J. Phys. A: Math. Gen. **23** (1990) L965–L968. Printed in the UK

LETTER TO THE EDITOR

On the relativistic Feynman–Kac–Ito formula

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Received 10 May 1990

Abstract. We construct a Feynman–Kac–Ito formula for the relativistic Hamiltonian

$$H = \{c^2(-i\hbar\nabla - e/cA)^2 + M^2c^4\}^{1/2} - Mc^2 + V.$$

The main ingredient of our approach is a suitable random time $\tau_c(t)$ which is used to turn the ordinary FKI formula into the relativistic one.

The Feynman–Kac–Ito (FKI) formula [1]:

$$\exp(-tH/\hbar)\psi(x) = \mathbb{E}\left[\psi(x+\sqrt{\nu}\,w_t)\exp(-1/\hbar)\left(\int_0^t V(x+\sqrt{\nu}\,w_s)\,ds + ie/cF(t,x,w,A)\right)\right]$$

(where $\nu = \hbar/M$ and $s \mapsto w_s$ is the three-dimensional Brownian motion starting at the origin) gives a probabilistic representation of the semigroup $t \mapsto \exp(-tH/\hbar)$ for the Schrödinger Hamiltonian $H = 1/2M(-i\hbar\nabla - e/cA)^2 + V$ (in a magnetic field). The vector potential A appears in the expectation $\mathbb{E}(\cdot)$ only through the phase factor $\exp -i(e/\hbar c)F$ where:

$$F(t,x,w,A) = \sqrt{\nu}\int_0^t A(x+\sqrt{\nu}\,w_s)\cdot dw_s + \nu/2\int_0^t \operatorname{div} A(x+\sqrt{\nu}\,w_s)\,ds.$$

A consequence of this fact is the diamagnetic inequality [1] which ensures that energy can only rise when the magnetic field is turned on. The stability of matter under Coulomb forces is therefore unaffected by an external magnetic field in non-relativistic quantum mechanics. The stability of matter has been also studied [2–5] when the non-relativistic kinetic energy operator $-(\hbar^2/2M)\Delta$ is replaced by the relativistic one $\{-\hbar^2c^2\Delta + M^2c^4\}^{1/2}$, but such a change leads to an unpleasant surprise: atoms are stable no more when the atomic number Z is larger than $Z_c = 2/\pi\alpha \simeq 87$, nevertheless stability can be proved when $Z \leqslant Z_c$. From a physical point of view this means, of course, that these relativistic quantum models with a fixed number of charged particles reach the boundary of their domain of validity when $Z = Z_c$. It is worthwhile observing that similar results also hold for the equations of Dirac ($Z_c = \alpha^{-1}$) and Klein–Gordon ($Z_c = 1/2\alpha$) in an electrostatic potential ϕ, therefore, on this ground, there are no qualitative reasons to prefer them to the quantum relativistic Hamiltonian $H = \{-\hbar^2c^2\Delta + M^2c^4\}^{1/2} + e\phi$.

0305-4470/90/180965+04$03.50

The main task of our paper is to provide a relativistic FKI formula for the Hamiltonian:

$$H=\{c^2(-\mathrm{i}\hbar\nabla-e/c\boldsymbol{A})^2+M^2c^4\}^{1/2}-Mc^2+V=H_0(\boldsymbol{A})+V \tag{1}$$

which is supposed to describe a spinless relativistic charged particle in the potential V and in a magnetic field $\boldsymbol{B}=\operatorname{rot}\boldsymbol{A}$. Despite the troublesome square root in (1) there is a simple way of turning the usual FKI formula into the relativistic one by using a probabilistic idea essentially due to Lévy. Let $s\mapsto w_s^0$ be an additional one-dimensional Wiener process independent from the three-dimensional Brownian motion $s\mapsto \boldsymbol{w}_s$ and let the random time $\tau_c(t)$ be the smallest s such that $cs+\sqrt{\nu}\,w_s^0=ct$

