

## Work exchange between quantum systems: The spin-oscillator model

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With the development of quantum thermodynamics it has been shown that relaxation to thermal equilibrium and with it the concept of heat flux may emerge directly from quantum mechanics. This happens for a large class of quantum systems if embedded into another quantum environment. In this paper, we discuss the complementary question of the emergence of work flux from quantum mechanics. We introduce and discuss two different methods to assess the work source quality of a system, one based on the generalized factorization approximation, the other based on generalized definitions of work and heat. By means of those methods, we show that small quantum systems can, indeed, act as work reservoirs. We illustrate this behavior for a simple system consisting of a spin coupled to an oscillator and investigate the effects of two different interactions on the work source quality. One case will be shown to allow for a work source functionality of arbitrarily high quality.

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### I. INTRODUCTION

Thermodynamics is a theory of impressive success and a wide range of applicability. This is true despite its origin as a purely phenomenological theory in the late 16th and 17th century. It took about 200 years until Boltzmann and Maxwell gave a foundation of thermodynamics in terms of statistical mechanics based on classical mechanics.

In the beginning 20th century, the invention of quantum mechanics has triggered various attempts to establish a theory of *quantum thermodynamics*, i.e., to explain and derive thermodynamics by quantum mechanics only. Starting with John von Neumann, those works first concentrated on proving the ergodic theorem for isolated quantum systems with a large number of degrees of freedom in the sense of the identity of time average and microcanonical ensemble average for certain (macroscopic) observables for a majority of the initial states [1,2]. Deutsch has shown in [3] that the ergodic theorem holds for extensive and intensive observables under the presence of a random perturbation. Results from quantum chaos are used in [4] to prove that thermalization occurs for a system of hard spheres in a box. Yet another view on the subject has been given by Reimann, arguing that limitations of control and measurement accuracy make statistical physics the appropriate description for typical large systems [5,6].

It was only in recent years that another approach to quantum thermodynamics has received increased attention. This approach focuses on the role of the partitioning of the universe into “system” and “environment” and how the entanglement between those parts and the properties of typical environments leads to a thermal state in the system even for almost any instant in time. In contrast to the previously mentioned works, this approach does not try to prove a (generalized) ergodic theorem and reaches its statements without invoking time averages. This approach was first developed by

Gemmer *et al.* [7–9], where the emergence of thermodynamic behavior from quantum mechanics for a wide class of quantum systems and typical embeddings has been established (see [10] for a similar but not as general result). Other recent papers have extended and clarified the results of the aforementioned authors [11–13]. The present paper is inspired by this approach although we do not make explicit use of its results.

The interest in a quantum approach to thermodynamics is twofold: first, it promises a deeper understanding of thermodynamic core concepts like relaxation, irreversibility, heat, work, and might elucidate connections between those and concepts known from quantum mechanics, e.g., entanglement. Second, such an approach should help to find generalizations for the mentioned concepts for nonequilibrium, finite systems and strong interaction.

The definition of work in quantum systems has been discussed in various papers [14–16] and has been applied successfully to quantum heat engines [17–21]. Still, all those investigations typically deal with quantum systems that are subject to driving by means of a time-dependent Hamiltonian operator of the system. Thus, the identification and definition of work is determined *a priori* by relating it to the presence of classical driving, while no microscopic derivation of the concept is given. In the present paper we deal with closed, finite quantum systems. For such systems the functionality of cooling has already been investigated (see, e.g., [22]). Here we are interested in the question under what conditions a quantum system coupled to another can exert the effect of a classical driver over the other system and thus be identified with a reversible work source. By our new approach based on a complete quantum modeling of the work source, we are able to show that classical driving and therefore work is not a concept bound to macroscopic devices.

The paper is organized as follows. In Sec. II, we present the factorization approximation (FA) and its generalization to the case of semimixed factorizing initial states. It is shown that the applicability of the FA allows one to identify quantum systems as classical drivers. In Sec. IV, we deal with the question of work source quality definition. Based on Sec. II, we introduce a measure inspired by the FA and establish its

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connection to work source functionality. In addition, we develop another work reservoir quality measure based on considerations of work and heat fluxes, if an appropriate definition of those is given. The definition of work and heat flux we chose to use throughout the paper is taken from [23] and outlined in Sec. III. In Sec. V we present the spin-oscillator model and its properties for two types of interactions. This simple quantum model is then used to illustrate the implementation of work sources of arbitrarily high quality in quantum mechanics in Sec. VI and to discuss the limits of two different work functionality quality measures in Sec. VII, where we also give an idea of the overall work source behavior of the second type of the model. Finally, we summarize our results in Sec. VIII.

## II. EFFECTIVE DYNAMICS: TIME-DEPENDENT DRIVING

The factorization approximation has been thoroughly discussed, e.g., in [24,25]. We will therefore only summarize the basic statements and give a generalization to the result of [24].

In its form stated in [24], the FA reads as follows. Let us consider a bipartite quantum system with Hamilton operator

$$\hat{H} = \hat{H}_1 + \hat{H}_{12} + \hat{H}_2 \quad (1)$$

acting on the joint Hilbert space  $\mathcal{H}_{12} = \mathcal{H}_1 \otimes \mathcal{H}_2$ . The operators  $\hat{H}_1$  and  $\hat{H}_2$  act on the respective local Hilbert spaces  $\mathcal{H}_1$  and  $\mathcal{H}_2$  only. Let the initial state factorize, i.e.,

$$|\Psi(0)\rangle = |\Psi_1(0)\rangle \otimes |\Psi_2(0)\rangle. \quad (2)$$

After some time  $t$ , the total state of the system either given by  $|\Psi(t)\rangle$  or its density matrix  $\hat{\rho}(t) = |\Psi(t)\rangle\langle\Psi(t)|$  gives rise to the reduced states of the two subsystems  $\hat{\rho}_1(t) = \text{tr}_2(|\Psi(t)\rangle\langle\Psi(t)|)$  and  $\hat{\rho}_2(t) = \text{tr}_1(|\Psi(t)\rangle\langle\Psi(t)|)$ . Although the state was assumed to factorize initially, in general, the subsystem states no longer will be pure states due to entanglement introduced by the interaction between the subsystems. As the total state is pure, the subsystem purities  $P[\hat{\rho}_1(t)] = \text{tr}\{[\hat{\rho}_1(t)]^2\}$  and  $P[\hat{\rho}_2(t)] = \text{tr}\{[\hat{\rho}_2(t)]^2\}$  are equal at any instant  $t$ . Now, as long as the purity of the subsystems is close to 1, it can be shown that the dynamics of the system are, in good approximation, given by the reduced density matrices  $\hat{\rho}_i = |\Psi_i(t)\rangle\langle\Psi_i(t)|$ ,  $i=1,2$ , where the  $|\Psi_i(t)\rangle$  obey the coupled differential equations

$$i\hbar|\dot{\Psi}_1(t)\rangle = (\hat{H}_1 + \langle\Psi_2(t)|\hat{H}_{12}|\Psi_2(t)\rangle)|\Psi_1(t)\rangle, \quad (3)$$

$$i\hbar|\dot{\Psi}_2(t)\rangle = (\hat{H}_2 + \langle\Psi_1(t)|\hat{H}_{12}|\Psi_1(t)\rangle)|\Psi_2(t)\rangle \quad (4)$$

up to an irrelevant relative phase (for a detailed derivation see [24]). Obviously, the reduced states of the system evolve under the action of time-dependent effective Hamiltonians  $\hat{H}_1 + \hat{H}_1^{\text{eff}}(t)$  and  $\hat{H}_2 + \hat{H}_2^{\text{eff}}(t)$ , respectively, with

$$\hat{H}_1^{\text{eff}}(t) = \text{tr}_2\{\hat{H}_{12}[\hat{1} \otimes \hat{\rho}_2(t)]\}, \quad (5)$$

$$\hat{H}_2^{\text{eff}}(t) = \text{tr}_1\{\hat{H}_{12}[\hat{\rho}_1(t) \otimes \hat{1}]\}, \quad (6)$$

and in the present case  $\hat{\rho}_j(t) = |\Psi_j(t)\rangle\langle\Psi_j(t)|$ ,  $j=1,2$ .

The above statement can be generalized for the case of factorizing semimixed initial states, that is, states of the form

$$\hat{\rho}(0) = \hat{\rho}_1(0) \otimes |\Psi_2(0)\rangle\langle\Psi_2(0)|. \quad (7)$$

If the purity  $P[\hat{\rho}_2(t)]$  of the initially pure system 2 remains close to unity, the dynamics of the system can be given approximately by the coupled differential equations

$$i\hbar\dot{\hat{\rho}}_1(t) = [\hat{H}_1 + \hat{H}_1^{\text{eff}}(t), \hat{\rho}_1(t)], \quad (8)$$

$$i\hbar|\dot{\Psi}_2(t)\rangle = [\hat{H}_2 + \hat{H}_2^{\text{eff}}(t)]|\Psi_2(t)\rangle, \quad (9)$$

with  $\hat{\rho}_2(t) = |\Psi_2(t)\rangle\langle\Psi_2(t)|$ . Again, the effect of the subsystems on each other is to induce a time-dependent effective Hamiltonian that governs the time evolution of the subsystems. For the derivation, see Appendix A.

Here, we would like to stress the fact that, as long as the prerequisites for the FA are met, Eqs. (8) and (9) present an alternative description of the system dynamics: The subsystems can be considered classical drivers for each other. It is remarkable that this feature is reciprocal and based on (approximate) constancy of the subsystem purities (entropies).

