Quantum Irreversibility and Chaos*

Bruce J. West, Paolo Grigolini, Luca Bonci, and Roberto Roncaglia

Department of Physics, University of North Texas, P.O. Box 5368,
Denton, Texas 76203 (817) 565-2630, USA

Herein we establish a relation between quantum irreversibility and the chaotic semi-classical solutions for a spin-boson Hamiltonian system. We obtain quantum averages by numerically integrating the appropriate Liouville-Von Neumann equations of motion and find these averages to be less erratic than the corresponding chaotic semi-classical trajectories. However, the quantum averages are shown to be dissipative as measured by the entropy of the spin subsystem and to suppress the phenomenon of "revivals".

1. Introduction

It was not until after I, (BJW), had completed graduate study and reached the erstwhile conclusion that subjects like Classical Mechanics were essentially 19th Century physics, that I chanced across Dr. Sudarshan's book on classical mechanics [1]. It was from his book that I discovered that classical mechanics was not only still vital and alive, but that there was also ample opportunity, for one to make research contributions in this area. Now nearly two decades later this observation appears almost trite with the new found emphasis on dynamics in physics [2], e.g., the phenomena of *chaos*. What we would like to discuss in this brief lecture is one way in which the properties of the classical equations of motion influence the corresponding quantum system. In particular we demonstrate on a model system how chaotic semiclassical trajectories lead to irreversibility in the quantum domain [3].

We consider a model system for which a great deal is known, that being a spin-1/2 particle coupled to a coherent magnetic field:

$$H = -\frac{1}{2}\,\omega_0\,\hat{\sigma}_z + \frac{g}{\sqrt{2\,\Omega}}\,\hat{\sigma}_x(\hat{b}+\hat{b}^\dagger) + \Omega\,\hat{b}^\dagger\,\hat{b}, \quad (1)$$

where $\hat{b}(\hat{b}^\dagger)$ is the annihilation (creation) operator with commutation relation $[\hat{b},\hat{b}^\dagger]=1$, and $\hat{q}=(\hat{b}+\hat{b}^\dagger)/\sqrt{2\,\Omega}$, $\hat{p}=i(\hat{b}^\dagger-\hat{b})\sqrt{\Omega/2}$ are the coordinate and momentum operators of our oscillator with frequency Ω. The equations of motion for this system are equivalent to the quantum optics model of Jaynes and Cummings

for a two-state atom interacting with the single mode of an electric field [4].

Here we do not follow the usual analysis of the system dynamics, but rather follow a course set by Wigner by introducing a quantum mechanical phase space and a quasi-probability density. In this approach the quantum operators are replaced by C-numbers: $\hat{\sigma}_j \to x_j$, $\hat{q} \to q$ and $\hat{p} \to p$. The original Wigner formalism only involved p's and q's and not spin variables, so we had to extend his approach somewhat to treat the present problem.

2. Extended Wigner Formalism

Here we adopt a suitable generalization of the Wigner method and write the equation of evolution for the Wigner quasi-probability ϱ_w:

$$\frac{\partial}{\partial t}\,\varrho_w(x_1, x_2, x_3, q, p; t) = (\mathscr{L}_{cl} + \mathscr{L}_{QGD})$$
$$\varrho_w(x_1, x_2, x_3, q, p; t), \quad (2)$$

where the Liouville operator has been separated into two parts,

$$\mathscr{L}_{cl} \equiv \omega_0\left(x_1\frac{\partial}{\partial x_2} - x_2\frac{\partial}{\partial x_1}\right)$$
$$+ 2gq\left(x_3\frac{\partial}{\partial x_2} - x_2\frac{\partial}{\partial x_3}\right)$$
$$+ \Omega^2 q\frac{\partial}{\partial p} - p\frac{\partial}{\partial q} + gx_1\frac{\partial}{\partial p} \quad (3)$$

and

$$\mathscr{L}_{QGD} \equiv g\frac{\partial}{\partial p}\left[\frac{\partial}{\partial x_1} - \frac{\partial}{\partial x_1}x_1^2 - \frac{\partial}{\partial x_2}x_1 x_2 - \frac{\partial}{\partial x_3}x_1 x_3\right]. \quad (4)$$