$$\tau_c(t)=\inf\{s\geqslant 0:\ cs+\sqrt{\nu}\,w_s^0=ct\}. \tag{2}$$

It is not difficult to see that the process $t\mapsto\tau_c(t)$ is a non-decreasing jump Markov process with independent and time homogeneous increments (Lévy process). We proved in [6] that:

$$\mathbb{E}(\exp(-\tau_c(t)\gamma/\hbar))=\exp(-t/\hbar)(\{2Mc^2\gamma+M^2c^4\}^{1/2}-Mc^2) \tag{3}$$

for all $\gamma\geqslant 0$. Therefore, if Γ is a non-negative self-adjoint operator, it follows by the spectral theorem that

$$\exp(-t/\hbar)(\{2Mc^2\Gamma+M^2c^4\}^{1/2}-Mc^2)=\mathbb{E}(\exp-\tau_c(t)\Gamma/\hbar) \tag{4}$$

in other words the semigroup $t\mapsto\exp(-tH/\hbar)$ for $H=\{2Mc^2\Gamma+M^2c^4\}^{1/2}-Mc^2$ can be constructed as the averaged semigroup of Γ after replacing the deterministic time t by the random one $\tau_c(t)$. By choosing Γ as the Schrödinger Hamiltonian:

$$\Gamma=1/2M(-\mathrm{i}\hbar\nabla-e/c\boldsymbol{A})^2 \tag{5}$$

and by recalling the FKI formula, we get from (4)

$$\exp(-tH_0(\boldsymbol{A})/\hbar)\psi(\boldsymbol{x})=\mathbb{E}[\psi(\boldsymbol{x}+\sqrt{\nu}\,\boldsymbol{w}_{\tau_c(t)})\exp-\mathrm{i}(e/\hbar c)F(\tau_c(t),\boldsymbol{x},\boldsymbol{w},\boldsymbol{A})] \tag{6}$$

where the expectation $\mathbb{E}(\cdot)$ is taken with respect both to $s\mapsto\boldsymbol{w}_s$ and $t\mapsto\tau_c(t)$ or, equivalently, with respect to the four-dimensional Brownian motion $s\mapsto w_s^\mu=(w_s^0,\boldsymbol{w}_s)$.

Now it is possible to extend this result to the more general Hamiltonian $H=H_0(\boldsymbol{A})+V$. The Trotter-Kato formula gives, in fact:

$$\exp(-tH/\hbar)\psi(\boldsymbol{x}) =\mathbb{E}\left[\psi(\boldsymbol{x}+\boldsymbol{\xi}_t)\exp(-1/\hbar)\times\left(\int_0^t V(\boldsymbol{x}+\boldsymbol{\xi}_s)\,\mathrm{d}s+\mathrm{i}e/cF(\tau_c(t),\boldsymbol{x},\boldsymbol{w},\boldsymbol{A})\right)\right] \tag{7}$$

where $\boldsymbol{\xi}_t=\sqrt{\nu}\,\boldsymbol{w}_{\tau_c(t)}$ (a jump Markov process with independent and time homogeneous increments). A simple consequence of (7) is that the diamagnetic inequality still holds. Of course the effect of spin is crucial for the stability of matter in a magnetic field. The extension of our technique to Dirac Hamiltonians with an external magnetic field is possible and it is the subject of a forthcoming paper. It should be remarked that Ichinose and Tamura proposed [7, 8] a different relativistic FKI formula based only upon the Markov process $t\mapsto\boldsymbol{\xi}_t$ which they introduced independently from any reference to Brownian motion. Unfortunately their Hamiltonian is not gauge invariant up to a unitary transformation. Without magnetic field both formulae coincide and assume the structure of the Feynman–Kac formula with $t \mapsto \xi_t$ replacing the diffusion $t \mapsto \sqrt{\nu}\, w_t$. We think that the construction of ξ_t as $\sqrt{\nu}\, w_{\tau_c(t)}$ is useful because it allows one to grasp more easily the probabilistic meaning of the non-relativistic limit: the random time $\tau_c(t)$ converges in probability to the deterministic time t when the speed of light c goes to infinity [6]. Now we want to recall the relations between the relativistic quantum mechanics described here and the Klein–Gordon equation as a first quantized theory. Let us consider, first, the Klein–Gordon equation in a purely magnetic external field:

