



## Quantum versus classical decoherence dynamics

Jiangbin Gong & Paul Brumer

To cite this article: Jiangbin Gong & Paul Brumer (2003) Quantum versus classical decoherence dynamics, Journal of Modern Optics, 50:15-17, 2411-2422, DOI: [10.1080/09500340308233572](https://doi.org/10.1080/09500340308233572)

To link to this article: <https://doi.org/10.1080/09500340308233572>



Published online: 24 Apr 2008.



Submit your article to this journal [↗](#)



Article views: 63



View related articles [↗](#)



Citing articles: 1 View citing articles [↗](#)

## Quantum versus classical decoherence dynamics

JIANGBIN GONG and PAUL BRUMER

Chemical Physics Theory Group, Department of Chemistry,  
University of Toronto, Toronto, Canada M5S 3H6  
e-mail: pbrumer@tikiva.chem.utoronto.ca

(Received 15 February 2003; revision received 1 May 2003)

**Abstract.** A direct classical analogue of quantum decoherence is introduced. Similarities and differences between decoherence dynamics examined quantum-mechanically and classically are exposed via a second-order perturbative treatment and via a strong decoherence theory, providing new insights both into the dynamics of decoherence described quantum mechanically and into the conditions for quantum-classical correspondence in decoherence dynamics.

### 1. Introduction

In quantum information processing [1] and in the optical control of atomic and molecular processes [2-4], quantum coherence is essential for the successful manipulations of the quantum dynamics of atomic, molecular and optical systems. However, almost all quantum systems of interest are coupled to some environment and as a result decoherence, that is the loss of quantum coherence in the subsystem of interest, occurs in most circumstances [5]. This results, in quantum control applications for example, in a diminution in allowed control (see for example [6]) As such, understanding decoherence and eventually controlling decoherence are of crucial importance in a wide variety of quantum-based research areas.

There has been considerable theoretical and experimental work demonstrating that quantum-classical correspondence (QCC) can be induced by decoherence (see for example [7-10]). That is, in the presence of decoherence, the quantum dynamics of the systems of interest will behave more classically than in the absence of decoherence. This fundamental result is believed to be generally useful in understanding a variety of decoherence-related issues. By contrast, little work has been done on examining the correspondence between classical and quantum descriptions of the time evolution of decoherence itself, that is, *decoherence dynamics*.

The formal Liouville-based theory of QCC in an isolated system (see for example [11]) makes clear that there is a strict analogy between quantum and classical dynamics in phase space. As in the quantum case, the classical Liouville dynamics of a closed system is unitary and we expect the reduced classical Liouville dynamics of a system coupled to a bath to be non-unitary. We therefore suspect that, owing to a bath's coarse-graining effects, the reduced dynamics of the system propagated classically will show decoherence dynamics that are, qualitatively,

parallel to those seen in quantum dynamics such as the loss of phase information and entropy production.

Here we quantitatively compare the dynamics of decoherence that are induced quantum mechanically to those induced classically. This is done by analytically examining the dynamics of an initial quantum state, in a system coupled to a bath, which are propagated either quantum mechanically or classically. By studying the similarities and differences between the classical and quantum decoherence dynamics we show in this paper that, firstly, one can introduce a direct classical analogue of quantum decoherence and, secondly, by examining the dynamics of decoherence classically, one gains new insights into both the dynamics of decoherence described quantum-mechanically and into the conditions for QCC of the dynamics of decoherence. For example, we show below that the extent of QCC in decoherence dynamics depends strongly on the nature of the system–bath coupling as well as the initial quantum state and far less upon  $\hbar$  than expected, that results assumed to be quantum mechanical may be obtained classically and that nonlinear system–bath coupling can cause non-classical decoherence dynamics even for macroscopic systems. This work also provides new insights into semiclassical descriptions of decoherence dynamics [12, 13] and has motivated purely classical descriptions of dynamics-induced intrinsic decoherence, with preliminary computations [14, 15] that support the analytical results presented here.

This paper is organized as follows. In section 2, we introduce classical analogues of some representation-independent and representation-dependent measures of decoherence. In section 3, we use a second-order perturbative treatment to examine QCC in early-time decoherence dynamics. We then introduce in section 4 a classical theory of strong decoherence that allows us to go beyond perturbation theory; the classical results are then compared with the corresponding quantum theory of strong decoherence. Discussions and conclusions are given in section 5. A brief report on our main results below can be found in [16].

## 2. Classical analogues of two decoherence measures

Consider a system with a time-independent Hamiltonian

$$H^s = \frac{P^2}{2m} + V(Q), \quad (1)$$

where  $(Q, P)$  are conjugate position and momentum variables; coupled to  $N$  independent harmonic bath modes described by the Hamiltonians

$$H_j^b = \frac{p_j^2}{2m_j} + \frac{1}{2}m_j\omega_j^2q_j^2, \quad (2)$$

where  $\{p_j, q_j\}$  ( $j = 1, 2, \dots, N$ ) are bath-mode phase space variables. The system–bath coupling potential is assumed to be

$$V^{sb} = \sum_{j=1}^N C_j f(Q) q_j, \quad (3)$$

so that the total Hamiltonian is given by

$$H = H^s + \sum_{j=1}^N \left[ H_j^b + C_j f(Q) q_j \right]. \quad (4)$$

The phase space distribution function evolved classically and the quantum Wigner function for the entire phase space are represented by  $\rho^c[Q, P, \{q_j, p_j\}, t]$  and  $\rho^w[Q, P, \{q_j, p_j\}, t]$  respectively. Their time evolution is given by

