,\sigma)-\sum_{i=1}^{3}A_i(\boldsymbol{x})\frac{\partial^2}{\partial x_i\,\partial y_i}\Psi(t,\boldsymbol{x},\boldsymbol{y},z,\sigma)$$

$$+\tfrac{1}{2}\sum_{i=1}^{3}A_i(\boldsymbol{x})^2\frac{\partial^2}{\partial y_i^2}\Psi(t,\boldsymbol{x},\boldsymbol{y},z,\sigma)+\frac{1}{\sqrt{2}}V_1(\boldsymbol{x},\sigma)\frac{\partial}{\partial z}\Psi(t,\boldsymbol{x},\boldsymbol{y},z,\sigma)$$

$$+\frac{1}{2}\frac{\partial^2}{\partial z^2}\Psi(t,\boldsymbol{x},\boldsymbol{y},z,\sigma)+\Psi\Big(t,\boldsymbol{x},\boldsymbol{y},z+\frac{1}{\sqrt{2}}C(\boldsymbol{x},\sigma),-\sigma\Big)$$

$$-\Psi(t,\boldsymbol{x},\boldsymbol{y},z,\sigma)=0 \tag{A2.6}$$

and has indeed the form of a BKE (Gihman and Skorohod 1972).

The solution of such an equation can be given in terms of the following processes:

$$\xi_{x,t}(s)=\boldsymbol{x}+\boldsymbol{W}_s-\boldsymbol{W}_t, \tag{A2.7}$$

$$\zeta_{xt}(s)=-\int_t^s\boldsymbol{A}(\boldsymbol{x}+\boldsymbol{W}_\tau-\boldsymbol{W}_t)\cdot\mathrm{d}\boldsymbol{W}_\tau, \tag{A2.8}$$

$$\eta_{x,\sigma,t}(s)=\int_t^s V_1(\boldsymbol{x}+\boldsymbol{W}_\tau-\boldsymbol{W}_t,\sigma(-)^{N_t-N_\tau})\,\mathrm{d}\tau, \tag{A2.9}$$

$$\theta_{x,\sigma,t}(s)=\frac{1}{\sqrt{2}}\int_t^s C(\boldsymbol{x}+\boldsymbol{W}_\tau-\boldsymbol{W}_t,\sigma(-)^{N_t-N_\tau})\,\mathrm{d}N_\tau. \tag{A2.10}$$

The solution of (A2.6) which takes the value $\psi_0(\boldsymbol{x},\sigma)\exp(\sqrt{2}z+\mathrm{i}\Sigma_{i=1}^3 y_i)$ at $t=T$ is given for $t<T$ according to Gihman and Skorohod (1972) by

$$\Psi(t,\boldsymbol{x},\boldsymbol{y},z,\sigma)$$

$$=\mathrm{e}^{T-t}\mathbb{E}\Big[\psi_0(\boldsymbol{x}+\boldsymbol{W}_T-\boldsymbol{W}_t,\sigma(-)^{N_T-N_t})$$

$$\times\exp\Big(-\mathrm{i}\int_t^T\boldsymbol{A}(\boldsymbol{x}+\boldsymbol{W}_\tau-\boldsymbol{W}_t)\,\mathrm{d}\boldsymbol{W}_\tau+\int_t^T V_1(\boldsymbol{x}+\boldsymbol{W}_\tau-\boldsymbol{W}_t,\sigma(-)^{N_\tau-N_t})\,\mathrm{d}\tau$$

$$+\int_t^T C(\boldsymbol{x}+\boldsymbol{W}_\tau-\boldsymbol{W}_t,\sigma(-)^{N_\tau-N_t})\,\mathrm{d}N_\tau+\sqrt{2}z+\mathrm{i}\sum_{i=1}^{3}y_i\Big)\Big]. \tag{A2.11}$$

We remark that the derivative with respect to t is minus the derivative with respect to T. Then in the previous formula one chooses $y = z = 0$ and $t = 0$. This coincides with (3.2).

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