The energy exchanged this way can aptly be called “work:” classically one would define the work  $W$  imparted over time  $t_S$  on a Hamiltonian system  $H(\lambda)$  with  $\lambda$  denoting the time-dependent control parameter as [26]

$$W = \int_0^{t_S} dt \frac{d\lambda}{dt} \frac{\partial H}{\partial \lambda}[\vec{z}(t)], \quad (10)$$

where  $\vec{z}(t)$  denotes the system’s state trajectory in phase space. One notes, however, that the energy exchange will, in general, be contaminated by contributions violating the constancy of local purity. This contamination is a characteristic feature of the underlying total (unitary) dynamics. Close to thermal equilibrium such a contribution would be called heat,  $dQ$ : Work and heat in open quantum systems are usually defined as [14,15,17–19]

$$dU = d\langle\hat{H}\rangle = \underbrace{\text{tr}(\hat{\rho}d\hat{H})}_{dW} + \underbrace{\text{tr}(\hat{H}d\hat{\rho})}_{dQ} \quad (11)$$

again recognizing the energy exchange in the FA scenario as work.

We emphasize here, that explicitly time-dependent Hamiltonians are not part of the fundamental description of nature as given by quantum mechanics. Therefore, there is no way how they could come about save by an effective description of a system like the FA. If one denied any physical significance of such an effective description and hence considered it only a mathematical simplification without physical meaning, one obviously would have to deny the physical existence of classical drivers altogether. This is not a reasonable option.

### III. LEMBAS PRINCIPLE

The effective dynamics according to Eqs. (8) and (9) allows for an intuitive approach to the concept of work: in general, however, only approximately; the deviations remain unquantified. Here, the LEMBAS approach [23] comes into play based on the following ideas: first, choose a partitioning of the total isolated system into system of interest (1) and its environment (2) and consider the exact local dynamics of the system (1). The state of the total system is

$$\hat{\rho} = \hat{\rho}_1 \otimes \hat{\rho}_2 + \hat{C}_{12}, \quad (12)$$

where  $\hat{\rho}_i$  are the respective reduced density operators. Then, the exact (effective) Liouville-von Neumann equation for subsystem (1) can be written as

$$\dot{\rho}_1(t) = -\frac{i}{\hbar}[\hat{H}_1 + \hat{H}_1^{\text{eff}}(t), \hat{\rho}_1(t)] + \mathcal{L}_1^{\text{eff}}[\hat{\rho}(t)] \quad (13)$$

with the superoperator  $\mathcal{L}_1^{\text{eff}}[\hat{\rho}(t)] = -i\hbar^{-1} \text{tr}_2\{\hat{H}_{12}, \hat{C}_{12}\}$ .

The local energy  $\hat{H}'_1$  is defined now based on considerations how the local system would appear to an experimenter (“local effective measurement basis,” LEMBAS). There is some ambiguity in the procedure, but it has proven useful in [23] to choose

$$\hat{H}'_1 = \hat{H}_1 + \hat{H}_{1,a}^{\text{eff}}(t), \quad (14)$$

where  $\hat{H}'_1 = \hat{H}_{1,a}^{\text{eff}}(t) + \hat{H}_{1,b}^{\text{eff}}(t)$  and  $\hat{H}_{1,a}^{\text{eff}}(t)$  is the part of  $\hat{H}_1^{\text{eff}}(t)$  that commutes with  $\hat{H}_1$ .

The final step is to discriminate energy changes of the system based on whether they change the local von Neumann entropy  $S_1$  or not, that is whether they are of coherent (work) or incoherent origin (heat). This leads to the following formulas for heat and work fluxes for any partitioning and any  $\hat{H}'_1$ :

$$\dot{W}(t) = \text{tr}\{\hat{H}'_{1,a}(t)\hat{\rho}_1(t) - i[\hat{H}'_1(t), \hat{H}_{1,b}^{\text{eff}}(t)]\hat{\rho}_1(t)\}, \quad (15)$$

$$\dot{Q}(t) = \text{tr}\{\hat{H}'_1(t)\mathcal{L}_1^{\text{eff}}[\hat{\rho}(t)]\}. \quad (16)$$

How do these generalized definitions connect to their thermodynamic analogs? In the thermodynamic limit, that is, close to the thermodynamic equilibrium, for infinitely sized systems and weak couplings, the von Neumann entropy of the respective subsystem and its thermodynamic entropy coincide and the LEMBAS definitions of work and heat blend in with their thermodynamic counterparts.

But also in far from equilibrium situations, the LEMBAS definitions can be associated with work and heat in the following sense: we know from the results of quantum thermodynamics [7–9] that thermodynamic behavior of a system can be seen to result from an embedding in an environment, which by itself needs not to be and usually is not thermodynamic (in equilibrium, infinite, weak coupling). Thus, validity of thermodynamic concepts is not a property of the total system but has to do with whether or not the system of interest is influenced by its environment in such a way that thermodynamic properties emerge, which is a purely local

consideration. The LEMBAS definitions take this concept to the extreme in the sense that they state that “what locally has a work effect  $\hat{H}_1^{\text{eff}}(t)$ , is work” and “what locally has a heat effect  $\mathcal{L}_1^{\text{eff}}[\hat{\rho}(t)]$ , is heat” even for nonthermodynamic (in the classical sense), far from equilibrium situations. Making the distinction in this way is justified by the fact that classical driving can be unambiguously identified as work even in the thermodynamic sense and, therefore, any effect  $\mathcal{L}_1^{\text{eff}}[\hat{\rho}(t)]$  not related to work is identified as heat.

Finally, we note that the LEMBAS definitions retain the properties that

(1) work is energy exchange due to changing parameters of the Hamilton operator that describes the system;

(2) heat is energy exchange associated with change of entropy, although here a generalized definition of entropy is to be used.

### IV. MEASURES OF WORK SOURCE QUALITY

#### A. Work reservoir

An ideal work reservoir can be defined as a system exchanging energy only in the form of work. It is obvious that this definition is too restrictive for the classification of realistic models, that is, models involving finite size, finite interaction and limited control. No realistic model can comply to the idea of such an ideal work source as even arbitrary small but finite deviations from this idealized concept would lead to a rejection of a model as a work source. Additional complications arise due to the fact that we have to consider processes, the properties of which may change with time.

Thus, there is need for a more differentiated measure of work reservoir functionality. In a nonideal world, special attention is to be paid to the definition and quantification of the quality of a work reservoir to be able to compare and to draw conclusions on justified grounds.

Basically, one can distinguish two types of measures depending on whether they refer to a single point in time or to a (finite or infinitely large) interval of time. We like to refer to them as *instantaneous* and *integral* measures and our main interest lies on the integral ones, defined with respect to some finite time interval (again because under realistic condition it is not expected that a system can be a work source for all times). In the following section, we present two different approaches to the problem based on two distinct physical reasonings.

#### B. Purity based measure

Comparing Eq. (13) to Eq. (8), one realizes that the applicability of the FA is equivalent to a vanishing  $\mathcal{L}_1^{\text{eff}}$ . Thus, if the total system was initially in a semimixed state,  $\mathcal{L}_1^{\text{eff}}$  is negligible if  $P[\hat{\rho}_2(t)] \approx 1$ . In this sense,  $P[\hat{\rho}_2(t)]$  is a measure of work reservoir functionality. The closer it is to 1, the smaller  $\mathcal{L}_1^{\text{eff}}$  has to be and the less energy may be exchanged as heat instead of work. Note, that acting as a work reservoir is a reciprocal property, i.e., each subsystem acts on its partner in an analogous way. This is in perfect agreement with what we know from thermodynamics. If we have two systems undergoing a process during which only work is ex-

changed between them, both systems obviously act as work reservoirs for each other although we may imagine one system to be the gas filling a box and the other system to be the piston capping the box and being connected to a spring.

At first glance, the purity therefore seems to be a good candidate for assessing work source quality: it is an easy quantity to compute—even analytically—and by its connection to the FA, the physical reasoning is clear.

However, as clear as the ideal situation with  $P[\hat{\rho}_2(t)]=1$  is, it is unclear to give a quantitative interpretation for purities lower than unity because there is neither an obvious relation between  $P[\hat{\rho}_2(t)]$  and  $\mathcal{L}_1^{\text{eff}}$  nor between  $\mathcal{L}_1^{\text{eff}}$  and the quality of the work reservoir functionality. Moreover, it is expected that the same purity decrease for different systems, especially of different size, has to be weighted differently. Thus, any concrete choice of a minimum purity beyond which a system will be accepted as a work reservoir will remain somewhat arbitrary and difficult to compare with other systems' purity behavior. If such a purity threshold was given, the respective system could be considered as a work source for any time interval during which the purity stays above the given threshold.

As will become evident in Sec. VB, there is another problem besides the arbitrary definition of the threshold when using this measure: the decrease in purity is linked to the size of  $\mathcal{L}_1^{\text{eff}}$  only. Thus, the purity does not contain any information about the relative effects of  $\hat{H}_1^{\text{eff}}(t)$  and  $\mathcal{L}_1^{\text{eff}}$ . Since the former is related to work and the latter to heat, a comparison of both in terms of their effect on the energy of the system is in general expected to be an important part of the assessment of work source quality.

### C. Work and heat flux based measure

We introduce the ratio

$$r(t) := \frac{|\dot{W}(t)|}{|\dot{W}(t)| + |\dot{Q}(t)|}, \quad (17)$$

which has the following convenient properties:

- (i)  $r(t)=1 \Leftrightarrow \dot{W}(t) \neq 0 \wedge \dot{Q}(t)=0$ : ideal work source;
- (ii)  $r(t)=0 \Leftrightarrow \dot{W}(t)=0 \wedge \dot{Q}(t) \neq 0$ : ideal heat source.

