

Picard Approximation of the Matrix Elements of Quantum Stochastic Differential Equations and Quantum Flows and Basic Error Estimates

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Abstract

We describe Picard approximation schemes for the computation of the matrix elements of solutions of unitary quantum stochastic evolutions and associated quantum flows. We also provide some basic error estimates for the convergence of the approximation schemes presented. A combination of numerical and symbolic computation is required.

1 Quantum Stochastic Calculus

Let $B_t = \{B_t(\omega)/\omega \in \Omega\}$, $t \geq 0$, be one-dimensional Brownian motion. Integration with respect to B_t was defined by Itô in [3]. A basic result of the theory is that stochastic integral equations of the form

$$X_t = X_0 + \int_0^t b(s, X_s) ds + \int_0^t \sigma(s, X_s) dB_s$$

can be viewed as stochastic differential equations of the form

$$dX_t = b(t, X_t) dt + \sigma(t, X_t) dB_t$$

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where differentials are handled with the use of Itô's formula

$$(dB_t)^2 = dt, \quad dB_t dt = dt dB_t = (dt)^2 = 0 .$$

In [2], Hudson and Parthasarathy obtained a Fock space representation of Brownian motion and Poisson process.

Definition 1.1. *The Boson Fock space $\Gamma = \Gamma(L^2(\mathbb{R}_+, \mathcal{C}))$ over $L^2(\mathbb{R}_+, \mathcal{C})$ is the Hilbert space completion of the linear span of the exponential vectors $\psi(f)$ under the inner product*

$$\langle \psi(f), \psi(g) \rangle = e^{\langle f, g \rangle}$$

where $f, g \in L^2(\mathbb{R}_+, \mathcal{C})$ and $\langle f, g \rangle = \int_0^{+\infty} \bar{f}(s) g(s) ds$ where, here and in what follows, \bar{z} denotes the complex conjugate of $z \in \mathbb{C}$.

The annihilation, creation and conservation operators $A(f)$, $A^\dagger(f)$ and $\Lambda(F)$ respectively, are defined on the exponential vectors $\psi(g)$ of Γ as follows.

Definition 1.2.

$$A_t \psi(g) = \int_0^t g(s) ds \psi(g); \quad A_t^\dagger \psi(g) = \frac{\partial}{\partial \epsilon} \Big|_{\epsilon=0} \psi(g + \epsilon \chi_{[0,t]}); \quad \Lambda_t \psi(g) = \frac{\partial}{\partial \epsilon} \Big|_{\epsilon=0} \psi(e^{\epsilon \chi_{[0,t]}} g) .$$

The basic quantum stochastic differentials dA_t , dA_t^\dagger , and $d\Lambda_t$ are defined as follows.

Definition 1.3.

$$dA_t = A_{t+dt} - A_t; \quad dA_t^\dagger = A_{t+dt}^\dagger - A_t^\dagger; \quad d\Lambda_t = \Lambda_{t+dt} - \Lambda_t .$$

The fundamental result which connects classical with quantum stochastics is that the processes B_t and P_t defined by

$$B_t = A_t + A_t^\dagger; \quad P_t = \Lambda_t + \sqrt{\lambda}(A_t + A_t^\dagger) + \lambda t$$

are identified through their vacuum characteristic functions

$$\langle \psi(0), e^{i s B_t} \psi(0) \rangle = e^{-\frac{s^2}{2} t}; \quad \langle \psi(0), e^{i s P_t} \psi(0) \rangle = e^{\lambda (e^{i s} - 1) t}$$

with Brownian motion and Poisson process of intensity λ respectively.

Hudson and Parthasarathy defined stochastic integration with respect to the noise differentials of Definition 3 and obtained the Itô multiplication table

\cdot	dA_t^\dagger	$d\Lambda_t$	dA_t	dt
dA_t^\dagger	0	0	0	0
$d\Lambda_t$	dA_t^\dagger	$d\Lambda_t$	0	0
dA_t	dt	dA_t	0	0
dt	0	0	0	0

Within the framework of Hudson-Parthasarathy Quantum Stochastic Calculus, classical quantum mechanical evolution equations take the form

$$dU_t = - \left(\left(iH + \frac{1}{2} L^* L \right) dt + L^* W dA_t - L dA_t^\dagger + (I - W) d\Lambda_t \right) U_t; U_0 = I, \tag{1.1}$$

where, for each $t \geq 0$, U_t is a unitary operator defined on the tensor product $\mathcal{H} \otimes \Gamma(L^2(\mathbb{R}_+, \mathcal{C}))$ of a system Hilbert space \mathcal{H} and the noise (or reservoir) Fock space Γ . Here H, L, W are in $\mathcal{B}(\mathcal{H})$, the space of bounded linear operators on \mathcal{H} , with W unitary and H self-adjoint. In all cases, I denotes the appropriate identity operator. Here and in what follows we identify time-independent, bounded, system space operators X with their ampliation $X \otimes I$ to $\mathcal{H} \otimes \Gamma(L^2(\mathbb{R}_+, \mathcal{C}))$. As in [2], all Hilbert space inner products are linear on the right.