$$c^{-2}\partial_t^2\varphi + (-\mathrm{i}\nabla - e/\hbar c A)^2\varphi + M^2c^2\hbar^{-2}\varphi = 0 \tag{8}$$

which can be transformed into the first-order equation:

$$\begin{aligned}\mathrm{i}\hbar\partial_t\begin{pmatrix}\phi_1\\ \phi_2\end{pmatrix} &= \hbar\omega\begin{pmatrix}0 & [-\mathrm{i}\hbar\omega/Mc^2]^{-1}\\ [-\mathrm{i}\hbar\omega/Mc^2] & 0\end{pmatrix}\begin{pmatrix}\phi_1\\ \phi_2\end{pmatrix}\\ &= K_0(A)\begin{pmatrix}\phi_1\\ \phi_2\end{pmatrix}\end{aligned} \tag{9}$$

where $\phi_1 = \varphi$, $\phi_2 = \hbar/Mc^2\partial_t\varphi$ and $\omega = c\{(-\mathrm{i}\nabla - e/\hbar c A)^2 + M^2c^2/\hbar^2\}^{1/2}$. It is well known that the Klein–Gordon Hamiltonian $K_0(A)$ can be diagonalized as $\left(\begin{smallmatrix}\hbar\omega & 0\\ 0 & -\hbar\omega\end{smallmatrix}\right)$ and therefore equation (9) decouples in two independent relativistic Schrödinger equations (corresponding to positive and negative frequencies) with $\pm H_0(A)$ as Hamiltonians. The link with the previous theory is therefore fully established in a purely magnetic external field but when an external electric field is also present, the two theories are no longer equivalent except to first order of perturbation theory. This fact is not astonishing since a large external electric field can create pairs of particles and antiparticles and one-body theories are not physically satisfactory in this context. Before ending this paper we show that our technique also works in the presence of an external static scalar field U. The Klein–Gordon equation takes, in this case, the form

$$\Box\varphi + M^2c^2\hbar^{-2}\varphi = -U\varphi \tag{10}$$

which can be transformed, as before, in the first-order equation (9) with $\omega = c\{-\Delta + U + M^2c^2/\hbar^2\}^{1/2}$ and then diagonalized. The resulting couple of equations are relativistic Schrödinger equations with Hamiltonians $\pm\{2Mc^2\Gamma + M^2C^4\}^{1/2}$ where $\Gamma = \hbar^2/2M(-\Delta + U)$. As a consequence of that a relativistic Feynman–Kac formula is constructed as:

$$\exp(-tH/\hbar)\psi(x) = \mathbb{E}\left(\psi(x+\xi_t)\exp -\hbar/2M\int_0^{\tau_c(t)} U(x+\sqrt{\nu}\, w_s)\,\mathrm{d}s\right) \tag{11}$$

when $H = \hbar c\{-\Delta + U + M^2c^2/\hbar^2\}^{1/2} - Mc^2$. We finally observe that the integrals involving the scalar potential U in (11) and the potential V in (7) are different, nevertheless they coincide in the non-relativistic limit as $\tau_c(t) \to t$. After the completion of this paper we discovered references [9, 10] on related but not overlapping subjects. In such articles is described how to construct a relativistic Feynman–Kac (not Ito) formula for Hamiltonians:

$$H = \{-c^2\hbar^2\Delta + M^2c^4\}^{1/2} - Mc^2 + V$$

by means of the random time (2) and some of its consequences. This was also part of the content of our previous work [6].

This work was partially supported by Consiglio Nazionale delle Ricerche (CNR).

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