$$\frac{\partial \rho^c}{\partial t} = \{H, \rho^c\}_P \quad (5)$$

and

$$\frac{\partial \rho^w}{\partial t} = \{H, \rho^w\}_M, \quad (6)$$

where  $\{\cdot\}_P$  denotes the classical Poisson bracket and  $\{\cdot\}_M$  denotes the quantum Moyal bracket. Further, we define the classical and quantum reduced distribution functions  $\tilde{\rho}_c(Q, P, t) \equiv \int \rho^c d\Gamma_b^N$  and  $\tilde{\rho}_w(Q, P, t) \equiv \int \rho^w d\Gamma_b^N$ , where  $d\Gamma_b^N \equiv \prod_{j=1}^N dq_j dp_j$ . Our interest is in the correspondence between the classical and quantum decoherence dynamics of initial states that can be either classical (i.e. positive Wigner density everywhere) or non-classical [17] (e.g. displaying regions of negative  $\rho^w[Q, P, \{q_j, p_j\}, t]$ ).

We consider two measures of decoherence in each of classical and quantum mechanics. One widely used and representation-independent measure is the linear entropy [18]

$$S_q \equiv 1 - \text{Tr}(\hat{\rho}^2), \quad (7)$$

where  $\hat{\rho}$  is the reduced density operator of the system. An increase in  $S_q$  causes  $1/(1 - S_q)$  to increase, corresponding to an increasing number of incoherently populated orthogonal quantum states. Since

$$S_q = 1 - 2\pi\hbar \int \tilde{\rho}_w^2(Q, P, t) d\Gamma_s, \quad (8)$$

where  $d\Gamma_s \equiv dQ dP$ , this entropy has a natural classical analogue (denoted  $S_c$ ) obtained by replacing  $\tilde{\rho}_w$  with  $\tilde{\rho}_c$ . That is,

$$S_c \equiv 1 - 2\pi\hbar \int \tilde{\rho}_c^2(Q, P, t) d\Gamma_s. \quad (9)$$

A more detailed but representation-dependent description of decoherence is the decay of off-diagonal density matrix elements such as  $\langle Q_1 | \hat{\rho}(t) | Q_2 \rangle$ . Significantly, we discover that the classical analogue of these matrix elements can also be constructed. Specifically, noting that

$$\langle Q_1 | \hat{\rho}(t) | Q_2 \rangle = \int dP \tilde{\rho}_w(\bar{Q}, P, t) \exp\left(i \frac{\Delta Q P}{\hbar}\right), \quad (10)$$

where  $\bar{Q} \equiv (Q_1 + Q_2)/2$  and  $\Delta Q = Q_1 - Q_2$ , we define the classical analogue (denoted  $\tilde{\rho}_c(Q_1, Q_2, t)$ ) of  $\langle Q_1 | \hat{\rho}(t) | Q_2 \rangle$  as the Fourier transformed classical distribution function, that is

$$\tilde{\rho}_c(Q_1, Q_2, t) \equiv \int dP \tilde{\rho}_c(\bar{Q}, P, t) \exp\left(i \frac{\Delta Q P}{\hbar}\right). \quad (11)$$

This approach can be readily extended to the momentum representation.

### 3. Early-time decoherence dynamics

Perturbative treatments have proved to very useful in understanding decoherence dynamics [14, 19, 20]. Here, to examine classical versus quantum decoherence dynamics at short times, a regime of great interest in the control of decoherence, we consider a second-order expansion with respect to time variable  $t$  for both  $S_c$  and  $S_q$ , that is

$$S_c(t) = S_c(0) + \frac{t}{\tau_{c,1}} + \frac{t^2}{\tau_{c,2}^2} + \dots, \quad (12)$$

and

$$S_q(t) = S_q(0) + \frac{t}{\tau_{q,1}} + \frac{t^2}{\tau_{q,2}^2} + \dots. \quad (13)$$

Using the definitions of Poisson and Moyal brackets and assuming that the initial distribution function is decorrelated with initial bath statistics, we obtain

$$\frac{1}{\tau_{c,1}} = \frac{1}{\tau_{q,1}} = 0, \quad (14)$$

$$\frac{1}{\tau_{c,2}^2} = \frac{C_b}{\hbar} \int dQ_1 dQ_2 |\tilde{\rho}_c(Q_1, Q_2, 0)|^2 \Delta Q^2 \left( \frac{df(\bar{Q})}{d\bar{Q}} \right)^2, \quad (15)$$

and

$$\frac{1}{\tau_{q,2}^2} = \frac{C_b}{\hbar} \int dQ_1 dQ_2 |\langle Q_1 | \hat{\rho}(0) | Q_2 \rangle|^2 \Delta Q^2 \left( \frac{\Delta f(\bar{Q})}{\Delta Q} \right)^2. \quad (16)$$

Here

$$C_b = \sum_{j=1}^N C_j^2 \frac{\coth(\beta \hbar \omega_j / 2)}{2m_j \omega_j}, \quad (17)$$

$$\frac{\Delta f(\bar{Q})}{\Delta Q} \equiv \frac{f(\bar{Q} + \Delta Q / 2) - f(\bar{Q} - \Delta Q / 2)}{\Delta Q}, \quad (18)$$

and  $\beta$  is the Boltzmann factor. Note that the factor  $\hbar$  appearing in the classical result (equation (15)) is just due to the definitions of  $S_c$  and  $\tilde{\rho}_c(Q_1, Q_2, 0)$ , and that the initial variances of the bath variables  $q_j$  have been evaluated using quantum statistics to ensure the same initial quantum state for the ensuing classical and quantum dynamics. Note also that the decoherence time scale indicated in the easily derived and simple quantum result of equation (16) is consistent with, but is more transparent than, a previous perturbation result (equation (5.6) in [21]) obtained using a sophisticated influence functional approach.

