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Heisenberg picture operators in the stochastic wave function approach to open quantum systems

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Abstract. A fast simulation algorithm for the calculation of multitime correlation functions of open quantum systems is presented. It is demonstrated that any stochastic process which "unravels" the quantum Master equation can be used for the calculation of matrix elements of reduced Heisenberg picture operators, and thus for the calculation of multitime correlation functions, by extending the stochastic process to a doubled Hilbert space. The numerical performance of the stochastic simulation algorithm is investigated by means of a standard example.

PACS. 42.50.Lc Quantum fluctuations, quantum noise, and quantum jumps – 02.70.Lq Monte Carlo and statistical methods

1 Introduction

The state of an open quantum system is conventionally described through a reduced density matrix $\rho(t)$ whose dynamics is given by a dissipative equation of motion – the quantum Master equation. From a numerical point of view this formalism has a major drawback: for a system whose state is described in a N-dimensional Hilbert space $\mathcal{H}$, the quantum Master equation is a set of $N(N+1)/2$ coupled differential equations. Hence the numerical evaluation of the quantum Master equation is in practice not feasible for large systems [1].

This difficulty does not arise in the stochastic wave function approach to open systems [2–9]: here, the state of an open quantum system is described by a stochastic wave function $\psi(t) \in \mathcal{H}$, *i.e.*, by a N-dimensional state vector. The stochastic time evolution of $\psi(t)$ is either defined through a stochastic Schrödinger equation [8,9] (which is a stochastic differential equation) or alternatively through a conditional transition probability $T[\psi,t|\psi_0,t_0]$ [6,7], which is the probability density of finding the system in the state ψ at time $t \geq t_0$ *under the condition* that the system is in the state ψ_0 at time t_0. The connection to the density matrix formalism is made through the relation

$$\rho(t) = \int D\psi D\psi^* \int D\psi_0 D\psi_0^* \; |\psi\rangle\langle\psi| \; T[\psi,t|\psi_0,t_0] P[\psi_0,t_0], \tag{1}$$

where $P[\psi_0,t_0]$ is the probability density of an ensemble of normalized pure states characterizing some initial density matrix ρ_0 and $D\psi D\psi^*$ is the Hilbert space volume element [6,7]. The integrals extend over the Hilbert space $\mathcal{H}$. This relation ensures that one-time expectation values of any system operators are calculated correctly. Note that this condition alone does not uniquely specify a stochastic process. Diffusion type stochastic processes [8,9] as well as piecewise deterministic jump processes [2–7] have been proposed in the literature. A unique stochastic process can only be derived by making further assumptions such as specifying a certain measurement scheme [10–12].

Especially in quantum optical systems one-time expectation values of system observables are not the only measurable quantities: for example, the spectrum of fluorescence of a two level system is the Fourier transform of the two-time correlation function $\langle\!\langle \sigma^+(\tau)\sigma^- \rangle\!\rangle_{\rm s}$ in the stationary state, where $\sigma^\pm$ denote the pseudo spin operators of the system. Thus, for a complete description of open quantum systems it is necessary to introduce Heisenberg picture operators. In the density matrix formalism this concept is well understood [13]: consider the quantum Master equation

$$\dot\rho(t) = L(t)\rho(t), \tag{2}$$

where the super-operator $L(t)$ is defined as

$$L(t)\rho(t) = -i\,[H(t),\rho(t)] + \frac{1}{2}\sum_i \gamma_i \Big\{ 2J_i\rho(t)J_i^\dagger - J_i^\dagger J_i \rho(t) - \rho(t) J_i^\dagger J_i \Big\}. \tag{3}$$

The operator $H(t)$ is essentially the Hamiltonian of the isolated system which contributes to the coherent part of

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the dynamics, and the rates γ_i and the Lindblad operators J_i describe the dissipative coupling of the system to its environment through the i-th decay channel. The solution of equation (2) with respect to the initial condition $\rho(t_0) = \rho_0$ can be expressed for $t \geq t_0$ in terms of the propagation super-operator $V(t, t_0)$ as [14]

$$\rho(t) = V(t, t_0)\rho_0, \tag{4}$$

where $V(t, t_0)$ is the solution of the differential equation

$$\frac{\mathrm{d}}{\mathrm{d}t}V(t, t_0) = L(t)V(t, t_0), \tag{5}$$

with the initial condition $V(t_0, t_0) = I$. For an arbitrary Schrödinger system operator A the matrix elements of the *reduced* Heisenberg picture operator are defined as

$$\begin{aligned} A_t(\phi_0, \psi_0) &\equiv \langle \phi_0, t_0 | A(t) | \psi_0, t_0 \rangle \\ &= \mathrm{Tr}_{\mathrm{sys}}\Big\{ AV(t, t_0)|\psi_0\rangle\langle\phi_0| \Big\}. \end{aligned} \tag{6}$$

