Stochastic calculus and non-relativistic QED

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We summarize recent results on stochastic differential equations associated with the standard model of non-relativistic quantum electrodynamics for an electron in an electrostatic potential interacting with the quantized electromagnetic field. Moreover, we present a Feynman-Kac formula for the corresponding semi-group – which is new in case the electron-spin is taken into account – and a new Feynman-Kac formula for an operator-valued integral kernel of the semi-group. Finally, we announce a proof of the norm-continuity of the integral kernel.

Keywords: Stochastic differential equation, Feynman-Kac, quantized radiation field

1. Introduction

In his famous work on quantum electrodynamics (QED) R. P. Feynman developed in particular a path integral description for the quantum mechanical dynamics of a non-relativistic (NR) electron interacting with the quantized (relativistic) electromagnetic radiation field.[2] It is equally well-known that Feynman's formalism can be justified mathematically for various models given by semi-bounded self-adjoint Hamiltonians, provided that one considers the associated semi-groups instead of the unitary groups representing the quantum mechanical time evolution. For instance, Feynman-Kac (FK) representations of semi-groups have been extensively exploited in the study of Schrödinger operators and led to many important – physically relevant – spectral theoretic results. A natural next step, therefore, is to study FK representations of the semi-group generated by the Hamiltonian of the standard model of NRQED which is a Schrödinger operator minimally coupled to the quantized radiation field.

Employing some ideas from earlier work on polynomial quantum field models (in particular Ref. 11), FK representations in NRQED have been derived first by

F. Hiroshima[4] in the scalar case, i.e., without electron spin. A formula which takes spin into account as well has been established more recently by F. Hiroshima and J. Lőrinczi.[6] In both articles the FK formula is derived by means of repeated Trotter product expansions. In principle it should, however, also be possible to verify and analyze FK formulas in NRQED by means of a suitable version of *stochastic calculus* in Hilbert spaces.[9,10] This approach is explored in a recent paper by the present authors,[3] whose main results are summarized in this review. Before we explain its organization we also mention that various mathematical questions in NRQED (such as self-adjointness properties, ergodic properties in the scalar case, uniqueness and localization of ground states, and Gibbs measures associated with ground states) have already been investigated by means of FK representations before, mainly by F. Hiroshima and his co-workers. We refer the reader to the monograph Ref. 8 for an exhaustive exposition of these issues and appropriate references.

The model considered here is explained in Sect. 2. In Sect. 3 we introduce new representations of FK integrands in NRQED in a form resembling the *annihilation-preservation-creation processes* playing a prominent role in quantum stochastic calculus.[7] As a crucial merit of the application of the stochastic calculus, the FK integrands are identified as solutions of *stochastic differential equations (SDE's)*, which may be exploited in further investigations of NRQED. To the best of our knowledge the analysis of these novel equations is non-standard due to the appearance of non-deterministic, unbounded, non-commuting operators in their coefficients. Our main existence and uniqueness theorem for these SDE's is also stated in Sect. 3. The final Sect. 4 is devoted to various FK formulas.

2. Definition of the model

The standard model of NRQED for one electron interacting with the quantized photon field is given by a Hamiltonian acting in the Hilbert space $\mathscr{H}$ defined by

$$\mathscr{H} := L^2(\mathbb{R}^3, \hat{\mathscr{H}}) = \int_{\mathbb{R}^3}^{\oplus} \hat{\mathscr{H}} \, \mathrm{d}\boldsymbol{x}, \quad \text{with } \hat{\mathscr{H}} := \mathbb{C}^2 \otimes \mathscr{F}.$$

Here $\mathscr{F} = \oplus_{n=0}^{\infty} \mathscr{F}^{(n)}$ is the bosonic Fock space modeled over $\mathfrak{h} := L^2(\mathbb{R}^3 \times \mathbb{Z}_2, \mathrm{d}k)$, i.e., $\mathscr{F}^{(n)}$ is the n-th symmetric tensor power of $\mathfrak{h}$; $\mathrm{d}k$ denotes the product of the Lebesgue measure and the counting measure on $\mathbb{Z}_2$. We write $\mathscr{E}[\mathfrak{v}] := \{\zeta(h) : h \in \mathfrak{v}\}$ for the set of exponential vectors corresponding to some subset $\mathfrak{v} \subset \mathfrak{h}$, where

$$\zeta(h) := \big(1, ih, \dots, (n!)^{-1/2} i^n h^{\otimes_n}, \dots\big) \in \mathscr{F}, \qquad h \in \mathfrak{h},$$

and denote its complex linear hull by $\mathscr{C}[\mathfrak{v}] := \mathrm{span}_{\mathbb{C}}(\mathscr{E}[\mathfrak{v}])$. The symbols $a^\dagger(f)$ and $a(f)$ denote the usual bosonic creation and annihilation operators of a photon state $f \in \mathfrak{h}$ satisfying the following canonical commutations relations on, e.g., $\mathscr{C}[\mathfrak{h}]$,

$$[a(f), a(g)] = [a^\dagger(f), a^\dagger(g)] = 0, \quad [a(f), a^\dagger(g)] = \langle f|g\rangle \, \mathbb{1}_{\mathscr{F}}, \quad f, g \in \mathfrak{h}.$$

The field operator $\varphi(f)$ is defined as the self-adjoint closure of $(a^\dagger(f) + a(f))\restriction_{\mathscr{C}[\mathfrak{h}]}$. For $\boldsymbol{f} = (f_1, f_2, f_3) \in \mathfrak{h}^3$, we write $\varphi(\boldsymbol{f}) := (\varphi(f_1), \varphi(f_2), \varphi(f_3))$ for short. Finally,

$\Gamma(T)$ denotes the second quantization of a bounded linear or anti-linear operator T defined on $\mathfrak{h}$ with norm $\leqslant 1$.

