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On the classical limits in the spin-boson model

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Abstract. We show that, while the classical equations of motion of Belobrov, Zaslavski and Tartakovski are rigorously obtained from the thermodynamic limit of the Heisenberg equations of motion of the many-atom version of the spin-boson model in suitable states, those of Milonni, Ackerhalt and Galbraith are derivable from a quantum Hamiltonian only if $s > \frac{1}{2}$, where s is the spin quantum number. Both equations are known to display chaotic behaviour for large coupling constants.

1. Introduction and summary

The spin-boson model is a very interesting model in physics, with application to a wide variety of phenomena in condensed matter physics [1-3], macroscopic quantum tunnelling [4, 5], quantum optics (where the spin represents a two-level atom and the boson the electromagnetic field) [6] and, more recently, in dynamical problems related to 'quantum chaos' ([7] and references therein). In the latter, however, several controversial problems arise, the most serious one being that the well known level-statistics criteria which have been applied with great success to autonomous particle systems (see, e.g., [8] for a review) are not applicable to the model [9]. This seems to be due to the fact that the spin is 'too small' a quantum object to display chaotic behaviour, although the applicability of other dynamical criteria of chaos to the model are not excluded. Due to the pioneering discovery of Belobrov *et al* [10] and Milonni *et al* [11], that a classical form of the equations of motion displays chaotic behaviour, one is tempted to study semiclassical versions of the model from the point of view of 'quantum chaos'. This has been done extensively by Graham and Höhnerbach [7] (see also [12, 13]), but even the semiclassical limits present problems (see [7, sections 3*c* and 3*d*]).

Our objective is to complement and clarify some aspects of the study of the classical limit in the above-mentioned references.

In section 2 we point out that, in the model with N two-level atoms, certain equations of motion, known to exhibit chaotic behaviour for large coupling constant [10], result if the thermodynamic limit ($N \to \infty$) is performed in a certain precise sense [14, 15]. In a loose sense this means that both the spin and field become classical, and the result has been conjectured (and assumed to be true) in [13]. The proof, which follows directly from the seminal work of Hepp and Lieb [14, 15] shows, however,

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the crucial role played by a property (2.6) of the initial state, which corresponds precisely to the 'factorisation property' invoked in [7] and other references in order to obtain the equations of motion of [10] from the Heisenberg equations of motion for the spin-boson model. Incidentally, this result is also of some relevance to understanding the problem of 'quantum chaos' in the spin-boson model [12, 13].

Another form of the equations of motion seems to be suggested by a (different) semiclassical treatment of the model, using Maxwell's equations for the classical external electric field; they were also shown to display chaotic behaviour for large coupling constant [11]. We show, however, in section 3 that the thus-defined classical model derives from the classical limit of a quantum Hamiltonian only if $s > \frac{1}{2}$, where s is the spin quantum number. Hence, the equations of motion of Milonni *et al* [11] are not compatible with quantisation for a two-level atom. Nevertheless, the same type of semiclassical treatment using Maxwell's equations for the 'displacement vector' $\boldsymbol{D}$ yields the equations of motion of Belobrov *et al* [10]. It seems therefore that this effect may be understood as an additional subtlety of the semiclassical limit related to the famous inequivalence of the '$\boldsymbol{d} \cdot \boldsymbol{E}$' and '$\boldsymbol{p} \cdot \boldsymbol{A}$' interactions [16], but its main interest in this context lies in showing the special role played by spin-$\frac{1}{2}$ in this semiclassical limit. As shown in section 2, the 'factorisation property' is a way of obtaining the classical limit which we use without further comment throughout section 3.

2. The limit of large numbers of atoms

The spin-boson model is described by the Hamiltonian

$$H = \omega a^+ a + \omega_0 S_z + \lambda S_x (a + a^+) \tag{2.1}$$

on the tensor product $\mathbb{C}^{2s+1} \otimes F$, where S_x, S_y, S_z are spin-s operators satisfying the usual commutation relations $[S_x, S_y] = \mathrm{i} S_z$, and a, a^+ are standard annihilation and creation operators with $[a, a^+] = \mathbb{1}$ acting on Fock space F, and the frequencies ω, ω_0 ($\hbar = 1$) and the coupling λ are real constants which we take to be positive.