Provided there is energy exchange at all (i.e., not both,  $\dot{W}$ ,  $\dot{Q}$  are zero),  $r$  is well behaved. As we took separate moduli in the denominator, there can be no compensation due to opposite sign.

Based on this instantaneous measure, we can develop an integral measure for finite time intervals  $[t_0, t_1]$ . Directly integrating over  $r(t)$  is not an option for this would completely ignore the time dependence of the total of the absolute fluxes and therefore the necessary weighting of  $r$ . It is straightforward to apply the necessary weight, integrate and then normalize the result defining

$$\begin{aligned} R(t_1, t_0) &:= \frac{\int_{t_0}^{t_1} r(t)(|\dot{W}(t)| + |\dot{Q}(t)|)dt}{\int_{t_0}^{t_1} (|\dot{W}(t)| + |\dot{Q}(t)|)dt} \\ &= \frac{\int_{t_0}^{t_1} |\dot{W}(t)|dt}{\int_{t_0}^{t_1} (|\dot{W}(t)| + |\dot{Q}(t)|)dt}. \end{aligned} \quad (18)$$

Defining the quantities

$$\mathcal{W}(t_1, t_0) := \int_{t_0}^{t_1} |\dot{W}(t)|dt, \quad \mathcal{Q}(t_1, t_0) := \int_{t_0}^{t_1} |\dot{Q}(t)|dt, \quad (19)$$

we can rewrite Eq. (18) in the form of Eq. (17) as

$$R(t_1, t_0) := \frac{\mathcal{W}(t_1, t_0)}{\mathcal{W}(t_1, t_0) + \mathcal{Q}(t_1, t_0)}. \quad (20)$$

This integral measure has the same special points like the instantaneous measure with the following interpretations:

(i)  $R(t)=1 \Leftrightarrow \dot{Q}(t)=0$  for all  $t \in [t_0, t_1]$  and  $\dot{W}(t) \neq 0$  for some  $t \in [t_0, t_1]$ : ideal work source;

(ii)  $R(t)=0 \Leftrightarrow \dot{W}(t)=0$  for all  $t \in [t_0, t_1]$  and  $\dot{Q}(t) \neq 0$  for some  $t \in [t_0, t_1]$ : ideal heat source.

We stress the fact here that a measure based on the integrated work  $W(t_1, t_0) = \int_{t_0}^{t_1} \dot{W}(t)dt$  and the (analogously) integrated heat is not able to accomplish such precise assessment of the work source quality: for oscillating fluxes, e.g.,  $Q(t_1, t_0)$  might reach 0 for some interval, although during the time interval there might have flown vast amounts of heat. By employing the integrals of the absolute fluxes in the chosen definition, we achieve a much stronger statement about the quality of a system.

Finally, let us note that there is also a drawback to this measure, namely, the difficulty of calculating it because of the integration over the absolute values of the fluxes.

### V. APPLICATION: SPIN-OSCILLATOR MODEL (SOM)

We turn now to the description of the model we will use to demonstrate the existence of small quantum systems that do act as work sources. We illustrate the features of FA and the various work measures we have discussed above and discuss the model and its properties with special focus on the dynamics of the purity.

The model is a single spin interacting with a harmonic oscillator (*spin-oscillator model*, SOM). On the one hand, the SOM serves as an allusion to a classical steam engine with a gas of some temperature (spin) and a piston periodically compressing and expanding the gas (oscillator). On the other hand, the SOM has been used in previous related works as a central element of quantum thermodynamic machines [18,19,27]. Also, the simplicity and therefore partially possible analytical treatment of the model has further motivated the choice.

The SOM is defined by the Hamiltonian

$$\hat{H} = \frac{\omega_s}{2} \hat{\sigma}_z + \hat{H}_{\text{int}} + \omega_o \left( \hat{a}^\dagger \hat{a} + \frac{1}{2} \right), \quad (21)$$

where we have set  $\hbar=1$ . We denote the spin and oscillator local Hamilton operators as  $\hat{H}_s$  and  $\hat{H}_o$ , respectively. The eigenstates of  $\hat{H}_s$  are  $|0\rangle$  and  $|1\rangle$  with the respective eigenvalues  $\mp \omega_s/2$ . The eigenstates of  $\hat{H}_o$  are defined as  $\{|k\rangle\}$  with eigenvalues  $\omega_o(k+1/2)$ , where  $k=0, 1, 2, \dots$

We will discuss the  $z$  and the  $xz$  interaction,  $\hat{H}_{\text{int}} = \{\hat{H}_z, \hat{H}_{xz}\}$ , where

$$\hat{H}_{\text{int}} = \hat{H}_z = \lambda \hat{\sigma}_z \hat{x}, \quad (22)$$

$$\hat{H}_{\text{int}} = \hat{H}_{xz} = \lambda (\hat{\sigma}_z + \kappa \hat{\sigma}_x) \hat{x}. \quad (23)$$

For the initial state of the total system, we assume that the spin has interacted in the past with some heat bath in order to establish a thermal state but now is decoupled from said bath (or the bath coupling is so weak that its influence may be neglected during the period of evolution one is interested in). The oscillator is prepared in a coherent state  $|\alpha\rangle$ . Thus, the initial state is given as

$$\hat{\rho}(0) = \begin{pmatrix} c & 0 \\ 0 & 1-c \end{pmatrix} \otimes |\alpha\rangle\langle\alpha| \quad (24)$$

where the spin's state is given in its energy eigenbasis. The self-generated process imposed on the spin via coupling to the oscillator might thus be called ‘‘adiabatic,’’ however, due to quantum mechanical interactions the local entropy (purity) will, in general, not be constant, see below.

#### A. $z$ -interaction ( $z$ -SOM)

Representing the Hamiltonian (21) in the eigenbasis of the spin, one finds that it has a block-diagonal structure,

$$\hat{H} = \begin{pmatrix} \hat{H}_o - \lambda \hat{x} - \frac{\omega_s}{2} & \\ & \hat{H}_o + \lambda \hat{x} + \frac{\omega_s}{2} \end{pmatrix} =: \begin{pmatrix} \hat{H}_- & \\ & \hat{H}_+ \end{pmatrix}. \quad (25)$$

The same obviously holds for the time-evolution operator and—by the block-diagonal structure of the initial state—also for the propagated state  $\hat{\rho}(t)$  of the total system,

$$\hat{\rho}(t) = \begin{pmatrix} c |\alpha_-(t)\rangle\langle\alpha_-(t)| & \\ & (1-c) |\alpha_+(t)\rangle\langle\alpha_+(t)| \end{pmatrix}. \quad (26)$$

Here we have used the definitions  $|\alpha_\pm(t)\rangle := \hat{U}_\pm(t, 0)|\alpha\rangle$  and  $\hat{U}_\pm(t_1, t_0) = \exp[-i\hat{H}_\pm(t_1 - t_0)]$ . Note that the dynamics of the system are periodic, because both Hamilton operators  $\hat{H}_\pm$  describe (displaced) harmonic oscillators with the same frequency  $\omega_o$ . Thus, we have  $\hat{U}(t_1 + 2\pi m \omega_o^{-1}, t_0 + 2\pi n \omega_o^{-1}) = \hat{U}(t_1, t_0)$  for integer numbers  $n, m$ .

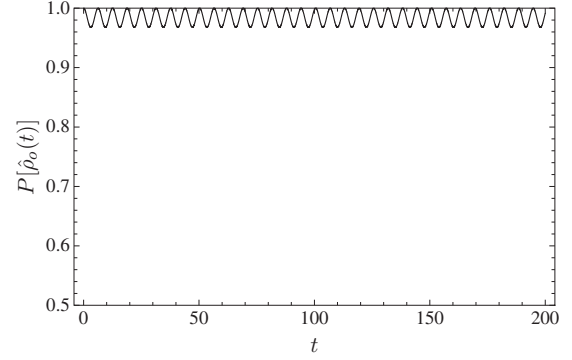


FIG. 1. Purity dynamics of the oscillator in the  $z$ -SOM for the special parameters  $\lambda=0.1$ ,  $c=0.7$ ,  $\alpha=0$ ,  $m=\omega_s=\omega_o=1$ .

Because of the simple structure of the time evolution of the system, the purity of the oscillator can be computed analytically and turns out to be given by

$$P[\hat{\rho}_o(t)] = c^2 + (1-c)^2 + 2c(1-c) |\langle\alpha_-(t)|\alpha_+(t)\rangle|^2 \quad (27)$$

with the time-dependent part

$$|\langle\alpha_-(t)|\alpha_+(t)\rangle|^2 = \exp\left[-8 \frac{\lambda^2}{m\omega_o^3} \sin^2\left(\frac{1}{2}\omega_o t\right)\right] \quad (28)$$

(for the derivation, see Appendix B;  $m$  is the oscillator mass). For pure initial spin states ( $c=0, 1$ ) we have  $P[\hat{\rho}_o(t)]=1$ . An example for  $P[\hat{\rho}_o(t)]$  for a mixed initial spin state is given in Fig. 1.

It is easy to see from Eqs. (27) and (28) that the minimum purity with respect to  $t$  and  $c$  is

$$P_o^{\min} = \frac{1}{2} [1 + \exp(-8\xi)], \quad (29)$$

where

$$\xi = \frac{\lambda^2}{m\omega_o^3}. \quad (30)$$

Therefore, one has to choose  $\xi \rightarrow 0$  and thus

$$1 - P_o^{\min} \ll 1 \quad (31)$$

in order to apply the FA.