Let $\omega(\boldsymbol{k}) := (\boldsymbol{k}^2 + \mu^2)^{1/2}$, $\boldsymbol{k} \in \mathbb{R}^3$, with $\mu \geqslant 0$, and let $\boldsymbol{m} = (m_1, m_2, m_3) : \mathbb{R}^3 \to \mathbb{R}^3$ be either the identity map on $\mathbb{R}^3$ or zero. Then the differential second quantization $\mathrm{d}\Gamma(\omega)$ is interpreted as the radiation field energy and $\mathrm{d}\Gamma(\boldsymbol{m}) := (\mathrm{d}\Gamma(m_1), \mathrm{d}\Gamma(m_2), \mathrm{d}\Gamma(m_3))$ is the field momentum operator, in case $\boldsymbol{m}(\boldsymbol{k}) = \boldsymbol{k}$. We introduce the following dense subspaces of $\mathfrak{h}$,

$$\mathfrak{d} := L^2\big(\mathbb{R}^3 \times \mathbb{Z}_2, [1 + (\omega + \tfrac{1}{2}\boldsymbol{m}^2)^2]\mathrm{d}k\big), \quad \mathfrak{k} := L^2\big(\mathbb{R}^3 \times \mathbb{Z}_2, [\tfrac{1}{\omega} + (\omega + \tfrac{1}{2}\boldsymbol{m}^2)^2]\mathrm{d}k\big).$$

If we interpret a Schrödinger operator acting in $L^2(\mathbb{R}^3)$ and $\mathrm{d}\Gamma(\omega)$ as operators in $\mathscr{H}$ in the canonical way, then the Hamiltonian of NRQED is a perturbation of their sum. To explain this more precisely, we introduce the interaction terms

$$\varphi(\boldsymbol{G}) := \int_{\mathbb{R}^3}^{\oplus} \mathbb{1}_{\mathbb{C}^2} \otimes \varphi(\boldsymbol{G}_{\boldsymbol{x}})\mathrm{d}\boldsymbol{x}, \quad \boldsymbol{\sigma} \cdot \varphi(\boldsymbol{F}) := \sum_{j=1}^{3} \int_{\mathbb{R}^3}^{\oplus} \sigma_j \otimes \varphi(F_{j,\boldsymbol{x}})\mathrm{d}\boldsymbol{x},$$

where σ_1, σ_2, and σ_3 are the $2{\times}2$ Pauli spin-matrices and the coupling functions $\boldsymbol{G}_{\boldsymbol{x}} = (G_{1,\boldsymbol{x}}, G_{2,\boldsymbol{x}}, G_{3,\boldsymbol{x}})$ and $\boldsymbol{F}_{\boldsymbol{x}} = (F_{1,\boldsymbol{x}}, F_{2,\boldsymbol{x}}, F_{3,\boldsymbol{x}})$ satisfy the following:

Assumption 2.1. *The map* $(\boldsymbol{x}, \boldsymbol{k}, \lambda) \mapsto (\boldsymbol{G}_{\boldsymbol{x}}, \boldsymbol{F}_{\boldsymbol{x}})(\boldsymbol{k}, \lambda)$ *is measurable,* $\boldsymbol{x} \mapsto \boldsymbol{G}_{\boldsymbol{x}}$ *belongs to* $C^2(\mathbb{R}^3, \mathfrak{h}^3)$*, and* $\boldsymbol{x} \mapsto \boldsymbol{F}_{\boldsymbol{x}} \in \mathfrak{h}^3$ *is globally Lipschitz continuous on* $\mathbb{R}^3$*. All components of* $\boldsymbol{G}_{\boldsymbol{x}}$*,* $\boldsymbol{F}_{\boldsymbol{x}}$*, and* $\partial_{x_\ell}\boldsymbol{G}_{\boldsymbol{x}}$ *belong to* $\mathfrak{k}$ *and the map*

$$\mathbb{R}^3 \ni \boldsymbol{x} \longmapsto (\boldsymbol{G}_{\boldsymbol{x}}, \partial_{x_1}\boldsymbol{G}_{\boldsymbol{x}}, \partial_{x_2}\boldsymbol{G}_{\boldsymbol{x}}, \partial_{x_3}\boldsymbol{G}_{\boldsymbol{x}}, \boldsymbol{F}_{\boldsymbol{x}}) \in \mathfrak{k}^{15}$$

is bounded and continuous. Moreover, there is a conjugation $C \colon \mathfrak{h} \to \mathfrak{h}$*, i.e., an anti-linear isometry with* $C^2 = \mathbb{1}_{\mathfrak{h}}$*, such that, for all* $t \geqslant 0$*,* $\boldsymbol{x} \in \mathbb{R}^3$*, and* $\ell = 1, 2, 3$*,*

$$[C, e^{-t\omega + i\boldsymbol{m}\cdot\boldsymbol{x}}] = 0, \quad G_{\ell,\boldsymbol{x}}, F_{\ell,\boldsymbol{x}} \in \mathfrak{h}_C := \{f \in \mathfrak{h} : Cf = f\}. \tag{1}$$