The Hamiltonian corresponding to (2.1) for N (for simplicity two-level, $s = \frac{1}{2}$) atoms is

$$H_N = \omega a^+ a + \omega_0 S_z^{(N)} + \frac{\lambda}{\sqrt{N}} S_x^{(N)} (a + a^+) \tag{2.2}$$

on the Hilbert space $\mathscr{H}_N = \mathscr{H}_N^S \otimes F$, where

$$\mathscr{H}_N^S = \bigotimes_{j=1}^{N} \mathbb{C}_j^2$$

with $\mathbb{C}_j^2$ a copy of $\mathbb{C}^2$ describing the jth atom. The spin-$\frac{1}{2}$ operators $S_{x,y,z;j}$ act on $\mathscr{H}_N^S$ and stand for

$$\tfrac{1}{2}\mathbb{1} \otimes \ldots \otimes \mathbb{1} \otimes \sigma_{x,y,z;j} \otimes \mathbb{1} \otimes \ldots \otimes \mathbb{1}$$

where $\sigma_{x,y,z;j}$ are Pauli matrices acting on just the jth copy $\mathbb{C}_j^2$. Finally

$$S_{x,y,z}^{(N)} = \sum_{j=1}^{N} S_{x,y,z;j} \, .$$

The scaling of λ by $1/\sqrt{N}$ in (2.2) derives from the $1/\sqrt{V}$ (V = volume) factor in the vector potential $\boldsymbol{A}$ of the electromagnetic field, the last operator term in (2.2) corresponding to the '$\boldsymbol{p}\cdot\boldsymbol{A}$' interaction [15]. As in [14, 15, 17], we define the 'intensive' operators

$$x_N, y_N, z_N \equiv \frac{S^{(N)}_{x,y,z}}{N} \qquad \alpha_N \equiv \frac{a}{\sqrt{N}} \qquad \alpha^+_N \equiv \frac{a^+}{\sqrt{N}}$$

which satisfy, by (2.2), the Heisenberg equations of motion:

$$\dot{x}_N = -\omega_0 y_N \tag{2.3a}$$

$$\dot{y}_N = \omega_0 x_N - \lambda z_N(\alpha_N + \alpha^+_N) \tag{2.3b}$$

$$\dot{z}_N = \lambda y_N(\alpha_N + \alpha^+_N) \tag{2.3c}$$

$$\dot{\alpha}_N = -\mathrm{i}\omega\alpha_N - \mathrm{i}\lambda x_N \tag{2.3d}$$

$$\dot{\alpha}^+_N = \mathrm{i}\omega\alpha^+_N + \mathrm{i}\lambda x_N. \tag{2.3e}$$

In the limit $N\to\infty$ the operators x_N, y_N, z_N, α_N, α^+_N become 'classical' in that their commutators tend to zero:

$$[x_N, y_N] = \frac{1}{N} z_N \qquad \text{(and cyclic permutations of } x, y, z)$$

$$[\alpha_N, \alpha^+_N] = \frac{\mathbb{1}}{N}$$

and the norms $\|x_N\|$, $\|y_N\|$, and $\|z_N\|$ are uniformly bounded (independently of N). These limits do not exist, however, in the sense of the norm, and in order to define them consider a set of density matrices ω^N on $\mathscr{H}_N$, such that the limits

$$x, y, z \equiv \lim_{N\to\infty} \omega^N(x_N, y_N, z_N) \tag{2.4}$$

$$\alpha = \lim_{N\to\infty} \omega^N(\alpha_N) \qquad \alpha^+ = \lim_{N\to\infty} \omega^N(\alpha^+_N) \tag{2.5}$$

exist. Let, for notational simplicity,

$$\rho^1_N \equiv x_N \qquad \rho^2_N \equiv y_N \qquad \rho^3_N \equiv z_N \qquad \rho^4_N \equiv \alpha_N \qquad \rho^5_N \equiv \alpha^+_N$$

with

$$\rho^1 \equiv x \qquad \rho^2 \equiv y \qquad \rho^3 \equiv z \qquad \rho^4 \equiv \alpha \qquad \rho^5 \equiv \alpha^+.$$

