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A Landau-Zener Lindblad equation and work extraction from coherences

Juzar Thingna,[1,*] Massimiliano Esposito,[1,2,†] and Felipe Barra[3,2,‡]

[1] *Complex Systems and Statistical Mechanics, Physics and Materials Science Research Unit, University of Luxembourg, L-1511 Luxembourg, Luxembourg*

[2] *Kavli Institute for Theoretical Physics, University of California, Santa Barbara, CA 93106 Santa Barbara, U.S.A.*

[3] *Departamento de Física, Facultad de Ciencias Físicas y Matemáticas, Universidad de Chile, Santiago, Chile*

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We show that the dynamics of a driven quantum system weakly coupled to a finite reservoir can be approximated by a sequence of Landau-Zener transitions if the level spacing of the reservoir is large enough. This approximation can be formulated as a repeated interaction dynamics and leads to a quantum master equation for the driven system which is of Lindblad form. The approach is validated by comparison with the numerically exact full system dynamics. To emphasize the role of coherence in the master equation, we propose a model-system which shows that in its presence, work can be extracted from a thermal reservoir while if the coherences vanish no work can be extracted.

I. INTRODUCTION

Establishing reliable kinetic descriptions for time-dependently driven open quantum systems is important in many contexts [1–8]. In recent years this became particularly true in quantum thermodynamics where work has been particulary focused for periodically driven systems [9–16] but not only [17–23]. We used a distinctive approach in Refs [24, 25], where we studied the thermodynamics and dynamics of a quantum dot with a time dependent energy level, coupled to a fermionic reservoir with finite spacing between energy levels. When the coupling is weak compared to that spacing, the dynamics can be described as a sequence of Landau-Zener transitions [26–29] occurring whenever the dot energy crosses a reservoir level. The resulting stochastic dynamics for the dot occupation was shown to agree very well with the numerically exact full quantum dynamics.

In these previous studies the initial state was thermal for the reservoir and diagonal in the energy basis of the dot. As a result coherences were absent from the description. In the first part of this work, Sec. II, we extend these previous works and consider initial states which may contain coherences. We formulate the problem in a different but equivalent physical setup. Our system is now a single spin 1/2 system interacting with a reservoir of L spin 1/2, that eventually will be thermal. We will show that the dynamical description we obtain for the system can be formulated in a repeated interaction framework [30–32]. The agreement with numerically exact results will again be shown to be very good.

In the second part of the paper, Sec. III, we use our results to propose a machine that can extract work from coherences, a topic that has attracted attention in recent years [33–35]. The machine is driven by spin-1/2 systems which are initially prepared in a thermally populated density matrix with non-vanishing coherences which repeatedly interacts with a spin 1/2 particle, in permanent contact with a thermal reservoir. Work extraction in this model is exclusively caused by coherences. Conclusions are drawn in Sec. IV.

II. QUANTUM DYNAMICAL MAP

We consider a spin-1/2 particle interacting with a finite number of spins whose Hamiltonian takes the form,

$$\begin{aligned} H(t) &= \varepsilon_t \sigma^z + \sum_{n=1}^{L} \epsilon_n \sigma_n^z + \sum_{n=1}^{L} \nu_n \sigma^+ \sigma_n^- + \text{H.c.}. \\ &= H_S(t) + H_B + V \end{aligned} \tag{1}$$

Above σ^α ($\alpha = x, y, z$) are Pauli spin-1/2 matrices and $\sigma^\pm = (\sigma^x \pm i\sigma^y)/2$. Hereon, we refer to the first spin (without subscript) as the system with time dependent $H_S(t) = \varepsilon_t \sigma^z$ and the remaining L spins as the reservoir with $H_B = \sum_{n=1}^{L} \epsilon_n \sigma_n^z$. When $L \to \infty$ we obtain a system interacting with a spin reservoir [36]. In this work we will set the Planck constant $\hbar$ and the Boltzmann constant k_B to unity.

As the energy level of the system, ε_t, is ramped in time at a rate $\dot{\varepsilon}_t$, it will cross the reservoir energy level ϵ_n (see Fig. 1) at time t_n and undergo an avoided crossing in the single spin magnetization (single-particle) basis with an energy gap of order $2\nu_n$. The level spacing between consecutive reservoir spin energies is assumed to be greater than the energy gap, i.e.,

$$\epsilon_{n+1} - \epsilon_n > 2|\nu_n| \tag{2}$$

and the ramping rate at crossing n, $\dot{\varepsilon}_n$, is assumed to change smoothly with n. The time between two consecutive levels $t_{n+1} - t_n = (\epsilon_{n+1} - \epsilon_n)/\dot{\varepsilon}_n$, is also assumed greater than the Landau-Zener validity time τ_n^{lz} [37, 38],