Equation (14) shows that zero first-order decoherence rate, that is  $1/\tau_{q,1} = 0$ , has a strict classical analogue. More interestingly, equations (15) and (16) show that, for the same fixed initial distribution function, the ratio of  $1/\tau_{q,2}^2$  to  $1/\tau_{c,2}^2$  is  $\hbar$  independent. As seen from equation (15) and (16),  $1/\tau_{q,2}^2 - 1/\tau_{c,2}^2$  arises from the difference between the derivative  $df/dQ$  and the finite-difference function  $\Delta f/\Delta Q$ , weighted by  $\Delta Q^2$  and the initial state. As a result, we have the following

- (i) For any given  $f(Q)$ , as long as  $\langle Q_1 | \hat{\rho}(0) | Q_2 \rangle$  decays fast enough with  $|\Delta Q|$  such that  $\Delta f/\Delta Q \approx df/dQ$ , there would be excellent QCC in early-time

decoherence dynamics. The smaller the  $\hbar$ , the more rigorous is this requirement.

- (ii) If  $f(Q)$  depends only linearly or quadratically upon the coupling coordinate  $Q$ , then  $1/\tau_{q,2}^2 - 1/\tau_{c,2}^2 = 0$  for any initial state. Significantly then, in all traditional decoherence models [22] where  $f(Q) = Q$  is assumed, there exists perfect QCC in early decoherence dynamics, regardless of  $\hbar$ , and irrespective of the system potential  $V(Q)$ . Indeed, in the case of  $f(Q) = Q$ , equation (15) reduces to an important result, previously obtained quantum-mechanically [19]:

$$\frac{1}{\tau_{c,2}^2} = \frac{1}{\tau_{q,2}^2} = 2 \frac{\delta^2 Q}{\hbar} \sum_{j=1}^N \frac{C_j^2}{2m_j \omega_j} \coth\left(\frac{\beta \hbar \omega_j}{2}\right), \quad (19)$$

where the initial state of the system is assumed to be pure, with the initial variance in  $Q$  given by  $\delta^2 Q$ .

- (iii) For nonlinear  $f(Q)$  where  $\Delta f/\Delta Q \neq df/dQ$  over the range of the initial state, QCC can be very poor.

The second-order perturbative treatment is most reliable at short times and for weak decoherence. The results are particularly significant for studies of decoherence control where early-time dynamics of weak decoherence is important. In these circumstances it should be useful in understanding the extent to which (quantum) decoherence is equivalent to classical entropy production, that is to increasing  $S_c(t)$ . In particular, if there exists good correspondence between classical and quantum decoherence dynamics, then the essence of decoherence control is equivalent to the suppression of classical entropy production, and various classical tools may be considered to achieve decoherence control. If not, then fully quantum tools are required.

To gain more insights into quantum–classical differences in decoherence dynamics, consider decoherence for an initial superposition state of two well-separated and strongly localized Gaussian wave packets located at  $Q_a = \bar{Q}_{ab} - \Delta Q_{ab}/2$  and  $Q_b = \bar{Q}_{ab} + \Delta Q_{ab}/2$  with  $\bar{Q}_{ab} = 0$ . For this initial state,  $1/\tau_{c,2}^2 \sim (C_b/\hbar) \Delta Q_{ab}^2 [df(\bar{Q}_{ab})/d\bar{Q}_{ab}]^2$ , and  $1/\tau_{q,2}^2 \sim (C_b/\hbar) \Delta Q_{ab}^2 [\Delta f(\bar{Q}_{ab})/\Delta Q_{ab}]^2$ . Then in a cubic decoherence model, for example, where  $f(Q) = Q^3$ , one would obtain  $1/\tau_{c,2}^2 \sim 0$  since  $df(\bar{Q}_{ab})/d\bar{Q}_{ab} = 0$ . However, here  $1/\tau_{q,2}^2 \gg 1/\tau_{c,2}^2$ , that is, there is appreciable *decoherence without classical entropy production*. By contrast, in another nonlinear decoherence model where  $f(Q) = \sin(2\pi Q/\Delta Q_{ab} + \pi/4)$ ,  $1/\tau_{q,2}^2 \sim 0$  since  $f(Q_a) = f(Q_b)$ . Here, however,  $1/\tau_{c,2}^2 \gg 1/\tau_{q,2}^2$ , that is, the system is *decoherence free but with substantial classical entropy production*. Since we find that the ratio of  $\tau_{q,2}^2$  to  $\tau_{c,2}^2$  in early-time decoherence dynamics is independent of  $\hbar$  for fixed initial state, these two examples lead to a rather counter-intuitive result; given a macroscopic object which is initially in a superposition state of two distinguishable states and is nonlinearly coupled with an environment, classical dynamics could totally fail to predict its initial entropy production or its decoherence rate. Indeed, equations (15) and (16) suggest that, as long as  $df(\bar{Q})/d\bar{Q} \neq 0$  and  $|f(Q)|$  is bounded, then  $1/\tau_{q,2}^2$  saturates with increasing  $\Delta Q_{ab}$ , whereas  $1/\tau_{c,2}^2$  does not. Thus, if the saturation behaviour of early-time decoherence rates is observed experimentally, one can then draw the conclusion that the decoherence dynamics must be quantum and that the system–environment coupling must be