A sequence of density matrices $\{\omega^N\}$ is called 2-classical [14, 15] with respect to the $\rho_N \equiv \{\rho^i_N\}^5_{i=1}$ with value at $\rho \equiv \{\rho^i\}^5_{i=1} \in (S^2 \times \mathbb{R}^2)$ where S^2 is the sphere $x^2+y^2+z^2 = \frac{1}{4}$, if

$$\lim_{N\to\infty} \sup_{i\in[1,5]} \omega^N((\rho^i_N - \rho^i)^\dagger(\rho^i_N - \rho^i)) = 0 \tag{2.6}$$

where the dagger denotes the adjoint operator.

By the Schwarz inequality:

$$\lim_{N\to\infty} \omega^N(\rho^i_N) = \rho^i \qquad i \in [1, 5] \tag{2.7}$$

$$\lim_{N\to\infty} \omega^N(\rho^i_N \rho^j_N) = \rho^i\rho^j \qquad i, j \in [1, 5] \tag{2.8}$$

and hence the observables ρ_N assume the classical value ρ at least in mean and covariance. We have [15, theorem 1, p 186] the following.

Theorem. If ω^N is 2-classical for ρ_N at $\rho \in (S^2 \times \mathbb{R}^2)$, then ω^N is 2-classical for all $\rho_N(t) \equiv \exp(\mathrm{i}H_N t)\rho_N \exp(-\mathrm{i}H_N t)$ at $\rho(t)$ where $\rho(t) \equiv (x(t), y(t), z(t), \alpha(t), \alpha^+(t))$ is the unique solution of the classical equations

$$\dot{x} = -\omega_0 y \tag{2.9a}$$

$$\dot{y} = \omega_0 x - \lambda z(\alpha + \alpha^+) \tag{2.9b}$$

$$\dot{z} = \lambda y(\alpha + \alpha^+) \tag{2.9c}$$

$$\dot{\alpha} = -\mathrm{i}\omega\alpha - \mathrm{i}\lambda x \tag{2.9d}$$

$$\dot{\alpha}^+ = \mathrm{i}\omega\alpha^+ + \mathrm{i}\lambda x \tag{2.9e}$$

(i.e. (2.3) in the 'limit' $N \to \infty$) with $\rho(0) = \rho \equiv (x, y, z, \alpha, \alpha^+)$.

The above theorem shows that the 'factorised form' of the equations for the spin-boson model (2.1) [7] follows rigorously from the large number of atoms limit $N \to \infty$ of the expectation value of (2.3) in a sequence of 2-classical density matrices. Indeed (2.7) and (2.8) correspond precisely to this 'factorisation property', and hence, although the final result has been stated in heuristic form in [13], the above shows the crucial role played by property (2.6) of the initial state. The scaling $\lambda \to \lambda/\sqrt{N}$ is consistent with the 'intensive' character of α_N, α_N^+, which means that the limit $N \to \infty$ is performed with photon energy $\omega a^+ a$ proportional to N (i.e. extensive). Hence, in this limit, in a sense, both the atoms and the field become 'classical', maintaining the extensive character of the interaction. An important class of states satisfying (2.6) is given by the product states

$$\omega^N(A) = (\Omega^N, A\Omega^N)$$

for any observable A, with

$$\Omega^N = \bigotimes_{j=1}^{N} (\delta|+\rangle_j + \beta|-\rangle_j) \otimes |f^N)$$

where $\delta, \beta \in \mathbb{C}$ such that $|\delta|^2 + |\beta|^2 = 1$; $|\pm\rangle_j$ is the usual basis of $\mathbb{C}_j^2$, i.e.

$$\sigma_{z;j}|\pm\rangle_j = \pm|\pm\rangle_j$$

and $|f^N) \in F$. Then (2.4) and (2.5) are also satisfied for a proper choice of $|f^N)$. Two standard choices are: $|f^N) = |\Omega)$ (the vacuum state in F) giving $\alpha = \alpha^+ = 0$, and $|f^N) = |\sqrt{N}\xi)$ (see [17]) giving $\alpha = \xi$, $\alpha^+ = \bar{\xi}$, where the bar denotes complex conjugate and $|\xi)$ is the usual [17] (normalised to one) Glauber coherent state.