The connection between the x_i's and the spin operators is given by

$$\langle \sigma_i(t) \rangle = T_r[\sigma_i \varrho(t)]$$
$$= \int dx \, dq \, dp \, x_i \varrho_w(x, q, p; t), \quad (5)$$

and similar relations connect the coordinates q and momentum p to the corresponding quantum operators $\hat{q}$ and $\hat{p}$. The operator $\mathcal{L}_{cl}$ is identical to the Liouvillian of a classical dipole interacting with a classical oscillator, i.e., this term alone corresponds to the semi-classical set of equations discussed by various authors [5, 6]. We refer to the calculations based on the study of the single trajectory solutions of the nonlinear dynamic equations as the semiclassical predictions. In this regard we point out a significant feature of the analysis that was apparently overlooked in previous investigations having to do with chaotic trajectories. These earlier studies focused on individual trajectories and gave them physical meaning, however, from (5) we see that even when $\mathcal{L}_{QGD}$ is neglected, it is only the ensemble that has physical significance not the individual trajectories.

The term $\mathcal{L}_{QGD}$ in (2) has a diffusion-like structure, but the state dependence of the "diffusion coefficient" results in its not being positive definite. It has recently been shown by Roncaglia et al. [7] that if the oscillator is coupled to a heat bath so as to transmit to the spin-1/2 dipole standard thermal fluctuations, then this term results in the mean value of the z-component of the dipole changing from a Langevin (classical) function to the hyperbolic tangent (quantum). In other words, this term, coined the Quantization Generating Diffusion (QGD) by Roncaglia et al. [7] insures that the dipole retains its quantum nature. The operator $\mathcal{L}_{QGD}$ acts as an anti-diffusional mechanism, it competes against thermal fluctuations and constrains the dipole, which otherwise would freely diffuse over all possible orientations, to vacillate between two possible orientations. It seems that in the absence of diffusion this term is inactive, it is only activated with the onset of thermal fluctuations.

Thus like the density matrix, ϱ_w describes an ensemble of systems and (2) describes the evolution of that ensemble in phase space. The initial state of the ensemble is described by the distribution

$$\varrho_w(x, p, q; t = 0) = \varrho_G(q, p) \, \delta(x_1) \, \delta(x_2) \, \delta(x_3 - 1), \quad (6)$$

being the product of a dipole distribution (polarization along the z-axis) and a Gaussian distribution (ϱ_G) for the oscillator. The Gaussian is dictated by the assumption that the initial state of the oscillator is a coherent state. In general the average trajectory obtained using the Wigner distribution

$$\langle \sigma_i(t) \rangle = \int dx \, dq \, dp \, x_i \, e^{-\mathcal{L}_{cl} t} \varrho_w(x, p, q; 0) \quad (7)$$

can be both qualitatively and quantitatively different from the single trajectories result.

3. Calculational Results

In Fig. 1 we compare the average z-component of the spin operator calculated using (7) with the theoretical prediction of Bonci, Grigolini, and Vitali [8], which we refer to as BGV. The BGV prediction is closely related to the well known treatment of quantum dissipation of Leggett and coworkers [9]. A detailed discussion of the merits and limitations of the former theoretical approach is given by Vitali and Grigolini [10], who stress that in these latter approaches the reaction of the field to the evolution of the spin is neglected, thereby suppressing an important nonlinear interaction. In Fig. 1a we observe that the "linearized" interacting system yields a BGV prediction which coincides with averaging over the semiclassical trajectories using (7). Both calculations yield results for the spin-field system in which the field does not react to the dynamics of the dipole, and which is characterized by collapses and revivals.