We can distinguish two different ways to enforce the limit  $\xi \rightarrow 0$ ,

$$m \rightarrow \infty, \omega_o = \text{const.}, \lambda = \text{const.} \quad (32)$$

$$\omega_o \rightarrow \infty, m = \text{const.}, \lambda^2/\omega_o = \text{const.} \quad (33)$$

Their relevance will become clear in Sec. VI. If one accepts the resulting finite  $P_o^{\min}$  for some finite  $\xi$ , the local coherence time may be called infinite.

#### B. $xz$ -interaction ( $xz$ -SOM)

We discuss now the more complicated case of an interaction of form Eq. (23). This interaction is motivated by the following considerations. First, the above case is very special

in that the minimum purity reached can be controlled completely by the system parameters. The more general  $xz$ -interaction case will show that this property is dependent on the interaction. Second, the chosen interaction allows us to study the effect of imperfect control over the exact form of the interaction as it might be the case for a more realistic experimental situation. Finally, the  $xz$  interaction exhibits a remarkable diversity of dynamics which serves to illustrate the pros and cons of the proposed work reservoir quality measures as well as the possibility to realize quantum work sources within the given model.

First, we show that a Hamiltonian

$$\hat{H} = \frac{\omega_s}{2} \hat{\sigma}_z + \lambda \hat{s} \hat{x} + \omega_o \left( \hat{a}^\dagger \hat{a} + \frac{1}{2} \right) \quad (34)$$

with an arbitrary operator  $\hat{s}$  acting on the spin's Hilbert space is equivalent to the  $xz$ -SOM. This is seen from the expansion of  $\hat{s}$  in the operator basis  $\{\hat{Q}_k | k=0, 1, 2, 3\} = \frac{1}{\sqrt{2}} \{\hat{1}, \hat{\sigma}_x, \hat{\sigma}_y, \hat{\sigma}_z\}$ , which reads

$$\hat{s} = \sum_{k=0}^3 \text{tr}(\hat{Q}_k^\dagger \hat{s}) \hat{Q}_k \quad (35)$$

(for details refer to [28], pp. 34–49). The  $\hat{1}$  term is local to the oscillator and can be absorbed in  $\hat{H}_o$ , while the  $\hat{\sigma}_k$  terms can always be transformed to the form  $\hat{s} = \lambda(\hat{\sigma}_z + \kappa \hat{\sigma}_x)$  by the local transformation  $\exp(-i\phi \hat{\sigma}_z)$  with appropriately chosen real  $\phi$ . This corresponds to a rotation around the  $z$  axis of the spin. The  $xz$ -SOM discussed here is therefore representative for the whole class of Hamiltonians of the form Eq. (34).

### C. Dynamics

Now, we want to look into the behavior of the system for  $|\kappa| \leq 1$ . To get insight into the dynamics, we invoke a rotating wave approximation (RWA). For that purpose, we first write the  $xz$ -SOM interaction Hamiltonian  $\hat{H}_{xz}$  in the interaction picture

$$\begin{aligned} \hat{H}_{xz} \propto & \hat{\sigma}_z \hat{a} \exp\left(i \frac{\Omega - \Delta}{2} t\right) + \hat{\sigma}_z \hat{a}^\dagger \exp\left(-i \frac{\Omega - \Delta}{2} t\right) \\ & + \kappa \hat{\sigma}_+ \hat{a} \exp(-i\Delta t) + \kappa \hat{\sigma}_- \hat{a} \exp(i\Omega t) \\ & + \kappa \hat{\sigma}_+ \hat{a}^\dagger \exp(-i\Omega t) + \kappa \hat{\sigma}_- \hat{a}^\dagger \exp(i\Delta t), \end{aligned} \quad (36)$$

where we have defined  $\Omega := \omega_s + \omega_o$  and  $\Delta := \omega_s - \omega_o$ . By restricting ourselves to the resonant case  $\Delta = 0$  and omitting all terms rotating with frequencies  $\Omega$  and  $\Omega/2$ , the  $xz$ -SOM Hamiltonian in RWA turns out to be

$$\hat{H}_{xz}^{\text{RWA}} = \frac{\omega}{2} \hat{\sigma}_z + g(\hat{\sigma}_+ \hat{a} + \hat{\sigma}_- \hat{a}^\dagger) + \omega \left( \hat{a}^\dagger \hat{a} + \frac{1}{2} \right) \quad (37)$$

in the Schrödinger picture. This is just the Hamiltonian  $\hat{H}_{\text{JC}}$  of the Jaynes-Cummings model (JCM) [29,30] with

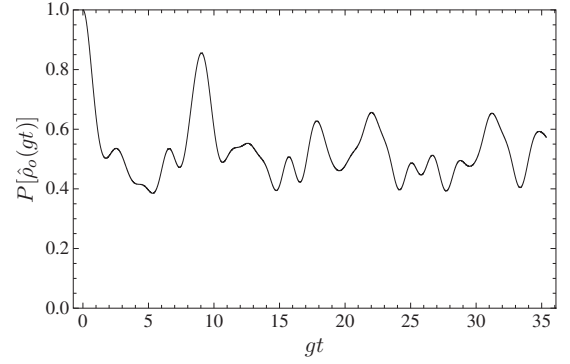


FIG. 2. Purity of the oscillator for numerically exact dynamics of the  $xz$ -SOM in RWA for arbitrary  $g$ . The parameters are:  $\lambda = 0.01$ ,  $\alpha = \omega_o = \omega_s = 1$ ,  $c = 0.7$ .

$$g = \frac{\lambda \kappa}{\sqrt{2m\omega}} \quad (38)$$

and  $\omega = \omega_s = \omega_o$ . According to [31,32], the RWA is accurate as long as  $g/\Omega \ll 1$ . This condition is met for all relevant cases, since we consider in the following a situation where the parameters  $m, \omega$ , and  $\lambda$  have been chosen such that for  $\kappa = 0$  ( $z$ -SOM) the FA holds for all times.

Now let us turn to the interpretation of the result. First, we note that by performing the RWA, in particular, the  $\hat{\sigma}_z$  term of the interaction Hamiltonian is removed. Therefore, the  $xz$ -SOM in RWA captures the effect of the  $\hat{\sigma}_x$  interaction alone and, in turn, this means that the main dynamics are governed by the  $\hat{\sigma}_x$  part of the interaction alone.

Second, the dynamics of the JCM (and therefore of the  $xz$ -SOM in RWA) scale in time with  $g^{-1}$ . This is most clear from the exact time-evolution operator for the JCM ([33], p. 205) in the case of exact resonance

$$\hat{U}_{\text{JC}}(t) = \begin{pmatrix} \cos(gt\hat{B}) & -i\hat{a}^\dagger \sin(gt\hat{A})\hat{A}^{-1} \\ -i\sin(gt\hat{A})\hat{A}^{-1}\hat{a} & \cos(gt\hat{A}) \end{pmatrix} \quad (39)$$

with  $\hat{A} = \sqrt{\hat{a}^\dagger \hat{a} + 1}$  and  $\hat{B} = \sqrt{\hat{a}^\dagger \hat{a}}$ .

The numerical results of the dynamics of the purity of the oscillator are given in Fig. 2 for the case of a coherent initial state with one photon in the cavity on average ( $\alpha = 1$ ). The deviations of the numerical results for the  $xz$ -SOM with and without RWA for three different orders of magnitude of  $g$  are given in Fig. 3.

From Fig. 3 one sees that the RWA yields good results (less than 10% relative deviation) up to  $\kappa \approx 10$ . This shows again that the RWA gives an accurate description of the  $xz$ -SOM dynamics in agreement with the expectation given above.

It is obvious from Figs. 1 and 2 that the purity behavior of the  $xz$ -SOM is fundamentally different from the  $z$  case. The decrease in the purity due to the additional  $\hat{\sigma}_x$  interaction term is several orders of magnitude stronger than what is expected from the  $\hat{\sigma}_z$  term alone and due to the approximate scaling behavior of the  $xz$ -SOM, the minimum does not depend on  $\kappa$ , as long as  $\kappa$  is not zero. We conclude from that, that in the presence of an arbitrarily small but nonvanishing

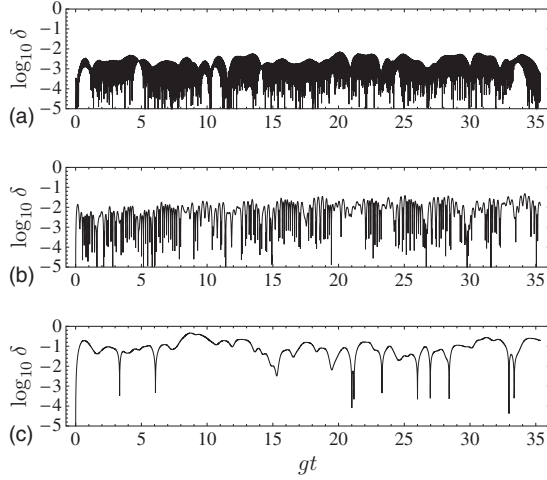


FIG. 3. Common logarithm of the absolute deviation  $\delta$  of the (numerically exact) purity dynamics with and without RWA for (top to bottom)  $g=-0.01, -0.1, -1$  corresponding to  $\kappa=\sqrt{2}, 10\sqrt{2}, 100\sqrt{2}$  according to Eq. (38) with the parameters  $\lambda=-0.01$ ,  $m=1$ ,  $\alpha=\omega_o=\omega_s=1$ ,  $c=0.7$ .

$\hat{\sigma}_x$  term the FA and with it the work reservoir quality of the oscillator will break down in finite time. Reduction of  $\kappa$  can only delay the breakdown and, thus, if  $\lambda, \kappa \neq 0$  no choice of the other model parameters can prevent the breakdown. This result is in agreement with the finding in [24] for the that the coherence time for the JCM depends on the interaction strength such that weaker interaction leads to longer coherence time.

