Cooling of quantum systems through optimal control and dissipation

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Based on an exact non-Markovian open systems quantum dynamics we demonstrate how to reduce the entropy of an open system through a cooperative effect of driving and dissipation. We illustrate the controlled dynamics in phase space in terms of Wigner functions and discuss the applicability of approximate approaches using master equations.

I. INTRODUCTION

Coherent control of quantum dynamics is a powerful tool to drive a system towards desired states and to optimize properties of the dynamics. Mature numerical methods exist for the control of non-dissipative dynamics [1–5]. Similar approaches to open quantum systems are urgently needed and evolving rapidly [6–8]. However, particular care is needed in this case, for which commonly used equations of motion are approximate. Strong driving does not only have an impact on the system, but the interaction between the control-modified system and the reservoir differs substantially from the case of autonomous dynamics. This basically calls Markovian and perturbative approaches into question. Instead of relying on these approaches, we propagate the quantum system using a fully non-Markovian, exact stochastic Liouville-von Neumann equation [9]. Uniting this approach with optimal control theory allows the consideration of control signals of arbitrary strength and complexity [10].

II. METHOD

In order to derive the exact dynamics we describe the driven open system by a Hamiltonian of the form

$$H = H_0 + H_C + H_I + H_R, \tag{1}$$

where the individual terms are defined as follows: The system Hamiltonian H_0 governs the autonomous dynamics of the system, which we assume to be characterized by a position q and a momentum p, or equivalent conjugate variables, such as phase and charge in a mesoscopic circuit. The control Hamiltonian $H_C = H_C(\mathbf{u}(t))$ describes the modification of this dynamics through classical controls $\mathbf{u}(t)$, typically fields assumed to be acting on the system only. The vector-valued function $\mathbf{u}(t)$ is the *independent quantity* to be varied in the control problem. The term H_I denotes the Hamiltonian of the system-reservoir-interaction, and H_R is the Hamiltonian governing the autonomous dynamics of the reservoir. As shown by Caldeira and Leggett [11], any reservoir with Gaussian fluctuations can be modeled by a set of harmonic oscillators,

$$H_I + H_R = \sum_i \frac{p_i^2}{2m_i} + \frac{m_i\omega_i^2}{2}\left(x_i - \frac{c_i}{m_i\omega_i^2}q\right)^2. \tag{2}$$

Here x_i, p_i, m_i and ω_i are the coordinates and parameters of the respective reservoir mode, q is the coordinate of the system and c_i is the coupling constant of the system and the respective reservoir mode.

An exact expression for the reduced dynamics in closed form requires the path integral formalism [11, 12], which is unsuitable for optimal control theory. However, the *stochastic* equation of motion

$$\begin{aligned}\dot\rho_{\nu,\xi} &= \mathcal{L}\rho_{\nu,\xi} \\ &:= -\frac{i}{\hbar}[H_0 + H_C, \rho_{\nu,\xi}] \\ &\quad + \frac{i}{\hbar}\xi(t)[q, \rho_{\nu,\xi}] + \frac{\mathrm{i}}{2}\nu(t)\{q, \rho_{\nu,\xi}\},\end{aligned} \tag{3}$$

which can be used in optimal control theory, has been shown to be fully equivalent [9]. The functions $\xi(t)$ and $\nu(t)$ are correlated complex-valued Gaussian stochastic processes [9] exactly matching the fluctuations and the dynamic response of the reservoir as given by the quantum correlation function $L(\tau)$ of the total environmental force,

$$L(t-t') = \left\langle \sum_i c_i x_i(t) \sum_j c_j x_j(t') \right\rangle. \tag{4}$$

Eq. (3) introduces the stochastic Liouvillian superoperator $\mathcal{L}$, defined through the second equality. For an environment in thermal equilibrium, $L(t-t')$ is fully determined by the spectral density $J(\omega)$ and the inverse thermal energy β of the reservoir:

$$\begin{aligned}L(t) &= \frac{\hbar}{\pi}\int_0^\infty \mathrm{d}\omega\ J(\omega) \\ &\quad \times \left(\coth\frac{\hbar\omega\beta}{2}\cos\omega t - i\sin\omega t\right).\end{aligned} \tag{5}$$