If the rotating-wave approximation [18] is made, the resulting classical equations analogous to (2.9) do not display chaotic behaviour [18]. In this case, it is possible to extend the class of states for which the theorem holds as being all ergodic states [19], but this result hinges on the existence of an additional conservation law and the effective boundedness of the boson operators when restricted to the appropriate subspace. Hence, whether the class of allowed states may be similarly extended in the present case is an open problem.

3. A different classical limit

Introducing in system (2.9) the notation $q = (\alpha + \alpha^+)/\sqrt{2}$ and $p = \mathrm{i}(\alpha^+ - \alpha)\sqrt{2}$ we obtain

$$\dot{x} = -\omega_0 y \tag{3.1a}$$

$$\dot{y} = \omega_0 x - \gamma q z \tag{3.1b}$$

$$\dot{z} = \gamma q y \tag{3.1c}$$

$$\dot{q} = \omega p \tag{3.1d}$$

$$\dot{p} = -\omega q - \gamma x \tag{3.1e}$$

where $\gamma = \sqrt{2}\lambda$. The last two equations (3.1*d*) and (3.1*e*) are equivalent to the following single second-order equation for q:

$$\ddot{q} + \omega^2 q = -\gamma\omega x. \tag{3.2}$$

These are the equations of Belobrov *et al* [10] and we now study the link between them and those of Milonni *et al* [11] mentioned in the introduction (see also [20]).

It is clear that one obtains exactly equations (3.1) from the Hamiltonian (2.1) (written in terms of the operators $\hat{q} = (a + a^+)/\sqrt{2}$ and $\hat{p} = \mathrm{i}(a^+ - a)/\sqrt{2}$) by taking expectation values $\langle\ \rangle$ of the Heisenberg equations, assuming that the expectation values for products factorise and identifying $x \equiv \langle S_x \rangle$, $y \equiv \langle S_y \rangle$, $z \equiv \langle S_z \rangle$, $q \equiv \langle \hat{q} \rangle$ and $p \equiv \langle \hat{p} \rangle$. We point out also that another approach consists in considering (3.1) as classical Hamiltonian equations. This is possible by performing the following change of variables:

$$\begin{aligned} x(Q, P) &= \sin\theta\, P + \cos\theta\, (\tfrac{1}{4} - P^2)^{1/2} \cos Q \\ y(Q, P) &= (\tfrac{1}{4} - P^2)^{1/2} \sin Q \\ z(Q, P) &= \cos\theta\, P - \sin\theta\, (\tfrac{1}{4} - P^2)^{1/2} \cos Q \end{aligned} \tag{3.3}$$

where θ is a fixed arbitrary angle and $0 \leqslant Q \leqslant 2\pi$, $-\frac{1}{2} \leqslant P \leqslant \frac{1}{2}$. Define now the Hamiltonian

$$H(q, p; Q, P) = \tfrac{1}{2}\omega(q^2 + p^2) + \gamma q x(Q, P) + \omega_0 z(Q, P)$$

with (q, p) and (Q, P) as pairs of conjugated variables. Writing now the canonical equations $\dot{q} = \partial H/\partial p$, $\dot{p} = -\partial H/\partial q$, $\dot{Q} = \partial H/\partial P$, $\dot{P} = -\partial H/\partial Q$ we obtain (3.1) by computing $\dot{x}$, $\dot{y}$ and $\dot{z}$ from them and (3.3). As remarked in the introduction, a set of equations different from (3.1) is obtained if the classical external electric field is assumed to satisfy Maxwell's equation

$$\ddot{q} + \omega^2 q = \frac{\gamma}{\omega} \ddot{x} \tag{3.4}$$

instead of (3.2). With equations (3.1*a, b, c*) remaining unchanged, this is the model of Milonni *et al* [11]. Remarking that (3.4) is equivalent to