Example 2.1. In the standard model of NRQED for one electron interacting with the quantized electromagnetic radiation field in Coulomb gauge and with a sharp ultra-violet cut-off one chooses $\omega(\boldsymbol{k}) = |\boldsymbol{k}|$, $\boldsymbol{m} = \boldsymbol{0}$, and $\boldsymbol{G}$ is given by

$$\boldsymbol{G}^{\Lambda}_{\boldsymbol{x}}(\boldsymbol{k}, \lambda) := (\alpha/2)^{1/2}(2\pi)^{-3/2}\omega(\boldsymbol{k})^{-1/2}\, 1_{\{\omega(\boldsymbol{k}) \leqslant \Lambda\}}\, e^{-i\boldsymbol{k}\cdot\boldsymbol{x}}\boldsymbol{\varepsilon}(\boldsymbol{k}, \lambda),$$

where $\alpha, \Lambda > 0$. Applying a suitable unitary transformation, we may achieve that $\boldsymbol{\varepsilon}(\boldsymbol{k}, 0) = |\boldsymbol{e} \times \boldsymbol{k}|^{-1}\boldsymbol{e} \times \boldsymbol{k}$ and $\boldsymbol{\varepsilon}(\boldsymbol{k}, 1) = |\boldsymbol{k}|^{-1}\boldsymbol{k} \times \boldsymbol{\varepsilon}(\boldsymbol{k}, 0)$, for a.e. $\boldsymbol{k}$ and some unit vector $\boldsymbol{e}$ in $\mathbb{R}^3$. If the electron spin is neglected, then we choose $\boldsymbol{F} = \boldsymbol{0}$; otherwise we set $\boldsymbol{F}$ equal to $\boldsymbol{F}^{\Lambda}_{\boldsymbol{x}}(k) := -\frac{i}{2}\boldsymbol{k} \times \boldsymbol{G}^{\Lambda}_{\boldsymbol{x}}(\boldsymbol{k}, \lambda)$. The choice $\boldsymbol{m}(\boldsymbol{k}) := \boldsymbol{k}$ appears in the definition of certain fiber Hamiltonians associated with the model. An appropriate conjugation is given by $(Cf)(\boldsymbol{k}, \lambda) := -(-1)^{\lambda}\overline{f(-\boldsymbol{k}, \lambda)}$.

Let $V \in L^1_{\mathrm{loc}}(\mathbb{R}^3, \mathbb{R})$. Then the *total Hamiltonian* for our model is given by

$$H^V := \tfrac{1}{2}(-i\nabla_{\boldsymbol{x}} - \varphi(\boldsymbol{G}))^2 - \boldsymbol{\sigma} \cdot \varphi(\boldsymbol{F}) + \mathrm{d}\Gamma(\omega) + V.$$

A priori it is interpreted as a quadratic form with dense domain $C_0^\infty(\mathbb{R}^3) \otimes \mathbb{C}^2 \otimes \mathscr{C}[\mathfrak{d}_C]$, where $\mathfrak{d}_C := \mathfrak{d} \cap \mathfrak{h}_C$. If this form is bounded from below, then we denote the unique self-adjoint operator representing its closure again by H^V. The SDE's discussed below involve the *generalized fiber Hamiltonians* defined, for fixed $\boldsymbol{\xi}, \boldsymbol{x} \in \mathbb{R}^3$, by

$$\widehat{H}^V(\boldsymbol{\xi},\boldsymbol{x}) := \mathbb{1}_{\mathbb{C}^2} \otimes \widehat{H}^V_{\mathrm{scal}}(\boldsymbol{\xi},\boldsymbol{x}) - \boldsymbol{\sigma}\cdot\varphi(\boldsymbol{F}_{\boldsymbol{x}}),$$
$$\widehat{H}^V_{\mathrm{scal}}(\boldsymbol{\xi},\boldsymbol{x}) := \tfrac{1}{2}\boldsymbol{v}(\boldsymbol{\xi},\boldsymbol{x})^2 - \tfrac{i}{2}\varphi(\mathrm{div}\boldsymbol{G}_{\boldsymbol{x}}) + \mathrm{d}\Gamma(\omega) + V(\boldsymbol{x}),$$

where $\boldsymbol{v}(\boldsymbol{\xi},\boldsymbol{x}) := \boldsymbol{\xi} - \mathrm{d}\Gamma(\boldsymbol{m}) - \varphi(\boldsymbol{G}_{\boldsymbol{x}})$. They act in $\widehat{\mathscr{H}}$ and $\mathscr{F}$, respectively. Essentially well-known, simple estimations reveal that they are closed on the domain $\widehat{\mathcal{D}}$, where