The specific properties of the Gaussian processes $\xi(t)$ and

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$\nu(t)$ are related to $L(t-t')$ as follows:

$$\mathbb{E}\left[\xi(t)\xi(t')\right] = \mathrm{Re}(L(t-t')) \quad (6a)$$

$$\mathbb{E}\left[\xi(t)\nu(t')\right] = 2\frac{i}{\hbar}\Theta(t-t') \times \mathrm{Im}(L(t-t')) \quad (6b)$$

$$\mathbb{E}\left[\nu(t)\nu(t')\right] = 0 \quad (6c)$$

$$\mathbb{E}\left[\xi(t)\right] = \mathbb{E}\left[\nu(t)\right] = 0. \quad (6d)$$

For computational purposes, eq. (3) is solved multiple times with numerical samples of ξ and ν generated according to Eq. (6). Averaging over samples yields the physical density matrix,

$$\rho = \mathbb{E}\left[\rho_{\nu,\xi}\right], \quad (7)$$

from which any physical observable may be obtained, in particular, the optimization objective.

Based on the exact dynamics we have generalized Krotov's iterative algorithm [13, 14] into a form applicable to Eqs. (3) and (7). Details are provided in Ref. [10] (including supplemental material).

The type of objective we are considering is minimizing an expectation value $\langle M\rangle$ of an observable M of the system at a final time t_f (a von Neumann measurement). In the minimization of the corresponding objective functional

$$F[\mathbf{u}(t),\{\rho_{\nu,\xi}\}] = \mathbb{E}\left[\mathrm{tr}\{\mathrm{M}\ \rho_{\nu,\xi}(\mathrm{t_f})\}\right], \quad (8)$$

the equation of motion (3) needs to be introduced as a constraint, valid for any realization of the stochastic variables $\xi(t)$ and $\nu(t)$.

Variational calculus leads to a characterization of local extrema that includes a stochastic equation of motion for the Lagrange multiplier Λ with a *terminal* boundary condition:

$$\dot{\Lambda}_{\nu,\xi}(t) = -\mathcal{L}^{\dagger}\Lambda_{\nu,\xi}(t) \quad (9a)$$

$$\Lambda_{\nu,\xi}(t_f) = -M \quad (9b)$$

where $\mathcal{L}^{\dagger}$ is the adjoint of the Liouvillian $\mathcal{L}$ (see Eq. (3)) and $M = -|\alpha\rangle\langle\alpha|$ is defined through a projection operator on a target state $|\alpha\rangle$ at final time t_f.

The Krotov algorithm relies on the coupled dynamics of the quantum state and a *costate* Λ, which can (for most purposes) be identified with the previously introduced Lagrange multiplier; most importantly, it also obeys the equation of motion (9a). The key step of the Krotov algorithm is an iterative update for the control fields, changing the components of the vector $\mathbf{u}(t)$ according to

$$u_i^{(new)}(t) = u_i^{(old)}(t) - \frac{1}{\lambda_i(t)} \times \mathbb{E}\left[\frac{2}{\hbar}\mathrm{Im}\left[tr\left\{\frac{\partial H_c}{\partial u_i}\left[\rho_{\nu,\xi},\Lambda^{\dagger}_{\nu,\xi}\right]\right\}\right]\right]. \quad (10)$$

Different choices for the function $\lambda_i(t)$ can be made in order to tune the convergence properties of the algorithm [14].

III. APPLICATION AND RESULTS

While coherent control of Hamiltonian dynamics still conserves entropy (a scalar invariant of unitary transformations), open-system dynamics generally brings about a change in entropy. Without external control, this results in thermalization, i.e., a rise in entropy when considering a pure initial state. In the following, we demonstrate that it is possible to *remove* entropy from an open quantum system by applying optimal control fields, without promoting the coupling to a low temperature reservoir, as is done, e.g., in sideband cooling.

