Stochastic Wave-Function Simulation of Irreversible Emission Processes for Open Quantum Systems in a Non-Markovian Environment

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Abstract. When conducting the numerical simulation of quantum transport, the main obstacle is a rapid growth of the dimension of entangled Hilbert subspace. The Quantum Monte Carlo simulation techniques, while being capable of treating the problems of high dimension, are hindered by the so-called “sign problem”. In the quantum transport, we have fundamental asymmetry between the processes of emission and absorption of environment excitations: the emitted excitations are rapidly and irreversibly scattered away. Whereas only a small part of these excitations is absorbed back by the open subsystem, thus exercising the non-Markovian self-action of the subsystem onto itself. We were able to devise a method for the exact simulation of the dominant quantum emission processes, while taking into account the small backaction effects in an approximate self-consistent way. Such an approach allows us to efficiently conduct simulations of real-time dynamics of small quantum subsystems immersed in non-Markovian bath for large times, reaching the quasistationary regime. As an example we calculate the spatial quench dynamics of Kondo cloud for a bozonized Kondo impurity model.

INTRODUCTION

Real-time dynamics of open quantum systems is actively studied in such diverse fields as quantum information/computing, solid state nanodevices, quantum biology and chemical physics [1]. The specific type of open quantum system, the Anderson impurity model, is also highly important in condensed matter physics, since it is a key component of the dynamical mean-field theory calculations [2, 3]. This stimulates the development of novel techniques for simulation of real-time open quantum dynamics. Currently these developments have resulted in the appearance of efficient simulation methods in such cases when: the total amount of excitations in the environment is not large; the memory of the environment is short; the system-environment coupling is weak; or the spectral density of the environment has special (Lorentzian) shape [1]. Nevertheless, recent experimental advances in fabrication of dispersion-engineered metamaterials urges us to develop techniques which are capable of handling the cases when: the memory of environment is long; the system-environment coupling is strong; we are interested in a long-time dynamics of a driven open system (or environment at finite temperature), so that the total amount of emitted/scattered excitations in the environment is unbounded.

There is no difficulty in simulating the relaxation dynamics of an excited open quantum system into the vacuum environment. In this case, only a few excitation quanta are emitted in the environment. Therefore, we may restrict the total Hilbert space of the environment to the several-quanta subspace, and then solve the Schrodinger equation exactly [1]. However, when there is driving of the open system, or when the environment is at finite temperature/chemical potential, the simulation quickly becomes intractable by exact numerical methods. The reason is that in the first case (driving) the number of emitted excitations grows (asymptotically) linearly with time, whereas in the second case (finite temperature/chemical potential) the number of scattered excitations is linearly growing. Since the dimension of the relevant Hilbert subspace grows combinatorially with the number of excitations, the dimension of the problem
grows exponentially with time, and thus we quickly run out of available memory and time resources.

In this work we investigate the idea that the growth of emitted/scattered environment excitations is the major factor of complexity of real-time quantum dynamics simulations. A way to eliminate this factor is considered. The environment excitations are divided into the two kinds: those which are irreversibly emitted/scattered (“output” quantum field of the environment) and those which will be eventually absorbed back by the open subsystem (quantum field of virtual excitations of the environment). We propose to conduct a numerically exact stochastic simulation of the output quantum field, and to evaluate quantum mechanically the virtual part with a certain approximation.

There is development in the literature which is similar in spirit: hybrid stochastic hierarchy equations of motion approach (sHEOM) [4]. However, the latter is limited to the Drude-Lorentz spectrum of environment, whereas our approach in principle may be applied to any spectral shape. Another distinction of our approach is that we make a physically-informed separation of the full quantum problem into the exact stochastic and the approximate deterministic parts.

In section a) we provide a precise meaning for the definitions of the irreversibly emitted output field and of the virtual excitation field. It is shown that the interaction with the output quantum field can be efficiently simulated without the sign problem by a stochastic wavefunction method analogous to that of Diosi, Gisin, and Strunz [5, 6]. However, the important distinction from the latter is that we explicitly keep the full quantum mechanical problem for virtual excitations. In section a) we discuss the approximations to the quantum virtual field and introduce the simplest zero-order approximation. Then, in section a) we apply our approach to the bozonized Kondo model and compute the spatial quench dynamics of the Kondo cloud. Finally, a conclusion is made in section a).