In the above sense, the work reservoir functionality in the given quantum scenario is quite sensitive to the quality of control of the interaction between spin and oscillator.

## VI. WORK SOURCE QUALITY IN THE $z$ -SOM

Considering the first case of  $z$ -SOM, let us assume that one has chosen the parameters of the system such that Eq. (31) is fulfilled. We can then apply the FA not only to describe the dynamics of the system up to any desired accuracy but moreover, we get a new level of description combined with new physical insight in the properties and characteristics of the system. This will be outlined below.

Applying the FA to the SOM, we find according to Eqs. (8) and (9) the following effective coupled equations:

$$i\dot{\hat{\rho}}_s = \left[ \left( \frac{\omega_s}{2} + \lambda \langle \hat{x} \rangle(t) \right) \hat{\sigma}_z, \hat{\rho}_s \right], \quad (40)$$

$$i|\dot{\Psi}(t)\rangle = (\hat{H}_o + \lambda(1-2c)\hat{x})|\Psi(t)\rangle, \quad (41)$$

where we have defined  $\langle \hat{x} \rangle(t) := \langle \Psi(t) | \hat{x} | \Psi(t) \rangle$ . Hence, the spin is driven by the oscillator displacement which acts like an additional time-dependent magnetic field, modulating the spin's Zeeman splitting. On the other hand, the spin dynamics lead to a constant displacement of the oscillator potential. In this sense there is asymmetry between the two subsystems: The effective Hamiltonian for the oscillator is modified but not time dependent.

Clearly, this result is in agreement with the result which one would obtain from applying the integral measure based on  $\mathcal{W}$  and  $\mathcal{Q}$ : the latter is zero, since according to Sec. V A and Eq. (40), the spin's state does not change and the oscillator only exerts classical driving on the spin. The local effective energy change of the spin resulting from the driving is 100% work. Hence, the oscillator acts as an ideal work source at least in the limits discussed in Sec. V A, Eqs. (32) and (33).

However, it has to be noted that the peak-to-peak amplitude  $\Delta\omega_s^{\text{eff}} = \lambda(\langle \hat{x} \rangle_{\text{max}} - \langle \hat{x} \rangle_{\text{min}})$  of the effective spin splitting is dependent on the system parameters (see Appendix C),

$$\Delta\omega_s^{\text{eff}} = 2\lambda \sqrt{\frac{2}{m\omega_o}} |\alpha + \gamma|, \quad (42)$$

where  $\gamma = \sqrt{\lambda^2/(2m\omega_o^3)(1-2c)} = \sqrt{\xi/2}(1-2c)$  [cf. Eq. (30)]. For the first limit proposed in Eq. (32), we therefore find that for both  $\gamma \rightarrow 0$  and  $\Delta\omega_s^{\text{eff}} \rightarrow 0$ , if all parameters besides  $m$  are kept constant. Thus, the work effect induced by the oscillator diminishes more and more for increasingly better fulfilled FA. This can be avoided, though, by additionally imposing  $\alpha \rightarrow \infty$ , such that  $|\alpha|^2/m$  remains constant, which then defines the splitting's amplitude. This is a classical limit in that the mass and average excitation number of the oscillator go to infinity.

There is also a true quantum limit, though, which is found to be realized exploiting the second limit given in Eq. (33). Here, by letting  $\omega_o \rightarrow \infty$ , we enforce that  $\xi \rightarrow 0$  so that the factorization approximation becomes exact. However, by requiring  $\lambda^2/\omega_o = \text{const.}$ , the prefactor of  $\Delta\omega_s^{\text{eff}}$  in Eq. (42),  $2\sqrt{2}\lambda^2/(m\omega_o)$ , becomes constant. Thus, although  $\gamma \rightarrow 0$ ,  $\Delta\omega_s^{\text{eff}}$  retains a finite value

$$\Delta\omega_s^{\text{eff}} \rightarrow 2\lambda \sqrt{\frac{2}{m\omega_o}} |\alpha| = \text{const.} \quad (43)$$

for arbitrary (small but finite)  $m$  and  $\alpha$  in the limit of exact FA.

By the preceding reasoning, we conclude that the oscillator is, indeed, a work reservoir for the spin, periodically changing the spin splitting and therefore transferring work to/from it. What is special about that finding is the fact that a true quantum system (the oscillator in the quantum limit of the  $z$ -SOM) can be set up as an ideal work source and, thus, the work concept is not tied to classical devices. Moreover, as long as we fulfill Eq. (31) the oscillator behaves as a work reservoir for any time period.

## VII. WORK SOURCE QUALITY IN THE $xz$ -SOM

In this section, we present and discuss our results for the work reservoir behavior in the more general  $xz$ -SOM presented in Sec. V B with focus on the suitability of the work source quality measures proposed in Sec. IV.

The numerical results used herein have been produced with the *Mathematica* package using the following techniques: we have computed the time evolution of the system by direct diagonalization of the Hamilton operator (with a cutoff chosen such that only states with occupation probab-

ity higher than  $10^{-6}$  are included). Integration of quantities—where necessary—has been performed using the rectangle rule and the error of integration has been controlled by cross-checking with results for the trapezoidal rule and/or for smaller time steps.

### A. Purity based approach

We need now to define a lower bound for the purity of the oscillator. The  $\hat{\sigma}_z$  coupling alone already leading to some limited purity loss in the oscillator can be considered as sort of a “natural” purity drop, which has to be accepted for any system that interacts at all and that is present even if the FA is good and the work source quality high.

The work source functionality is considered to fail when the purity decrease of the RWA dynamics (caused by the  $\hat{\sigma}_x$  interaction term) reaches the maximum purity drop  $P_o^{\min}$  of the  $\hat{\sigma}_z$  dynamics alone found for the given system parameters  $(\lambda, \omega_s, \omega_0, m)$ . This allows us to define a breakdown time  $t^*$  by  $P[\hat{\rho}_o(t^*)] = P_o^{\min}$ .

The close connection of the  $xz$ -SOM dynamics to the JCM dynamics seems to suggest an analytical approach based on the standard approximations made to solve the JCM (see, e.g., [34], Ch. 6): approximation of the occupation probability of the coherent state with a Gaussian and linearization of the spectrum of the JCM around its peak. With those approximations a fairly accurate description of the JCM’s typical collapse and revival behavior of the spin polarization for high initial photon numbers ( $|\alpha| \gg 1$ ) is possible. After the initial collapse of polarization, the spin reaches its minimum purity [30] and the oscillator purity will as well have dropped significantly.

Unfortunately, even in the high photon number limit the accuracy of this approach in the relevant time interval up to this point of the evolution is insufficient: typical values of the purity drop due to the  $\hat{\sigma}_z$  interaction are of the order of  $10^{-2}$ , while the error of the mentioned approximations is of around the same order during the collapse. This renders the application of those approximations futile and since a full analytical analysis is much too involved, we will only exemplify some results based on numerics.

To this end, we choose the following parameters for the  $xz$ -SOM:  $\omega_o = \omega_s = 1$  (resonant case),  $m_o = 1$ ,  $\lambda = \kappa = 0.1$ . In the following, we consider the results of two special cases:

- (a)  $\alpha = 0$ ,  $c = 0.5$ ;
- (b)  $\alpha = 2$ ,  $c = 1$ .

These two examples are drawn from a set of results for initial states with parameters  $\alpha \in [0, 4]$  and  $c \in [0.5, 1.0]$  and have been chosen for they represent in some sense extremal cases, that will be seen to illustrate the features of the different work source quality measures. A short overview about the more general behavior of the  $xz$ -SOM is given in Sec. VII C.

The purity behavior of the examples is shown in Fig. 4. The time after which the FA is estimated to fail is roughly  $t_{(a)}^* \approx 28$  and  $t_{(b)}^* \approx 73$ . Although this means that the second case is expected to exhibit work reservoir functionality about three times longer than the first case, one would conclude from the curves that for both cases, the oscillator’s work

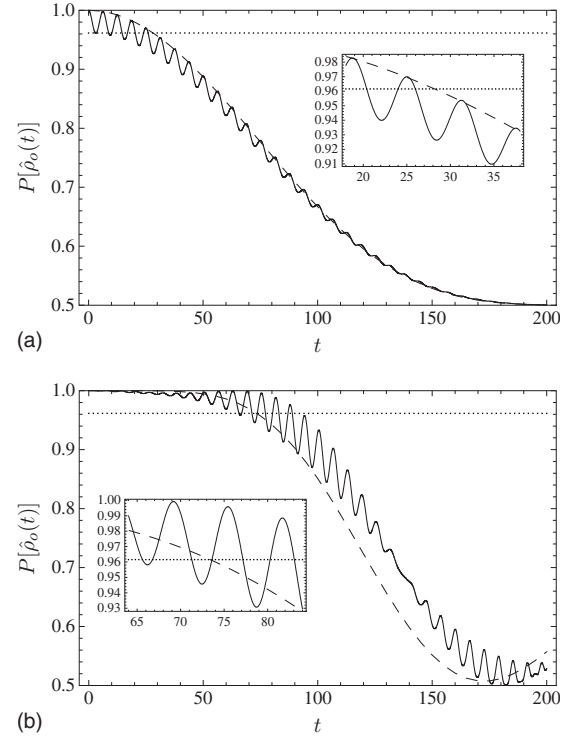


FIG. 4. Oscillator purity behavior of two special cases [(a)  $\alpha = 0$ ,  $c = 0.5$  and (b)  $\alpha = 2$ ,  $c = 1$ ] of  $xz$ -SOM and comparison with minimum purity of  $z$ -SOM for the given system parameters: Numerical exact result (solid line), numerical result with RWA (dashed), minimum  $z$ -SOM purity (dotted), which—according to Eq. (29)—is  $[1 + \exp(-2/25)]/2 \approx 0.962$ . The insets show the crossings of RWA-purity with minimum  $z$ -SOM purity.

source functionality degrades quickly after the initial high purity phase and is virtually absent at least for  $t > 100$ .