nonlinear. Although this kind of experiment is quite difficult to carry out in many quantum systems, we note that the saturation behaviour of decoherence rates with the separation of two pointer states has been observed experimentally using an optical analogue of quantum wave mechanics [23]. Further, it is clear that, in the limit of large  $\Delta Q_{ab}$ , classical decoherence dynamics in the general case of nonlinear system–environment coupling predicts much faster decoherence than does quantum decoherence dynamics. This leads to the rather surprising inference that initial superposition states of well-separated wave packets would be more susceptible to nonlinear system–environment coupling if they are propagated by classical dynamics than by quantum mechanics.

#### 4. Strong decoherence dynamics

To go beyond the perturbation results, in this section we consider a strong decoherence model in which decoherence is assumed to be much faster than the system dynamics, so that  $H^s$  can be set to zero [5]. We consider both the ‘off-diagonal elements’  $\tilde{\rho}_c(Q_1, Q_2, t)$  as well as the entropy  $S_c(t)$  and compare them with the quantum results.

In this case the classical Liouville equation is given by

$$\begin{aligned} \frac{\partial \rho^c[\bar{Q}, P, \{q_j, p_j\}, t]}{\partial t} = & \sum_{k=1}^N \frac{\partial H_k^b}{\partial q_k} \frac{\partial \rho^c[\bar{Q}, P, \{q_j, p_j\}, t]}{\partial p_k} \\ & - \sum_{k=1}^N \frac{\partial H_k^b}{\partial p_k} \frac{\partial \rho^c[\bar{Q}, P, \{q_j, p_j\}, t]}{\partial q_k} + \sum_{k=1}^N C_k f(\bar{Q}) \frac{\partial \rho^c[\bar{Q}, P, \{q_j, p_j\}, t]}{\partial p_k} \\ & + \sum_{k=1}^N C_k \frac{df(\bar{Q})}{d\bar{Q}} q_k \frac{\partial \rho^c[\bar{Q}, P, \{q_j, p_j\}, t]}{\partial P}. \end{aligned} \quad (20)$$

To solve equation (20) for  $\tilde{\rho}_c(Q_1, Q_2, t)$  we first apply a Fourier transformation  $\int dP \exp(i \Delta Q P / \hbar)$  to both sides of equation (20), yielding

$$\begin{aligned} \frac{\partial F_c[\bar{Q}, \Delta Q, \{q_j, p_j\}, t]}{\partial t} = & \sum_{k=1}^N \frac{\partial H_k^b}{\partial q_k} \frac{\partial F_c[\bar{Q}, \Delta Q, \{q_j, p_j\}, t]}{\partial p_k} \\ & - \sum_{k=1}^N \frac{\partial H_k^b}{\partial p_k} \frac{\partial F_c[\bar{Q}, \Delta Q, \{q_j, p_j\}, t]}{\partial q_k} \\ & + \sum_{k=1}^N C_k f(\bar{Q}) \frac{\partial F_c[\bar{Q}, \Delta Q, \{q_j, p_j\}, t]}{\partial p_k} \\ & - \frac{i}{\hbar} \Delta Q \sum_{k=1}^N C_k \frac{df(\bar{Q})}{d\bar{Q}} q_k F_c[\bar{Q}, \Delta Q, \{q_j, p_j\}, t], \end{aligned} \quad (21)$$

where

$$F_c(\bar{Q}, \Delta Q, \{q_j, p_j\}, t) \equiv \int dP \exp\left(i \frac{\Delta Q P}{\hbar}\right) \rho^c[\bar{Q}, P, \{q_j, p_j\}, t]. \quad (22)$$

Since  $\dot{Q} = 0$  because  $H_s = 0$ , and  $\Delta Q$  is a time-independent parameter introduced in the Fourier transformation, equation (21) leads to

$$\begin{aligned} \frac{dF_c[\bar{Q}, \Delta Q, \{q_j(t), p_j(t)\}, t]}{dt} &= \frac{\partial F_c[\bar{Q}, \Delta Q, \{q_j(t), p_j(t)\}, t]}{\partial t} \\ &+ \sum_{k=1}^N \frac{\partial F_c[\bar{Q}, \Delta Q, \{q_k(t), p_k(t)\}, t]}{\partial q_k(t)} \dot{q}_k(t) \\ &+ \sum_{k=1}^N \frac{\partial F_c[\bar{Q}, \Delta Q, \{q_k(t), p_k(t)\}, t]}{\partial p_k(t)} \dot{p}_k(t) \\ &= -\frac{i}{\hbar} \Delta Q \sum_{k=1}^N C_k q_k(t) \frac{df(\bar{Q})}{d\bar{Q}} F_c[\bar{Q}, \Delta Q, \{q_j(t), p_j(t)\}, t], \end{aligned} \quad (23)$$

where  $\{q_j(t), p_j(t)\}$  satisfy

$$\dot{q}_j(t) = \frac{\partial H_j^b}{\partial p_j(t)}, \quad (24)$$

and

$$\dot{p}_j(t) = -\frac{\partial H_j^b}{\partial q_j(t)} - C_j f(\bar{Q}). \quad (25)$$