* juzar.thingna@uni.lu
† massimiliano.esposito@uni.lu
‡ fbarra@dfi.uchile.cl

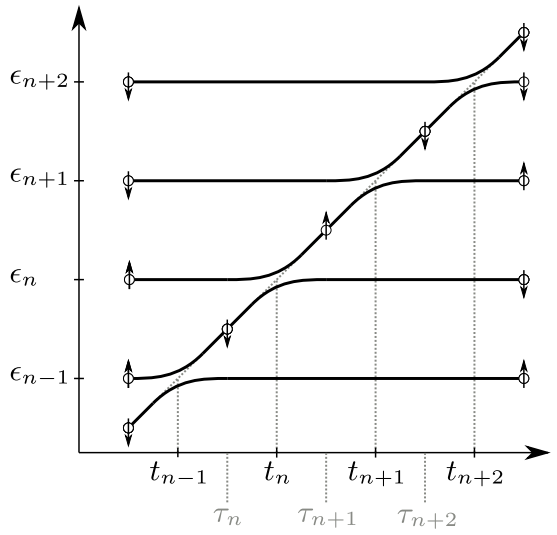

FIG. 1. Schematics of the model with ε_t linearly ramped.

the time necessary for the standard asymptotic Landau-Zener formulas to hold. This implies a second condition

$$\epsilon_{n+1} - \epsilon_n > \sqrt{\dot{\varepsilon}_n}\max\left[1, 2|\nu_n|/\sqrt{\dot{\varepsilon}_n}\right]. \tag{3}$$

These assumptions will allow us to treat the dynamics as a repeated interaction problem [30–32], where the system interacts with the spins of the reservoir *sequentially*. Indeed, over times $\tau_{n+1} > t > \tau_n$ where $\tau_n = (t_n + t_{n-1})/2$ for $n > 1$ and $\tau_1 = 0$, the Hamiltonian can be approximated as

$$H(t) \approx H_n + H_{\neq n} \tag{4}$$

with

$$\begin{aligned} H_n &= \varepsilon_t\sigma^z + \epsilon_n\sigma_n^z + \left(\nu_n\sigma^+\sigma_n^- + \text{H.c.}\right), \\ H_{\neq n} &= \sum_{n'\neq n}\epsilon_{n'}\sigma_{n'}^z. \end{aligned} \tag{5}$$

The corresponding unitary evolution operator in full space between τ_n and τ_{n+1} is thus given by $U_n \otimes U_{\neq n}$, with $U_x = \exp_+\left[-i\int_{\tau_n}^{\tau_{n+1}} dt H_x\right]$ ($x = n, \neq n$ and the subscript + indicates the time-ordered exponential). We will only consider initial states at time $t = 0$ of the total system of the form $\varrho_1 \bigotimes_{n=1}^{L}\rho_n^B(0)$, where ϱ_1 is an arbitrary system density matrix and $\rho_n^B(0)$ an arbitrary density matrix for spin n of the reservoir. Therefore, as long as the ramping of the system level occurs only in one direction (to avoid multiple crossings with the same reservoir level and thus ensure that at every crossing the system encounters a free reservoir spin), the system density matrix at time τ_n, denoted ϱ_n, will be given by the iterative relation (valid for $n \geq 1$)

$$\varrho_{n+1} = \text{Tr}_n[U_n(\varrho_n \otimes \rho_n^B(\tau_n))U_n^\dagger], \tag{6}$$

where $\rho_n^B(\tau_n) = e^{-i\epsilon_n\sigma_n^z\tau_n}\rho_n^B(0)e^{i\epsilon_n\sigma_n^z\tau_n}$ is the freely evolved reservoir spin n and Tr_n is the trace over the space of the spin n of the reservoir.

Thus, the problem of evaluating the quantum dynamical map of the system density matrix boils down to obtain an expression for the evolution operator U_n. To do so, we begin by expressing H_n in the basis that diagonalize $\sigma^z \otimes \sigma_n^z$

$$\begin{aligned} H_n|\uparrow\uparrow_n\rangle &= (\varepsilon_t + \epsilon_n)|\uparrow\uparrow_n\rangle, \\ H_n|\uparrow\downarrow_n\rangle &= (\varepsilon_t - \epsilon_n)|\uparrow\downarrow_n\rangle + \nu_n^*|\downarrow\uparrow_n\rangle, \\ H_n|\downarrow\uparrow_n\rangle &= -(\varepsilon_t - \epsilon_n)|\downarrow\uparrow_n\rangle + \nu_n|\uparrow\downarrow_n\rangle, \\ H_n|\downarrow\downarrow_n\rangle &= -(\varepsilon_t + \epsilon_n)|\downarrow\downarrow_n\rangle, \end{aligned} \tag{7}$$

where $\sigma_z|\uparrow\rangle = |\uparrow\rangle$, $\sigma_z|\downarrow\rangle = -|\downarrow\rangle$, and $|\uparrow\downarrow_n\rangle = |\uparrow\rangle\otimes|\downarrow_n\rangle$ with the first ket corresponding to the system spin and the second corresponding to the nth reservoir spin. This shows that nontrivial dynamics will only happen in the subspace $\{|\uparrow\downarrow_n\rangle, |\downarrow\uparrow_n\rangle\}$ and that it coincides with the standard Landau-Zener problem [26–29].