### B. Work/heat based approach

However, taking a look at the result for the integral quality measure  $R$  shown in Fig. 5 one comes to a completely different conclusion: in case (a) the oscillator starts as a perfect heat source rather than a perfect work source and only in the course of time a work source effect arises, whereas in

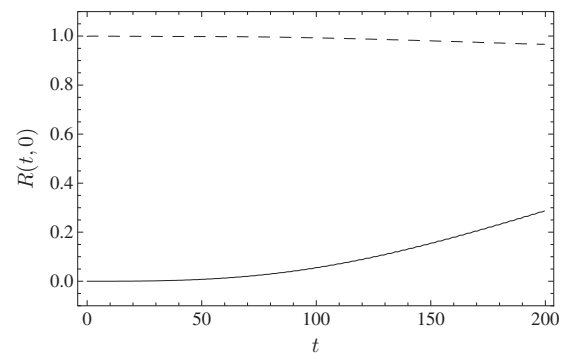


FIG. 5. Results of the integral work reservoir quality measure  $R(t, 0)$  for the examples as of Fig. 4: (a)  $\alpha = 0$ ,  $c = 0.5$  (solid line), (b)  $\alpha = 2$ ,  $c = 1$  (dashed)



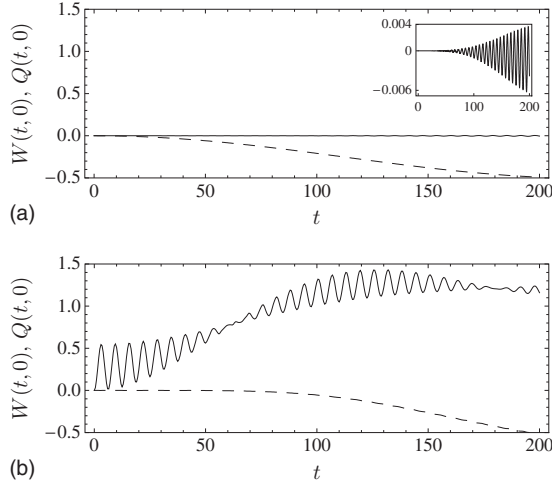


FIG. 6. Integrated work  $W(t,0)$  (solid line) and heat  $Q(t,0)$  (dashed) for the two chosen examples, as of Fig. 5. The inset of case (a) shows  $W(t,0)$  alone.

case (b) the oscillator is recognized as a nearly ideal work source during the whole interval. It is astonishing to see that the purity based measure gives such a different picture since the reasoning based on the FA is valid: During the initial phase,  $\mathcal{L}_s^{\text{eff}}$  is close to 0.

The reason for this seemingly contradictory characterization becomes evident when examining the results for the integrated work and heat,  $W(t)$  and  $Q(t)$  (see Fig. 6). In both presented cases, the total heat flow in the beginning of the dynamics is small as expected from the FA argument. Also, the heat becomes significant not before  $t_{(a)}^*$  and  $t_{(b)}^*$ , respectively, which again demonstrates the strong connection between heat and purity.

However, the work exhibits a completely different behavior for the two cases: in the first case, the work remains almost constant at zero until oscillations set in at around  $t \approx 100$  [see the inset of Fig. 6(a)]. Those oscillations lead to the slow increase in work source quality in the second half of the considered time interval. Although the oscillations have only small amplitude, their work source effect becomes significant due to their frequency, which is high when compared to the time scale of heat dynamics.

In case (b),  $W(t,0)$  shows strong oscillations of an amplitude orders of magnitude larger than in case (a) from the very beginning of the dynamics. Thus, the reason for the contradiction to the purity measure result is traced back to the problem already touched on in Sec. VII A: although the purity can be used as a measure for the size of incoherent part of the effective dynamics of the spin,  $\mathcal{L}_s^{\text{eff}}$ , which is associated with the heat flow, it is completely insensitive to the size and effects of the coherent part  $\hat{H}_s^{\text{eff}}$  and thus the actual work source effect.

From this result, we can draw the conclusion that due to the fact that the purity measure is only linked to  $\mathcal{L}_s^{\text{eff}}$  alone, it can only be used as a necessary condition for work source functionality. In order to get the full picture, a more detailed analysis of the work and heat fluxes via the measure  $R$  is necessary.

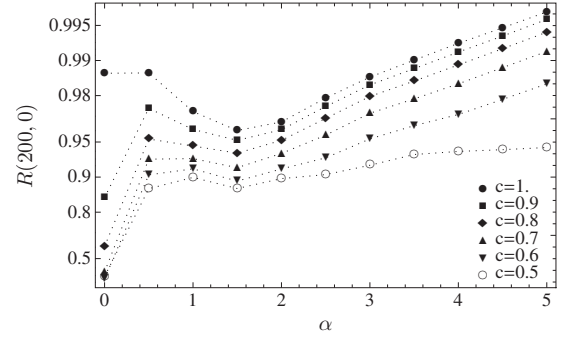


FIG. 7. Log-scale plot of the overall work source quality  $R$  for the time interval  $[0,200]$ . The behavior of  $R(200,0)$  is shown depending on the initial state determined by the parameters  $\alpha$  and  $c$ .  $R$  is defined in Eq. (20),  $\alpha$  and  $c$  in Eq. (24).

### C. Work source quality overview

Computing  $R$  as defined in Eq. (20) for a low photon number parameter window ( $\alpha \in [0,4]$ ) and initial spin temperatures ranging from 0 to  $\infty$  ( $c \in [0.5, 1]$ ), we find the following trends (cf. Fig. 7):

For  $\alpha=0$ , the overall work source quality of the considered interval  $t \in [0,200]$  is generally significantly lower than for the corresponding (with respect to  $c$ ) cases for  $\alpha>0$ , and  $R(200,0)$  ranges from roughly 0.8 to 0.2 with decreasing  $c$ , except for the particular initial state  $c=1$ ,  $\alpha=0$ . Initial states with  $\alpha=0$  lead to a significant work effect despite their lack of initial excitation of the oscillator. This is easily explained in view of Eq. (41): for  $c \neq 0.5$ , the oscillator is subject to an effective displacement of its potential. In the new set of the new eigenstates, the initial state  $|0\rangle$  is a coherent superposition state again.

For  $\alpha>0$ ,  $R(200,0)$  takes on values close to or above 0.9, with a slow increase for higher  $\alpha$  and  $c$ . The first increase can be related to the higher excitation of the oscillator and the resulting bigger amplitude of the position expectation. The second trend has to do with a special property of the initial states  $|0\rangle|\alpha\rangle$  and  $|1\rangle|\alpha\rangle$  of which the initial state of the  $xz$ -SOM is a statistical mixture.

In order to explain the trend for increasing  $c$ , we invoke the first-order perturbation theory for the extremal initial states  $|0\rangle|\alpha\rangle$  and  $|1\rangle|\alpha\rangle$  which is applicable to the beginning of the dynamics, as long as  $gt^* \ll 1$  holds with  $g=10^{-2}/\sqrt{2}$ . The calculation is carried out in Appendix D. Here, we only make use of the result

$$\hat{U}^I(t)|0\rangle|\alpha\rangle = (|0\rangle - i\alpha gt|1\rangle)|\alpha\rangle + \mathcal{O}(g^2), \quad (44)$$

$$\hat{U}^I(t)|1\rangle|\alpha\rangle = \left( |1\rangle - i\frac{\alpha^*}{2}gt|0\rangle \right)|\alpha\rangle - igt|0\rangle\frac{\partial}{\partial\alpha^*}|\alpha\rangle + \mathcal{O}(g^2), \quad (45)$$

and  $\alpha^*$  denotes the complex conjugate of  $\alpha$ . From this form of the state  $\partial_{\alpha^*}|\alpha\rangle$ , we easily see that in first order  $\hat{U}^I(t)|0\rangle|\alpha\rangle$  factorizes contrary to  $\hat{U}^I(t)|1\rangle|\alpha\rangle$ . The purity behavior of the initial state  $\rho(0)=[c|0\rangle\langle 0|+(1-c)|1\rangle\langle 1|] \otimes |\alpha\rangle\langle\alpha|$  continuously changes from the  $|0\rangle|\alpha\rangle$  case to the  $|1\rangle|\alpha\rangle$  case. As the

$|1\rangle|\alpha\rangle$  state becomes more and more mixed into the initial state with decreasing  $c$ , a significant purity drop happens at earlier times of the evolution. The same is true for the heat flow, which is tied to the purity drop. With this increased heat flow at the early stage of the evolution,  $Q(200,0)$  reaches higher values for decreasing  $c$ .

Moreover, the size of work flux for the same change of effective splitting of the spin decreases with decreasing  $c$  until it reaches 0 for  $c=0.5$ . Thus, in the beginning and as long as the spin's state is close to its initial occupation, the work source effect of the oscillator is reduced or suppressed additionally. Clearly, this reduces the work source quality and explains the trend seen in the numerical results.

### VIII. SUMMARY

Work and heat are related to (thermodynamic) processes, which seem to require external control. In this paper, we have argued that work functionality may show up in closed bipartite quantum systems, even down to the nanoscale. We have shown under what general conditions the respective subsystem dynamics may be described via time-dependent effective Hamiltonians and in this sense act as classical driver for each other.

