Dissipation of classical energy in nonlinear quantum systems

Cite as: J. Chem. Phys. 128, 134107 (2008); https://doi.org/10.1063/1.2844597
Submitted: 29 October 2007 . Accepted: 23 January 2008 . Published Online: 03 April 2008

Andrey Pereverzev, Yuriy V. Pereverzev, and Oleg V. Prezhdo

ARTICLES YOU MAY BE INTERESTED IN

Correlation functions in quantized Hamilton dynamics and quantal cumulant dynamics
The Journal of Chemical Physics 129, 144104 (2008); https://doi.org/10.1063/1.2990005

Quantized Hamilton dynamics for a general potential
The Journal of Chemical Physics 116, 4450 (2002); https://doi.org/10.1063/1.1451060

Quantized Hamilton dynamics
The Journal of Chemical Physics 113, 6557 (2000); https://doi.org/10.1063/1.1290288
Dissipation of classical energy in nonlinear quantum systems

Andrey Pereverzev,¹,a) Yuriy V. Pereverzev,² and Oleg V. Prezhdo²,a,c)
¹Department of Chemistry and Center for Materials Chemistry, University of Houston, Houston, Texas 77204, USA
²Department of Chemistry, University of Washington, Seattle, Washington 98195, USA

(Received 29 October 2007; accepted 23 January 2008; published online 3 April 2008)

We show using two simple nonlinear quantum systems that the infinite set of quantum dynamical variables, as introduced in quantized Hamilton dynamics [O. V. Prezhdo and Y. V. Pereverzev, J. Chem. Phys. 113, 6557 (2000)], behave as a thermostat with respect to the finite number of classical variables. The coherent classical component of the evolution decays by coupling to the chaotic quantum reservoir. The classical energy, understood as the part of system energy expressible through the average values of coordinates and momenta, is transferred to the quantum energy expressible through the higher moments of coordinates and momenta and other quantum variables. At long times, the classical variables reach equilibrium, and the classical energy fluctuates around the equilibrium value. These phenomena are illustrated with the exactly solvable Jaynes–Cummings model and a nonlinear oscillator. © 2008 American Institute of Physics. [DOI: 10.1063/1.2844597]

I. INTRODUCTION

The idea of introducing classical and quantum dynamical variables to study evolution of a quantum system finds many applications in chemical physics. In semiclassical approaches, quantum dynamics is approximated by a finite number of variables, as exemplified by the center and width parameters of wave packets.¹⁻⁹ Quantum-classical approaches treat part of the system fully quantum mechanically and approximate the remaining degrees of freedom by classical mechanics. Surface hopping and related schemes provide an important illustration of this idea.¹⁰⁻¹² In surface hopping, a finite number of quantum levels interact with classical ionic motion. In this paper, we focus the quantized hopping, a finite number of quantum levels interact with quantum reservoir energies.²⁰,²⁶

The main goal of this paper is to show that there is an irreversible flow of energy from the classical to the quantum reservoir in nonlinear quantum systems. The separation of energy into the two reservoirs is based on the possibility to describe quantum systems in the space of classical and quantum variables.¹³⁻²⁷ This description allows one to study time evolution of the quantum system using Heisenberg equations, which reduce to the Hamilton equations in the classical limit. The main challenge of this approach is the unbounded growth in the number of quantum variables when their equations of motion are written down. In order to obtain a finite closed system of equations, the higher-order quantum variables have to be approximated through the lower-order variables. Note that in the case of a harmonic oscillator, there is no interaction between classical and quantum variables. Moreover, there exist noninteracting blocks of quantum variables. Therefore, it is natural that in this simple system, there is no flow of energy from the classical to quantum reservoir. A similar situation is found in pure spin systems. However, when the potential energy is not quadratic, the equations of motion become nonlinear, classical, and quantum variables begin to interact, and the flow of energy between them becomes possible.