The quantum stochastic differential equation satisfied by the *quantum flow*

$$j_t(X) = U_t^* X U_t \tag{1.2}$$

where X is a bounded system space operator, is

$$\begin{aligned} dj_t(X) &= j_t \left(i [H, X] - \frac{1}{2} (L^* L X + X L^* L - 2L^* X L) \right) dt \\ &\quad + j_t ([L^*, X] W) dA_t + j_t (W^* [X, L]) dA_t^\dagger + j_t (W^* X W - X) d\Lambda_t, \\ j_0(X) &= X, \quad t \in [0, T]. \end{aligned}$$

The commutation relations associated with the operator processes A_t, A_t^\dagger are the Canonical (or Heisenberg) Commutation Relations (CCR), namely

$$[A_t, A_t^\dagger] = t I.$$

Applications of quantum stochastic calculus to the control of quantum evolutions and Langevin equations (quantum flows) can be found, for example, in [1] and the references within it. However, to the author's best knowledge, no work has been done in the direction of performing actual numerical

computations, most likely with the use of a computer. That would require the implementation of suitable algorithms whose reliability depends on the existence of good norm estimates. It is that gap that this paper aspires to close.

2 Matrix Elements and Approximation Schemes

The fundamental theorems of the Hudson-Parthasarathy quantum stochastic calculus give formulas for expressing the matrix elements of quantum stochastic integrals in terms of ordinary Riemann-Lebesgue integrals.

Theorem 2.1. *Let*

$$M(t) = \int_0^t E(s) d\Lambda(s) + F(s) dA(s) + G(s) dA^\dagger(s) + H(s) ds$$

where E, F, G, H are adapted processes. Let also $u \otimes \psi(f)$ and $v \otimes \psi(g)$ be in the exponential domain of $\mathcal{H} \otimes \Gamma$. Then

$$\begin{aligned} &< u \otimes \psi(f), M(t) v \otimes \psi(g) > = \\ &\int_0^t < u \otimes \psi(f), (\bar{f}(s) g(s) E(s) + g(s) F(s) + \bar{f}(s) G(s) + H(s)) v \otimes \psi(g) > ds . \end{aligned}$$

Proof. See Theorem 4.1 of [2]. □

Theorem 2.2. *Let*

$$M(t) = \int_0^t E(s) d\Lambda(s) + F(s) dA(s) + G(s) dA^\dagger(s) + H(s) ds$$

and

$$M'(t) = \int_0^t E'(s) d\Lambda(s) + F'(s) dA(s) + G'(s) dA^\dagger(s) + H'(s) ds$$

where $E, F, G, H, E', F', G', H'$ are adapted processes. Let also $u \otimes \psi(f)$ and $v \otimes \psi(g)$ be in the exponential domain of $\mathcal{H} \otimes \Gamma$. Then

$$\begin{aligned} &< M(t) u \otimes \psi(f), M'(t) v \otimes \psi(g) > = \\ &\int_0^t (< M(s) u \otimes \psi(f), (\bar{f}(s) g(s) E'(s) + g(s) F'(s) + \bar{f}(s) G'(s) + H'(s)) v \otimes \psi(g) > \\ &+ < (\bar{g}(s) f(s) E(s) + f(s) F(s) + \bar{g}(s) G(s) + H(s)) u \otimes \psi(f), M'(s) v \otimes \psi(g) > \\ &+ < (f(s) E(s) + G(s)) u \otimes \psi(f), (g(s) E'(s) + G'(s)) v \otimes \psi(g) >) ds . \end{aligned}$$

Proof. See Theorem 4.3 of [2]. □

We are interested in defining approximation schemes which can be used to compute the matrix elements

$$\langle u \otimes \psi(f), U_t v \otimes \psi(g) \rangle, \quad \langle u \otimes \psi(f), j_t(X) v \otimes \psi(g) \rangle$$

related to the quantum flow (1.2) and the Hudson-Parthasarathy stochastic differential equation

$$dU_t = \left(K dt + B dA_t + C dA_t^\dagger + D d\Lambda_t \right) U_t; \quad U_0 = I \quad (2.3)$$

with initial condition where $t \in [0, T]$ for some $T > 0$, and K, B, C, D are bounded system space operators of the form appearing in (1.1), i.e

$$K = - \left(iH + \frac{1}{2} L^* L \right); \quad B = -L^* W; \quad C = L; \quad D = W - I.$$

2.1 Unitary Evolutions

Equation (2.3) has the integral form

$$U_t = I + \int_0^t K U_s ds + B U_s dA_s + C U_s dA_s^\dagger + D U_s d\Lambda_s \quad (2.4)$$

defined (see [2], Proposition 7.1) as the $[0, T]$ -uniform limit of the sequence $U_n = \{U_{n,t} / t \geq 0\}$ defined recursively on the exponential domain of $\mathcal{H} \otimes \Gamma$ by

$$U_{0,t} = I \quad (2.5)$$

and, for $n \geq 1$,

$$U_{n,t} = I + \int_0^t K U_{n-1,s} ds + B U_{n-1,s} dA_s + C U_{n-1,s} dA_s^\dagger + D U_{n-1,s} d\Lambda_s. \quad (2.6)$$

By Theorem 1, the matrix elements of (2.6) are given, for $n \geq 1$, by the recursion scheme

$$\begin{aligned} & \langle u \otimes \psi(f), U_{n,t} v \otimes \psi(g) \rangle \quad (2.7) \\ & = \langle u \otimes \psi(f), v \otimes \psi(g) \rangle + \int_0^t (\bar{f}(s)g(s) \langle u \otimes \psi(f), D U_{n-1,s} v \otimes \psi(g) \rangle \\ & + g(s) \langle u \otimes \psi(f), B U_{n-1,s} v \otimes \psi(g) \rangle + \bar{f}(s) \langle u \otimes \psi(f), C U_{n-1,s} v \otimes \psi(g) \rangle \\ & + \langle u \otimes \psi(f), K U_{n-1,s} v \otimes \psi(g) \rangle) ds. \end{aligned}$$