Since the ramping has been assumed to vary smoothly with n, close to the crossing, the energy of the system spin can be assumed to change linearly in time, i.e., $\varepsilon_t = \dot{\varepsilon}_n t$. Using this assumption, one can solve the dynamics exactly. The so-called adiabatic impulse approximation [37] (see also [41–45]) consists in matching the exact analytic solution for $t \to \infty$ to the finite time adiabatic evolution to obtain a simple but accurate expression. In this way, one obtains that

$$\begin{aligned} U_n|\uparrow\uparrow_n\rangle &= e^{-i\alpha_n}|\uparrow\uparrow_n\rangle, \\ U_n|\uparrow\downarrow_n\rangle &= \sqrt{R_n}|\uparrow\downarrow_n\rangle - \sqrt{1-R_n}e^{i\varphi_n}|\downarrow\uparrow_n\rangle, \\ U_n|\downarrow\uparrow_n\rangle &= \sqrt{R_n}|\downarrow\uparrow_n\rangle + \sqrt{1-R_n}e^{-i\varphi_n}|\uparrow\downarrow_n\rangle, \\ U_n|\downarrow\downarrow_n\rangle &= e^{i\alpha_n}|\downarrow\downarrow_n\rangle, \end{aligned} \tag{8}$$

with

$$\alpha_n = \frac{\dot{\varepsilon}_n}{2}\left(\tau_{n+1}^2 - \tau_n^2\right) + \epsilon_n\left(\tau_{n+1} - \tau_n\right), \tag{9}$$

$$R_n = e^{-2\pi\delta_n}, \quad \delta_n = \frac{|\nu_n|^2}{2\dot{\varepsilon}_n}, \tag{10}$$

$$\varphi_n = \frac{\pi}{4} + \delta_n\left(\ln\delta_n - 1\right) + \arg\left[\Gamma(1 - i\delta_n)\right], \tag{11}$$

and $\Gamma(x)$ being the Gamma function of x. The parameter φ_n above is the Stokes phase [40] that is independent of all the details of the evolution and only depends on what happens at the avoided crossing. The phase α_n keeps track of the finite time.

Representing ϱ_n in the basis $\{|\uparrow\rangle, |\downarrow\rangle\}$ as

$$\varrho_n = \begin{pmatrix} p_n & k_n \\ k_n^* & 1 - p_n \end{pmatrix}, \tag{12}$$

using Eq. (6) and Eq. (8), we find that

$$\begin{aligned} p_{n+1} &= R_n p_n + a_n(1 - R_n) \\ &\quad + \sqrt{R_n(1-R_n)}\left[e^{i\varphi_n}q_n k_n^* + \text{H.c.}\right], \end{aligned} \tag{13}$$

$$\begin{aligned} k_{n+1} &= \sqrt{R_n}e^{-i\alpha_n}k_n \\ &\quad - \sqrt{1-R_n}e^{-i(\alpha_n - \varphi_n)}q_n(2p_n - 1), \end{aligned} \tag{14}$$