One of the simplest models that introduces nonlinearity into the potential energy is the Jaynes–Cummings model,²⁸⁻⁳⁰ in which an oscillator interacts with a two-level spin system. This model is exactly solvable and, therefore, the process of energy flow between classical and quantum reservoirs can be studied exactly. In order to demonstrate the generality of the irreversible classical energy flow in nonlinear systems, we consider as another example a nonlinear oscillator with quartic term in the potential energy.

This paper is organized as follows. First, we introduce classical variables and classical reservoir energy for the Jaynes–Cummings model. The time dependence of the classical energy is investigated for different strengths of the spin-phonon coupling and detuning. The notion of the time-averaged classical energy is introduced. Then, we consider the Heisenberg equations of motion for classical and quantum variables of a nonlinear oscillator. Two ways to truncate the Heisenberg hierarchy are investigated. In each case, we obtain time dependence of the classical energy by solving a simple closed system of equations. The approximate results are compared to the exact numerical solution of the Schrödinger equation for the nonlinear oscillator. In all models that we study, the initial state of the oscillator is taken to be a coherent state since these states can be considered the most classical with the maximum possible classical energy. The paper concludes with a brief summary and further thoughts on classical variables coupled to a quantum variable reservoir.

¹Authors to whom correspondence should be addressed.
²Electronic mail: andrey.pereverzev@mail.uh.edu.
³Electronic mail: prezhdo@u.washington.edu.
II. JAYNES–CUMMINGS MODEL

The Jaynes–Cummings model\textsuperscript{28–30} is of the simplest and exactly solvable examples of a nonlinear quantum system. Below, we derive the exact expressions for the time evolution of the observables of interest here, and then analyze the behavior of these observables for several sets of model parameters.

A. Exact evolution of classical energy and spin polarization

The Jaynes–Cummings Hamiltonian describes a harmonic oscillator interacting with a two-level system. The Hamiltonian of the oscillator

\[ H_0 = p^2/2 + x^2/2 \]

is given in the dimensionless form by using $\hbar/m\omega$ as the unit of length and $\hbar/\omega$ as the unit of momentum. Here, $\hbar$ is Planck’s constant, $m$ is the oscillator mass, and $\omega$ is its frequency. In the following discussion we use the Heisenberg representation for operators in which time limits. The two-level system that interacts with the oscillator is described by the time evolution operator $\exp(-iHt/\hbar)$, because of its interaction with the two-level system that is exactly solvable due to the presence of $S_z$, with the eigenvalue $1/2$, and $|n\rangle$ is the eigenstate of $a^\dagger a$ with the eigenvalue $n$. Parameter $\alpha$ can be expressed through the average initial coordinate and momentum: $\alpha = x_0/\sqrt{2}\xi$ and $\Im\alpha = p_0/\sqrt{2}\xi[x_0 = x_c(0)$ and $p_0 = p_c(0)]$. In the following discussion, we use $\xi$ for simplicity that $p_0 = 0$, i.e., $\alpha$ is real.

The classical energy from Eqs. (6), (2), (4), and (7) has the form

\[ E_{cl}(t) = E_{cl}(0)\exp(-x_c^2/\xi) \times \left\{ \sum_{n=0}^{\infty} \left( \frac{x_c^2}{2}\xi \right)^n \frac{n!}{n!} \left( \cos b(n)t \cos b(n+1)t \right. \right. \]

\[ + \frac{b(n+1)}{b(n)} \sin b(n)t \sin b(n+1)t \right\} \}

\[ \left. + \frac{\delta t}{4} \sum_{n=0}^{\infty} \left( \frac{x_c^2}{2}\xi \right)^n \frac{n!}{n!} \left( \cos b(n)t \sin b(n+1)t \right. \right. \]

\[ \left. \left. - \frac{b(n+1)}{b(n)} \sin b(n)t \cos b(n+1)t \right\} \right\}, \]

where $b(n) = (x_c^2/\xi)(n+1) + \delta t/4$ and $E_{cl}(0) = x_c^2/2$ is the classical energy at $t = 0$. Note that the time dependence of the classical energy is given in terms of the frequencies $b(n)$ which depend on the interaction strength $g$, the quantum parameter $\xi$, and detuning $\delta$. In order to better understand the long time behavior of the classical energy, it is useful to look at the time-averaged classical energy defined as

\[ \langle E_{cl} \rangle = \lim_{T \to \infty} \frac{1}{T} \int_0^T E_{cl}(t)dt. \]