$$\widehat{\mathcal{D}} := \mathcal{D}(\mathrm{d}\Gamma(\boldsymbol{m})^2) \cap \mathcal{D}(\mathrm{d}\Gamma(\omega)), \quad \|\psi\|^2_{\widehat{\mathcal{D}}} := \|\psi\|^2 + \big\|\big(\tfrac{1}{2}\mathrm{d}\Gamma(\boldsymbol{m})^2 + \mathrm{d}\Gamma(\omega)\big)\psi\big\|^2; \quad (2)$$

cf. App. B of Ref. 3 and the references given there. If $\mathrm{div}\boldsymbol{G}_{\boldsymbol{x}} = 0$, then they are self-adjoint on $\widehat{\mathcal{D}}$. Moreover, $\mathbb{C}^2 \otimes \mathscr{C}[\mathfrak{d}_C]$ (resp. $\mathscr{C}[\mathfrak{d}_C]$) is an operator core.

Example 2.2. In the situation of Ex. 2.1 the SDE's involving $\widehat{H}^0(\boldsymbol{\xi},\boldsymbol{0})$ are of direct physical interest, as H^0 is unitarily equivalent to the direct integral $\int^{\oplus}_{\mathbb{R}^3} \widehat{H}^0(\boldsymbol{\xi},\boldsymbol{0})\mathrm{d}\boldsymbol{\xi}$.

3. Annihilation-preservation-creation processes and SDE's

In what follows, the interval I is either $[0,\mathcal{T}]$ with $0 < \mathcal{T} < \infty$ or $[0,\infty)$ and we fix a stochastic basis $\mathbb{B} := (\Omega, \mathfrak{F}, (\mathfrak{F}_t)_{t\in I}, \mathbb{P})$ satisfying the usual assumptions.[9] If $\mathscr{K}$ is a Hilbert space, then $\mathsf{S}_I(\mathscr{K})$ denotes the space of *continuous* $\mathscr{K}$-valued semi-martingales w.r.t. $\mathbb{B}$. The bold letter $\boldsymbol{B}$ denotes a $\mathbb{B}$-Brownian motion in $\mathbb{R}^3$ (with covariance matrix $\mathbb{1}$) and $\boldsymbol{X} \in \mathsf{S}_I(\mathbb{R}^3)$ is a solution of the Itô equation

$$\boldsymbol{X}_\bullet = \boldsymbol{q} + \boldsymbol{B}_\bullet + \int_0^\bullet \boldsymbol{\beta}(s, \boldsymbol{X}_s)\,\mathrm{d}s, \quad (3)$$

for some $\mathfrak{F}_0$-measurable $\boldsymbol{q} : \Omega \to \mathbb{R}^3$, under the following convention:

- If $I = [0,\mathcal{T}]$, then $\boldsymbol{\beta}(t,\boldsymbol{x}) = \frac{\boldsymbol{y}-\boldsymbol{x}}{\mathcal{T}-t}$, so that $\boldsymbol{X}$ is a Brownian bridge from $\boldsymbol{q}$ to $\boldsymbol{y}$.
- If $I = [0,\infty)$, then $\boldsymbol{\beta} : I \times \mathbb{R}^3 \to \mathbb{R}^3$ is continuous and $\boldsymbol{\beta}(t,\cdot)$ is globally Lipschitz continuous with Lipschitz constant L_t, where $[0,\infty) \ni t \mapsto L_t$ is non-decreasing.

Moreover, we always assume that $\mathbb{P}\{V(\boldsymbol{X}_\bullet) \in L^1_{\mathrm{loc}}(I)\} = 1$.

Definition 3.1. We define a process of isometries $\iota_t \colon \mathfrak{h} \to L^2(\mathbb{R}^4 \times \mathbb{Z}_2)$, $t \in \mathbb{R}$,

$$\iota_t f(k_0, \boldsymbol{k}, \lambda) := \pi^{-1/2} e^{-itk_0 - i\boldsymbol{m}\cdot(\boldsymbol{X}_t - \boldsymbol{X}_0)} \omega(\boldsymbol{k})^{1/2} (\omega(\boldsymbol{k})^2 + k_0^2)^{-1/2} f(\boldsymbol{k}, \lambda),$$

a.e. $(k_0, \boldsymbol{k}, \lambda) \in \mathbb{R}^4 \times \mathbb{Z}_2$. As usual ι^τ is ι stopped at τ, and we set $w_{\tau,t} := \overline{w}^*_{\tau,t}$ with

$$\overline{w}_{\tau,t} := (\iota^\tau_t)^* \iota_t = e^{-(t-\tau)\omega - i\boldsymbol{m}\cdot(\boldsymbol{X}_t - \boldsymbol{X}_\tau)}\, 1_{t>\tau} + 1_{t\leqslant\tau} : \Omega \to \mathscr{B}(\mathfrak{h}_C), \quad t, \tau \in I.$$

In the case $\boldsymbol{m} = \boldsymbol{0}$, the isometry ι_t has been introduced by Nelson.[11]