Equation (6) can be interpreted in the following way: for the calculation of the matrix element $A_t(\phi_0, \psi_0)$ start with the initial "density matrix" $|\psi_0\rangle\langle\phi_0|$ and propagate it up to the time t. Then calculate the expectation value of A with respect to the propagated "density matrix". However, since $|\psi_0\rangle\langle\phi_0|$ is in general not a positive matrix and thus not a true density matrix, it can not be characterized by a probability density $P[\psi_0, t_0]$ of normalized pure states in $\mathcal{H}$ (*cf.* Eq. (1)). Hence a direct application of the stochastic wave function approach to the calculation of Heisenberg picture operators is not possible.

2 Heisenberg picture operators in the stochastic wave function approach

In a closed system where the time evolution of states is given through the unitary propagator $U(t, t_0)$ we can calculate arbitrary matrix elements $A_t(\phi_0, \psi_0)$ of a Heisenberg operator $A(t)$ in the following way (*cf.* Fig. 1): propagate ϕ_0 and ψ_0 to obtain $\phi = U(t, t_0)\phi_0$ and $\psi = U(t, t_0)\psi_0$, respectively and then evaluate the scalar product $\langle\phi|A|\psi\rangle$. This method is easily generalized to the calculation of matrix elements of a *reduced* Heisenberg picture operator, *i.e.*, to open systems: instead of propagating the state vectors $\phi_0 \in \mathcal{H}$ and $\psi_0 \in \mathcal{H}$ separately, we can construct a stochastic process in the *doubled* Hilbert space $\widetilde{\mathcal{H}} = \mathcal{H} \oplus \mathcal{H}$ which propagates the normalized *pair* of state vectors $\theta_0 = (\phi_0, \psi_0)^{\mathrm{T}}/\sqrt{2} \in \widetilde{\mathcal{H}}$ simultaneously in such a way that the following condition holds:

$$A_t(\phi_0, \psi_0) = 2 \int D\theta D\theta^* \langle\phi|A|\psi\rangle \widetilde{T}[\theta, t|\theta_0, t_0], \tag{7}$$

where $\theta = (\phi, \psi)^{\mathrm{T}}$ and we introduced the conditional transition probability $\widetilde{T}$ for the stochastic process in the doubled Hilbert space $\widetilde{\mathcal{H}}$. Throughout this letter, the superscript T denotes the transpose of a vector. This condition

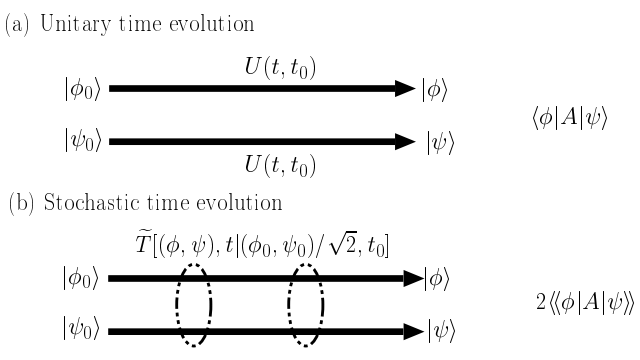

Fig. 1. Calculation of Heisenberg operator matrix elements: (a) for a closed system and (b) for an open system.

states that matrix elements of arbitrary Heisenberg operators are calculated correctly. It is important to note that equation (7) alone does not specify the stochastic time evolution in the doubled Hilbert space uniquely. In fact, each stochastic process which can be used to simulate the quantum Master equation (2) can be extended to the doubled Hilbert space and used for the calculation of the matrix elements of arbitrary Heisenberg picture operators. We will first demonstrate this for the piecewise deterministic jump process proposed in [2–7] and then generalize the result. A derivation of the simulation algorithm for the stochastic time evolution in the doubled Hilbert space which is based on a microscopic system-reservoir model can be found in reference [15].

For the piecewise deterministic jump process the simulation algorithm reads as follows.

1) Start with the normalized state $\theta_0 = (\phi_0, \psi_0)^{\mathrm{T}}/\sqrt{2}$ at t_0.