The solution to equations (24) and (25) is given by

$$q_j(t) = \frac{C_j f(\bar{Q})}{m_j \omega_j^2} [\cos(\omega_j t) - 1] + q_j(0) \cos(\omega_j t) + \frac{p_j(0)}{m_j \omega_j} \sin(\omega_j t) \quad (26)$$

and

$$p_j(t) = m_j \dot{q}_j(t). \quad (27)$$

Based on this, equation (23) can be readily integrated and we have

$$\begin{aligned} F_c[\bar{Q}, \Delta Q, \{q_j(t), p_j(t)\}, t] &= \exp\left(-\frac{i}{\hbar} \int_0^t dt \Delta Q \sum_{k=1}^N C_k q_k(t) \frac{df(\bar{Q})}{d\bar{Q}}\right) \\ &\times F_c[\bar{Q}, \Delta Q, \{q_j(0), p_j(0)\}, 0]. \end{aligned} \quad (28)$$

Further using  $d\Gamma_b^N(t) = d\Gamma_b^N(0)$  and

$$\tilde{\rho}_c(Q_1, Q_2, t) = \int d\Gamma_b^N(t) F_c[\bar{Q}, \Delta Q, \{q_j(t), p_j(t)\}, t], \quad (29)$$

we obtain

$$\begin{aligned} \tilde{\rho}_c(Q_1, Q_2, t) &= \int d\Gamma_b^N(0) F_c[\bar{Q}, \Delta Q, \{q_j(0), p_j(0)\}, 0] \\ &\times \exp\left(-\frac{i}{\hbar} \int_0^t dt \Delta Q \sum_{k=1}^N C_k q_k(t) \frac{df(\bar{Q})}{d\bar{Q}}\right). \end{aligned} \quad (30)$$

Substituting equation (26) into equation (30), using the initial quantum state of the bath that is initially uncorrelated with the system, and assuming that the equilibrium state of the bath is maintained, we finally have

$$\frac{\tilde{\rho}_c(Q_1, Q_2, t)}{\tilde{\rho}_c(Q_1, Q_2, 0)} = \exp \left[ i\phi_c(t) - (\Delta Q)^2 \left( \frac{df(\bar{Q})}{d\bar{Q}} \right)^2 B_2(t) \right], \quad (31)$$

where

$$\phi_c(t) \equiv \frac{\Delta Q}{\hbar} f(\bar{Q}) \frac{df(\bar{Q})}{d\bar{Q}} B_1(t), \quad (32)$$

with

$$B_1(t) = \sum_{j=1}^N C_j^2 \frac{\omega_j t - \sin(\omega_j t)}{m_j \omega_j^3} \quad (33)$$

and

$$B_2(t) = \sum_{j=1}^N C_j^2 \frac{\coth(\beta \hbar \omega_j / 2) [1 - \cos(\omega_j t)]}{2 m_j \hbar \omega_j^3}. \quad (34)$$

Interestingly, the classical result (equation (31)) displays two dynamic aspects of  $\tilde{\rho}_c(Q_1, Q_2, t)$ , that is, coherent dynamics of its phase  $\phi_c(t)$ , and incoherent decay due to bath statistics. The classical linear entropy  $S_c(t)$  can then be obtained from equation (31) as

$$S_c(t) = 1 - \int dQ_1 dQ_2 |\tilde{\rho}_c(Q_1, Q_2, 0)|^2 \exp \left[ -2(\Delta Q)^2 \left( \frac{df(\bar{Q})}{d\bar{Q}} \right)^2 B_2(t) \right]. \quad (35)$$

The quantum strong decoherence dynamics can be considered using similar manipulations. In particular, the quantum Liouville equation in the Wigner representation is given by

$$\begin{aligned} \frac{\partial \rho^W[\bar{Q}, P, \{q_j, p_j\}, t]}{\partial t} &= \sum_{k=1}^N \frac{\partial H_k^b}{\partial q_k} \frac{\partial \rho^W[\bar{Q}, P, \{q_j, p_j\}, t]}{\partial p_k} \\ &\quad - \sum_{k=1}^N \frac{\partial H_k^b}{\partial p_k} \frac{\partial \rho^W[\bar{Q}, P, \{q_j, p_j\}, t]}{\partial q_k} + \sum_{k=1}^N C_k f(\bar{Q}) \frac{\partial \rho^W[\bar{Q}, P, \{q_j, p_j\}, t]}{\partial p_k} \\ &\quad + \sum_{k=1}^N C_k q_k \sum_{l \geq 0} \left( \frac{\hbar}{2i} \right)^{2l} \frac{1}{(2l+1)!} \frac{d^{(2l+1)} f(\bar{Q})}{d\bar{Q}^{(2l+1)}} \frac{\partial^{(2l+1)} \rho^W[\bar{Q}, P, \{q_j, p_j\}, t]}{\partial P^{(2l+1)}}. \end{aligned} \quad (36)$$