QUANTUM FIELD OF ENVIRONMENT: CLASSICAL INTERPRETATION OF THE IRREVERSIBLY EMITTED AND THERMAL PARTS

We consider the following Hamiltonian

$$\hat{H} = \hat{H}_{\text{sys}} + \hat{a} \hat{b}^\dagger + \hat{a}^\dagger \hat{b} + \hat{H}_{\text{env}}, \quad (1)$$

where $\hat{H}_{\text{env}}$ is an environment with quadratic Hamiltonian,

$$\hat{H}_{\text{env}} = \int_{-\infty}^{+\infty} d\omega \omega \hat{b}^\dagger(\omega) \hat{b}(\omega), \quad (2)$$

which is coupled bilinearly to the open system $\hat{H}_{\text{sys}}$ through a certain system operator $\hat{a}$ and the environment’s collective degree of freedom $\hat{b}$.

$$\hat{b} = \int_{-\infty}^{+\infty} d\omega c(\omega) \hat{b}(\omega). \quad (3)$$

Observe that in our representation the frequency dependence of the density-of-states is transferred to the coefficient $c(\omega)$.

Suppose that initially the open system is in a pure state $|\psi_{\text{sys}}\rangle$, and the environment is initially in a thermal state at inverse temperature $\beta$, with the mode occupations

$$n(\omega) = \text{Tr} \{ \hat{b}^\dagger(\omega) \hat{b}(\omega) \rho_{\text{env}} \}. \quad (4)$$

For the real-time evolution during time interval $[0, t]$, we may write the Keldysh contour partition function as a formal path integral over the forward/backward fields of open system $a_\pm(\tau)$, and over the environment $b_\pm(\tau)$,

$$Z[0, t] = \int D[a_\pm] D[b_\pm] \exp \{ S[a_\pm, b_\pm] \}, \quad (5)$$

with an appropriate Keldysh action $S[a_\pm, b_\pm]$. We integrate out the environment’s degrees of freedom $b_\pm(\tau)$, and obtain

$$Z[0, t] = \int D[a_\pm] \exp \{ S_{\text{eff}}[a_\pm] \}, \quad (6)$$
where the resulting effective action $S_{\text{eff}}[a_\omega]$ has the form

$$S_{\text{eff}}[a_\omega] = S_{\text{sys}}[a_\omega] - \int_0^T d\tau d\tau' \left[ \frac{-a_\omega^\dagger(\tau)}{a_\omega(\tau')} \right]^T K(\tau - \tau') \left[ \frac{-a_\omega(\tau')}{a_\omega^\dagger(\tau')} \right], \quad (7)$$

and in the second hybridization term the matrix $K(\tau - \tau')$ is the Keldysh function of the bath. We divide it into three parts:

$$K(t - t') = K_{\text{virt}}(t - t') + K_{\text{emit}}(t - t') + K_{\text{therm}}(t - t'), \quad (8)$$

where the term

$$K_{\text{virt}}(t - t') = \begin{bmatrix} \theta(t - t') & 0 \\ 0 & \theta(t' - t) \end{bmatrix} M(t - t') \quad (9)$$

describes the effect of the virtual environmental excitations (like Lamb shift);

$$K_{\text{emit}}(t - t') = \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix} M(t - t') \quad (10)$$

describes the irreversible emission of observable excitations;

$$K_{\text{therm}}(t - t') = \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} M_{\text{therm}}(t - t') \quad (11)$$

represents the effects of thermal fluctuations of environment. Here the environment memory function is

$$M(t - t') = \int_{-\infty}^{+\infty} d\omega |c(\omega)|^2 e^{-i\omega(t-t')}, \quad (12)$$

and the thermal noise memory function is

$$M_{\text{therm}}(t - t') = \int_{-\infty}^{+\infty} d\omega n(\omega)|c(\omega)|^2 e^{-i\omega(t-t')}. \quad (13)$$