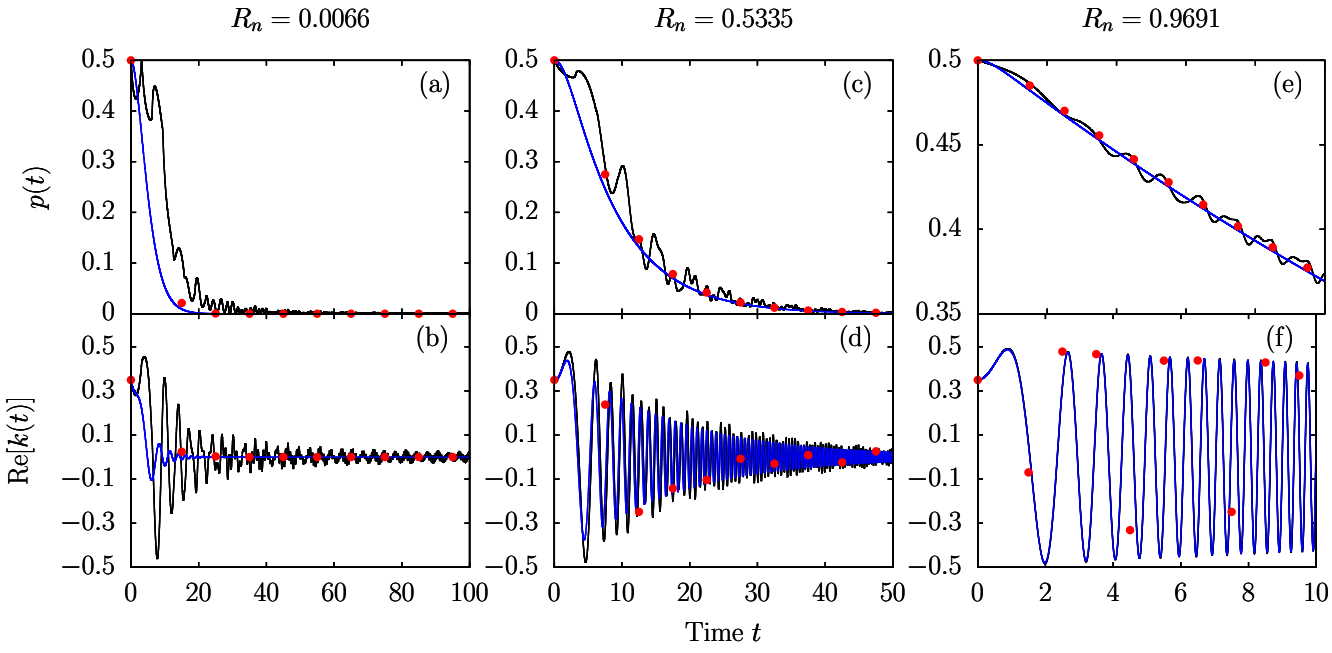

FIG. 2. Comparison between exact quantum dynamics (black solid line), Landau-Zener Markov chain [red closed circles, Eqs. (16) and (17)], and continuous time Landau-Zener master equation [blue solid line, Eqs. (22) and (23)] for different values of Landau-Zener transition probability $1 - R_n$. The parameters for panels: (a) and (b) are $\nu_n = 0.4$ and $\dot{\varepsilon}_n = 0.1$, (c) and (d) are $\nu_n = 0.2$ and $\dot{\varepsilon}_n = 0.2$, and (e) and (f) are $\nu_n = 0.1$ and $\dot{\varepsilon}_n = 1.0$. The spin reservoir with $L = 10$ is set initially at inverse temperature $\beta = 2$, $\mu = 0$, and energies $\epsilon_n = n\,\epsilon$ with $\epsilon = 1$.

where

$$\rho_n^B(\tau_n) = \begin{pmatrix} a_n & q_n \\ q_n^* & 1 - a_n \end{pmatrix}, \tag{15}$$

with $a_n = \langle\uparrow\ |\rho_n^B(0)|\ \uparrow\rangle$ and $q_n = \langle\uparrow\ |\rho_n^B(0)|\ \downarrow\rangle \exp[-2i\epsilon_n\tau_n]$. This completely positive trace preserving (CPTP) map forms the first main result of this work. The population and coherence dynamics are clearly coupled to each other.

In the rest of this section we consider the particular case where the reservoir density matrix is initially grand canonical $\rho^B(0) = \exp\left[-\beta(H_B - \mu M_B)\right]/Z_B$ where $M_B = \sum_{n=1}^{L} \sigma_n^z$ is the net magnetization of the reservoir and μ the associated spin-chemical potential. This means that Eq. (15) is diagonal, $q_n = 0$, whereas $a_n = f_n = \{\exp[2\beta(\epsilon_n - \mu)] + 1\}^{-1}$ is a Fermi-Dirac distribution for spins. As a result, Eq. (13) and Eq. (14) simplify to

$$p_{n+1} = R_n p_n + f_n(1 - R_n) \tag{16}$$

$$k_{n+1} = \sqrt{R_n} e^{-i\alpha_n} k_n. \tag{17}$$

The populations and coherences are now decoupled. The coherences will vanish as the number of crossings increases since R_n is a positive real number smaller than one. The population dynamics in turn obeys a stochastic jump process master equation which was previously derived in Ref. [24]. We note that our spin model is formally equivalent to the fermionic model used in that reference (this can be seen using the mapping: $\sigma_z \to c^\dagger c$, $\sigma^+ \to c^\dagger$ in the Hamiltonian [Eq. (1)] and $\beta \to \beta/2$, $\dot{\varepsilon}_n \to \dot{\varepsilon}_n/2$ for the dynamical map in Eqs. (16) and (17)).