Fourier transforming  $\int dP \exp(i\Delta Q P/\hbar)$ , both sides of equation (36) gives

$$\begin{aligned} \frac{\partial F_q[\bar{Q}, \Delta Q, \{q_j, p_j\}, t]}{\partial t} &= \sum_{k=1}^N \frac{\partial H_k^b}{\partial q_k} \frac{\partial F_q[\bar{Q}, \Delta Q, \{q_j, p_j\}, t]}{\partial p_k} - \sum_{k=1}^N \frac{\partial H_k^b}{\partial p_k} \frac{\partial F_q[\bar{Q}, \Delta Q, \{q_j, p_j\}, t]}{\partial q_k} \\ &\quad + \sum_{k=1}^N C_k f(\bar{Q}) \frac{\partial F_q[\bar{Q}, \Delta Q, \{q_j, p_j\}, t]}{\partial p_k} - \frac{i}{\hbar} \sum_{k=1}^N C_k q_k \frac{\Delta f(\bar{Q})}{\Delta Q} F_q[\bar{Q}, \Delta Q, \{q_j, p_j\}, t], \end{aligned} \quad (37)$$

where

$$F_q(\bar{Q}, \Delta Q, \{q_j, p_j\}, t) \equiv \int dP \exp\left(i \frac{\Delta Q P}{\hbar}\right) \rho^W[\bar{Q}, P, \{q_j, p_j\}, t]. \quad (38)$$

Based on equation (37) the full time derivative of  $F_q(\bar{Q}, \Delta Q, \{q_j(t), p_j(t)\}, t)$  can be derived:

$$\frac{dF_q[\bar{Q}, \Delta Q, \{q_j(t), p_j(t)\}, t]}{dt} = -\frac{i}{\hbar} \sum_{k=1}^N C_k q_k(t) \frac{\Delta f(\bar{Q})}{\Delta Q} F_q[\bar{Q}, \Delta Q, \{q_j(t), p_j(t)\}, t], \quad (39)$$

where  $q_j(t)$  and  $p_j(t)$  are still given by equations (26) and (27). Directly integrating equation (39) yields

$$F_q[\bar{Q}, \Delta Q, \{q_j(t), p_j(t)\}, t] = \exp\left(-\frac{i}{\hbar} \int_0^t dt \Delta Q \sum_{k=1}^N C_k q_k(t) \frac{\Delta f(\bar{Q})}{\Delta Q}\right) \times F_q[\bar{Q}, \Delta Q, \{q_j(0), p_j(0)\}, 0]. \quad (40)$$

Further, using the fact that

$$\langle Q_1 | \hat{\rho}(t) | Q_2 \rangle = \int d\Gamma_b^N(t) F_q[\bar{Q}, \Delta Q, \{q_j(t), p_j(t)\}, t] \quad (41)$$

and comparing equation (40) with equation (28), one obtains the quantum result

$$\frac{\langle Q_1 | \hat{\rho}(t) | Q_2 \rangle}{\langle Q_1 | \hat{\rho}(0) | Q_2 \rangle} = \exp\left[i\phi_q(t) - \Delta Q^2 \left(\frac{\Delta f(\bar{Q})}{\Delta Q}\right)^2 B_2(t)\right], \quad (42)$$

where

$$\phi_q(t) \equiv \frac{\Delta Q}{\hbar} f(\bar{Q}) \frac{\Delta f(\bar{Q})}{\Delta Q} B_1(t), \quad (43)$$

and

$$S_q(t) = 1 - \int dQ_1 dQ_2 |\langle Q_1 | \hat{\rho}(0) | Q_2 \rangle|^2 \exp\left[-2(\Delta Q)^2 \left(\frac{\Delta f(\bar{Q})}{\Delta Q}\right)^2 B_2(t)\right]. \quad (44)$$

These results extend those in [24] to nonlinear  $f(Q)$  using a simple approach and demonstrate a direct classical analogue of quantum strong decoherence dynamics.

Since  $dB_2(t)/dt(t=0) = 0$  and  $d^2B_2(t)/dt^2(t=0) = C_b/\hbar$ , one finds that, in the short-time limit, equations (35) and (44) reduce to previous perturbation results of  $1/\tau_{c,1}$ ,  $1/\tau_{c,2}^2$ ,  $1/\tau_{q,1}$  and  $1/\tau_{q,2}^2$ . Furthermore, the classical results (equation (31) and (35) are again very similar to the quantum results (equation (42) and (44)), with the only difference being that  $\Delta f/\Delta Q$  in the quantum expression is replaced by  $df/dQ$  in the classical result.

This result makes clear that our previous QCC results based upon second-order perturbation theory are generalizable to all orders of time in the strong decoherence case. In particular, defining  $\gamma_c(t) \equiv d[\ln |\tilde{\rho}_c(Q_1, Q_2, t)|]/dt$  and  $\gamma_q(t) \equiv d[\ln |\langle Q_1 | \hat{\rho}(t) | Q_2 \rangle|]/dt$ , we have  $\gamma_c(t) = -(\Delta Q)^2 [df(\bar{Q})/d\bar{Q}]^2 [dB_2(t)/dt]$  and  $\gamma_q(t) = -(\Delta Q)^2 [\Delta f(\bar{Q})/\Delta Q]^2 [dB_2(t)/dt]$ . Then, in the case of linear and/or quadratic coupling, for example  $f(Q) = aQ + bQ^2$ , one has  $\gamma_c(t) = \gamma_q(t)$  and

$S_c(t) = S_q(t)$ , showing that there is perfect QCC in decoherence dynamics for all times.