According to the BGV interpretation the collapse observed in Fig. 1 depends on a "multiplicative stochastic" process formally equivalent to Kubo's stochastic oscillator [11]. Unlike the Kubo oscillator, where the stochastic coefficient (frequency) is based on random fluctuations external to the system, in the present model the multiplicative fluctuations are generated by the dynamics of a single quantum oscillator. Semiclassical trajectories with different initial conditions are characterized by slightly different "oscillation frequencies" in the non-chaotic case and interference between these different members of the ensemble yields a Gaussian-like decay of the average spin-1/2 operators [11]. This functional form of the collapse was also obtained by Kubo for his stochastic oscillator, and by Cummings [12] for the JCM. It has therefore been concluded that this phenomenon corresponds to a relaxation process.

We test the above interpretation by numerically integrating the Liouville-Von Neumann equations for the density matrix and taking the trace over the field
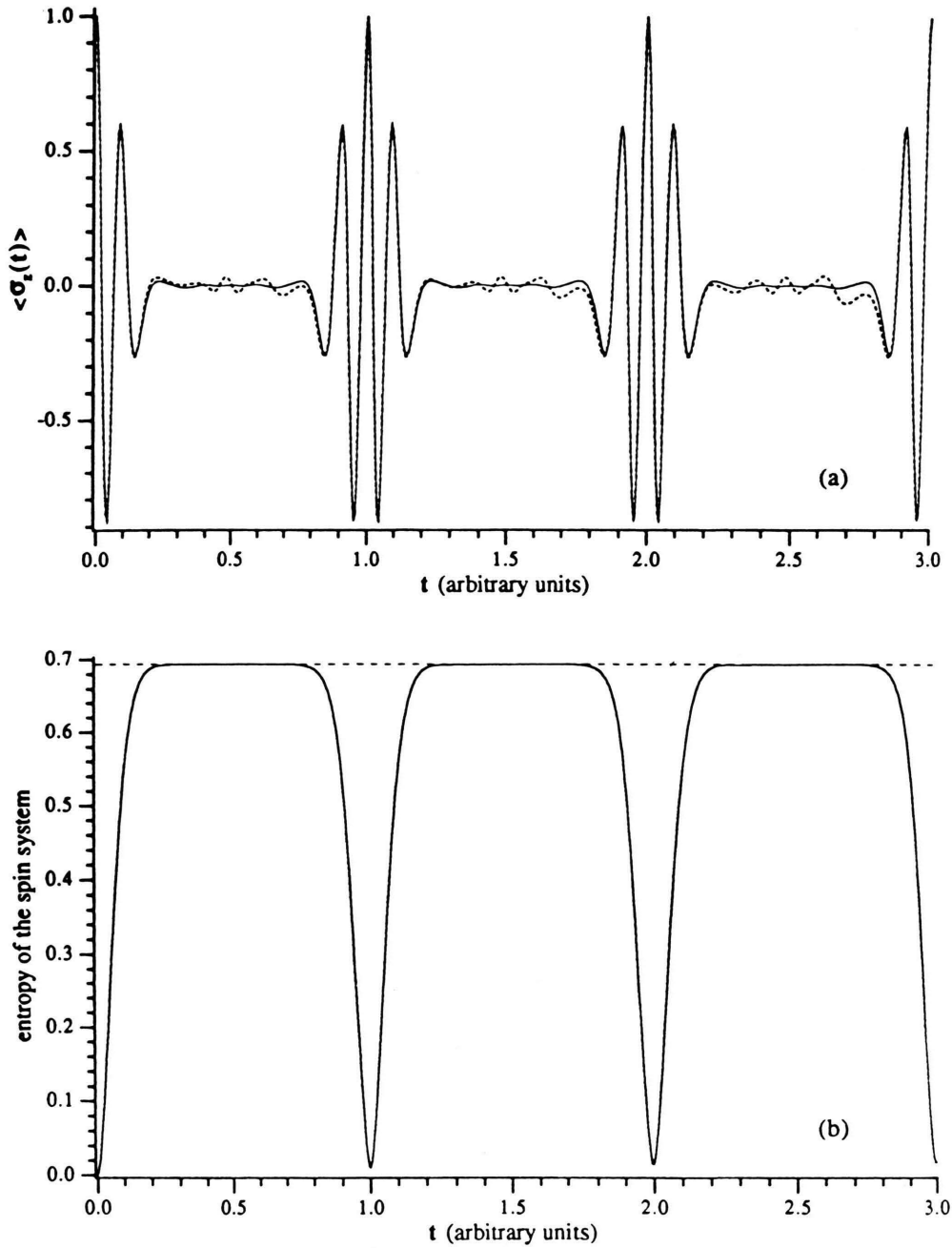