Letting

$$u_{D^*} = D^*u; u_{B^*} = B^*u; u_{C^*} = C^*u; u_{K^*} = K^*u$$

we can rewrite approximation scheme (2.7) as:

Approximation Scheme 1. (*Unitary Evolution*)

$$\begin{aligned} & \langle u \otimes \psi(f), U_{n,t} v \otimes \psi(g) \rangle = & (2.8) \\ & \langle u \otimes \psi(f), v \otimes \psi(g) \rangle + \int_0^t (\bar{f}(s)g(s) \langle u_{D^*} \otimes \psi(f), U_{n-1,s} v \otimes \psi(g) \rangle \\ & + g(s) \langle u_{B^*} \otimes \psi(f), U_{n-1,s} v \otimes \psi(g) \rangle + \bar{f}(s) \langle u_{C^*} \otimes \psi(f), U_{n-1,s} v \otimes \psi(g) \rangle \\ & + \langle u_{K^*} \otimes \psi(f), U_{n-1,s} v \otimes \psi(g) \rangle) ds \end{aligned}$$

with

$$\langle u \otimes \psi(f), U_{0,t} v \otimes \psi(g) \rangle = \langle u \otimes \psi(f), v \otimes \psi(g) \rangle .$$

The limit form of (2.8) as $n \rightarrow +\infty$ is:

$$\begin{aligned} & \langle u \otimes \psi(f), U_t v \otimes \psi(g) \rangle = \\ & \langle u \otimes \psi(f), v \otimes \psi(g) \rangle + \int_0^t (\bar{f}(s)g(s) \langle u_{D^*} \otimes \psi(f), U_s v \otimes \psi(g) \rangle \\ & + g(s) \langle u_{B^*} \otimes \psi(f), U_s v \otimes \psi(g) \rangle + \bar{f}(s) \langle u_{C^*} \otimes \psi(f), U_s v \otimes \psi(g) \rangle \\ & + \langle u_{K^*} \otimes \psi(f), U_s v \otimes \psi(g) \rangle) ds \end{aligned}$$

which, by subtraction of the cases $t = t_n$ and $t = t_{n-1}$ where $t_{n-1} \leq t_n$, implies

$$\begin{aligned} & \langle u \otimes \psi(f), U_{t_n} v \otimes \psi(g) \rangle - \langle u \otimes \psi(f), U_{t_{n-1}} v \otimes \psi(g) \rangle \\ & = \int_{t_{n-1}}^{t_n} (\bar{f}(s)g(s) \langle u_{D^*} \otimes \psi(f), U_s v \otimes \psi(g) \rangle + g(s) \langle u_{B^*} \otimes \psi(f), U_s v \otimes \psi(g) \rangle \\ & + \bar{f}(s) \langle u_{C^*} \otimes \psi(f), U_s v \otimes \psi(g) \rangle + \langle u_{K^*} \otimes \psi(f), U_s v \otimes \psi(g) \rangle) ds , \end{aligned}$$

or as:

Approximation Scheme 2. (*Time Approximation of Unitary Evolution*)

$$\begin{aligned} & \langle u \otimes \psi(f), U_{t_n} v \otimes \psi(g) \rangle = \\ & \langle u \otimes \psi(f), U_{t_{n-1}} v \otimes \psi(g) \rangle + \int_{t_{n-1}}^{t_n} (\bar{f}(s)g(s) \langle u_{D^*} \otimes \psi(f), U_s v \otimes \psi(g) \rangle \\ & + g(s) \langle u_{B^*} \otimes \psi(f), U_s v \otimes \psi(g) \rangle + \bar{f}(s) \langle u_{C^*} \otimes \psi(f), U_s v \otimes \psi(g) \rangle \\ & + \langle u_{K^*} \otimes \psi(f), U_s v \otimes \psi(g) \rangle) ds . \end{aligned}$$

2.2 Quantum Flows

The integral form of the quantum flow equation (1.2) is

$$j_t(X) = X + \int_0^t j_s(\hat{K}) ds + j_s(\hat{B}) dA_s + j_s(\hat{C}) dA_s^\dagger + j_s(\hat{D}) d\Lambda_s$$

where

$$\hat{K} = i[H, X] - \frac{1}{2}(L^* LX + XL^* L - 2L^* XL); \hat{B} = [L^*, X]W; \hat{C} = W^*[X, L]; \hat{D} = W^* X W - X.$$

The corresponding approximation scheme is

$$j_{0,t}(X) = X \quad (2.9)$$

and for $n \geq 1$

$$j_{n,t}(X) = X + \int_0^t j_{n-1,s}(\hat{K}) ds + j_{n-1,s}(\hat{B}) dA_s + j_{n-1,s}(\hat{C}) dA_s^\dagger + j_{n-1,s}(\hat{D}) d\Lambda_s. \quad (2.10)$$

The matrix element form of the approximation scheme (2.9) and (2.10) is

$$\begin{aligned} & \langle u \otimes \psi(f), j_{n,t}(X) v \otimes \psi(g) \rangle = \langle u \otimes \psi(f), X v \otimes \psi(g) \rangle + \quad (2.11) \\ & \langle u \otimes \psi(f), \left(\int_0^t j_{n-1,s}(\hat{K}) ds + j_{n-1,s}(\hat{B}) dA_s + j_{n-1,s}(\hat{C}) dA_s^\dagger + j_{n-1,s}(\hat{D}) d\Lambda_s \right) v \otimes \psi(g) \rangle \end{aligned}$$

which by Theorem 1 yields:

Approximation Scheme 3. (*General Quantum Flow*)

$$\begin{aligned} & \langle u \otimes \psi(f), j_{n,t}(X) v \otimes \psi(g) \rangle = \langle u \otimes \psi(f), X v \otimes \psi(g) \rangle \\ & + \int_0^t \left(\bar{f}(s)g(s) \langle u \otimes \psi(f), j_{n-1,s}(\hat{D}) v \otimes \psi(g) \rangle + g(s) \langle u \otimes \psi(f), j_{n-1,s}(\hat{B}) v \otimes \psi(g) \rangle \right. \\ & \left. + \bar{f}(s) \langle u \otimes \psi(f), j_{n-1,s}(\hat{C}) v \otimes \psi(g) \rangle + \langle u \otimes \psi(f), j_{n-1,s}(\hat{K}) v \otimes \psi(g) \rangle \right) ds. \end{aligned}$$

Notice that for $n = 1$ recursion (2.11) becomes

$$\begin{aligned}
& \langle u \otimes \psi(f), j_{1,t}(X) v \otimes \psi(g) \rangle \\
&= \langle u \otimes \psi(f), X v \otimes \psi(g) \rangle + \langle u \otimes \psi(f), \left(\int_0^t \hat{K} ds + \hat{B} dA_s + \hat{C} dA_s^\dagger + \hat{D} d\Lambda_s \right) v \otimes \psi(g) \rangle \\
&= \langle u \otimes \psi(f), X v \otimes \psi(g) \rangle + \int_0^t \left(\bar{f}(s)g(s) \langle u \otimes \psi(f), \hat{D} v \otimes \psi(g) \rangle \right. \\
&\quad \left. + g(s) \langle u \otimes \psi(f), \hat{B} v \otimes \psi(g) \rangle + \bar{f}(s) \langle u \otimes \psi(f), \hat{C} v \otimes \psi(g) \rangle + \langle u \otimes \psi(f), \hat{K} v \otimes \psi(g) \rangle \right) ds \\
&= \langle u \otimes \psi(f), X v \otimes \psi(g) \rangle + \int_0^t \left(\bar{f}(s)g(s) \langle u_{\hat{D}} \otimes \psi(f), v \otimes \psi(g) \rangle \right. \\
&\quad \left. + g(s) \langle u_{\hat{B}} \otimes \psi(f), v \otimes \psi(g) \rangle + \bar{f}(s) \langle u_{\hat{C}} \otimes \psi(f), v \otimes \psi(g) \rangle + \langle u_{\hat{K}} \otimes \psi(f), v \otimes \psi(g) \rangle \right) ds
\end{aligned}$$

and so, letting $u_{X^*} = X^* u$, we have

$$\begin{aligned}
& \langle u \otimes \psi(f), j_{1,t}(X) v \otimes \psi(g) \rangle \\
&= \langle u_{X^*} \otimes \psi(f), v \otimes \psi(g) \rangle + \int_0^t \bar{f}(s)g(s) ds \langle u_{\hat{D}} \otimes \psi(f), v \otimes \psi(g) \rangle \\
&\quad + \int_0^t g(s) ds \langle u_{\hat{B}} \otimes \psi(f), v \otimes \psi(g) \rangle + \int_0^t \bar{f}(s) ds \langle u_{\hat{C}} \otimes \psi(f), v \otimes \psi(g) \rangle \\
&\quad + \int_0^t ds \langle u_{\hat{K}} \otimes \psi(f), v \otimes \psi(g) \rangle .
\end{aligned}$$

The general theory of quantum flows, in the context of Hudson-Parthasarathy calculus, can be found in [4]. We now consider flows $\{j_t(X) / t \geq 0\}$ of the standard quantum mechanical form

$$j_t(X) = U_t^* X U_t$$

where U_t is, for each $t \geq 0$, a unitary operator.

Proposition 2.3. *Let X be a bounded system space operator, let U_t and $U_{n,t}$ be, for each $t \in [0, T]$ and $n \geq 1$, as in (2.4) and (2.6) respectively, and let U_t^* and $U_{n,t}^*$ be their adjoints. If*

$$j_t(X) = U_t^* X U_t$$

and

$$j_{n,t}(X) = U_{n,t}^* X U_{n,t} \tag{2.12}$$

then

$$\lim_{n \rightarrow \infty} \langle u \otimes \psi(f), j_{n,t}(X) v \otimes \psi(g) \rangle = \langle u \otimes \psi(f), j_t(X) v \otimes \psi(g) \rangle$$

for all $u \otimes \psi(f)$ and $v \otimes \psi(g)$ in the exponential domain of $\mathcal{H} \otimes \Gamma$. Convergence is uniform on $[0, T]$.