We have explicitly

\[ S_z(t) = \exp(i\lambda t)A_1 + \exp(-i\lambda t)B_1 - \delta C, \]

where $\lambda = \sqrt{4g^2/\xi + 4g^2/\xi}$, $A_1 + B_1 = S_z$, and $A_1 - B_1 = -g\sqrt{\delta C}$. We are interested in the time dependence of the classical energy of the oscillator. This energy can be interpreted as the classical analogue of Eq. (1) in which coordinate and momentum operators are replaced by their average values. Thus, we define the classical energy as

\[ E_{cl}(t) = p_{cl}(t)^2/2 + x_{cl}(t)^2/2, \]

with $|\Psi_0\rangle = |\alpha\rangle |1/2\rangle$ being the wave function of our system at time $t = 0$, $|\alpha\rangle = \exp(-|\alpha|^2/2)\sum_n (\alpha^n/\sqrt{n!})|n\rangle$ is a coherent state of the harmonic oscillator, $|1/2\rangle$ is the eigenstate of $S_z$ with the eigenvalue $1/2$, and $|n\rangle$ is the eigenstate of $a^\dagger a$ with the eigenvalue $n$. Parameter $\alpha$ can be expressed through the average initial coordinate and momentum: $\Re\alpha = x_0/\sqrt{2}\xi$ and $\Im\alpha = p_0/\sqrt{2}\xi[x_0 = x_c(0)$ and $p_0 = p_c(0)]$. In the following discussion, we use $\xi$ for simplicity that $p_0 = 0$, i.e., $\alpha$ is real.

The classical energy from Eqs. (6), (2), (4), and (7) has the form

\[ E_{cl}(t) = E_{cl}(0)\exp(-x_c^2/\xi) \times \left\{ \sum_{n=0}^{\infty} \left( \frac{x_c^2}{2}\xi \right)^n \frac{n!}{n!} \left( \cos b(n)t \cos b(n+1)t \right. \right. \]

\[ + \frac{b(n+1)}{b(n)} \sin b(n)t \sin b(n+1)t \right\} \}

\[ \left. + \frac{\delta t}{4} \sum_{n=0}^{\infty} \left( \frac{x_c^2}{2}\xi \right)^n \frac{n!}{n!} \left( \cos b(n)t \sin b(n+1)t \right. \right. \]

\[ \left. \left. - \frac{b(n+1)}{b(n)} \sin b(n)t \cos b(n+1)t \right\} \right\}, \]

where $b(n) = (x_c^2/\xi)(n+1) + \delta t/4$ and $E_{cl}(0) = x_c^2/2$ is the classical energy at $t = 0$. Note that the time dependence of the classical energy is given in terms of the frequencies $b(n)$ which depend on the interaction strength $g$, the quantum parameter $\xi$, and detuning $\delta$. In order to better understand the long time behavior of the classical energy, it is useful to look at the time-averaged classical energy defined as

\[ \langle E_{cl} \rangle = \lim_{T \to \infty} \frac{1}{T} \int_0^T E_{cl}(t)dt. \]
We perform the summations numerically, and the corresponding series converge rapidly within $n = 100$.