2) Draw a random number η_1 from a uniform distribution on $[0, 1]$; this random number will determine the time of the first jump.

3) Propagate θ_0 according to the Schrödinger-type equation

$$i\frac{\mathrm{d}}{\mathrm{d}s}\hat{\theta}(s) = \widetilde{H}_{\mathrm{eff}}(s)\hat{\theta}(s) \tag{8}$$

where the extensions of the Hamiltonian H and Lindblad operators J_i to the doubled Hilbert space are defined as

$$\widetilde{H}(s) = \begin{pmatrix} H(s) & 0 \\ 0 & H(s) \end{pmatrix}, \quad \widetilde{J}_i = \begin{pmatrix} J_i & 0 \\ 0 & J_i \end{pmatrix}, \tag{9}$$

and the non-Hermitian effective Hamiltonian is defined as

$$\widetilde{H}_{\mathrm{eff}}(s) = \widetilde{H}(s) - \frac{i}{2}\sum_i \gamma_i \widetilde{J}_i^{\dagger}\widetilde{J}_i. \tag{10}$$

4) The time T_1 of the first jump is determined by the condition

$$\eta_1 = \|\hat{\theta}(T_1)\|^2. \tag{11}$$

5) Select a particular type of jump with probability $\gamma_i w_i / \sum_i \gamma_i w_i$, where $w_i = \|\widetilde{J}_i\hat{\theta}(T_1)\|^2$. The state of the

system immediately after the first jump is given by

$$\theta(T_1) = \widetilde{J}_i\hat{\theta}(T_1)/\|\widetilde{J}_i\hat{\theta}(T_1)\|. \tag{12}$$

6) Draw a second random number η_2 to determine the time T_2 of the next jump and propagate $\theta(T_1)$ according to the differential equation (8) and so on until $s = t$.

7) The state of the system at time t is given by

$$\theta(t) \equiv (\phi(t), \psi(t))^{\mathrm{T}} = \hat{\theta}(t)/\|\hat{\theta}(t)\|. \tag{13}$$

The matrix elements of the reduced Heisenberg picture operator $A(t)$ are then obtained by computing

$$A_t(\phi_0, \psi_0) = 2\Big\langle\Big\langle \langle\phi(t)|A|\psi(t)\rangle\Big\rangle\Big\rangle, \tag{14}$$

where the angular brackets $\langle\langle\cdots\rangle\rangle$ denote the average over the realizations of the stochastic process.

In order to show that this algorithm leads to the correct result, we introduce the density matrix

$$\widetilde{\rho}(t) = \begin{pmatrix} \widetilde{\rho}_{11}(t) & \widetilde{\rho}_{12}(t) \\ \widetilde{\rho}_{21}(t) & \widetilde{\rho}_{22}(t) \end{pmatrix} \tag{15}$$

on the doubled Hilbert space $\widetilde{\mathcal{H}}$ which is a solution of the extended quantum Master equation

$$\begin{aligned} \dot{\widetilde{\rho}}(t) = &- i\Big[\widetilde{H}(t), \widetilde{\rho}(t)\Big] \\ &+ \frac{1}{2}\sum_i \gamma_i \Big\{2\widetilde{J}_i\widetilde{\rho}(t)\widetilde{J}_i^{\dagger} - \widetilde{J}_i^{\dagger}\widetilde{J}_i\widetilde{\rho}(t) - \widetilde{\rho}(t)\widetilde{J}_i^{\dagger}\widetilde{J}_i\Big\}, \end{aligned} \tag{16}$$

with the initial condition

$$\widetilde{\rho}(t_0) = |\theta_0\rangle\langle\theta_0| \equiv \frac{1}{2}\begin{pmatrix} |\phi_0\rangle\langle\phi_0| & |\phi_0\rangle\langle\psi_0| \\ |\psi_0\rangle\langle\phi_0| & |\psi_0\rangle\langle\psi_0| \end{pmatrix}. \tag{17}$$

By definition of the extended operators $\widetilde{H}$ and $\widetilde{J}_i$ each component $\widetilde{\rho}_{ij}(t)$ which is an operator on $\mathcal{H}$ is a solution of the original quantum Master equation (2). Since $\widetilde{\rho}_{21}(t)$ is a solution of equation (2) with the initial condition $\widetilde{\rho}_{21}(t_0) = |\psi_0\rangle\langle\phi_0|/2$ the matrix elements $A_t(\phi_0, \psi_0)$ of a reduced Heisenberg picture operator $A(t)$ can be written as (*cf.* Eq. (6))

$$A_t(\phi_0, \psi_0) = 2\mathrm{Tr}_{\mathrm{sys}}\Big\{A\widetilde{\rho}_{21}(t)\Big\}. \tag{18}$$