Continuous time Landau-Zener quantum master equation

In order to obtain a continuous time Landau-Zener quantum master equation for a system interacting with a thermal reservoir, we consider that during a small interval of time dt the system interacts with n reservoir spins. Thus, the populations take the form [24, 25],

$$\frac{p_n - p_1}{dt} = \frac{1}{dt} \sum_{l=1}^{n} (1 - R_l)(f_l - p_l). \tag{18}$$

Neglecting the variation of $(1 - R_l)(f_l - p_l)$ under the sum, we obtain

$$\frac{dp(t)}{dt} = \dot{\varepsilon}_t \bar{D}_t [1 - R_t][f(\varepsilon_t) - p(t)], \tag{19}$$

with $R_t = \exp\left[-2\pi\delta_t\right]$, $\delta_t = |\nu_t|^2/2\dot{\varepsilon}_t$, and $f(\varepsilon_t) = \{\exp[2\beta(\varepsilon_t - \mu)] + 1\}^{-1}$, $\dot{\varepsilon}_t$ being the instantaneous linearized speed of the system at any time t. The factor $\dot{\varepsilon}_t \bar{D}_t$ is an estimation of the number of spins that have interacted with the system in a small interval dt with $\bar{D}_t$ being the reservoir density of states. We next do the same for the coherences map by expressing it in terms of

initial condition k_1 as,

$$\begin{aligned} k_{n+1} &= k_1 \Pi_{j=1}^{n} \sqrt{R_j} e^{-i\alpha_j} \\ &= k_1 \exp\left[\sum_{j=1}^{n}\left(\frac{\ln R_j}{2} - i\alpha_j\right)\right]. \end{aligned} \tag{20}$$

using the fact that in the continuous time limit $\tau_{j+1} - \tau_j = dt'$, $\tau_{j+1} + \tau_j = 2t'$, and $\sum_{j=1}^{n}$ becomes $\int_0^t$, we obtain

$$k(t) = k(0) \exp\left[\int_0^t dt' \left\{ |\dot{\varepsilon}_{t'}| \bar{D}_{t'} \frac{\ln R_{t'}}{2} - 2i\varepsilon_{t'} \right\}\right]. \tag{21}$$

If we furthermore assume to operate in the diabatic regime where R_t is close to one, we can expand R_t in Eqs. (19) and (21) to obtain,

$$d_t p(t) = T^+[1 - p(t)] - T^- p(t), \tag{22}$$

$$d_t k(t) = -2i\varepsilon_t k(t) - \frac{\Xi_t}{2} k(t). \tag{23}$$

with $T^+ = \Xi_t f(\varepsilon_t)$, $T^- = \Xi_t[1 - f(\varepsilon_t)]$, and $\Xi_t = \pi \bar{D}_t |\nu_t|^2$. This equation is of Lindblad form. It is also equivalent to the Markovian Redfield equation [46] when applied to our model. The coherence are decoupled from the population and undergo damped oscillations with a rate Ξ_t.

We now compare in Fig. 2 our Landau-Zener dynamics with the exact quantum dynamics obtained by solving the Schrödinger equation using the Crank-Nicolson method [47]. The reservoir is thermal and consists of only 10 spins with equally spaced energy levels $\epsilon_n = n\,\epsilon$ and thus a uniform density of states $\bar{D}_t = \epsilon^{-1}$. The Landau-Zener Markov chain results are depicted as red closed circles [Eqs. (16) and (17)] and match well with the exact dynamics (black solid lines) irrespective of the Landau-Zener transition probability $1 - R_n$, for both populations [Fig. 2(a), (c), and (e)] and coherence [Fig. 2(b), (d), and (f)]. In the regime of fast driving [Fig. 2(e) and (f)], the continuous time approach [Eqs. (22) and (23)] always coincides at discrete times with the Markov chain results and thus with the exact results for both populations and coherences. But the oscillations in between the avoided crossings are not supposed to be captured. This is indeed the case for populations but the coherence oscillations are surprisingly well reproduced. As expected, the agreement becomes bad in the slow driving regime [Fig. 2(a) and (b)] since R_n is not anymore close to one. Overall, within its regime of applicability the Landau-Zener approach reproduces very well the exact quantum dynamics for both populations and coherence. We are limited by the computational resources to go beyond 10 spins in the reservoir, but as observed for the populations [25], one may expect a better agreement between the Landau-Zener approach and the exact quantum dynamics as the number of spins in the reservoir increases.

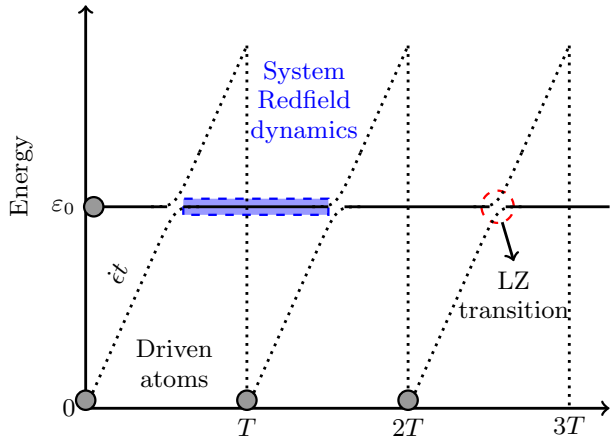

FIG. 3. An illustration of the work machine that utilizes coherences from the atoms to extract work. The energy of the atoms is linearly driven across a spin system connected to a thermal reservoir. The resonant coupling between the nonthermal atoms and the system generates a Landau-Zener transition which sustain coherences in the system and enables work extraction.