**B. Analysis of classical energy and spin polarization**

Consider the time evolution of the classical energy [Eqs. (9) and (11)] and spin polarization [Eqs. (12)–(14)] for various sets of model parameters and initial conditions. The model parameters include the spin-phonon coupling $g$ and detuning $\delta$. As discussed above, the initial conditions for the harmonic oscillator are chosen in the form of the coherent state [Eq. (8)] with the initial momentum set to zero. Thus, the only varying parameter is the initial position $x_0$. The initial value of the spin polarization is set to $+\frac{1}{2}$. The dimensionless quantum parameter $\xi$ allows us to consider the quantum ($\xi = 1$) and classical ($\xi = 0$) limits. It enters both Hamiltonian (3) and the solutions (9)–(14).

Figure 1(a) shows the time dependence of the reduced classical energy $E_{\text{cl}}(t)/E_{\text{cl}}(0)$ for the following values of parameters $x_0 = 7$, $g = 0.1$, $\delta = 0$, and $\xi = 1$. The classical energy shows an oscillatory decay with time. It is transformed into the quantum energy $E_{\text{qp}}(t)$, defined by

$$E_{\text{qp}}(t) = \frac{1}{2} \langle \Psi_0 | \exp(iHt) [p - p_{\text{cl}}(t)]^2 + (q - q_{\text{cl}}(t))^2 \rangle \exp(-iHt) | \Psi_0 \rangle.$$  

The quantum energy can be interpreted as the difference between the average oscillator Hamiltonian given by Eq. (1) and the classical energy $E_{\text{cl}}(t)$. An explicit expression for the quantum energy [Eq. (15)] is easy to find using the integral of motion $\gamma$ defined above. On the one hand, $\xi(\Psi_0 | \gamma | \Psi_0) = x_0^2/2 + \xi$, and on the other hand, $\xi(\Psi_0 | \gamma | \Psi_0) = E_{\text{cl}}(t) + E_{\text{qp}}(t) + \xi \sigma(t)$ and, therefore,

$$E_{\text{qp}}(t) = x_0^2/2 + \xi (1 - \sigma(t)) - E_{\text{cl}}(t).$$  

The time dependence of $E_{\text{qp}}(t)$ is shown on Fig. 2. It is almost a mirror image of the classical energy in Fig. 1(a). This is because the zero point energy and the energy of the two-level system are small relative to the initial classical energy. Numerical calculations of expressions (9) and (16)
were conducted for time intervals that are much longer then the time scale of the classical energy relaxation shown in Figs. 1(a) and 2. No recurrence phenomena were observed for these longer time scales. Hence, our results can be interpreted as an irreversible flow of energy into the quantum reservoir.

The behavior of the two-level system shows a strong correlation with the transfer of the classical energy to the quantum energy. Figure 1(b) gives the time dependence of $\sigma(t)$, which shows a nontrivial evolution only for as long as there is a substantial amount of classical energy in the system. Once this energy is transferred into the quantum reservoir, the behavior of $\sigma(t)$ appears to be chaotic.

The time dependence of $E_{c}(t)/E_{c}(0)$ and $\sigma(t)$ in the case of nonzero detuning is shown on Figs. 3(a) and 3(b). There are the following differences from the resonant case. First, the energy transfer proceeds more slowly. Second, the minimum values of the classical energy are rather large during the initial oscillations, demonstrating that some of the energy is retained in the quantum reservoir already in the initial time interval, in contrast to the resonant case [Fig. 1(a)]. This peculiarity of the nonresonant case can also be seen in the behavior of spin polarization: $\sigma(t)$ oscillates around a nonzero value in Fig. 3(b).

The effect of changing the quantum parameter $\xi$ is illustrated in Figs. 4(a) and 4(b). By taking $\xi=0.5$, we shift the system toward the classical limit ($\xi=0$). As can be expected for this system, the energy transfer becomes much slower. This effect increases with decreasing $\xi$ so that for $\xi\rightarrow 0$, $E_{c}(t)\rightarrow \text{const.}$