In this context, we look at systems with at most a few bound states thermally accessible, usually well described in the harmonic approximation, with an environment characterized by a spectral density of the form $J(\omega) = \eta\omega/(1+\frac{\omega^2}{\omega_c^2})^2$ with large UV cutoff ω_c, corresponding to Stokes (or Ohmic) friction with friction constant η in the classical limit. Still, we emphasize our method is not restricted to harmonic systems. In the following, we use natural units ($\hbar = 1; k_B = 1$). At the initial time $t = 0$ the system is thermalized with the reservoir (inverse thermal energy $\beta = 1$), and a moderate value $\eta = 0.1$ is chosen for the friction constant. The objective is defined by chosing the ground state as target state $|\alpha\rangle$.

The parametric control

$$H_C(t) = \frac{\Delta(t)}{2}q^2 \quad (11)$$

is chosen as the simplest time-dependent modification of the potential with non-trivial effects on the dynamics. The single control field $\Delta(t)$ takes the place of $\mathbf{u}(t)$. With a Gaussian initial state, all stochastic samples remain Gaussian over time; therefore Eqs. (3) and (9a) can be replaced by ordinary differential equations for the expectation values of position and momentum and for the matrix elements of the covariance matrix associated with the Wigner function. We emphasize, however, that the more general case of an anharmonic system can be treated on an equal footing. In either case the optimal control dynamics in phase space can be investigated in terms of the Wigner function of the system.

A. stochastic Liouville–von Neumann equation

In Fig. 1 we show the time evolution of the Wigner function of the system for the optimal control field obtained from Eqs. (10) and (11). In natural units, the initial Wigner function has rotational symmetry, characteristic of a thermal state, later evolving through various squeezed states. The optimal control solution (Fig. 1, right) shows two main features: First there is a long ramp-like rise, followed by a steep descent, with virtually no transition. On the other hand the signal carries also a periodic modulation which, in this case matches both on the timescale of the original system ($\omega_0 = 1$) and the

thermal time $\hbar\beta = 1$. During the gradual rise, the Wigner function gets more and more squeezed in the direction q as the applied control narrows the potential, indicating that the energy added by the work performed is dissipated to the reservoir, also transferring entropy to the environment in the process. The effective temperature of the system, roughly estimated from the level populations and the characteristic energy scale of $H_0 + H_C$, decreases. The rapid decrease of the control towards the end of the propagation is fast enough to preserve this cooling effect (i.e. to prevent the full re-thermalization of the energy levels). In addition, the small modulations visible in the numerically determined optimal control, serve to drive the squeezed state back towards a state again isotropic in phase space.

In Fig. 2 we compared our optimal control signal with a simplified one lacking the oscillatory parts, approximating the numerical solution by two linear ramps. This simplified signal, while also achieving a significant overlap with the ground state, results in a Wigner much less isotropic. One might be interested in replacing the exact but computationally expensive equation of motion Eq. (3) with simpler approaches to the dynamics. The consequences will be outlined in the following section.

B. Quantum optical master equation

Surprisingly, the quantum optical master equation, one of the standard approaches to the dynamics of open quantum systems, fails to account for the cooling effect described above. Since the level structure of the time-independent Hamiltonian H_0 is, so to speak "hard-coded" into the dissipative terms, these terms describe relaxation towards the canonical ensemble, $\rho = Z^{-1}\exp(-\beta H_0)$ even for strong changes to the potential. Using the system Hamiltonian $H_0 + H_C$ and standard Lindblad operators (obtained solely from H_0) cannot reproduce the cooling effect. The fact that the resulting solutions always describe heating, never cooling [10], underscores the inconsistency of this approach.