We have then brought forward the argument that energy exchanged under such conditions has to be considered as work from the viewpoint of thermodynamics. In addition, we have introduced purity based and work/heat based work source quality measures and discussed their usefulness. We have demonstrated that due to the lack of sensitivity to the effects of  $\hat{H}_1^{\text{eff}}$ , the purity based measure is only a necessary condition for work source functionality, in general.

To give an example for a quantum work source and to illustrate the properties of the given work source quality measures, we have applied these results to the SOM confirming that a system as small and simple as a single harmonic oscillator coupled to a spin can act as a work reservoir for the latter.

Finally, with regard to quantum thermodynamic machines, we note that the implementation of a full thermodynamic process within a closed quantum system will require driving as well as thermalizing embeddings.

### ACKNOWLEDGMENTS

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### APPENDIX A: GENERALIZED FACTORIZATION APPROXIMATION

In its original form the FA is formulated for a bipartite system [cf. [24], Eq. (3) and (4)]. Let us now consider a tripartite system defined by the Hamiltonian

$$\hat{H} = \hat{H}_0 + \hat{H}_1 + \hat{H}_{12} + \hat{H}_2. \quad (\text{A1})$$

Let us assume that system 0 has interacted with system 1 in the past but is now decoupled from system 1. System 2, however, is supposed to have been uncoupled in the past and is now being coupled to system 1 alone. Finally, we assume that the combined system 01 and system 2 are now in a pure state. We are then left with an initial state for the whole system of the form

$$\hat{\rho}(0) = \hat{\rho}_{01}(0) \otimes \hat{\rho}_2(0), \quad (\text{A2})$$

with  $\hat{\rho}_{01}(0) = |\Psi_{01}(0)\rangle\langle\Psi_{01}(0)|$  and  $\hat{\rho}_2(0) = |\Psi_2(0)\rangle\langle\Psi_2(0)|$ .

We now consider the dynamics of this system with respect to the given initial state. In the case that  $\text{tr}[\hat{\rho}_2^2(t)] \approx 1$  holds, the FA is applicable to the whole system yielding the two coupled equations

$$i\hbar|\dot{\Psi}_{01}(t)\rangle = [\hat{H}_0 + \hat{H}_1 + \langle\Psi_2(t)|\hat{H}_{12}|\Psi_2(t)\rangle]|\Psi_{01}(t)\rangle, \quad (\text{A3})$$

$$i\hbar|\dot{\Psi}_2(t)\rangle = (\hat{H}_2 + \langle\Psi_{01}(t)|\hat{H}_{12}|\Psi_{01}(t)\rangle)|\Psi_2(t)\rangle. \quad (\text{A4})$$

By restating Eq. (A3) in the form

$$i\hbar\dot{\hat{\rho}}_{01}(t) = [\hat{H}_0 + \hat{H}_1 + \langle\Psi_2(t)|\hat{H}_{12}|\Psi_2(t)\rangle, \hat{\rho}_{01}(t)] \quad (\text{A5})$$

and taking the trace of the Hilbert space of the ancillary system 0, we arrive at the result

$$i\hbar\dot{\hat{\rho}}_1(t) = [\hat{H}_1 + \langle\Psi_2(t)|\hat{H}_{12}|\Psi_2(t)\rangle, \hat{\rho}_1(t)]. \quad (\text{A6})$$

To get this result, we have made use of the two partial trace relations

$$\text{tr}_0[\hat{A} \otimes \hat{1}_1, \hat{B}] = 0, \quad (\text{A7})$$

$$\text{tr}_0[\hat{1}_0 \otimes \hat{A}, \hat{B}] = [\hat{A}, \text{tr}_0\hat{B}]. \quad (\text{A8})$$

Note that in contrast to the case of the FA for a bipartite system, the criterion for the applicability of the FA is the purity dynamics of system 2 alone.

### APPENDIX B: PURITY OF THE OSCILLATOR

The purity dynamics of the oscillator in the case of the pure  $\hat{\sigma}_z \hat{x}$  interaction can be derived from the solution of the Liouville-von Neumann equation given in Eq. (26),

$$\hat{\rho}(t) = \begin{pmatrix} c|\alpha_-(t)\rangle\langle\alpha_-(t)| & \\ & (1-c)|\alpha_+(t)\rangle\langle\alpha_+(t)| \end{pmatrix}.$$

Thus, the oscillator reduced state is

$$\hat{\rho}_o(t) = c|\alpha_-(t)\rangle\langle\alpha_-(t)| + (1-c)|\alpha_+(t)\rangle\langle\alpha_+(t)| \quad (\text{B1})$$

and taking the square and the trace of this expression, we end up with the result for the purity given in Eq. (27),

$$P[\hat{\rho}_o(t)] = c^2 + (1-c)^2 + 2c(1-c)|\langle\alpha_-(t)|\alpha_+(t)\rangle|^2.$$

For the time-dependent term we find

$$|\langle \alpha_{-}(t) | \alpha_{+}(t) \rangle|^2 = |\langle \alpha | \hat{U}_{-}^{\dagger}(t, 0) \hat{U}_{+}(t, 0) | \alpha \rangle|^2, \quad (\text{B2})$$

$$= |\langle \alpha | \exp(i\hat{H}_{-}t) \exp(-i\hat{H}_{+}t) | \alpha \rangle|^2 \quad (\text{B3})$$

with  $\hat{H}_{\pm} = \hat{H}_o \pm \lambda \hat{x} \pm \frac{\omega_s}{2}$ . Making use of the displacement operator  $\hat{D}(\alpha) = \exp(\alpha \hat{a}^{\dagger} - \alpha^* \hat{a})$  and its properties

$$\hat{D}(-\alpha) \hat{x} \hat{D}(\alpha) = \hat{x} + \sqrt{\frac{2}{m\omega_o}} \text{Re}(\alpha), \quad (\text{B4})$$

$$\hat{D}(-\alpha) \hat{p} \hat{D}(\alpha) = \hat{p} + \sqrt{2m\omega_o} \text{Im}(\alpha), \quad (\text{B5})$$

we can express  $\hat{H}_{\pm}$  as

$$\hat{H}_{\pm} = \hat{D}(-\beta_{\pm}) \hat{H}_o \hat{D}(\beta_{\pm}) + C \quad (\text{B6})$$

and therefore have

$$\hat{U}_{\pm}(t, 0) = e^{-iCt} \hat{D}(-\beta_{\pm}) \exp(-i\hat{H}_o t) \hat{D}(\beta_{\pm}) \quad (\text{B7})$$

with  $\beta_{\pm} = \mp \lambda / \sqrt{2m\omega_o^3}$  up to constant factors or a phase, respectively, which are irrelevant for the computation of the modulus in Eq. (B2). With the help of the relations

$$\hat{D}(\alpha) \hat{D}(\beta) = \exp[i \text{Im}(\alpha\beta^*)] \hat{D}(\alpha + \beta), \quad (\text{B8})$$

$$\exp(-i\hat{H}_o t) | \alpha \rangle = \exp(-i\omega_o t/2) | \alpha \rangle \exp(-i\omega_o t), \quad (\text{B9})$$

we arrive at

$$|\alpha_{\pm}(t)\rangle = \exp[i\phi_{\pm}(t)] | (\alpha + \beta_{\pm}) \exp(-i\omega_o t) - \beta_{\pm} \rangle. \quad (\text{B10})$$

Finally making use of the relation  $|\langle \alpha | \alpha' \rangle|^2 = \exp(-|\alpha - \alpha'|^2)$  yields the result

$$|\langle \alpha_{-}(t) | \alpha_{+}(t) \rangle|^2 = \exp\left[-8 \frac{\lambda^2}{m\omega_o^3} \sin^2\left(\frac{1}{2}\omega_o t\right)\right]. \quad (\text{B11})$$

### APPENDIX C: AMPLITUDE OF THE SPIN'S EFFECTIVE SPLITTING IN THE $z$ -SOM

In the case of the  $z$ -SOM and applicable FA, the effective Hamiltonians of the spin and oscillator are found to be [Eqs. (40) and (41)]

$$\hat{H}_s^{\text{eff}}(t) = \left( \frac{\omega_s}{2} + \lambda \langle \hat{x} \rangle(t) \right) \hat{\sigma}_z, \quad (\text{C1})$$

$$\hat{H}_o^{\text{eff}} = (\hat{H}_o + \lambda(1 - 2c)\hat{x}), \quad (\text{C2})$$

and the latter may be rewritten in the form

$$\hat{H}_o^{\text{eff}} = \frac{1}{2} \omega_o (\hat{X}^2 + \hat{P}^2) + \text{const} \quad (\text{C3})$$

with the dimensionless position and momentum operators

$$\hat{X} = \hat{X} + \sqrt{\frac{\lambda^2}{m\omega_o}} (1 - 2c) \quad (\text{C4})$$

$$\hat{P} = \hat{P}, \quad (\text{C5})$$

where  $\hat{X} = \sqrt{m\omega_o} \hat{x}$ ,  $\hat{P} = \hat{p} / \sqrt{m\omega_o}$ . Making use of the properties of the displacement operator  $\hat{D}(\alpha)$  in Eqs. (B4) and (B5), one finds that

$$\hat{H}_o^{\text{eff}} = \hat{D}(-\gamma) \hat{H}_o \hat{D}(\gamma) \quad (\text{C6})$$

with

$$\gamma = \sqrt{\frac{\lambda^2}{2m\omega_o}} (1 - 2c). \quad (\text{C7})$$

In order to compute the peak-to-peak amplitude of the effective spin splitting

$$\Delta\omega_s^{\text{eff}} = \lambda (\langle \hat{x} \rangle_{\text{max}} - \langle \hat{x} \rangle_{\text{min}}) \quad (\text{C8})$$