Definition 3.2 (Basic processes). *Let $\tau \in I$. Then we $\mathbb{P}$-a.s. define, for all $t \in I$,*

$$K_{\tau,t} := \int_0^t 1_{s>\tau}\, \iota_s \boldsymbol{G}_{\boldsymbol{X}_s}\, \mathrm{d}\boldsymbol{X}_s + \frac{1}{2}\int_0^t 1_{s>\tau}\, \iota_s(\mathrm{div}\boldsymbol{G}_{\boldsymbol{X}_s} - i\boldsymbol{m}\cdot\boldsymbol{G}_{\boldsymbol{X}_s})\,\mathrm{d}s,$$

as well as $K_t := K_{0,t}$, $U^-_{\tau,t} := (\iota^\tau_t)^* K_{\tau,t}$, $U^-_t := U^-_{0,t}$, $U^+_t := \iota^*_t K_t$, *and*

$$u^V_{\boldsymbol{\xi},t} := \frac{1}{2}\,\|K_t\|^2 + \int_0^t V(\boldsymbol{X}_s)\,\mathrm{d}s - i\boldsymbol{\xi}\cdot(\boldsymbol{X}_t - \boldsymbol{X}_0), \quad \boldsymbol{\xi}\in\mathbb{R}^3.$$

The process K defined above appears in Ref. 4. In the next definition $\exp\{\cdots\}$ abbreviates exponential series of operators which are strongly convergent on $\mathscr{C}[\mathfrak{h}]$.

Definition 3.3 (Annihilation-preservation-creation process). *We set*

$$\begin{aligned} W^V_{\boldsymbol{\xi},t}\,\zeta(h) &:= e^{-u^V_{-\boldsymbol{\xi},t}} \exp\{ia^\dagger(U^+_t)\}\,\Gamma(w_{0,t})\,\exp\{ia(U^-_t)\}\zeta(h) \\ &= e^{-u^V_{-\boldsymbol{\xi},t} - \langle U^-_t|h\rangle}\zeta\big(w_{0,t}\,h + U^+_t\big), \quad t\in I,\ h\in\mathfrak{d}_C, \end{aligned} \tag{4}$$

which, by linear extension, uniquely defines linear operators $W^V_{\boldsymbol{\xi},t}$ *on* $\mathscr{C}[\mathfrak{d}_C]$.

Proposition 3.1. *Let* $h\in\mathfrak{d}_C$. *Then* $W^V_{\boldsymbol{\xi}}\zeta(h)\in\mathsf{S}_I(\mathscr{F})$ *and,* $\mathbb{P}$*-a.s.,*

$$W^V_{\boldsymbol{\xi},\bullet}\zeta(h) = \zeta(h) - i\int_0^\bullet \boldsymbol{v}(\boldsymbol{\xi},\boldsymbol{X}_s)W^V_{\boldsymbol{\xi},s}\zeta(h)\mathrm{d}\boldsymbol{X}_s - \int_0^\bullet \widehat{H}^V_{\mathrm{scal}}(\boldsymbol{\xi},\boldsymbol{X}_s)W^V_{\boldsymbol{\xi},s}\zeta(h)\mathrm{d}s$$

on $[0,\sup I)$. *Moreover,* $\mathbb{P}$*-a.s., all operators* $W^V_{\boldsymbol{\xi},t}$, $t\in I$, *extend uniquely to elements of* $\mathscr{B}(\mathscr{F})$ *– again denoted by the same symbols – such that* $\|W^V_{\boldsymbol{\xi},t}\| \leqslant e^{-\int_0^t V(\boldsymbol{X}_s)\mathrm{d}s}$.

Proof. The expression in the second line of (4) is essentially an exponential function of basic processes. Moreover, it is possible to show that $U^\pm\in\mathsf{S}_I(\mathfrak{h}_C)$, $u^V_{\boldsymbol{0}}\in\mathsf{S}_I(\mathbb{R})$, and to represent these processes as stochastic integrals w.r.t. the process $(t,\boldsymbol{X}_t)_{t\in I}$. The Itô formula and the rules of stochastic calculus for *real* Hilbert spaces proved in Ref. 10 apply in this situation and eventually lead to the asserted SDE. In the computations we exploit that $\langle U^+|\boldsymbol{G}_{\boldsymbol{X}}\rangle$, $\langle U^+|\mathrm{div}\boldsymbol{G}_{\boldsymbol{X}}\rangle$, and $\langle U^+|i\boldsymbol{m}\cdot\boldsymbol{G}_{\boldsymbol{X}}\rangle$ are real as a consequence of (1). □

Remark 3.1. The adjoint of $W^0_{\boldsymbol{0},t}$ (with $\boldsymbol{m}=\boldsymbol{0}$) appears in Hiroshima's FK formula[4] for the scalar semi-group where it is represented as $W^{0\,*}_{\boldsymbol{0},t} = \Gamma(\iota^*_0)e^{-i\varphi(K_t)}\Gamma(\iota_t)$. As noted in Ref. 4, the isometries ι_t are not strongly differentiable w.r.t. t, which seems to prevent an application of Itô's formula at first sight. However, the application of Itô's formula to the more regular representation of $W^0_{\boldsymbol{0},t}$ as an annihilation-preservation-creation process is fairly straightforward.