C. Caldeira-Leggett master equation

The shortcomings of the quantum optical master equation are related to the inapplicability of the Born-Markov approximation and the rotating-wave approximation in their conventional form. One attempt to circumvent this difficulty while maintaining the simplicity of a master equation is the use of the Caldeira-Leggett master equation [11].

$$\frac{d}{dt}\rho = -\frac{i}{\hbar}[H_0, \rho] - \frac{i\eta}{2m\hbar}[q, \{p, \rho\}] - \frac{\eta}{\hbar^2\beta}[q, [q, \rho]] \quad (12)$$

This approach replaces the Born-Markov approximation (separation of time scales between environmental fluctuations and relaxation) with a stronger Markovian approximation, assuming the decay of environmental fluctuations to be virtually instantaneous compared to any other time scale of the dynamics. It does not rely on the rotating-wave approximation.

In Fig.3 we show the optimal control solution obtained through the Caldeira-Leggett Master equation. The resulting control signal shows some qualitative features of the one calculated without approximations. Again, there is a gradual rise of the control signal, superimposed with oscillations of increasing amplitude. However, the growth of this amplitude is much stronger than in the exact dynamics, and the final drop of the signal is virtually instantaneous. This indicates that the Markovian approximation of the dynamics reproduces the essence of the effect, but overestimates the effectiveness of high-frequency components in the control signal. The final states shown on the r.h.s. of Fig. 3 also show that the Caldeira-Leggett master equation tends to overstate the effect: The predicted phase-space density is concentrated in a *smaller* area than that of the ground state. In retrospect, this misfeature is less than surprising: When Eq. (12) is translated into an equation of motion for the Wigner function, the special case of an harmonic potential yields a result identical to the classical Klein-Kramers equation. The quantum mechanical zero-point motion is missing from this picture. This anomalous result is also closely related to the previous observation that the Caldeira-Leggett master equation violates positivity [15]. Reliable results can be expected of the Caldeira-Leggett master equation only for temperatures far above the range of interest for the cooling effect considered here.

However, the observation that cooling can be observed in classical dynamics as well, is interesting in itself. Preliminary results indicate that both Markovian and non-Markovian classical dynamics allow cooling through optimal control [16].

IV. OUTLOOK

Controlling an open quantum system not only changes the dynamics of the system but has an equally important indirect impact on mechanisms of dissipation. We demonstrate that driving can partly reverse the natural heat flow a reservoir to a system as a drastic manifestation. This opens the door to a rigorous treatment to non-equilibrium mesoscopic heat engines.