Proof. We have

$$\begin{aligned} & | \langle u \otimes \psi(f), j_t(X) v \otimes \psi(g) \rangle - \langle u \otimes \psi(f), j_{n,t}(X) v \otimes \psi(g) \rangle | \\ &= | \langle u \otimes \psi(f), (j_t(X) - j_{n,t}(X)) v \otimes \psi(g) \rangle | \\ &= | \langle u \otimes \psi(f), (U_t^* X U_t - U_{n,t}^* X U_{n,t}) v \otimes \psi(g) \rangle | \\ &= | \langle u \otimes \psi(f), ((U_t^* - U_{n,t}^*) X U_t + U_{n,t}^* X (U_t - U_{n,t})) v \otimes \psi(g) \rangle | \\ &\leq | \langle u \otimes \psi(f), (U_t^* - U_{n,t}^*) X U_t v \otimes \psi(g) \rangle | + | \langle u \otimes \psi(f), U_{n,t}^* X (U_t - U_{n,t}) v \otimes \psi(g) \rangle | \\ &= | \langle (U_t - U_{n,t}) u \otimes \psi(f), X U_t v \otimes \psi(g) \rangle | + | \langle U_{n,t} u \otimes \psi(f), X (U_t - U_{n,t}) v \otimes \psi(g) \rangle | \\ &\leq \| (U_t - U_{n,t}) u \otimes \psi(f) \| \| X \| \| U_t \| \| v \otimes \psi(g) \| + \| U_{n,t} u \otimes \psi(f) \| \| X \| \| (U_t - U_{n,t}) v \otimes \psi(g) \| \\ &\leq \| (U_t - U_{n,t}) u \otimes \psi(f) \| \| X \| \| v \otimes \psi(g) \| + \| U_{n,t} u \otimes \psi(f) \| \| X \| \| (U_t - U_{n,t}) v \otimes \psi(g) \| \end{aligned}$$

since $\|U_t\| = 1$. Since $U_{n,t}$ converges to U_t on the exponential domain of $\mathcal{H} \otimes \Gamma$ uniformly with respect to t and $\|U_{n,t} u \otimes \psi(f)\|$ is bounded, it follows that

$$| \langle u \otimes \psi(f), j_{n,t}(X) v \otimes \psi(g) \rangle - \langle u \otimes \psi(f), j_t(X) v \otimes \psi(g) \rangle | \rightarrow 0$$

as $n \rightarrow +\infty$. □

The approximation scheme for the matrix element associated with (2.12) is

obtained, with the use of Theorems 1 and 2 as follows:

$$\begin{aligned}
& \langle u \otimes \psi(f), U_{n,t}^* X U_{k,t} v \otimes \psi(g) \rangle = \langle U_{n,t} u \otimes \psi(f), X U_{k,t} v \otimes \psi(g) \rangle \\
& = \langle \left(I + \int_0^t K U_{n-1,s} ds + B U_{n-1,s} dA_s + C U_{n-1,s} dA_s^\dagger + D U_{n-1,s} d\Lambda_s \right) u \otimes \psi(f), \\
& X \left(I + \int_0^t K U_{k-1,s} ds + B U_{k-1,s} dA_s + C U_{k-1,s} dA_s^\dagger + D U_{k-1,s} d\Lambda_s \right) v \otimes \psi(g) \rangle \\
& = \langle u \otimes \psi(f), (X v) \otimes \psi(g) \rangle + \\
& + \langle u \otimes \psi(f), \left(\int_0^t X K U_{k-1,s} ds + X B U_{k-1,s} dA_s + X C U_{k-1,s} dA_s^\dagger + X D U_{k-1,s} d\Lambda_s \right) v \otimes \psi(g) \rangle \\
& + \langle \left(\int_0^t K U_{n-1,s} ds + B U_{n-1,s} dA_s + C U_{n-1,s} dA_s^\dagger + D U_{n-1,s} d\Lambda_s \right) u \otimes \psi(f), (X v) \otimes \psi(g) \rangle \\
& + \langle \left(\int_0^t K U_{n-1,s} ds + B U_{n-1,s} dA_s + C U_{n-1,s} dA_s^\dagger + D U_{n-1,s} d\Lambda_s \right) u \otimes \psi(f),
\end{aligned}$$

$$\begin{aligned}
& \left(\int_0^t X K U_{k-1,s} ds + X B U_{k-1,s} dA_s + X C U_{k-1,s} dA_s^\dagger + X D U_{k-1,s} d\Lambda_s \right) v \otimes \psi(g) \rangle \\
& = \langle u \otimes \psi(f), (X v) \otimes \psi(g) \rangle \\
& + \int_0^t \langle u \otimes \psi(f), (\bar{f}(s) g(s) X D + g(s) X B + \bar{f}(s) X C + X K) U_{k-1,s} v \otimes \psi(g) \rangle ds \\
& + \int_0^t \langle (\bar{g}(s) f(s) X^* D + f(s) X^* B + \bar{g}(s) X^* C + X^* K) U_{k-1,s} u \otimes \psi(f), v \otimes \psi(g) \rangle ds \\
& + \int_0^t \langle (U_{n,s} - 1) u \otimes \psi(f), (\bar{f}(s) g(s) X D + g(s) X B + \bar{f}(s) X C + X K) U_{k-1,s} v \otimes \psi(g) \rangle \\
& + \langle (\bar{g}(s) f(s) D + f(s) B + \bar{g}(s) C + K) U_{n-1,s} u \otimes \psi(f), X (U_{k,s} - 1) v \otimes \psi(g) \rangle \\
& + \langle (f(s) D + C) U_{n-1,s} u \otimes \psi(f), (g(s) X D + X C) U_{k-1,s} v \otimes \psi(g) \rangle ds .
\end{aligned}$$

Using (2.6) we obtain:

Approximation Scheme 4. (*Quantum Mechanical Flows*) For $n, k \geq 1$

$$\begin{aligned}
 & \langle u \otimes \psi(f), U_{n,t}^* X U_{k,t} v \otimes \psi(g) \rangle = \langle u \otimes \psi(f), (X v) \otimes \psi(g) \rangle \quad (2.13) \\
 & + \int_0^t (\bar{f}(s) g(s) \langle u \otimes \psi(f), U_{n,s}^* X D U_{k-1,s} v \otimes \psi(g) \rangle \\
 & + g(s) \langle u \otimes \psi(f), U_{n,s}^* X B U_{k-1,s} v \otimes \psi(g) \rangle \\
 & + \bar{f}(s) \langle u \otimes \psi(f), U_{n,s}^* X C U_{k-1,s} v \otimes \psi(g) \rangle + \langle u \otimes \psi(f), U_{n,s}^* X K U_{k-1,s} v \otimes \psi(g) \rangle \\
 & + \bar{f}(s) g(s) \langle u \otimes \psi(f), U_{n-1,s}^* D^* X U_{k,s} v \otimes \psi(g) \rangle + \bar{f}(s) \langle u \otimes \psi(f), U_{n-1,s}^* B^* X U_{k,s} v \otimes \psi(g) \rangle \\
 & + g(s) \langle u \otimes \psi(f), U_{n-1,s}^* C^* X U_{k,s} v \otimes \psi(g) \rangle + \langle u \otimes \psi(f), U_{n-1,s}^* K^* X U_{k,s} v \otimes \psi(g) \rangle \\
 & + \bar{f}(s) g(s) \langle u \otimes \psi(f), U_{n-1,s}^* D^* X D U_{k-1,s} v \otimes \psi(g) \rangle \\
 & + \bar{f}(s) \langle u \otimes \psi(f), U_{n-1,s}^* D^* X C U_{k-1,s} v \otimes \psi(g) \rangle \\
 & + g(s) \langle u \otimes \psi(f), U_{n-1,s}^* C^* X D U_{k-1,s} v \otimes \psi(g) \rangle \\
 & + \langle u \otimes \psi(f), U_{n-1,s}^* C^* X C U_{k-1,s} v \otimes \psi(g) \rangle) ds .
 \end{aligned}$$

Letting $n = k$ in (2.13) we obtain the value of the matrix element

$$\langle u \otimes \psi(f), j_{n,t}(X) v \otimes \psi(g) \rangle .$$

3 Basic Error Estimates

Proposition 3.1. *Let $\epsilon > 0$, and let U_t and $U_{n,t}$, where $0 \leq t \leq T < +\infty$, be defined respectively by (2.4) and (2.6). Then for all $u \otimes \psi(f)$ and $v \otimes \psi(g)$ in the exponential domain of $\mathcal{H} \otimes \Gamma$, with g locally bounded and $u, v \neq 0$:*

$$| \langle u \otimes \psi(f), U_t v \otimes \psi(g) \rangle - \langle u \otimes \psi(f), U_{n,t} v \otimes \psi(g) \rangle | < \epsilon \quad (3.14)$$

for all $t \in [0, T]$ provided that

$$\sqrt{\frac{\lambda^{n+1} T^{n+1}}{(n+1)!}} < \frac{\epsilon}{\|u\| \|v\| e^{\frac{\|f\|^2}{2}} e^{\frac{\|g\|^2}{2}}} \quad (3.15)$$

where $\epsilon > 0$ is the required degree of accuracy and

$$\begin{aligned}
 \|f\|^2 &= \int_0^{+\infty} |f(s)|^2 ds; \quad \|g\|^2 = \int_0^{+\infty} |g(s)|^2 ds; \quad \lambda = 6 \alpha(T)^2 e^T M \\
 M &= \max(\|K\|, \|B\|, \|C\|, \|D\|); \quad \alpha(T) = \sup_{0 \leq s \leq T} \max(|g(s)|^2, |g(s)|, 1) .
 \end{aligned}$$

Proof.

$$\begin{aligned}
& | \langle u \otimes \psi(f), U_t v \otimes \psi(g) \rangle - \langle u \otimes \psi(f), U_{n,t} v \otimes \psi(g) \rangle |^2 \\
&= | \langle u \otimes \psi(f), (U_t - U_{n,t}) v \otimes \psi(g) \rangle |^2 \leq \|u \otimes \psi(f)\|^2 \|(U_t - U_{n,t}) v \otimes \psi(g)\|^2 \\
&= \|u \otimes \psi(f)\|^2 \left\| \left(\int_0^t K(U_{s_1} - U_{n-1,s_1}) ds_1 + B(U_{s_1} - U_{n-1,s_1}) dA_{s_1} + C(U_{s_1} - U_{n-1,s_1}) dA_{s_1}^\dagger \right. \right. \\
&\quad \left. \left. + D(U_{s_1} - U_{n-1,s_1}) d\Lambda_{s_1} \right) v \otimes \psi(g) \right\|^2
\end{aligned}$$