Figures 5 and 6 show the time-averaged classical energy and spin polarization versus the initial coordinate $x_0$. The time averaged $\sigma(t)$ is given for nonzero detuning because only in this case, it is nonvanishing. The square of $x_0$ determines the initial classical energy [Eq. (6)] and, for sufficiently large $x_0$, the overall energy contained in the system. Since the classical energy decays with time, its time average effectively represents the remainder of this energy in the system for long times. As can be seen from Fig. 5, the time-averaged classical energy grows with $x_0$. In contrast, the time averaged $\sigma(t)$ decreases with increasing $x_0$. This indicates that when the energy transfer into the quantum reservoir is complete, the system is chaotic and can be characterized by some sort of effective “temperature.” The value of the effective temperature increases as the initial classical energy increases. In case of zero detuning, the phenomenon can be observed in the spin subsystem, if one considers the time-averaged square of $\sigma(t)$ given by Eq. (14).

Concluding this section, we would like to note that nontriviality of the Jaynes–Cummings model, in which the interaction between the oscillator and spin subsystem is bilinear, is due to the fact that the commutator of the spin operators is not a $c$-number. This leads to the coupling of the classical and quantum dynamical variables for the oscillator. This phenomenon will not be observed in a system of two bilinearly coupled oscillators because the commutator of the coordinate and momentum of each oscillator is a $c$-number. Thus, interaction between classical and quantum reservoirs of energy can become possible in oscillatory systems only if the Hamiltonian contains nonlinear terms.
III. NONLINEAR OSCILLATOR

In order to demonstrate the generality of the irreversible classical energy transfer in nonlinear quantum systems, we consider as another example a nonlinear oscillator with the Hamiltonian

$$H = p^2/2 + x^2/2 + gx^4/4.$$  \hspace{1cm} (17)

If the oscillator system in Eq. (3) is nonlinear as a consequence of interaction with another system, the nonlinearity is present in Eq. (17) explicitly through the quartic term involving constant $g > 0$. Our interest is in the time dependence of the classical energy.

In order to analyze this system using QHD,13–16 it is convenient to rewrite Hamiltonian ((17)) in the form that contains the classical energy explicitly,

$$H = E_{cl}(t) + p_{cl}(t)\bar{p} + x_{cl}(t)\bar{x} + \frac{1}{2}(\bar{p}^2 + \bar{x}^2)$$

$$+ \frac{g}{4}(\bar{x}^4 + 4x_{cl}(t)\bar{x}^3 + 5x_{cl}(t)^2\bar{x}^2 + 4x_{cl}(t)^3\bar{x}),$$  \hspace{1cm} (18)

where $\bar{x} = x - x_{cl}(t)$, $\bar{p} = p - p_{cl}(t)$, and $x_{cl}(t), p_{cl}(t)$ are defined similarly to Eq. (7), but now the initial state is just the oscillator coherent state $|\Psi_0\rangle = |\alpha\rangle$ and the operators $a(t)$ and $a^*(t)$ are in the Heisenberg representation corresponding to Hamilton (18). The classical energy of the nonlinear oscillator is

$$E_{cl}(t) = p_{cl}(t)^2/2 + x_{cl}(t)^2/2 + gx_{cl}(t)^4/4.$$  \hspace{1cm} (19)

The remaining part of energy is the quantum energy,

$$E_{qu}(t) = (\langle \bar{p}^2 \rangle/2 + \langle \bar{x}^2 \rangle/2 + (g/4)\langle x^4 \rangle + 4x_{cl}(t)\langle \bar{x}^3 \rangle + 5x_{cl}(t)^2\langle \bar{x}^2 \rangle).$$  \hspace{1cm} (20)

The sum of these two energies is time independent.

We investigate the time-evolution of the classical and quantum energies [Eqs. (19) and (20)] approximately using QHD (Refs. 13–16) and exactly by numerical solution.