Next, let $t\triangle_n := \{(s_1,\ldots,s_n)\in\mathbb{R}^n:\ 0\leqslant s_1\leqslant\ldots\leqslant s_n\leqslant t\}$. If $t_1,\ldots,t_n\in\mathbb{R}$ and $\mathcal{A}\subset[n]:=\{1,\ldots,n\}$, then we set $t_{\mathcal{A}} := (t_{a_1},\ldots,t_{a_m})$ where $\mathcal{A}=\{a_1,\ldots,a_m\}$, $a_1<\ldots<a_m$, and analogously for a multi-index $\alpha\in[3]^n=\{1,2,3\}^n$.

Definition 3.4 (Time-ordered integral processes). *Let* $t,t_1,\ldots,t_n\in I$, $\alpha\in[3]^n$, *and* $\mathcal{A},\mathcal{B}\subset[n]$. *We put* $\mathscr{L}^{\alpha_\varnothing}_t(t_\varnothing) := \mathscr{R}_{\alpha_\varnothing}(t_\varnothing) := \mathbb{1}$ *and, if* $\mathcal{A}\neq\varnothing\neq\mathcal{B}$,

$$\begin{aligned} \mathscr{L}^{\alpha_{\mathcal{A}}}_t(t_{\mathcal{A}}) &:= \prod_{a\in\mathcal{A}}\{a^\dagger(w_{t_a,t}F_{\alpha_a,\boldsymbol{X}_{t_a}}) + i\langle U^-_{t_a,t}|F_{\alpha_a,\boldsymbol{X}_{t_a}}\rangle\}, \\ \mathscr{R}_{\alpha_{\mathcal{B}}}(t_{\mathcal{B}}) &:= \prod_{b\in\mathcal{B}}\{a(\overline{w}_{0,t_b}F_{\alpha_b,\boldsymbol{X}_{t_b}}) + i\langle F_{\alpha_b,\boldsymbol{X}_{t_b}}|U^+_{t_b}\rangle\}, \end{aligned}$$

on $\mathscr{C}[\mathfrak{d}_C]$. *If* $\mathcal{C} \subset [n]$ *with* $\#\mathcal{C} \in 2\mathbb{N}_0$, *then we further set* $\mathscr{I}_{\alpha_\varnothing}(t_\varnothing) := 1$ *and*

$$\mathscr{I}_{\alpha_\mathcal{C}}(t_\mathcal{C}) := \sum_{\substack{\mathcal{C}=\cup\{c_p,c_p'\}\\ c_p<c_p'}} \prod_{p=1}^{\#\mathcal{C}/2} \langle F_{\alpha_{c_p'},\boldsymbol{x}_{t_{c_p'}}} | w_{t_{c_p},t_{c_p'}} F_{\alpha_{c_p},\boldsymbol{x}_{t_{c_p}}} \rangle, \quad \text{if } \mathcal{C} \neq \varnothing.$$

Here the sum runs over all possibilities to split $\mathcal{C}$ *into disjoint subsets* $\{c_p, c_p'\} \subset \mathcal{C}$ *with* $c_p < c_p'$, $p = 1, \ldots, \#\mathcal{C}/2$. *Writing* $dt_{[n]} := \mathrm{d}t_1 \ldots \mathrm{d}t_n$, *we finally define*

$$\mathbb{W}^{V,(n)}_{\boldsymbol{\xi},t}\psi := \sum_{\alpha\in[3]^n} \sigma_{\alpha_n} \ldots \sigma_{\alpha_1} \otimes \sum_{\substack{\mathcal{A}\cup\mathcal{B}\cup\mathcal{C}=[n]\\ \#\mathcal{C}\in 2\mathbb{N}_0}} \int_{t\triangle_n} \mathscr{I}_{\alpha_\mathcal{C}}(t_\mathcal{C})\, \mathscr{L}^{\alpha_\mathcal{A}}_t(t_\mathcal{A}) W^V_{\boldsymbol{\xi},t} \mathscr{R}_{\alpha_\mathcal{B}}(t_\mathcal{B})\, \psi\, \mathrm{d}t_{[n]},$$

for $\psi \in \mathbb{C}^2 \otimes \mathscr{C}[\mathfrak{d}_C]$, $n \in \mathbb{N}$, *and* $\mathbb{W}^{V,(0)}_{\boldsymbol{\xi},t} := \mathbb{1}_{\mathbb{C}^2} \otimes W^V_{\boldsymbol{\xi},t}$. *Here the second sum runs over all* disjoint *partitions of* $[n]$, *where* $\mathcal{A}$, $\mathcal{B}$, *or* $\mathcal{C}$ *may be empty and* $\#\mathcal{C}$ *is even.*

We can now state our fundamental existence and uniqueness result for the SDE associated with the generalized fiber Hamiltonian; recall that $\widehat{\mathcal{D}}$ is normed by (2).