III. WORK EXTRACTION USING COHERENCES

In this section we study a simple model illustrating that work can be extracted from coherences.

We first consider a system H_S in contact with a thermal harmonic reservoir H_R via H_{SR}. The total Hamiltonian reads $H_S + H_R + H_{SR}$, where

$$\begin{aligned} H_S &= \varepsilon_0 \sigma^z \\ H_R &= \sum_k \frac{p_k^2}{2m_k} + \frac{1}{2} m_k \omega_k^2 x_k^2, \\ H_{SR} &= (\sigma_0^x + \sigma_0^z) \sum_k c_k x_k. \end{aligned} \tag{24}$$

The system density matrix ϱ follows the well known Markovian Redfield quantum master equation [46, 48] which, given the form of the term H_{SR}, couples populations and coherences and is given by,

$$d_t \varrho_{nm} = -i\Delta_{nm}\varrho_{nm} + \sum_{i,j} \mathcal{R}_{nm}^{ij} \varrho_{ij}, \tag{25}$$

$$\begin{aligned} \mathcal{R}_{nm}^{ij} =& S_{ni} S_{jm} (W_{ni} + W_{mj}) - \delta_{j,m} \sum_l S_{nl} S_{li} W_{li} \\ & - \delta_{n,i} \sum_l S_{jl} S_{lm} W_{lj}. \end{aligned}$$

Note that there is no general theorem guaranteeing the positivity of the state ϱ for every t under a Redfield evolution. However, we check that this is the case in our computation. In Eq.(25), the only non-zero elements of Δ_{nm} are $\Delta_{12} = -\Delta_{21} = 2\varepsilon_0$. The operator $S = \sigma_0^x + \sigma_0^z$ has elements $S_{11} = S_{12} = S_{21} =$

$-S_{22} = 1$, and the Markovian rates read $W_{12} = J(2\varepsilon_0)n(2\varepsilon_0)$, $W_{21} = J(2\varepsilon_0)\left[n(2\varepsilon_0)+1\right]$ and $W_{11} = W_{22} = \lim_{x\to 0} J(x)n(x)$ (the Lamb-shift are ignored). Also, $J(\omega) = \eta\omega/\left[1+(\omega/\omega_c)^2\right]$ is an ohmic spectral density with a Lorentz-Drude cutoff ω_c and $n(\omega) = [\exp(\beta\omega)-1]^{-1}$ is the Bose-Einstein distribution. Because H_{SR} is assumed weak, the heat flow from the reservoir to the system is obtained by integrating over time the heat rate $\dot{Q} = \mathrm{Tr}_S H_S d_t \varrho$.

We now assume that the system H_S is also subjected to a short interaction every period T with a driven atom $H_A(t)$, described by an interaction term H_{SA}, i.e., $H_{SA}(t) = H_S + H_A(t) + V_{SA}$, where

$$\begin{aligned} H_A(t) &= \epsilon(t)\sigma^z, \\ V_{SA} &= \nu\sigma_0^+\sigma^- + \text{H.c.}. \end{aligned} \tag{26}$$

We will also assume that during a time interval T which starts in between two interactions (see Fig. 3), the energy of the incoming atom $\epsilon(t)$ is ramped linearly in time from 0 to $2\varepsilon_0$ and suddenly switched off back to 0 at the end of the interval T. The process is then repeated with a fresh statistically identical incoming atom. The interaction is assumed to be much shorter than the typical relaxation time $\tau_R \sim 1/J(2\varepsilon_0)$ induced by the reservoir on the system. In that way, the effect of the reservoir can be neglected during the system atom interaction. The Landau-Zener map Eq. (13) and Eq. (14) can thus be applied to describe the effect of the crossing on the system density matrix. For consistency, the period T between two successive system-atom interactions must be longer than the Landau-Zener time τ^{lz} which in turn must be shorter than the typical relaxation time induced by the reservoir τ_R. As a result of the repeated interactions with statistically identical atoms, the system will reach a steady state regime of period T. If τ_R is comparable or smaller than T, the system will always thermalize between successive system-atom interactions. But more interesting effects will be obtained when τ_R is larger than T.