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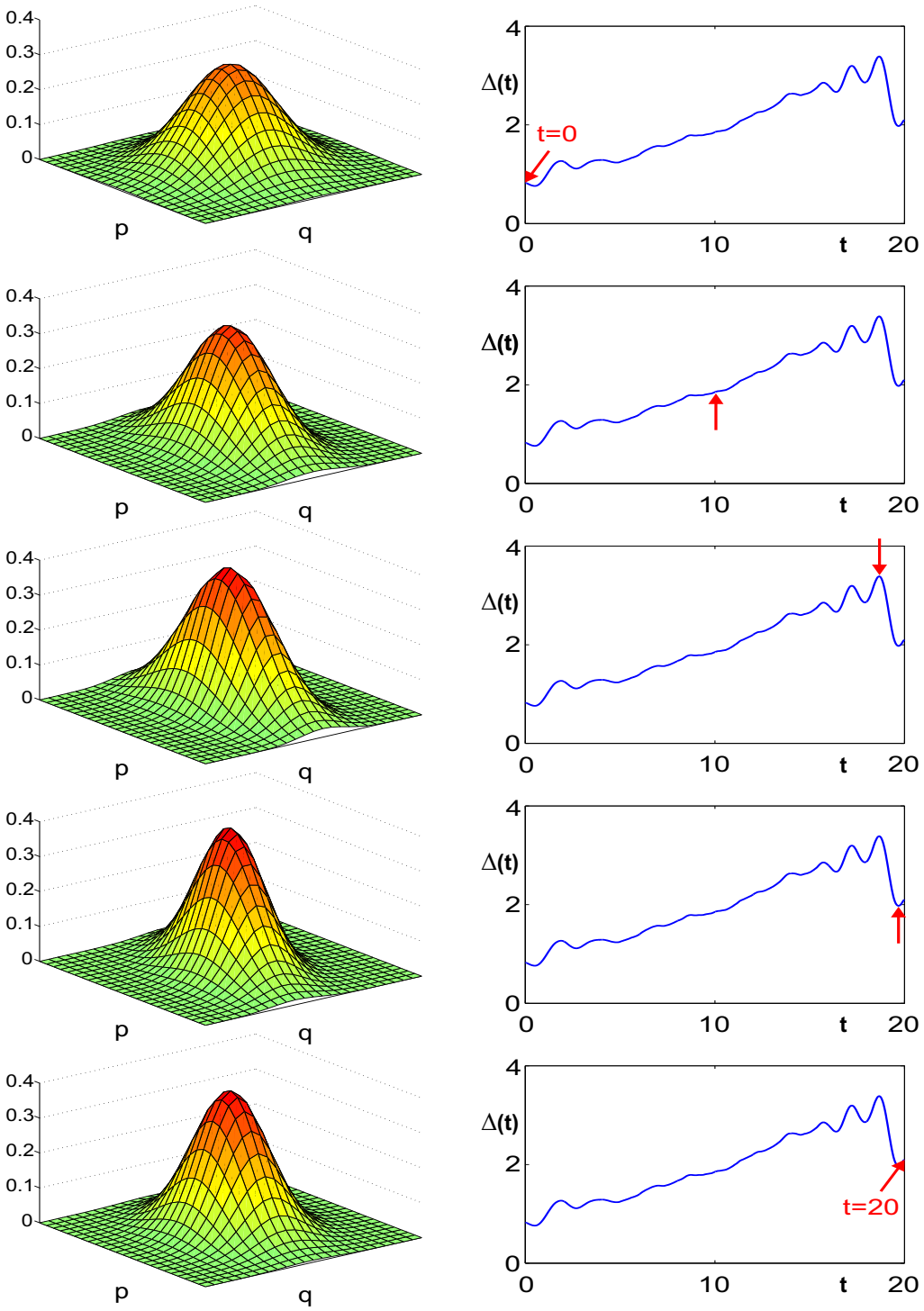

Figure 1:(color online) Control of an open quantum system with parametric control: For the time steps $t = 0,\ 10,\ 18.7,\ 19.7$ and 20 each. Left hand side: Wigner function, right hand side: control signal $\Delta(t)$. Parameters: inverse thermal energy of the reservoir: $\beta = 1$, friction constant $\eta = 0.1$