Fig. 1. In all curves $g = 20$, $\omega_0 = 10^{-2}$, $\Omega = 2\pi$ and the average number of photons in the field $\bar{n} = 10$. a) The solid curve is the analytic prediction of BGV theory which coincides with the numerically integrated results. The dashed curve is the average z-component of the spin using the Wigner distribution without $\mathscr{L}_{QGD}$. b) The solid curve is the entropy of the spin system numerically calculated using the Liouville-Von Newmann equations of motion. The dashed line is the theoretical maximum value of the entropy ($\ell n\, 2$).
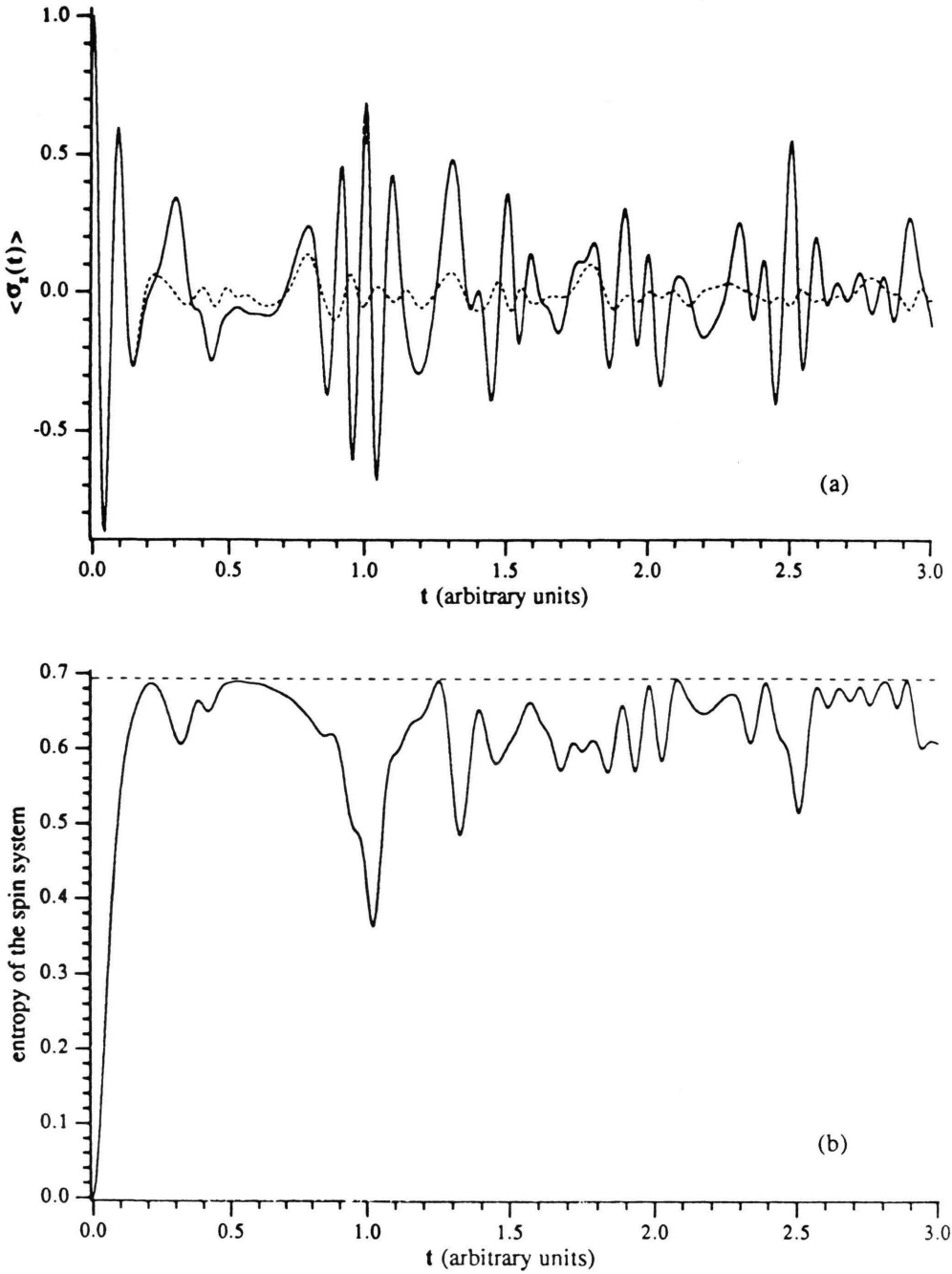
Fig. 2. In all curves $g = 20$, $\omega_0 = \Omega = 2\pi$ and the average number of photons in the field $\bar{n} = 10$. a) The solid curve is the prediction from the numerically integrated equations of motion. The dashed curve is the average z-component of the spin using the Wigner distribution without $\mathscr{L}_{QGD}$. b) The solid curve is the entropy of the spin system numerically calculated using the Liouville-Von Newmann equations of motion. The dashed curve is the theoretical maximum value of the entropy ($\ell n\, 2$).