which by Corollary 1 and Theorem 4.4 of [2] is

$$\begin{aligned}
&\leq 6\alpha(T)^2 \|u \otimes \psi(f)\|^2 \int_0^T e^{t-s_1} \{ \|K(U_{s_1} - U_{n-1,s_1}) v \otimes \psi(g)\|^2 \\
&\quad + \|B(U_{s_1} - U_{n-1,s_1}) v \otimes \psi(g)\|^2 + \|C(U_{s_1} - U_{n-1,s_1}) v \otimes \psi(g)\|^2 \\
&\quad + \|D(U_{s_1} - U_{n-1,s_1}) v \otimes \psi(g)\|^2 \} ds_1 \\
&\leq 6\alpha(T)^2 (\max\{\|K\|, \|B\|, \|C\|, \|D\|\})^2 \|u \otimes \psi(f)\|^2 \int_0^T e^{t-s_1} \|(U_{s_1} - U_{n-1,s_1}) v \otimes \psi(g)\|^2 ds_1 \\
&= \lambda \|u \otimes \psi(f)\|^2 \int_0^T \|(U_{s_1} - U_{n-1,s_1}) v \otimes \psi(g)\|^2 ds_1 \\
&\leq \lambda^2 \|u \otimes \psi(f)\|^2 \int_0^T \int_0^{s_1} \|(U_{s_2} - U_{n-2,s_2}) v \otimes \psi(g)\|^2 ds_2 ds_1 \\
&\leq \lambda^3 \|u \otimes \psi(f)\|^2 \int_0^T \int_0^{s_1} \int_0^{s_2} \|(U_{s_3} - U_{n-3,s_3}) v \otimes \psi(g)\|^2 ds_3 ds_2 ds_1 \\
&\vdots \\
&\leq \lambda^n \|u \otimes \psi(f)\|^2 \int_0^T \int_0^{s_1} \int_0^{s_2} \dots \int_0^{s_{n-1}} \|(U_{s_n} - U_{0,s_n}) v \otimes \psi(g)\|^2 ds_n \dots ds_3 ds_2 ds_1
\end{aligned}$$

which using

$$\begin{aligned}
U_{s_n} &= I + \int_0^{s_n} K U_{s_{n+1}} ds_{n+1} + B U_{s_{n+1}} dA_{s_{n+1}} + C U_{s_{n+1}} dA_{s_{n+1}}^\dagger + D U_{s_{n+1}} d\Lambda_{s_{n+1}} \\
U_{0,s_n} &= I
\end{aligned}$$

and the unitarity of $U_{s_{n+1}}$, becomes

$$\begin{aligned}
 &\leq \lambda^{n+1} \|u \otimes \psi(f)\|^2 \int_0^T \int_0^{s_1} \int_0^{s_2} \dots \int_0^{s_{n-1}} \int_0^{s_n} \|U_{s_{n+1}} v \otimes \psi(g)\|^2 ds_{n+1} ds_n \dots ds_3 ds_2 ds_1 \\
 &= \lambda^{n+1} \|u \otimes \psi(f)\|^2 \int_0^T \int_0^{s_1} \int_0^{s_2} \dots \int_0^{s_{n-1}} \int_0^{s_n} \|v \otimes \psi(g)\|^2 ds_{n+1} ds_n \dots ds_3 ds_2 ds_1 \\
 &= \|u \otimes \psi(f)\|^2 \|v \otimes \psi(g)\|^2 \lambda^{n+1} \int_0^T \int_0^{s_1} \int_0^{s_2} \dots \int_0^{s_{n-1}} \int_0^{s_n} ds_{n+1} ds_n \dots ds_3 ds_2 ds_1 \\
 &= \|u \otimes \psi(f)\|^2 \|v \otimes \psi(g)\|^2 \lambda^{n+1} \frac{T^{n+1}}{(n+1)!} \\
 &= \|u\|^2 \|v\|^2 e^{\|f\|^2} e^{\|g\|^2} \lambda^{n+1} \frac{T^{n+1}}{(n+1)!}
 \end{aligned}$$

which is less than ϵ^2 provided that (3.15) is satisfied. □

Corollary 3.2. *In the notation of Proposition 2*

$$| | \langle u \otimes \psi(f), U_t v \otimes \psi(g) \rangle | - | \langle u \otimes \psi(f), U_{n,t} v \otimes \psi(g) \rangle | | < \epsilon$$

for all $t \in [0, T]$ and u, v, f, g with $u, v \neq 0$, provided that

$$\sqrt{\frac{\lambda^{n+1} T^{n+1}}{(n+1)!}} < \frac{\epsilon}{\|u\| \|v\| e^{\frac{\|f\|^2}{2}} e^{\frac{\|g\|^2}{2}}} .$$

Proof. The proof follows by applying the triangle inequality to (3.14). □

Proposition 3.3. *In the notation of Proposition 1*

$$| \langle u \otimes \psi(f), j_{n,t}(X) v \otimes \psi(g) \rangle - \langle u \otimes \psi(f), j_t(X) v \otimes \psi(g) \rangle | < \epsilon \quad (3.16)$$

for all $t \in [0, T]$ and u, v, f, g with $u, v \neq 0$, provided that

$$\max \left(\sqrt{\frac{\lambda^{n+1} T^{n+1}}{(n+1)!}}, \frac{\lambda^{n+1} T^{n+1}}{(n+1)!} \right) < \frac{\epsilon}{3 \|u\| \|v\| e^{\frac{\|f\|^2}{2}} e^{\frac{\|g\|^2}{2}} \|X\|} .$$

Proof.