In Fig. 1 we present the hybridization expansion of partition function with respect to $K_{\text{virt}}(t - t')$ and $K_{\text{emit}}(t - t')$, which is the basis for our physical interpretation. It is seen that $K_{\text{virt}}(t - t')$ corresponds to the contractions inside one branch of Keldysh contour (virtual excitations which are ultimately absorbed back), and $K_{\text{emit}}(t - t')$ corresponds to contractions across different branches (irreversibly emitted excitations which contribute to the trace over the environment’s states). It turns out that $K_{\text{emit}}(t - t')$ and $K_{\text{therm}}(t - t')$ can be interpreted in a classical way. Indeed, in the spirit of stochastic wavefunction method of Diosi, Gisin, and Strunz [5, 6], we introduce a c-number stochastic fields

$$z_{\text{emit}}(t) = \int_{-\infty}^{+\infty} d\omega c(\omega) e^{-i\omega t} \xi(\omega) \quad (14)$$

and

$$v_{\text{therm}}(t) = \int_{-\infty}^{+\infty} d\omega \sqrt{n(\omega)} c(\omega) e^{-i\omega t} \eta(\omega), \quad (15)$$

where $\xi(\omega)$ and $\eta(\omega)$ are complex independent white noises:

$$\xi^\dagger(\omega)\xi(\omega') = \delta(\omega - \omega'), \quad \eta^\dagger(\omega)\eta(\omega') = \delta(\omega - \omega'). \quad (16)$$

The following stochastic Hamiltonian is introduced

$$\tilde{H}_{\text{stoch}}(z_{\text{emit}}(t), v_{\text{therm}}(t)) = \tilde{H}_{\text{sys}} + \hat{a}^\dagger \left[ z_{\text{emit}}^\dagger(t) + v_{\text{therm}}^\dagger(t) \right] + \hat{a} \left[ z_{\text{emit}}(t) + v_{\text{therm}}(t) \right] + \tilde{H}_{\text{env}}. \quad (17)$$
Here we see that the effect of the finite temperature can be exactly represented as a classical fluctuating field \( v_{\text{therm}}(t) \). Then, since the thermal bath state is Gaussian, when we calculate the averages, the Wick theorem rules apply for all the occurrences of the bath operators \( \hat{b}(t) \) and \( \hat{b}^\dagger(t) \). However, according to the stochastic wavefunction method, the Wick theorem rules do not change if we replace \( \hat{H} \) by \( \hat{H}_{\text{stoch}}(t) \) and instead of the full trace we compute the environment vacuum-vacuum amplitude:

\[
Z[0,t] = \left| \langle 0_{\text{env}}, \psi_{\text{sys}} | \mathcal{T} \exp \left[ -i \int_{0}^{t} d\tau \hat{H}_{\text{stoch}}(\tau), v_{\text{therm}}(\tau) \right] | 0_{\text{env}}, \psi_{\text{sys}} \rangle \right|^{2} \tag{18}
\]

Note that we consider the virtual excitations component \( K_{\text{virt}}(t-t') \) as a genuinely quantum object. Indeed, all the attempts to employ a stochastic sampling of \( K_{\text{virt}}(t-t') \) lead to an exponential growth of complexity of calculations, numerical instabilities, etc, which we call a “generalized sign problem”. Therefore, we propose to compute the influence of \( K_{\text{virt}}(t-t') \) quantum-mechanically, within a certain approximation.

The exact stochastic evaluation of real-time dynamics of a certain observable system \( \hat{O}_{\text{sys}} \) proceeds in the following way. We solve the stochastic Schrodinger equation with bath degrees of freedom

\[
\partial_t |\Psi(t)\rangle = -i\hat{H}_{\text{stoch}}(\zeta_{\text{emit}}(t), v_{\text{therm}}(t)) |\Psi(t)\rangle, \tag{19}
\]

for a given realization of noises \( \zeta_{\text{emit}} \) and \( v_{\text{therm}} \) and for the initial condition \( |0_{\text{env}}, \psi_{\text{sys}}\rangle \). Then, the observable average is calculated as

\[
\langle \hat{O}_{\text{sys}} \rangle = \langle \Psi(t) | 0_{\text{env}} \rangle \hat{O}_{\text{sys}} (0_{\text{env}} | \Psi(t)\rangle)_{\zeta_{\text{emit}}, v_{\text{therm}}} \tag{20}
\]