In summary, in between system-atom interactions the system dynamics is described by the Redfield equation (25) while the effect of the interaction on both the system and the atoms will be described for $n \geq 1$ by

$$\begin{aligned} p_{n+1} &= Rp_n + a(1-R) \\ &\quad + \sqrt{R(1-R)}\left[e^{i\varphi}qk_n^* + \text{H.c.}\right], \end{aligned} \tag{27}$$

$$\begin{aligned} k_{n+1} &= \sqrt{R}e^{-i\alpha_n}k_n \\ &\quad - \sqrt{1-R}e^{-i(\alpha_n-\varphi)}q(2p_n-1), \end{aligned} \tag{28}$$

$$\begin{aligned} a'_{n+1} &= Ra + p_n(1-R) \\ &\quad - \sqrt{R(1-R)}\left[e^{i\varphi}qk_n^* + \text{H.c.}\right], \end{aligned} \tag{29}$$

$$\begin{aligned} q'_{n+1} &= \sqrt{R}e^{-i\alpha_n}q \\ &\quad + \sqrt{1-R}e^{-i(\alpha_n+\varphi)}k_n(2a-1) \end{aligned} \tag{30}$$

where a and q (resp. a'_n and q'_n) denote the populations and coherence of the atom before (resp. after) the interaction. The phase $2\alpha_n = \dot{\epsilon}\left(\tau_{n+1}^2 - \tau_n^2\right) + 2\varepsilon_0\left(\tau_{n+1}-\tau_n\right)$, $\varphi = \pi/4 + \delta\left(\ln\delta - 1\right) + \arg\left[\Gamma(1-i\delta)\right]$ with $\delta = |\nu|^2/2\dot{\epsilon}$, and the probability $R = \exp[-2\pi\delta]$ [similar to Eqs. (9), (10), and (11)].

In what follows, we will assume that the atoms are initially not thermal. The initial populations are thermal $a = f$ but the coherences q are nonvanishing. This will allow us to isolate the effect of coherences. Mechanical work is the work produced by the external time dependent Hamiltonian and obtained by integrating over time the work rate $\dot{W}_{mech} = \mathrm{Tr}\rho_{SA} d_t H_{SA} = \mathrm{Tr}\rho_A d_t H_A$. We want to see if mechanical work can be extracted (extracted work is negative by convention) over one period T. The mechanical work over one period T centered around the nth system-atom interaction can be decomposed into three parts: From 0 to the avoided crossing at $T/2$, it is given by the average energy change occurring when ramping the atom level from 0 to ε_0

$$W^{(1)} = 2\varepsilon_0 a - \varepsilon_0(1-a). \tag{31}$$

From after the avoided crossing at $T/2$ up to time T it is given by the average energy change occurring when ramping the atom level from ε_0 to $2\varepsilon_0$

$$W_n^{(2)} = \varepsilon_0 a'_{n+1} - \varepsilon_0(1-a'_{n+1}). \tag{32}$$

We note that a'_{n+1} [Eq. (29)] implicitly contains information about all previous coherence due to Redfield evolution that mixes the populations and coherence. From the sudden switch of the atom level from $2\varepsilon_0$ back to 0 at time T it is given by

$$W_n^{(3)} = -2\varepsilon_0 a'_{n+1} + 2\varepsilon_0(1-a'_{n+1}). \tag{33}$$

Thus, the mechanical work done over the period T centered around the nth system-atom interaction is

$$\begin{aligned} W_n^{mech} &= W^{(1)} + W_n^{(2)} + W_n^{(3)}, \\ &= 2\varepsilon_0(a - a'_{n+1}). \end{aligned} \tag{34}$$

This work is thus exactly plus (resp. minus) the energy change in the system (resp. atom) occurring at the crossing since the Landau-Zenner map preserves total energy. Energy conservation at every instant reads $d_t(\mathrm{Tr}\rho_{SA}H_{SA}) = \dot{W}_{mech} + \dot{Q}$. Integrated over a period, we thus see that the system energy change over a period ΔE^S plus the atom energy change ΔE^A, is the system energy change due to the crossing, W^{mech}, plus the energy entering the system from the (Redfield) reservoir as heat Q. Since the system energy of the atom at the beginning and end of a period has been set to zero, $\Delta E^A = 0$ and does not appear in the energy balance over the period. When the system reaches a periodic steady state, the energy change of the system over a period vanishes, and the minus work equals heat. Work extraction in this case means that heat is absorbed from the reservoir. As we will see this is made possible by the initial atom coherences. Indeed, in the absence of coherence $k_0 = 0$