$$\begin{aligned}
 &| \langle u \otimes \psi(f), j_{n,t}(X) v \otimes \psi(g) \rangle - \langle u \otimes \psi(f), j_t(X) v \otimes \psi(g) \rangle | \\
 &\leq \|(U_t - U_{n,t}) u \otimes \psi(f)\| \|X\| \|v \otimes \psi(g)\| \\
 &+ (\|(U_t - U_{n,t}) u \otimes \psi(f)\| + \|u \otimes \psi(f)\|) \|X\| \|(U_t - U_{n,t}) v \otimes \psi(g)\|
 \end{aligned}$$

and using, as in the proof of Proposition 2, the inequality

$$\|(U_t - U_{n,t}) a \otimes \psi(b)\|^2 \leq \|a \otimes \psi(b)\|^2 \frac{\lambda^{n+1} T^{n+1}}{(n+1)!}$$

we obtain

$$\begin{aligned} & | \langle u \otimes \psi(f), j_{n,t}(X) v \otimes \psi(g) \rangle - \langle u \otimes \psi(f), j_t(X) v \otimes \psi(g) \rangle | \\ & \leq \|u \otimes \psi(f)\| \|v \otimes \psi(g)\| \|X\| \left(2 \sqrt{\frac{\lambda^{n+1} T^{n+1}}{(n+1)!}} + \frac{\lambda^{n+1} T^{n+1}}{(n+1)!} \right) \\ & \leq 3 \max \left(\sqrt{\frac{\lambda^{n+1} T^{n+1}}{(n+1)!}}, \frac{\lambda^{n+1} T^{n+1}}{(n+1)!} \right) \|u\| \|v\| e^{\frac{\|f\|^2}{2}} e^{\frac{\|g\|^2}{2}} \|X\| < \epsilon \end{aligned}$$

from which (3.16) follows. \square

Corollary 3.4. *In the notation of Proposition 3*

$$| | \langle u \otimes \psi(f), j_{n,t}(X) v \otimes \psi(g) \rangle | - | \langle u \otimes \psi(f), j_t(X) v \otimes \psi(g) \rangle | | < \epsilon \quad (3.17)$$

for all $t \in [0, T]$ and u, v, f, g with $u, v \neq 0$, provided that

$$\max \left(\sqrt{\frac{\lambda^{n+1} T^{n+1}}{(n+1)!}}, \frac{\lambda^{n+1} T^{n+1}}{(n+1)!} \right) < \frac{\epsilon}{3 \|u\| \|v\| e^{\frac{\|f\|^2}{2}} e^{\frac{\|g\|^2}{2}} \|X\|}.$$

Proof. The proof follows by applying the triangle inequality to (3.16). \square

Remark 3.5. In the case of unitary evolutions and quantum flows, to produce a numerical result for the matrix elements symbolic and numerical computations should be run in parallel. That is because, for example, the numerical computation for specific t and u, v, f, g of the matrix element of U_n at the n -th step requires the symbolic calculation, i.e. for general s , of the matrix element at the previous step, with u transformed by the adjoints of K, B, C, D .

4 Example

In (2.4), let $K = (i - \frac{1}{2}) I$, $B = C = iI$ and $D = 0$, corresponding to $L = iI$ and $W = -H = I$. Then, letting

$$\phi(t) := \langle u \otimes \psi(f), U_t v \otimes \psi(g) \rangle; \quad \phi_n(t) := \langle u \otimes \psi(f), U_{n,t} v \otimes \psi(g) \rangle$$

(2.4) and (2.6) become

$$\phi(t) = \langle u \otimes \psi(f), v \otimes \psi(g) \rangle + \int_0^t \left(-\frac{1}{2} + i(g(s) + \overline{f(s)} + 1) \right) \phi(s) ds \quad (4.18)$$

and

$$\phi_n(t) = \langle u \otimes \psi(f), v \otimes \psi(g) \rangle + \int_0^t \left(-\frac{1}{2} + i(g(s) + \overline{f(s)} + 1) \right) \phi_{n-1}(s) ds \quad (4.19)$$

respectively.

The exact solution of (4.18) is

$$\phi(t) = \langle u \otimes \psi(f), v \otimes \psi(g) \rangle e^{\int_0^t (-\frac{1}{2} + i(g(s) + \overline{f(s)} + 1)) ds} .$$

Taking $u = v = e_{n_0}$ where $\{e_n : n = 1, 2, \dots\}$ is an orthonormal basis for \mathcal{H} , and $f(s) = g(s) = e^{-s}$ we have

$$\langle u \otimes \psi(f), v \otimes \psi(g) \rangle = \langle u, v \rangle \langle \psi(f), \psi(g) \rangle = e^{\frac{1}{2}}$$

so

$$\phi(t) = e^{\frac{1}{2} + 2i} e^{(i - \frac{1}{2})t} e^{-2ie^{-t}} .$$

For example, for $T = 2$ we have

$$\|f\|^2 = \|g\|^2 = \frac{1}{4} ; \|K\| = \frac{\sqrt{5}}{2} ; \|B\| = \|C\| = 1 ; \|D\| = 0 ; M = \frac{\sqrt{5}}{2} ; \alpha(2) = 1 ; \lambda = 3\sqrt{5}e^2$$

and (3.15) becomes

$$\frac{(6\sqrt{5}e^2)^{n+1}}{(n+1)!} < \frac{\epsilon^2}{e^{\frac{1}{2}}}$$

which for $\epsilon = 0.000001$ is seen (using Mathematica) to be satisfied for $n \geq 292$. However, iterating (4.19) we find, for example for $t = 1$,

$$\phi(1) = -0.6391901814352063 + i 0.7690487058417224$$

and

$$\phi_{14}(1) = -0.6391900891154059 + i 0.7690483524915057$$

with

$$|\phi_{14}(1) - \phi(1)| = 3.65211 * 10^{-7} < 0.000001$$

so, in this case, convergence within the required error bound is actually faster than predicted by formula (3.15).

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