From the commutation relations it can also be shown that the environment’s observables \( \hat{O}_{\text{env}} \) in the antinormally ordered form can be computed by substituting

\[
\hat{b}(\omega) \to e^{-i\omega t} \left( \xi(\omega) + \sqrt{n(\omega)} \eta(\omega) \right), \tag{21}
\]

\[
\hat{b}^\dagger(\omega) \to e^{i\omega t} \left( \xi^*(\omega) + \sqrt{n(\omega)} \eta^*(\omega) \right) \tag{22}
\]

in the operator expression for \( \langle \hat{O}_{\text{env}} \rangle \), obtaining a c-number function \( O_{\text{env}}(\xi, \eta) \). Then, the average is computed as

\[
\langle \hat{O}_{\text{env}} \rangle = \langle \Psi(t) | 0_{\text{env}} \rangle O_{\text{env}}(\xi, \eta) (0_{\text{env}} | \Psi(t)\rangle)_{\zeta_{\text{emit}}, v_{\text{therm}}} \tag{23}
\]

Note that this ordering prescription closely resembles the Husimi Q-function representation of the environment’s state (in the interaction picture).

**ZERO-ORDER APPROXIMATION TO VIRTUAL EXCITATIONS**

The simplest approximation is to completely neglect the intrabranch contractions \( K_{\text{virt}}(t-t') \). This corresponds to neglecting all the diagrams with the intrabranch contractions in Fig. 1, and neglecting completely the environment degrees of freedom in the stochastic Schrodinger equation (19). We obtain the following stochastic recipe:

\[
\partial_t |\psi_{\text{sys}}(t)\rangle = -i\hat{H}_{\text{sys}} |\psi_{\text{sys}}(t)\rangle - i\hat{a} \left[ \zeta_{\text{emit}}(t) + v_{\text{therm}}(t) \right] |\psi_{\text{sys}}(t)\rangle - i\hat{a}^\dagger v_{\text{therm}}(t) |\psi_{\text{sys}}(t)\rangle. \tag{24}
\]

Note that the virtual excitations play the following two roles. a) by drawing the analogy with Lindblad equation in the Markovian case, we argue that they ensure the balance of probability density distribution of quantum trajectories: they vary the norm of the quantum trajectory to take into account the probability flux into other trajectories. b) they take into account the dynamical effects of virtual excitations, e.g. Lamb shift of levels. Therefore, by discarding these virtual terms, we break a) and b). In order to fix approximately a), when computing observables for the trajectories Eq. (24), we divide by the average norm of the ensemble of trajectories:

\[
\langle \hat{O}_{\text{sys}} \rangle = \frac{|\psi_{\text{sys}}(t) \hat{O}_{\text{sys}} \psi_{\text{sys}}(t)\rangle_{\zeta_{\text{emit}}, v_{\text{therm}}}}{|\psi_{\text{sys}}(t) \psi_{\text{sys}}(t)\rangle_{\zeta_{\text{emit}}, v_{\text{therm}}}}. \tag{25}
\]

These two equations, (24) and (25), is the resulting zero-order approximation (without virtual excitations).

\[\text{[End of text]}\]
BOSONIZATION OF KONDO MODEL

In this section we apply our method to the spin-1/2 Kondo model which describes a localized magnetic moment interacting with electron gas [8, 9, 10, 11]. The characteristic property of this model is that in the ground state the electron gas becomes correlated with the impurity, the so called Kondo screening cloud, which forms a spin singlet round impurity. The 1d chiral Kondo problem has the following Hamiltonian

\[
\tilde{H} = \sum_{k\mu} \epsilon_k c_{k\mu}^\dagger c_{k\mu} + \frac{J_\perp}{2} \sum_{k,k'} \left( c_{k\uparrow}^\dagger c_{k'\downarrow} S^\perp_{\mathrm{imp}} + c_{k\downarrow}^\dagger c_{k'\uparrow} S^\uparrow_{\mathrm{imp}} \right) + \frac{J_\parallel}{2} \left( c_{k\uparrow}^\dagger c_{k'\downarrow} - c_{k\downarrow}^\dagger c_{k'\uparrow} \right) S^z_{\mathrm{imp}},
\]

where

\[
k = 2\pi n / L, \quad -\infty < n < \infty,
\]