variables to obtain the spin distribution $\varrho_s(t)$ and defining the entropy for the spin-1/2 dipole as

$$S = - \text{Tr}_{\text{spin}} [\varrho_s \, \ell n \, \varrho_s]. \tag{8}$$

We see in Fig. 1b that the entropy S monotonically increases until it reaches its maximum value; the so-called "collapse" process. However, once attained the maximum entropy is eventually lost, the order of the spin system being restored by the oscillator. The entropy monotonically decreases beyond its maximum to a minimum in the interval of revival. This behavior of the entropy clearly indicates that the dynamics of the mixed state of the spin-1/2 dipole is reversible. The phenomenon of "collapse and revival" of quantum state vectors has attracted increasing interest in the past decade [3, 8, 13–17]. A straightforward discussion of the physical origins of both collapses and revivals in the context of the JCM is given by Phoenix and Knight [17], who used the concept of entropy to describe the appearance of disorder resulting from the interaction between the two-level system and the infinite quantum states necessary to simulate the electromagnetic field in a coherent state.

Let us now study the resonance case wherein $\omega_0 = \Omega$, and first of all turn our attention to the semi-classical trajectories that solve the dynamic equations corresponding to $\mathscr{L}_{cl}$. In accordance with the results of [5] and [6], we find that the individual semi-classical trajectories can exhibit chaos for specific values of the system parameters. Using the method of Benettin et al. [18], we evaluate the Lyapunov coefficient λ which in the case of Fig. 2 turns out to be $\lambda = 2.1$. On the other hand, we have seen that the generalization of the Wigner theory leads us to conclude that single trajectories do not have a direct physical interpretation, only quantities averaged over the initial conditions (6) are physically significant. By definition chaotic trajectories that are initially close together diverge exponentially in time. Thus, the decorrelation mechanism is given by the internal dynamics of the system rather than being external as in the stochastic fluctuations of Kubo.

In Fig. 2 we depict two results of averaging in which the effects of chaotic trajectories are included. One uses (7) in which $\mathscr{L}_{\text{QGD}}$ is neglected and another where the full Hamiltonian dynamics are taken into account by numerical integration of the Liouville-Von Neumann equations of motion. We refer to the latter as the exact calculation. We see in Fig. 2a that at the end of the standard relaxation process the system reaches a

sort of thermodynamic equilibrium and that all revivals after the first are suppressed. It is clear that the collapse is now irreversible due to the subsequent incoherence of the chaotic trajectories. This is even more evident in the dashed curve for the Wigner distribution, since only the chaotic effects are included therein, the QGD effects are not. The entropy (8) is now calculated using the spin distribution, numerically determined by the full nonlinear dynamical equations, i.e., the back reaction of the field is included. We note that the entropy in Fig. 2b monotonically approaches a plateau as it should for an irreversible process. However, in the vicinity of the first revival, a ghost is observed in the form of a slight decrease in the entropy. This blip indicates a competition between the irreversible effects of chaos and the reversible effects of QGD, both of which are in the "exact" calculation.