Now consider a particular "unraveling" of the *extended* quantum Master equation (16) which is characterized by a conditional transition probability $\widetilde{T}[\theta, t|\theta_0, t_0]$ in the doubled Hilbert space. For the density matrix $\widetilde{\rho}(t)$ we then obtain in analogy to equation (1)

$$\widetilde{\rho}(t) = \int D\theta D\theta^*\ |\theta\rangle\langle\theta|\ \widetilde{T}[\theta, t|\theta_0, t_0], \tag{19}$$

and hence for $\widetilde{\rho}_{21}(t)$

$$\widetilde{\rho}_{21}(t) = \int D\theta D\theta^*\ |\psi\rangle\langle\phi|\ \widetilde{T}[\theta, t|\theta_0, t_0], \tag{20}$$

where $\theta = (\phi, \psi)^{\mathrm{T}}$. By inserting equation (20) into equation (18) we recover equation (7). Thus we have shown that matrix elements of reduced Heisenberg picture operators are calculated correctly (*i.e.*, Eq. (7) holds) if the stochastic process in the doubled Hilbert space can be used to simulate the extended quantum Master equation (16). Since this is the case for the simulation algorithm presented above we have completed the proof.

It is important to note that the above proof does not rely on a specific "unraveling" of the quantum Master equation (16). On the contrary, it is valid for any stochastic process the covariance matrix (see Eq. (19)) of which is governed by equation (16).

3 Multitime correlation functions

The simulation algorithm in the doubled Hilbert space can also be used for the calculation of multitime correlation functions. Consider for example the two-time correlation function

$$g(\phi_0, t_1, t_2) = \langle\phi_0, t_0|A(t_2)B(t_1)|\phi_0, t_0\rangle, \tag{21}$$

where $t_1 \leq t_2$. Here, the stochastic simulation algorithm would read as follows.

1) Start in the state ϕ_0 at time t_0 and use the stochastic time evolution in the Hilbert space $\mathcal{H}$ to obtain the stochastic wave function $\phi(t_1)$.

2) Propagate the state

$$\theta(t_1) = (\phi(t_1), B\phi(t_1))^{\mathrm{T}}/\|(\phi(t_1), B\phi(t_1))\| \tag{22}$$

using the stochastic time evolution in the doubled Hilbert space to obtain the state vector $\theta(t_2) = (\phi(t_2), \psi(t_2))^{\mathrm{T}}$. The multitime correlation function is then obtained by computing

$$\begin{aligned} &g(\phi_0, t_1, t_2) = \\ &\qquad \Big\langle\Big\langle \big\|\big(\phi(t_1), B\phi(t_1)\big)\big\|^2 \langle\phi(t_2)|A|\psi(t_2)\rangle\Big\rangle\Big\rangle. \end{aligned} \tag{23}$$

The generalization of this scheme to the calculation of arbitrary time-ordered multitime correlation functions of the form

$$\begin{aligned} &g(\phi_0, t_0, t_1, ..., t_n, s_1, ..., s_m) = \\ &\langle\phi_0, t_0|A_1(t_1)\cdots A_n(t_n)B_m(s_m)\cdots B_1(s_1)|\phi_0, t_0\rangle, \end{aligned} \tag{24}$$

where $t_0 \leq \cdots \leq t_n$, and $t_0 \leq s_1 \leq \cdots \leq s_m$, and A_i and B_i are arbitrary system operators is straightforward: order the set of times $\{t_1, \cdots t_n, s_1, \cdots s_m\}$ and rename them r_i such that $r_1 < \cdots < r_q$ where q is the number of distinct time points. Then define a set of Schrödinger operators F_l and G_l as

$$\begin{cases} F_l = A_i^{\dagger},\ G_l = \ I, & \text{if } r_l = t_i \neq s_j \text{ for some } i \text{ and all } j, \\ G_l = I, \quad F_l = B_j, & \text{if } r_l = s_j \neq t_i \text{ for some } j \text{ and all } i, \\ G_l = A_i^{\dagger},\ F_l = B_j, & \text{if } r_l = t_i = s_j \text{ for some } i \text{ and } j. \end{cases} \tag{25}$$

The multitime correlation function $g(\phi_0, t_0, t_1, ..., t_n, s_1, ..., s_m)$ is then obtained in the following way.