Theorem 3.1. (a) $\mathbb{P}$-*a.s., all operators* $\mathbb{W}^{V,(n)}_{\boldsymbol{\xi},t}$ *with* $n \in \mathbb{N}_0$ *and* $t \in I$ *extend uniquely to elements of* $\mathscr{B}(\hat{\mathscr{H}})$, *which are henceforth again denoted by the same symbols. Furthermore,* $\mathbb{P}$-*a.s., the limit* $\mathbb{W}^V_{\boldsymbol{\xi},t} := \lim_{N\to\infty} \sum_{n=0}^N \mathbb{W}^{V,(n)}_{\boldsymbol{\xi},t}$ *exists in* $\mathscr{B}(\hat{\mathscr{H}})$ *locally uniformly in* $t \in I$, *and* $\|\mathbb{W}^V_{\boldsymbol{\xi},t}\| \leqslant e^{\mathfrak{c}t-\int_0^t V(\boldsymbol{X}_s)\mathrm{d}s}$ *with* $\mathfrak{c} \propto \sup_{\boldsymbol{x}} \|\omega^{-1/2}\boldsymbol{F}_{\boldsymbol{x}}\|^2$.
(b) *Let* $\eta : \Omega \to \widehat{\mathcal{D}}$ *be* $\mathfrak{F}_0$-*measurable. Then* $\mathbb{W}^V_{\boldsymbol{\xi}}\,\eta \in \mathsf{S}_I(\hat{\mathscr{H}})$ *and, up to indistinguishability,* $\mathbb{W}^V_{\boldsymbol{\xi}}\,\eta$ *is the unique element of* $\mathsf{S}_I(\hat{\mathscr{H}})$ *whose paths belong* $\mathbb{P}$-*a.s. to* $C(I, \widehat{\mathcal{D}})$ *and which* $\mathbb{P}$-*a.s. solves*

$$\mathscr{X}_\bullet = \eta - i\int_0^\bullet \boldsymbol{v}(\boldsymbol{\xi}, \boldsymbol{X}_s)\, \mathscr{X}_s\, \mathrm{d}\boldsymbol{X}_s - \int_0^\bullet \widehat{H}^V(\boldsymbol{\xi}, \boldsymbol{X}_s)\, \mathscr{X}_s\, \mathrm{d}s \quad \text{on } [0, \sup I). \tag{5}$$

If V is bounded and continuous, then we infer the following from Thm. 3.1:

- The existence of a stochastic flow for the system comprised of (3) and (5).
- The existence of a family of transition operators associated with the flow, which enjoys the Feller and Markov properties.
- A Blagoveščensky-Freidlin type theorem, i.e., the existence of strong solutions.

4. Feynman-Kac representations

The construction of $\mathbb{W}^V_{\boldsymbol{\xi}}$ depends on the choice of $\boldsymbol{X}$. Since we are dealing with different choices of $\boldsymbol{X}$ at the same time in this section, we indicate this by adding the variable $[\boldsymbol{X}]$ to the symbol $\mathbb{W}^V_{\boldsymbol{\xi}}$.

Theorem 4.1 (FK formula: fiber case). *Assume that* $\boldsymbol{G}$ *and* $\boldsymbol{F}$ *do not depend on* $\boldsymbol{x}$, *and let* $\boldsymbol{\xi} \in \mathbb{R}^3$ *and* $t \geqslant 0$. *Then* $e^{-t\widehat{H}^0(\boldsymbol{\xi},\boldsymbol{0})} = \mathbb{E}[\mathbb{W}^0_{\boldsymbol{\xi},t}[\boldsymbol{B}]^*]$.

Remark 4.1. In the earlier literature FK formulas for fiber Hamiltonians have been deduced from the FK formula for the total Hamiltonian by inserting suitable peak functions.[5,6,8] By a standard procedure, based on Thm. 3.1, we are able to avoid this detour and treat the fiber case directly. For non-zero $\boldsymbol{F}$, Thm. 4.1 is new as the earlier formulas involved an additional regularization procedure;[6,8] compare Rem. 4.2 (a) below.

For $\boldsymbol{x},\boldsymbol{y}\in\mathbb{R}^3$, we set $\boldsymbol{B}^{\boldsymbol{x}}:=\boldsymbol{x}+\boldsymbol{B}$ and let $\boldsymbol{b}^{t;\boldsymbol{y},\boldsymbol{x}}\in\mathsf{S}_{[0,t]}(\mathbb{R}^3)$ denote the Brownian bridge from $\boldsymbol{y}$ to $\boldsymbol{x}$ in time $t>0$, defined as the solution of $\boldsymbol{b}_\bullet=\boldsymbol{B}^{\boldsymbol{y}}_\bullet+\int_0^\bullet\frac{\boldsymbol{x}-\boldsymbol{b}_s}{t-s}\mathrm{d}s$.