A. Quantized Hamilton dynamics solution

The QHD approach is based on approximating complex dynamical variables through simpler ones. QHD uses dynamical equations in the Heisenberg representation, and in the case of the quartic oscillator deals with various combinations of operators $\bar{x}$ and $\bar{p}$ according to

$$i\langle \alpha | \frac{\partial A(t)}{\partial t} | \alpha \rangle = \frac{1}{\xi} \langle \alpha | [A,H](t) | \alpha \rangle,$$  \hspace{1cm} (21)

where $A(t)$ is the Heisenberg representation for an arbitrary operator $A$ and $|\alpha\rangle$ is the initial coherent state of oscillator [Eq. (8)].

Using Eq. (21) with Hamiltonian (18), we obtain for operators $\bar{x}$ and $\bar{p}$

$$\frac{dx_{cl}(t)}{dt} = p_{cl}(t),$$  \hspace{1cm} (22)

$$\frac{dp_{cl}(t)}{dt} = -[x_{cl}(t) + gx_{cl}(t)^3 + g(\langle \bar{x}^3 \rangle + 3x_{cl}(t)\langle \bar{x}^2 \rangle)].$$

The second equation contains quantum variables $\langle \bar{x}^3 \rangle$ and $\langle \bar{x}^2 \rangle$. If these variables are neglected, then Eq. (22) reduces to the ordinary classical Hamilton equations which follow from the classical Hamiltonian corresponding to Eq. (19). Obviously, the classical energy is conserved in the classical limit of Eq. (22). The presence of the quantum variables in Eq. (22) leads to coupling between the classical and quantum energy reservoirs. The coupling occurs through the nonlinearity parameter $g$.

In order to advance further, it is necessary to write equations for the three quantum variables $\langle \bar{x}^3 \rangle$, $\langle \bar{p}^2 \rangle$, and $\langle \bar{\Delta} \rangle = \frac{1}{2} \langle \bar{\Delta}^2 \rangle$ as in Refs. 13–16. Here is one of these equations,

$$\frac{d\langle \bar{\Delta} \rangle}{dt} = \langle \bar{p}^2 \rangle - [(\langle \bar{x}^3 \rangle(1 + 2.5g x_{cl}(t)^2) + g(\langle \bar{x}^4 \rangle + 3x_{cl}(t)\langle \bar{x}^3 \rangle)].$$  \hspace{1cm} (23)

Similar to the second equation in Eq. (22), Eq. (23) contains variables of higher orders $\langle \bar{x}^3 \rangle$ and $\langle \bar{x}^2 \rangle$. Equations of motion for these variables will contain variables of even higher orders and so on.

QHD truncates the infinite hierarchy by expressing higher order variables through lower-order ones and neglecting the irreducible variables of certain order (see, for example, Ref. 31). If we limit our description to quadratic

![Figure 5](image1.png)

FIG. 5. Time-averaged classical energy ($E_{cl}$) vs the initial coordinate $x_0$ in the Jaynes–Cummings model: $g=0.1$, $\delta=0$, and $\xi=1$.

![Figure 6](image2.png)

FIG. 6. Time-averaged spin polarization $\langle \sigma \rangle$ vs the initial coordinate $x_0$ in the Jaynes–Cummings model: $g=0.1$, $\delta=0.5$, and $\xi=1$. 

quantum variables, the higher-order variables in Eqs. (22) and (23) are expressed through the lower order ones in the following form $\langle \tilde{x}^3 \rangle = 0, \langle \tilde{x}^4 \rangle = 3 \langle \tilde{x}^2 \rangle^2$. In this approximation, the system of equations becomes closed and contains five equations of motion for the two classical and three quantum variables. This system of equations is only slightly more complex than the classical Hamilton’s equations and can be solved numerically. The time dependence of the classical energy is shown by the dotted line in Fig. 7(a) for the following values of parameters $x_0=5, p_0=0, g=0.05$, and $\xi=1$. We can see that for times up until $t \sim 10$, the energy flow between the classical and quantum reservoirs is almost periodic, and the classical part of energy attenuates only slightly. Note that the observed oscillation period $T \sim 2.25$ depends on the interaction between the classical and quantum variables through the anharmonicity constant $g$. This period is smaller than the period of the corresponding classical anharmonic oscillator which for the chosen parameter values equals to $\sim 3.7$. For $t > 10$, the classical energy begins to increase again. However, as we will show below, this increase is due to the approximate nature of the decoupling scheme that takes into account only three quantum variables.