1) Start with the state ϕ_0 at time t_0 and propagate it up to the time r_1 to obtain $\phi(r_1)$.

2) Propagate the state

$$\theta(r_1) = (F_1\phi(r_1), G_1\phi(r_1))^{\mathrm{T}} / \|(F_1\phi(r_1), G_1\phi(r_1))\| \quad (26)$$

to obtain $\theta(r_2) = (\phi(r_2), \psi(r_2))^{\mathrm{T}}$.

3) Jump to the state

$$\theta(r_2) = (F_2\phi(r_2), G_2\psi(r_2))^{\mathrm{T}} / \|(F_2\phi(r_2), G_2\psi(r_2))\| \quad (27)$$

and propagate it up to r_3 and so on. $g(\phi_0, t_0, t_1, ..., t_n, s_1, ..., s_m)$ is then given by

$$\begin{aligned} g(\phi_0, t_0, t_1, ..., t_n, s_1, ..., s_m) = \\ \Big\langle\Big\langle \big\| \big(F_1\phi(r_1), G_1\phi(r_1)\big)\big\|^2 \\ \times \big\| \big(F_2\phi(r_2), G_2\psi(r_2)\big)\big\|^2 \cdots \\ \times \big\| \big(F_{q-1}\phi(r_{q-1}), G_{q-1}\psi(r_{q-1})\big)\big\|^2 \\ \times \langle\phi(r_q)|F_q^\dagger G_q|\psi((r_q)\rangle\Big\rangle\Big\rangle. \end{aligned} \quad (28)$$

It is important to note, that also for higher order correlation functions, we only have to propagate two state vectors.

Finally, let us remark that the choice of the initial condition (23) (or (26), respectively) is not unique. We can also multiply the operator B by a constant ε and define the state vector $\theta_\varepsilon(t_1)$ as

$$\theta_\varepsilon(t_1) = (\phi(t_1), \varepsilon B\phi(t_1))^{\mathrm{T}} / \|(\phi(t_1), \varepsilon B\phi(t_1))\| \quad (29)$$

and accordingly the correlation function $g(\phi_0, t_1, t_2)$ as

$$g(\phi_0, t_1, t_2) = \frac{1}{\varepsilon}\Big\langle\Big\langle \big\| \big(\phi(t_1), \varepsilon B\phi(t_1)\big)\big\|^2 \langle\phi_\varepsilon(t_2)|A|\psi_\varepsilon(t_2)\rangle\Big\rangle\Big\rangle, \quad (30)$$

where $\theta_\varepsilon(t_2) = (\phi_\varepsilon(t_2), \psi_\varepsilon(t_2))^{\mathrm{T}}$ is obtained by propagating $\theta_\varepsilon(t_1)$ according to the simulation algorithm in the doubled Hilbert space. Again, the unnormalized deterministic motion is governed by the equation of motion

$$i\frac{\mathrm{d}}{\mathrm{d}t}\hat{\phi}_\varepsilon(t) = H_{\mathrm{eff}}(t)\hat{\phi}_\varepsilon(t) \quad (31)$$

$$i\frac{\mathrm{d}}{\mathrm{d}t}\hat{\psi}_\varepsilon(t) = H_{\mathrm{eff}}(t)\hat{\psi}_\varepsilon(t) \quad (32)$$

but in the limit $\varepsilon \to 0$, we find

$$\|\hat{\theta}_\varepsilon(t)\| \to \|\hat{\phi}_\varepsilon(t)\| \quad (33)$$

$$w_i = \|\widetilde{J}_i\hat{\theta}_\varepsilon(T)\|^2 \to \|J_i\hat{\phi}_\varepsilon(T)\|^2, \quad (34)$$

and hence the jumps of the trajectory $\theta_\varepsilon(t)$ are completely governed by the jumps of $\phi_\varepsilon(t)$, which evolves according to the "usual" stochastic time evolution in $\mathcal{H}$ (*cf.* Eqs. (11, 12)). In this limit we obtain a procedure first proposed by Dum *et al.* in reference [5], which is based on "probing the system with δ kicks" (see Append. D of Ref.[5]). For further discussions of this method see for example the references [16–18].