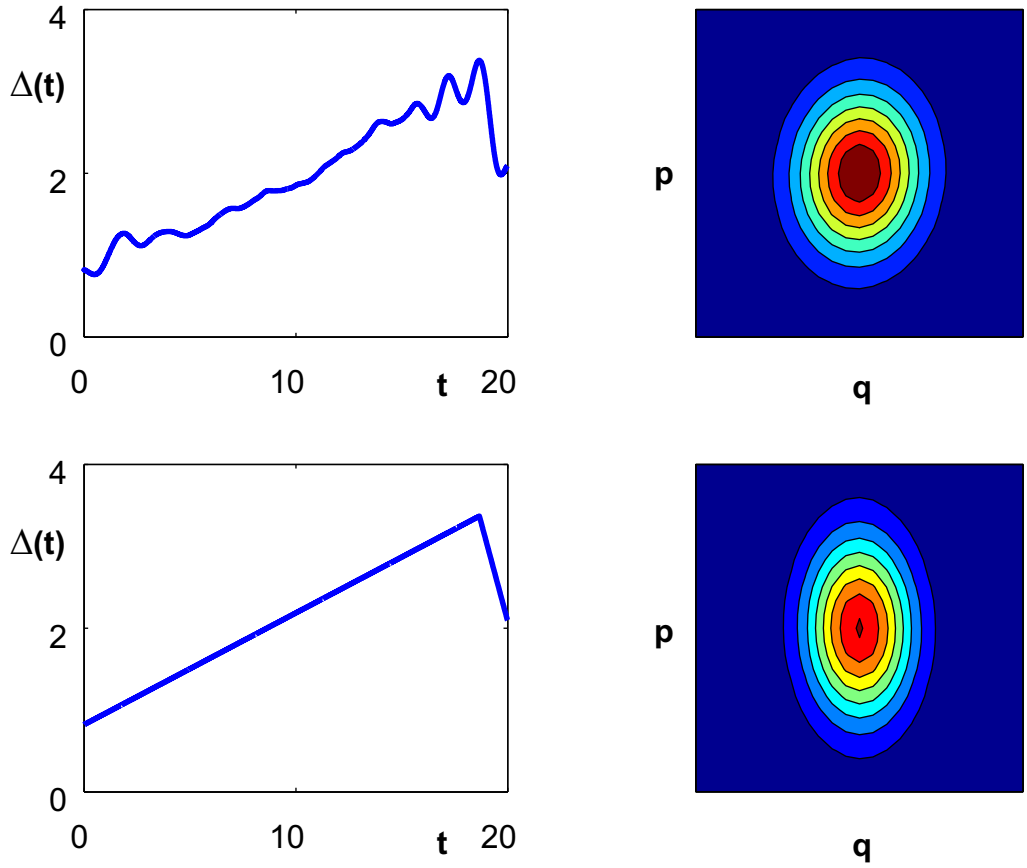

Figure 2: (color online) Comparison between original control signal $\Delta(t)$ (upper left) with respective contour plot of the Wigner function of the system (upper right) at $t = t_f$ and a simplification of the control signal (lower left) with respective contour plot of the Wigner function of the system (lower right) at $t = t_f$. While achieving compareable overlap with the objective, the simplified control fails to reduce the squeezing of intermediate states.

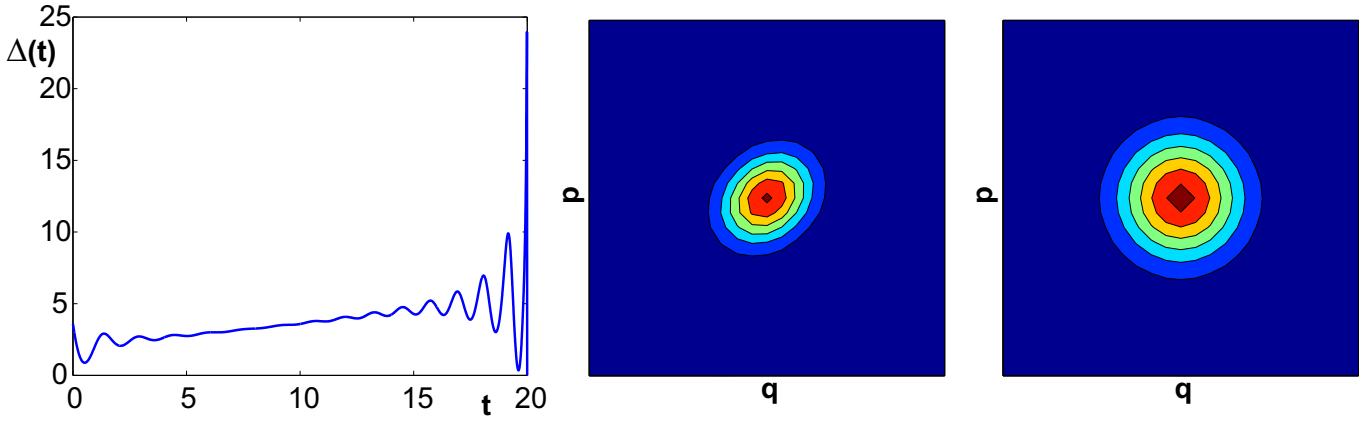

Figure 3: (color online) Results of optimal control with a classical Caldeira-Leggett-Master equation: The computed control signal $\Delta(t)$ (left hand side) carries the main features of the control signals of the quantum treatment. The Wigner function of the classical dynamics shows cooling (middle), but violates the uncertainty relation: the ground state (right hand side) covers a larger area in phase space