We also investigated truncation of the system at the next level, taking into account quantum variables of the third order: $\langle \tilde{x}^3 \rangle, \langle \tilde{p}^3 \rangle, \langle \tilde{x}\tilde{p}^2 \rangle$, and $\langle \tilde{p}\tilde{x}\tilde{p} \rangle$. Equations for these variables contain higher-order variables that are expressed through the lower-order variables as follows:

$$\langle \tilde{x}^3 \rangle \approx 10\langle \tilde{x}^2 \rangle\langle \tilde{x} \rangle, \quad \langle \tilde{p}^3 \rangle \approx 3\langle \tilde{p}\tilde{x} \rangle\langle \tilde{x}^2 \rangle,$$

$$\langle \tilde{p}^2\tilde{x}^2 \rangle \approx \langle \tilde{p}^2 \rangle\langle \tilde{x}^2 \rangle + 2\langle \tilde{p}\tilde{x} \rangle^2,$$

$$\langle \tilde{p}\tilde{x}\tilde{p} \rangle \approx 4\langle \tilde{p}\tilde{x} \rangle\langle \tilde{x}^2 \rangle + 6\langle \tilde{x} \rangle^2\langle \tilde{p}^2 \rangle,$$

$$\langle \tilde{p}\tilde{x}\tilde{p} \rangle \approx \langle \tilde{p}^2 \rangle\langle \tilde{x}^2 \rangle + 6\langle \tilde{p}\tilde{x} \rangle\langle \tilde{x}^2 \rangle + 3\langle \tilde{x} \rangle^2\langle \tilde{p}^2 \rangle.$$

The nonsymmetrized forms were symmetrized using the commutation relations for the coordinate and momentum. In this case, the closed system of equations contains nine variables. The results are shown in Fig. 7(a) by the dashed line. The increase in the number of quantum variables compared to the previous case leads to the following changes. First, the time during which the classical energy decays is slightly longer. Second, the amount of classical energy that is transferred into the quantum reservoir during the time interval considered in Fig. 7(a) is considerably larger: $\sim 0.4$ for the three quantum variables versus $\sim 0.6$ for the seven quantum variables.

B. Exact numerical solution

The exact numerical solution of the evolution of the nonlinear oscillator [Eq. (17)] demonstrates that QHD approaches the exact result when the number of quantum variables is increased [Fig. 7(a)]. In the exact simulation, the time evolution of the wave function was found by numerically solving the Schrödinger equation $i\hbar \frac{d\psi}{dt} = H\psi$, and the wave function was used to obtain $x_0(t)$ and $p_0(t)$, and finally, $E_0(t)$. The exact result for the time interval from 0 to 30 is given in Fig. 7(b). The classical energy completely decays by $t \sim 25$. As in the approximate solution, there are partial periodic revivals of the classical energy. By expanding the number of the quantum variables, we can expect to get yet better approximations of the exact time evolution [Fig. 7(a)].

Note the short-time increase of the classical energy [Figs. 7(a) and 7(b)]. This happens because the quantum energy [Eq. (20)] contains terms that depend on the classical coordinate. The initial decrease of the classical coordinate makes the quantum energy smaller for short times. If the initial coherent state is chosen to have $x_0=0$ and $p_0 \neq 0$, then the classical energy decreases already at $t=0$.

A typical relaxation time of the classical energy is much shorter for the nonlinear oscillator than for the Jaynes–Cummings model, compare $t=25$ in Fig. 7(b) versus $t = 2500$ in Fig. 1(a), even though the Jaynes–Cummings interaction parameter is rather large. This is due to the fact that the anharmonicity parameter of the nonlinear oscillator manifests itself already in the first order equations, whereas in the Jaynes–Cummings model, the interaction parameter appears in the classical energy starting only at the second order.