\( L \) is the quantization volume, \( L \to \infty \). The 1d chiral Kondo is mapped onto the spin-boson model [8, 9, 10, 11]

\[
\tilde{H} = \frac{J_\perp}{4\pi a} \sigma_x + v_F \sum_q q b_q^\dagger b_q + \left( \frac{J_\parallel}{4\pi} - v_F \right) \sqrt{\frac{\sigma_z}{2}} \sum_{q < 0} \sqrt{\frac{2\pi q}{L}} \left( b_q + b_q^\dagger \right) e^{-aq/2},
\]

for the spectral regularization parameter \( a \to 0 \).

\[
q = 2\pi n_q / L, \quad 0 < n_q < \infty,
\]

The bosonic operators are related to the fermionic ones as

\[
b_{q\mu}^\dagger = in_q^{-1/2} \sum_k c_{k+q\mu}^\dagger c_k.
\]

In this work we employed the following parameters: \(|n| \leq 1600, L = 60, J_\perp = J_\parallel = 2\pi \times 0.3, v_F = 1, a = 0.01\). According to the approximate stochastic algorithm (24)-(25), we have the open system and the environment Hamiltonians

\[
\tilde{H}_{\mathrm{sys}} = \frac{J_\perp}{4\pi a} \sigma_x, \quad \tilde{H}_{\mathrm{env}} = v_F \sum_q q b_q^\dagger b_q.
\]
The time and spatially dependent spin-spin correlation function $\langle \sigma_z(t) S_z(x,t) \rangle$ between the impurity and the Kondo cloud as a color contour plot. After the initial coupling is switched on at $t = 0$, the correlation propagates with the Fermi velocity $v_F$.

The system is coupled through its operator $\hat{a} = \sigma_z$, (32)

and the bath’s collective degree of freedom

$$\hat{x} = \left( \frac{J_x}{4\pi} - v_F \right) \sum_{q>0} \frac{2\pi q}{L} (b_q + b_q^\dagger) e^{-aq^2/2}. \quad (33)$$

Let us take the vacuum initial state of the environment, and the impurity spin initially directed towards $z$-axis. We switch on the coupling at $t = 0$ and conduct the stochastic Monte Carlo simulation of the resulting quench dynamics. In Fig. 2 we present the results of calculation of spin-spin correlation function $\langle \sigma_z(t) S_z(x,t) \rangle$.

In Fig. 3 we present simulation result when an additional quench is done: an external field $\hat{H}_{\text{ext}} = 500\sigma_x$ (34)

is smoothly switched on by the time moment $t = 3$. Such a strong field suppresses orientational fluctuations of the impurity spin, which are important for sustaining the Kondo cloud. As a consequence, the Kondo cloud detaches from the impurity and flies away.

**CONCLUSION**

In this work we propose the idea of how to advance in the development of real-time simulation techniques for open quantum systems. Our approach is to calculate in a numerically exact way all the observable effects of the environment: irreversibly emitted excitations and the thermal field. Due to this observability, we obtain true probabilities for Monte Carlo simulation at long times without the sign problem. However, we argue that the genuinely quantum virtual excitations cannot be interpreted in a classical way without the sign problem, and should be computed quantum mechanically in a certain approximate way. In this work we demonstrate the simplest approximation: to completely neglect the virtual terms. On the example of chiral Kondo model we easily obtain interesting semiquantitative results. In particular, the stochastic simulation demonstrates how the process of Kondo cloud formation propagates in space at the Fermi velocity. Another simulated effect is that if the impurity spin fluctuations are suppressed by a strong external field, the Kondo cloud detaches and flies away.
FIGURE 3. The time and spatially dependent spin-spin correlation function \( \langle \sigma_z(t) S_z(x,t) \rangle \) between the impurity and the Kondo cloud as a color contour plot. When the orientational fluctuations of the impurity spin are suppressed by a strong external field at time moment around \( t = 3 \), the Kondo cloud cannot be sustained, it detaches from the impurity and flies away at the speed \( v_F \).

Higher order approximations for the quantum field of virtual excitations may be implemented by e.g. including a truncated basis of environment states into the stochastic Schrodinger equation (24); by employing (multi)polaronic expansion [12, 13] etc.

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