By contrast, in the case of nonlinear coupling,  $\gamma_c(t)$  in general does not saturate with increasing  $\Delta Q$  whereas  $\gamma_q(t)$  does saturate for bounded  $|f(Q)|$ . As such, in the limit of large  $\Delta Q$ , one has  $|\gamma_c(t)| \gg |\gamma_q(t)|$  and thus  $[1 - S_c(t)] \ll [1 - S_q(t)]$  as  $t$  increases, with  $|\gamma_c(t)/\gamma_q(t)|$  independent of  $\hbar$ . This observation is of conceptual importance; it says that decoherence can dramatically improve QCC but, as far as some detailed characteristics of decoherence dynamics are concerned, decoherence itself does not necessarily suffice to ensure that the dynamics of quantum entropy production equal those of classical entropy production. That is, even in the presence of strong decoherence, subtle quantum–classical differences may persist in some measures (e.g.  $1/[1 - S_q(t)]$  versus  $1/[1 - S_c(t)]$ ) for all finite times. Note, however, that entropy measures such as  $1/[1 - S_q(t)]$  are not quantum-mechanical observables and hence do not allow one to measure directly the subtle difference between classical and quantum decoherence dynamics at later times. Another interesting observation from equations (32) and (43) is that

$$\gamma_c(t)[\phi_q(t)]^2 = \gamma_q(t)[\phi_c(t)]^2. \quad (45)$$

Hence, QCC in strong decoherence dynamics is directly related to the dynamics of the phase associated with off-diagonal density matrix elements.

## 5. Discussion and conclusion

From both the perturbation results in section 3 and the strong decoherence results in section 4, we see that QCC in decoherence dynamics depends critically upon the initial quantum state and upon the nature of the system–environment coupling. Indeed, the quantum–classical difference in decoherence time scale arises directly from the difference between  $df(\bar{Q})/d\bar{Q}$  and  $\Delta f(\bar{Q})/\Delta Q$  over the coordinate scale of the initial state. Hence, exact correspondence exists for linear or quadratic coupling. For the case of general nonlinear coupling, correspondence may significantly break down; for example, quantum entropy production can be totally unrelated to classical entropy production.

The case of exact QCC in decoherence dynamics is worthy of further discussion. Physically, linear system–environment coupling, previously introduced to allow analytical results [22], is just an over-simplified version of realistic system–environment couplings. In this sense, the exact QCC in decoherence dynamics for linear or quadratic system–environment coupling is just a formal result. Furthermore, it is not surprising, in retrospect, that the classical and quantum results are in perfect agreement in cases where the bath is harmonic, the coupling is linear or quadratic, and the system can be neglected as in the perturbative treatment and in the strong decoherence theory. In such cases, one expects that the quantum and classical Liouville dynamics are identical because their time evolution equations take the same form. What is surprising and important, however, is that this equivalence can be extended to the process of decoherence, a phenomenon generally assumed to be solely quantum in nature, and that excellent QCC may also exist for nonlinear system–environment couplings.

Both the perturbation and the strong decoherence results can be interpreted as follows. Quantum-mechanically, the system, which is coupled with the environment through  $f(Q)$ , is essentially subject to a quantum measurement of  $f(Q)$  by the

environment. In the case when  $f(Q_1) = f(Q_2)$ , measurement results cannot tell which pointer state (i.e.  $|Q_1\rangle$  or  $|Q_2\rangle$ ) that the system is in. Thus, this measurement induces no decoherence. In the case when  $f(Q_1) \neq f(Q_2)$ , quantum information leaks into the environment and decoherence occurs. By contrast, from the viewpoint of classical Liouville dynamics, the same environment also decoheres the system, however, through a 'measurement' of  $(Q_1 - Q_2) df(\bar{Q})/d\bar{Q}$  rather than  $\Delta f(\bar{Q}) = f(Q_1) - f(Q_2)$ . The quantum-classical difference will be most significant for larger distributions in the case of nonlinear system-environment coupling.

A number of interesting extensions of this work are under consideration. Firstly, we propose to consider cases in which the system-environment coupling depends upon both position and momentum using canonical transformation in phase space. Secondly, we propose to investigate further the role of the dynamics of the system. Indeed, one important implication of this work is that the relationship between classical Lyapunov exponents and decoherence rates in classically chaotic systems should be re-examined for the case of nonlinear system-environment coupling, since previous studies [25] only dealt with the linear case. Thirdly, as in many other studies we have assumed that the bath is made up of independent harmonic oscillators. Clearly, the extension to anharmonic bath modes is of considerable theoretical interest. We note that considering anharmonic bath modes is straightforward in the second-order perturbative treatment but may substantially change the physical picture of QCC in strong decoherence dynamics. Fourthly, it is interesting to study QCC in decoherence dynamics in terms of the decay of off-diagonal density matrix elements in arbitrary representations.

In conclusion, we have examined, using analogous measures, the decoherence dynamics of an initial quantum state coupled to a bath that is subjected to either classical or quantum dynamics. Within the framework of a second-order perturbative treatment and a strong decoherence theory, we have exposed the system-independent conditions under which the quantum decoherence dynamics are either well, or poorly, approximated by classical dynamics. Most significantly, the nature of system-environment coupling and the character of the initial state are shown to play decisive roles. Further studies are ongoing to assess QCC in cases beyond the short time and strong decoherence approximations. Preliminary computational results [14, 15] support the conclusions drawn herein.