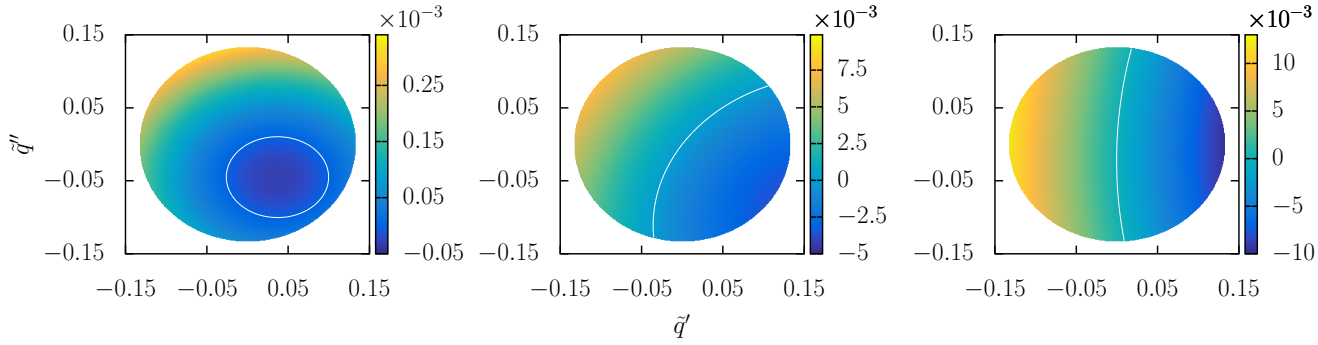

FIG. 4. Average power per cycle, $P_{mech} = W_{mech}/T$, as a function of the initial coherence $q = \tilde{q}' + i\tilde{q}''$ of the atoms. The panels represent different Landau-Zener interaction strengths $\nu = 0.1$ (left panel), $\nu = 0.45$ (middle panel), and $\nu = 1$ (right panel) that affect the Landau-Zener transition probability $R \approx 1, 0.5, 0$ from left to right. The white solid line represents the contour for $P_{mech} = 0$. The parameters used are: $\varepsilon_0 = 1$, $\eta = 0.1$, $\beta = 2$, $\mu = 0$, $\omega_c = 10$, $T = 2$.

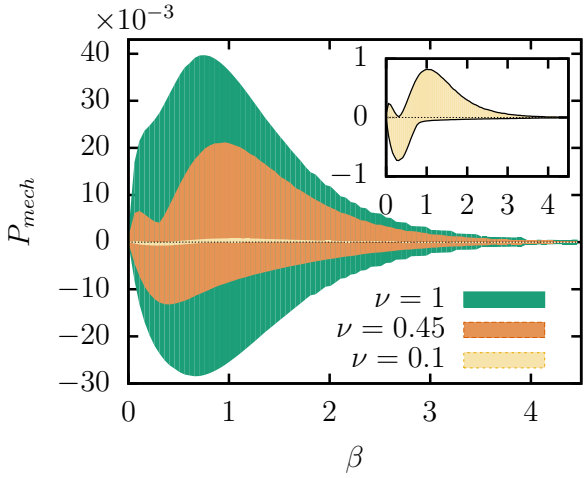

FIG. 5. Range of mechanical power, plotted as the shaded region, between maximum and minimum power as a function of inverse temperature β for the same parameters as in Fig. 4. The inset is a zoom in for $\nu = 0.1$.

and $q = 0$, the steady-state populations for the Redfield dynamics would be $p_n = a$ leading to $W_{mech} = 0$.

We plot the steady-state mechanical power $P_{mech} = W_{mech}/T$ per unit cycle in Fig. 4 for different values of Landau-Zener interaction strength ν as a function of the real and imaginary part of the initial atom coherence. The uncolored (white) parts of Fig. 4 are the regions where the initial density matrix is not physical. The power profile is not symmetric with respect to the real and imaginary parts of the initial coherence. Higher work extraction occurs for positive real parts. The maximum work is extracted when the Landau-Zener interaction is the strongest due to a high probability of exchange $1 - R$ between the system and the atom.

As the temperature β is varied, the populations of the atoms vary and hence the positivity range of the initial density matrix changes. Thus, the global maximum mechanical work done ($P_{mech} > 0$) and extracted ($P_{mech} < 0$) per cycle taken with respect to the real and imaginary part of coherence would vary as a function of β. In Fig. 5 the shade represents the entire range of mechanical power P_{mech} accessible at each value of the inverse temperature β. The inset shows that at weak to moderate Landau-Zener interactions, the maximum power extraction occurs in the high temperature (low β) regime, whereas the maximum power spent occurs in the low temperature regime. This could be a possible control strategy to tune the machine to either extract or spend power depending only on the temperature of operation. At strong Landau-Zener interactions this asymmetry disappears and the maximum extracted and spent power both occur close to $\beta = \varepsilon_0$.

IV. CONCLUSIONS AND DISCUSSION

In this paper we extended the Landau-Zener master equation studied in [24, 25] by incorporating the coherence dynamics and showing that the resulting quantum master equation is of Lindblad form. The main idea is to approximate the system-reservoir interaction as a repeated interaction problem where every interaction is described as a Landau-Zener crossing. We showed that the theory agrees very well with the numerically exact full quantum simulations. To illustrate the theory and the role of coherences, we proposed a toy model where a system can extract work from a single thermal reservoir bcause it is repeatedly interacting with atoms with thermal populations but nonvanishing coherences. While presented on a specific model, the method used to derive our Landau-Zener quantum master equation should be generalizable to any noninteracting open quantum system. The extension to interacting models is an interesting future research avenue.

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