we need to evaluate

$$\begin{aligned} \langle \hat{x} \rangle(t) &= \langle \alpha(t) | \hat{x} | \alpha(t) \rangle = \langle \alpha | \exp(i\hat{H}_o^{\text{eff}} t) \hat{x} \exp(-i\hat{H}_o^{\text{eff}} t) | \alpha \rangle \\ &= \langle \alpha | \hat{D}(-\gamma) \exp(i\hat{H}_o t) \hat{D}(\gamma) \hat{x} \hat{D}(-\gamma) \\ &\quad \times \exp(-i\hat{H}_o t) \hat{D}(\gamma) | \alpha \rangle \\ &= \langle \alpha + \gamma | \exp(i\hat{H}_o t) \hat{x} \\ &\quad \times \exp(-i\hat{H}_o t) | \alpha + \gamma \rangle + \tilde{\gamma}, \end{aligned} \quad (\text{C9})$$

where we have used Eqs. (B4), (B8), and (C6) assuming  $\alpha \in \mathbb{R}$  and defining  $\tilde{\gamma} = \sqrt{2/(m\omega_o)} \gamma$ . Now, we can see that the first term is just the time evolution of the expectation value of the position of the original oscillator described by  $\hat{H}_o$  for a coherent initial state  $|\alpha + \gamma\rangle$ . With the help of Eq. (B9) it is straightforward to show that  $\langle \hat{X} \rangle_{\text{max}} - \langle \hat{X} \rangle_{\text{min}} = 2\sqrt{2} |\alpha + \gamma|$  and therefore

$$\Delta\omega_s^{\text{eff}} = 2\lambda \sqrt{\frac{2}{m\omega_o}} |\alpha + \gamma|. \quad (\text{C11})$$

Note that this result is only exact if the Hamiltonian governing the oscillator's dynamics is  $\hat{H}_o^{\text{eff}}$  and  $\mathcal{L}_o^{\text{eff}}[\hat{\rho}(t)] = 0$ , that is if the FA is exact. Still, if the FA holds in good approximation, Eq. (C11) is a good approximation as well.

### APPENDIX D: FIRST-ORDER TIME-DEPENDENT PERTURBATION THEORY FOR PURE INITIAL STATES OF JCM

It is convenient to apply the perturbation theory in the interaction picture. All interaction picture quantities are denoted by a superscript "I." The expansion of the time-evolution of the state is given by

$$|\Psi^I(t)\rangle = |\Psi(0)\rangle + \hat{U}_1^I(t) |\Psi(0)\rangle + \mathcal{O}(g^2) \quad (\text{D1})$$

and the first-order contribution to the time-evolution operator  $\hat{U}_1^I(t)$  is given by (see, e.g., [35], p. 207ff)

$$\hat{U}_1^I(t) = -i \int_0^t d\tau \hat{V}^I(\tau) \quad (\text{D2})$$

and

$$\begin{aligned} \hat{V}^I(t) &= \hat{U}_0^\dagger(t) \hat{V} \hat{U}_0(t) \\ &= g \exp[i(\hat{H}_s + \hat{H}_o)t] (\hat{\sigma}_+ \hat{a} + \hat{\sigma}_- \hat{a}^\dagger) \exp[-i(\hat{H}_s + \hat{H}_o)t] \\ &= g(\hat{\sigma}_+ \hat{a} + \hat{\sigma}_- \hat{a}^\dagger) \end{aligned} \quad (\text{D3})$$

is the interaction operator in the interaction picture. According to the RWA, only terms of the interaction are kept which are time-independent in the interaction picture, thus the last equality. From Eqs. (D3) and (D2), it follows that

$$\hat{U}_1^I(t) = -igt(\hat{\sigma}_+ \hat{a} + \hat{\sigma}_- \hat{a}^\dagger). \quad (\text{D4})$$

The time evolution of a state in the JCM is therefore given in first-order perturbation by

$$|\Psi^I(t)\rangle = [\hat{I} - igt(\hat{\sigma}_+ \hat{a} + \hat{\sigma}_- \hat{a}^\dagger)] |\Psi(0)\rangle + \mathcal{O}(g^2). \quad (\text{D5})$$

Here, we consider  $|0\rangle|\alpha\rangle$  and  $|1\rangle|\alpha\rangle$  as initial states. Together with

$$\hat{a}^\dagger|\alpha\rangle = \left( \frac{\partial}{\partial \alpha^*} + \frac{\alpha^*}{2} \right) |\alpha\rangle \quad (\text{D6})$$

(see [36]) we find for those states

$$\hat{U}^I(t)|0\rangle|\alpha\rangle = (|0\rangle - igt|1\rangle)|\alpha\rangle + \mathcal{O}(g^2), \quad (\text{D7})$$

$$\hat{U}^I(t)|1\rangle|\alpha\rangle = \left( |1\rangle - i\frac{\alpha^*}{2}gt|0\rangle \right) |\alpha\rangle - igt|0\rangle \frac{\partial}{\partial \alpha^*} |\alpha\rangle + \mathcal{O}(g^2), \quad (\text{D8})$$

where

$$\frac{\partial}{\partial \alpha^*} |\alpha\rangle := \frac{\partial}{\partial \alpha^*} \left[ \exp\left(-\frac{|\alpha|^2}{2}\right) \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} |n\rangle \right] \quad (\text{D9})$$

( $\alpha^*$  is the complex conjugate of  $\alpha$ ).

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- [1] J. v. Neumann, *Z. Phys. A: Hadrons Nucl.* **57**, 30 (1929).  
[2] P. Bocchieri and A. Loinger, *Phys. Rev.* **114**, 948 (1959).  
[3] J. M. Deutsch, *Phys. Rev. A* **43**, 2046 (1991).  
[4] M. Srednicki, *Phys. Rev. E* **50**, 888 (1994).  
[5] P. Reimann, *Phys. Rev. Lett.* **99**, 160404 (2007).  
[6] P. Reimann, *Phys. Rev. Lett.* **101**, 190403 (2008).  
[7] J. Gemmer, A. Otte, and G. Mahler, *Phys. Rev. Lett.* **86**, 1927 (2001).  
[8] P. Borowski, J. Gemmer, and G. Mahler, *Eur. Phys. J. B* **35**, 255 (2003).  
[9] J. Gemmer, M. Michel, and G. Mahler, *Quantum Thermodynamics* (Springer, New York, 2004).  
[10] H. Tasaki, *Phys. Rev. Lett.* **80**, 1373 (1998).  
[11] S. Popescu, A. J. Short, and A. Winter, *Nat. Phys.* **2**, 754 (2006).  
[12] N. Linden, S. Popescu, A. J. Short, and A. Winter, *Phys. Rev. E* **79**, 061103 (2009).  
[13] S. Goldstein, J. L. Lebowitz, R. Tumulka, and N. Zanghi, *Phys. Rev. Lett.* **96**, 050403 (2006).  
[14] R. Alicki, *J. Phys. A* **12**, L103 (1979).  
[15] R. Kosloff and M. A. Ratner, *J. Chem. Phys.* **80**, 2352 (1984).  
[16] P. Talkner, E. Lutz, and P. Hänggi, *Phys. Rev. E* **75**, 050102(R) (2007).  
[17] T. D. Kieu, *Phys. Rev. Lett.* **93**, 140403 (2004).  
[18] M. J. Henrich, M. Michel, and G. Mahler, *Europhys. Lett.* **76**, 1057 (2006).  
[19] M. J. Henrich, G. Mahler, and M. Michel, *Phys. Rev. E* **75**, 051118 (2007).  
[20] M. J. Henrich, F. Rempp, and G. Mahler, *Eur. Phys. J. Spec. Top.* **151**, 157 (2007).  
[21] A. E. Allahverdyan, R. S. Johal, and G. Mahler, *Phys. Rev. E* **77**, 041118 (2008).  
[22] N. Linden, S. Popescu, and P. Skrzypczyk, e-print arXiv:0908.2076.  
[23] H. Weimer, M. J. Henrich, F. Rempp, H. Schröder, and G. Mahler, *Europhys. Lett.* **83**, 30008 (2008).  
[24] J. Gemmer and G. Mahler, *Eur. Phys. J. D* **17**, 385 (2001).  
[25] C. R. Willis and R. Picard, *Phys. Rev. A* **9**, 1343 (1974).  
[26] C. Jarzynski, *Phys. Rev. E* **56**, 5018 (1997).  
[27] F. Tonner and G. Mahler, *Fortschr. Phys.* **54**, 939 (2006).  
[28] G. Mahler and V. A. Weberruß, *Quantum Networks—Dynamics of Open Nanostructures*, 2nd ed. (Springer, New York, 1998).  
[29] E. Jaynes and F. Cummings, *Proc. IEEE* **51**, 89 (1963).  
[30] B. W. Shore and P. L. Knight, *J. Mod. Opt.* **40**, 1195 (1993).  
[31] J. H. Shirley, *Phys. Rev.* **138**, B979 (1965).  
[32] J. Larson, *Phys. Scr.* **76**, 146 (2007).  
[33] M. O. Scully and M. S. Zubairy, *Quantum Optics* (Cambridge University Press, Cambridge, England, 1997).  
[34] J.-L. Basdevant and J. Dalibard, *The Quantum Mechanics Solver: How to Apply Quantum Theory to Modern Physics* (Springer, New York, 2000).  
[35] A. Messiah, *Quantenmechanik*, 3rd ed. (Walter de Gruyter, Berlin, 1990), Vol. 2.  
[36] W. Vogel and D.-G. Welsch, *Quantum Optics*, 3rd ed. (Wiley-VCH Verlag GmbH & Co. KGaA., Weinheim, 2006).