Figure 8 shows the time dependence of the classical energy for a long time up to $t=1400$. In the case of the Jaynes–Cummings model, we observed long time fluctuations of the classical energy. A similar behavior is seen with the nonlinear oscillator. Some characteristic structure can be detected in Fig. 8 for times up to $t=600$. After that, only small changes in the classical energy take place. This regime can be regarded as fluctuations. To see the fluctuations more...
clearly, we present the values of the classical energies for two initial states with $x_0=5$ [Fig. 9(a)] and $x_0=7$ [Fig. 9(b)] for very long times up to $3 \times 10^5$. The values are taken every 100 time units. Both figures show a fluctuating behavior. The fluctuations are considerably smaller than the initial values of the classical energies, which are 20.3 and 54.5, respectively, and which extend far beyond the scales of the figures. Comparison of Figs. 9(a) and 9(b) shows that an increase in the initial energy leads to an increase of the fluctuations.

In order to estimate the intensity of the fluctuations quantitatively, we performed numerical averaging of the classical energy over a long time interval. Figure 10 shows how this averaged fluctuating classical energy depends on the initial coordinate $x_0$. The magnitude of the time-averaged classical energy is greater for the nonlinear oscillator than for the Jaynes–Cummings model (see Fig. 5). This is not surprising since the classical energy of the nonlinear oscillator contains a nonlinear term, i.e., the last term of Eq. (19), which accumulates the additional energy. Note that the higher the initial energy, the more time it takes for energy to flow from the classical to the quantum reservoir.

IV. SUMMARY

We have investigated the decay of the classical energy in two nonlinear quantum systems, including the Jaynes–Cummings model and the quartic oscillator. The decay is a consequence of the system nonlinearity as well as of the infinite number of quantum variables that are coupled to the classical variables. We have shown for both models that only a weak background of classical energy remains in the long-time limit. It is suggested that the transfer of classical energy to the quantum reservoir is a general phenomenon for nonlinear systems with infinite dimensional Hilbert spaces.

The time dependence of the energy of the two-level subsystem in Jaynes–Cummings model is nontrivial only when a noticeable amount of classical energy remains in the oscillator subsystem. Two approximate QHD truncations of the equations of motion have been considered for the quartic oscillator. Going from the second to the third order improves agreement with the numerical quantum result.

The energy flow studied in this paper is reminiscent of the behavior of an isolated high-energy particle interacting with a bath consisting of many particles. The isolated particle transfers energy to the surrounding particles, raising their temperature. In the cases considered here, everything happens with only one quantum particle! Infinitely, many quantum dynamical variables interact with the two classical variables. The analogy between the usual system-bath coupling and the coupling of the classical-variable system with the quantum-variable bath within just one particle is not complete, however, since the quantum energy depends on a finite number of quantum variables, while the energy of the usual bath depends on infinitely many bath variables. Nevertheless,
as the system evolves, this quantum energy becomes the major part of the initial energy. For example, according to the data in Fig. 10, when \( x_0 = 10 \), the initial value of the classical energy for the nonlinear oscillator equals \( E_{cl}(0) = 175 \), whereas the value of the remaining time-averaged classical energy is only \( \approx 1.9 \).

It remains to be seen whether one can introduce a notion of temperature in this case. Another interesting problem for this approach is introduction of a quantity similar to entropy, which would describe the irreversible flow of energy from the classical to the quantum reservoir.

We conclude by noting that the notion of the quantum energy reservoir observed here with the Jaynes–Cummings model and the quartic oscillator is very important in more complex interacting systems. For example, it was shown in Ref. 26 that the energy of electrons is transformed into the quantum part of the ionic kinetic energy. Ionic quantum degrees of freedom are likely to be important in the general energy balance of systems consisting of ions and electrons.10,11

**ACKNOWLEDGMENTS**

The funding was provided by grants from NSF (CHE-0701517) and PRF (46772-AC6).