Theorem 4.2 (FK formula). *Assume that $V=V_+-V_-$, where $V_\pm:\mathbb{R}^3\to[0,\infty)$ such that $V_+\in L^1_{\mathrm{loc}}(\mathbb{R}^3)$ and V_- is $-\frac{1}{2}\Delta$-form bounded with form bound $b\leqslant 1$. Then $\Psi\in\mathcal{Q}(H^{V_+})\subset\mathscr{H}=L^2(\mathbb{R}^3,\hat{\mathscr{H}})$ implies $\|\Psi(\cdot)\|=\|\Psi(\cdot)\|_{\hat{\mathscr{H}}}\in\mathcal{Q}(-\frac{1}{2}\Delta+V_+)$ with*

$$\big\langle\|\Psi(\cdot)\|\big|(-\tfrac{1}{2}\Delta+V_+)\|\Psi(\cdot)\|\big\rangle\leqslant\big\langle\Psi\big|\big(H^{V_+}+\mathfrak{c}\sup_{\boldsymbol{x}}\|\omega^{-1/2}\boldsymbol{F}_{\boldsymbol{x}}\|^2\big)\Psi\big\rangle.\qquad(6)$$

In particular, V_- is H^{V_+}-form bounded with form bound b as well, so that H^V has a distinguished self-adjoint realization defined via quadratic forms (which is again denoted by H^V). For all $t>0$, $\Psi\in\mathscr{H}$, and a.e. $\boldsymbol{x}\in\mathbb{R}^3$, we then have

$$(e^{-tH^V}\Psi)(\boldsymbol{x})=\mathbb{E}\big[\mathbb{W}^V_{\boldsymbol{0},t}[\boldsymbol{B}^{\boldsymbol{x}}]^*\Psi(\boldsymbol{B}^{\boldsymbol{x}}_t)\big]=\int_{\mathbb{R}^3}\frac{e^{-|\boldsymbol{x}-\boldsymbol{y}|^2/2t}}{(2\pi t)^{3/2}}\mathbb{E}\big[\mathbb{W}^V_{\boldsymbol{0},t}[\boldsymbol{b}^{t;\boldsymbol{y},\boldsymbol{x}}]\big]\Psi(\boldsymbol{y})\mathrm{d}\boldsymbol{y}.\quad(7)$$

Proof. Let $V\in C(\mathbb{R}^3)$ be bounded. Employing (inter alia) the Markov property of the stochastic flow we check that $(T_t\Psi)(\boldsymbol{x}):=\mathbb{E}[\mathbb{W}^V_{\boldsymbol{0},t}[\boldsymbol{B}^{\boldsymbol{x}}]^*\Psi(\boldsymbol{B}^{\boldsymbol{x}}_t)]$ defines a strongly continuous semi-group of self-adjoint operators $T_t\in\mathscr{B}(\mathscr{H})$. Then we use (5) to verify that the generator of this semi-group agrees with H^V on a suitable core of H^V. This yields the first identity in (7) and the second one follows from Thm. 3.1 and well-known relations for Brownian motions and Brownian bridges. Invoking standard extension procedures we then get (6) and (7) for general V. □

Remark 4.2. (a) In the scalar case ($\boldsymbol{F}=\boldsymbol{0}$), and under slightly more restrictive conditions on $\boldsymbol{G}$, the first equality in (7) has been proved by F. Hiroshima in Ref. 4 while the second one is new. For a spin-1/2 electron, the sesqui-linear form of the semi-group has been represented earlier only as a *limit* of expectation values of certain *regularized* FK integrands involving a Poisson jump process to account for the spin degrees of freedom.[6] Hence, both identities in (7) are new for non-zero $\boldsymbol{F}$.
(b) The assumptions of Thm. 4.2 imply $\mathbb{P}\{V(\boldsymbol{B}^{\boldsymbol{x}}_\bullet)\in L^1_{\mathrm{loc}}([0,\infty))\}=1$, for a.e. $\boldsymbol{x}$.
(c) In Thm. 4.2, the integral $\mathbb{E}\big[\mathbb{W}^V_{\boldsymbol{0},t}[\boldsymbol{b}^{t;\boldsymbol{y},\boldsymbol{x}}]\big]\in\mathscr{B}(\hat{\mathscr{H}})$ is defined only for a.e. $(\boldsymbol{x},\boldsymbol{y})\in\mathbb{R}^6$. The condition on V of Thm. 4.3 implies its existence for *all* $\boldsymbol{x},\boldsymbol{y}\in\mathbb{R}^3$.
(d) The condition on V_- in Thm. 4.2 ensures the validity of the FK formula for the Schrödinger operator with potential V_-,[12] which is what we really use in the proof.

Let us announce the next theorem as a first application. Its proof combines arguments from Ref. 1 with certain weighted estimates on $\mathbb{W}^0_{\boldsymbol{0},t}$ inferred from Thm. 3.1. Here the weights are given by unbounded functions of $\mathrm{d}\Gamma(\omega)$.

Theorem 4.3. *Assume that $V = V_+ - V_-$, where $V_- \geqslant 0$ belongs to the Kato class and $V_+ \geqslant 0$ is in the local Kato class. Then the following map is continuous w.r.t. the norm topology on $\mathscr{B}(\hat{\mathscr{H}})$,*

$$(0,\infty) \times \mathbb{R}^3 \times \mathbb{R}^3 \ni (t, \boldsymbol{x}, \boldsymbol{y}) \longmapsto \mathbb{E}\big[\mathbb{W}^V_{\mathbf{0},t}[\boldsymbol{b}^{t;\boldsymbol{y},\boldsymbol{x}}]\big] \in \mathscr{B}(\hat{\mathscr{H}}).$$

Remark 4.3. **(a)** All results presented above hold true for several electrons as well. **(b)** Suitable analogs of all results stated here are available for Nelson's model.

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