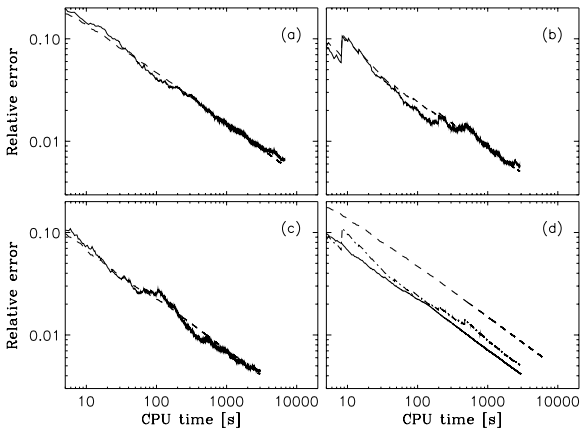

Fig. 2. Calculation of the first order correlation function $\langle\langle\sigma^+(\tau)\sigma^-\rangle\rangle_{\mathrm{s}}$ for a coherently driven two level atom on resonance. This figure shows the relative error *versus* the CPU time in seconds for the simulation algorithms proposed in reference [2] (a), reference [2] (b), and for our algorithm in the doubled Hilbert space (c). The solid lines represent the mean square deviation of the numerical solution from the exact solution and the dashed lines show the estimated standard deviation of the numerical solution. In Figure 2d, we compare the estimated standard deviation for the three algorithms.

4 Numerical results

In order to investigate the numerical performance of our simulation algorithm, we compare it with the method proposed by Dum *et al.* in reference [5] and with an alternative method proposed by Dalibard *et al.* which is based on a decomposition of the stochastic trajectory into four sub-trajectories [2]. Note that all procedures are fully consistent with the quantum regression theorem [14,19] and hence lead to the same result for the multitime correlation function. However, the numerical performance of the algorithms is quite different. We demonstrate this by means of a standard example of quantum optics – the calculation of the spectrum of resonance fluorescence of a two level system. In Figures 2a-c we show the computational time necessary to achieve a given accuracy (measured by the relative error of the correlation function $\langle\langle\sigma^+(\tau)\sigma^-\rangle\rangle_{\mathrm{s}}$ in the stationary state) for a coherently driven two level atom with Rabi frequency $\Omega = 10\gamma$ obtained on a RS6000 workstation. The solid lines represent the mean square deviation of the numerical solution from the exact solution [20] and the dashed lines show the mean estimated standard deviation of the numerical solution. Obviously, the latter quantity provides for all algorithms a very good measure of the accuracy of the numerical simulation. In Figure 2d we compare the estimated standard deviation for the three algorithms. Obviously, the numerical performance of the algorithms proposed by Dum *et al.* and our algorithm is quite similar, although the convergence of our algorithm is smoother. On the other hand, for a given accuracy the stochastic simulation in the doubled Hilbert space is by a factor of 3 faster than the algorithm proposed in reference [2]. We expect this result to be even better for higher order correlation functions since for a multitime

correlation function of the type of equation (24) one has to propagate in general 4^{n+m-1} different state vectors in each realization using the method of Castin *et al.*, whereas in our approach it is only necessary to propagate two state vectors.

Let us briefly summarize the main results of this letter: we have shown that starting from a stochastic simulation algorithm for the quantum Master equation (2) it is possible to obtain a fast simulation algorithm for the calculation of matrix elements of arbitrary Heisenberg picture operators and time-ordered multitime correlation functions by making the substitutions

$$\psi \in \mathcal{H} \longrightarrow \theta \in \widetilde{\mathcal{H}}, \quad H \longrightarrow \widetilde{H}, \quad J_i \longrightarrow \widetilde{J}_i, \tag{35}$$

i.e., we replace the stochastic wave function $\psi(t)$ by a stochastic wave function $\theta(t)$ in the doubled Hilbert space and extend accordingly the operators H and J_i which are present in the quantum Master equation to the doubled Hilbert space (*cf.* Eq. (9)). We emphasize that these replacements can be done for *any* "unraveling" of the quantum Master equation, *e.g.*, also for the quantum state diffusion model [8,9]. The resulting stochastic process in the doubled Hilbert space is then similar to a process first proposed by Gisin in reference [21]. However, the latter process is only well defined, when the initial states ϕ_0 and ψ_0 are *non-orthogonal*, *i.e.*, if $\langle\phi_0|\psi_0\rangle \neq 0$. This problem does not occur in the ansatz presented here.

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