The curve labeled exact in Fig. 2 includes the antidiffusional effects of QGD and shows a clear peak where the revival is depicted in Figure 1. It has already been remarked that the QGD mechanism becomes activated in the presence of thermal fluctuations. It is possible to show that in the resonant case the QGD mechanism might be significant even in the case of weak oscillator-field coupling. Our numerical results indicate that the same parameter values that trigger chaos in the semiclassical trajectories also stimulate the QGD mechanism. We are led to conclude that the QGD mechanism reacts against the spreading of chaotic semiclassical trajectories and tends to recover, at least in part, the original correlations just as it did for thermal fluctuations.

4. Conclusions

We conclude by contrasting the above results with the traditional picture of a quantum system coupled to a heat bath. Quantum dissipation in these earlier models arises from the infinite number of degrees of freedom in the bath, which for technical reasons is generally treated as being linear [19]. In this paper, however, dissipation is found to be also a quantum manifestation of the chaos in the semiclassical trajectories. This mechanism has nothing do to with the traditional concept of a "heat bath" and is a consequence of the non-integrability of the spin-boson Hamiltonian. Thus, quantum irreversibility is herein not only a many-body effect, but an effect of chaos. This new mechanism (chaos) augments the usual dissipation associated with the many degrees of freedom of the heat bath.

[1] E. C. G. Sudarshan and N. Mukunda, Classical Dynamics: A Modern Perspective, John-Wiley, New York 1974.
[2] See eq., J. Gleik, Chaos: Making a New Science, Viking, New York 1988.
[3] R. Roncaglia, L. Bonci, P. Grigolini and B. J. West, J. Stat. Phys. **646,** 321 (1992).
[4] E. T. Jaynes and F. W. Cummings, Proc. IEEE **51,** 89 (1963).
[5] P. I. Belobrov, G. M. Zaslavsky, and G. Th. Tartakovsky, Sov. Phys. JETP **44,** 945 (1976); P. M. Milonni, J. R. Ackerhalt and H. W. Galbraith, Phys. Rev. Lett. **50,** 966 (1983).
[6] R. Graham and M. Höhnerbach, Z. Phys.-Cond. Matt. **57,** 233 (1984); R. F. Fox and J. Eidson, Phys. Rev. A **34,** 482, 3288 (1986).
[7] R. Roncaglia, R. Mannella, D. Vitali, and P. Grigolini, Phys. Rev. E **51,** 5524 (1995).
[8] L. Bonci, P. Grigolini and D. Vitali, Phys. Rev. A **42,** 4452 (1990); L. Bonci and P. Grigolini.
[9] A. J. Leggett, S. Chakravartz, A. T. Dorsey, M. P. A. Fisher, A. Gorg, and W. Zwerger, Rev. Mod. Phys. **59,** 1 (1987).
[10] D. Vitali and P. Grigolini, Phys. Rev. A **42,** 4452 (1990).
[11] R. Kubo, J. Math. Phys. **4,** 174 (1963).
[12] F. W. Cummings, Phys. Rev. A **140,** 1051 (1965).
[13] R. R. Puri and G. S. Agarwal, Phys. Rev. A **33,** 3610 (1986).
[14] S. M. Barnett and P. L. Knight, Phys. Rev. A **33,** 2444 (1986).
[15] J. Gea-Banacloche, Phys. Rev. Lett. **65,** 3385 (1990).
[16] N. B. Narozhny, J. J. Sánchez-Mondragón, and J. H. Eberly, Phys. Rev. A **23,** 236 (1981).
[17] S. J. D. Phoenix and P. L. Knight, Ann. Physics **186,** 381 (1988).
[18] G. Benettin, L. Galgani, and J. M. Strelcyn, Phys. Rev. A **14,** 2338 (1976).
[19] K. Lindenberg and B. J. West, The Nonequilibrium Statistical Mechanics of Open and Closed Systems, VCH Publishers, New York 1990.