## Acknowledgements

This work was supported by the US Office of Naval Research and the Natural Sciences and Engineering Research Council of Canada.

## References

- [1] NIELSEN, M. A., and CHUANG, I. L., 2000, *Quantum Computation and Quantum Information* (Cambridge University Press).
- [2] RICE, S. A., and ZHAO, M., 2000, *Optical Control of Molecular Dynamics* (New York: Wiley).
- [3] SHAPIRO, M., and BRUMER, P., 2000, *Adv. Atom. Molec. Opt. Phys.*, **42**, 287.
- [4] SHAPIRO, M., and BRUMER, P., 2003, *Principles of the Quantum Control of Molecular Processes* (New York: Wiley).
- [5] ZUREK, W. H., 2003, *Rev. Mod. Phys.*, **75**, 715.

- [6] SHAPIRO, M., and BRUMER, P., 1989, *J. Chem. Phys.*, **90**, 6179; JIANG, X-P., BRUMER, P., and SHAPIRO, M. 1996, *J. Chem. Phys.*, **104**, 607.
- [7] GIULINI, D., JOOS, E., KIEFER, C., KUPSCH, J., STAMATESCU, I. O., and ZEH, H. D., 1996, *Decoherence and the Appearance of a Classical World in Quantum Theory* (New York: Springer).
- [8] HABIB, S., SHIZUME, K., and ZUREK, W. H., 1998, *Phys. Rev. Lett.*, **80**, 4361.
- [9] GONG, J., and BRUMER, P., 1999, *Phys. Rev. E*, **60**, 1643.
- [10] MILNER, V., STECK, D. A., OSKAY, W. H. and RAIZEN, M. G., *Phys. Rev. E*, **61**, 7223; D'ARCY, M. B., GOOLUN, R. M., OBERTHALER, M. K., SUMMY, G. S., and BURNETT, K., 2001, *Phys. Rev. E*, **64**, 056 233.
- [11] WILKIE, J., and BRUMER, P., 1997a, *Phys. Rev. A*, **55**, 27; 1997b, *ibid.*, **55**, 43.
- [12] WANG, H., THOSS, M., SORGE, K. L., GIMÉNEZ, R. X., and MILLER, W. H., 2001, *J. Chem. Phys.*, **114**, 2562; GROSSMANN, F. 1995, *J. Chem. Phys.*, **103**, 3696; DE ALMEIDA, A. M. O. 2003, *J. Phys. A*, **36**, 67.
- [13] BATISTA, V. S., and BRUMER, P., 2002, *Phys. Rev. Lett.*, **89**, 143 201.
- [14] GONG, J., and BRUMER, P., 2003, *Phys. Rev. A*, **68**, 022101.
- [15] HAN, H., GONG, J., and BRUMER, P., 2003 (to be published).
- [16] GONG, J., and BRUMER, P., 2003, *Phys. Rev. Lett.*, **90**, 050 402.
- [17] JAFFÉ, C., KANFER, S., and BRUMER, P., 1985, *Phys. Rev. Lett.*, **54**, 8.
- [18] LICHTNER, P. C., and GRIFFIN, J. J., 1976, *Phys. Rev. Lett.*, **37**, 1521; ZUREK, W. H., HABIB, S., and PAZ, J. P., 1993, *Phys. Rev. Lett.*, **70**, 1187; JIANG, X-P., and BRUMER, P., 1993, *Chem. Phys. Lett.*, **208**, 179; ISAR, A., SANDULESCU, A., and SCHEID, W., 1999, *Phys. Rev. E*, **60**, 6371; MANFREDI, G., and FEIX, M. R., 2000, *Phys. Rev. E*, **62**, 4665.
- [19] KIM, J. I., NEMES, M. C., DE TOLEDO PIZA, A. F. R., and BORGES, H. E., 1996, *Phys. Rev. Lett.*, **77**, 207.
- [20] DUAN, L. M., and GUO, G. C., 1997, *Phys. Rev. A*, **56**, 4466; BACON, D., LIDER, D. A., and WHALEY, K. B. 1999, *Phys. Rev. A*, **60**, 1944.
- [21] HU, B. L., PAZ, J. P., and ZHANG, Y., 1993, *Phys. Rev. D*, **47**, 1576.
- [22] FEYNMAN, R. P., and VERNON, F. L., 1963, *Ann. Phys. (N.Y.)*, **24**, 118 (1963); CALDERIA, A. O., and LEGGETT, A. J., 1983, *Ann. Phys. (N.Y.)*, **149**, 374; UNRUH, W. G., and ZUREK, W. H., 1989, *Phys. Rev. D*, **40**, 1071; HU, B. L., PAZ, J. P., and ZHANG, Y., 1992, *Phys. Rev. D*, **45**, 2843.
- [23] CHENG, C. C., and RAYMER, M. G., 1999, *Phys. Rev. Lett.*, **82**, 4807.
- [24] BRAUN, D., HAAKE, F., and STRUNZ, W. T., 2001, *Phys. Rev. Lett.*, **86**, 2913.
- [25] ZUREK, W. H., and PAZ, J. P., 1994, *Phys. Rev. Lett.*, **72**, 2508; PATTANAYAK, A. K., 1999, *Phys. Rev. Lett.*, **83**, 4526; MONTEOLIVA, D., and PAZ, J. P., 2000, *Phys. Rev. Lett.*, **85**, 3373.