$$\begin{aligned} \dot{q} &= \omega p + \frac{\gamma}{\omega} \dot{x} = \omega p - \frac{\gamma\omega_0}{\omega} y \\ \dot{p} &= -\omega q \end{aligned} \tag{3.5}$$

our first result is that the system described by these last two equations and (3.1*a, b, c*) is Hamiltonian. Indeed, using again the transformation (3.3) as above, we consider the classical Hamiltonian

$$H'(q', p'; Q, P) = \tfrac{1}{2}\omega(p'^2 + q'^2) + \gamma q' x(Q, P) + \frac{\gamma^2}{2\omega} x^2(Q, P) + \omega_0 z(Q, P). \tag{3.6}$$

It is easy to see that the equations

$$\dot{x} = -\omega_0 y$$

$$\dot{y} = \omega_0 x - \gamma q' z - \frac{\gamma^2}{\omega} xz$$

$$\dot{z} = \gamma q' y + \frac{\gamma^2}{\omega} xy \tag{3.7}$$

$$\dot{q}' = \omega p'$$

$$\dot{p}' = -\omega q' - \gamma x$$

follow directly from (3.6) as canonical equations $\dot{q}' = \partial H'/\partial p'$, $\dot{p}' = -\partial H'/\partial q'$, $\dot{Q} = \partial H'/\partial P$, $\dot{P} = -\partial H'/\partial Q$. Writing now $q' = q - \gamma\omega^{-1}x$ and $p' = p$ one obtains exactly (3.1*a*, *b*, *c*) and (3.5).

Our second result answers the following question: is it possible to write down a quantum Hamiltonian depending on the $\hat{q}$, $\hat{p}$ operators and the spin-$\frac{1}{2}$ operators S_x, S_y, S_z yielding equations (3.1*a*, *b*, *c*) and (3.5) upon taking expectation values $\langle\ \rangle$ of the Heisenberg equations and assuming that the expectation values for products factorise?

The most general Hamiltonian for this case can be written as

$$H = h_0(\hat{p}, \hat{q}) + h_1(\hat{p}, \hat{q})S_x + h_2(\hat{p}, \hat{q})S_y + h_3(\hat{p}, \hat{q})S_z \tag{3.8}$$

where $h_\mu(\hat{p}, \hat{q})$, $\mu = 0, \ldots, 3$, are general functions of the operators $\hat{q}$ and $\hat{p}$.

The Heisenberg equations for the spin operators can be easily computed:

$$\dot{S}_x = \mathrm{i}[H, S_x] = h_2(\hat{p}, \hat{q})S_z - h_3(\hat{p}, \hat{q})S_y$$

$$\dot{S}_y = \mathrm{i}[H, S_y] = -h_1(\hat{p}, \hat{q})S_z + h_3(\hat{p}, \hat{q})S_x \tag{3.9}$$

$$\dot{S}_z = \mathrm{i}[H, S_z] = h_1(\hat{p}, \hat{q})S_y - h_2(\hat{p}, \hat{q})S_x.$$

Having in mind the identification $x \equiv \langle S_x \rangle$, $y \equiv \langle S_y \rangle$, $z \equiv \langle S_z \rangle$, $q \equiv \langle \hat{q} \rangle$ and $p \equiv \langle \hat{p} \rangle$, we impose that

$$\dot{S}_x = -\omega_0 S_y$$

$$\dot{S}_y = \omega_0 S_x - \gamma \hat{q} S_z$$

$$\dot{S}_z = \gamma \hat{q} S_y.$$

From this and (3.9), it follows that $h_1(\hat{p}, \hat{q}) = \gamma\hat{q}$, $h_2(\hat{p}, \hat{q}) = 0$ and $h_3(\hat{p}, \hat{q}) = \omega_0$ are uniquely determined. Then the two remaining Heisenberg equations are

$$\dot{\hat{p}} = \mathrm{i}[H, \hat{p}] = \mathrm{i}[h_0(\hat{p}, \hat{q}), \hat{p}] - \gamma S_x$$

$$\dot{\hat{q}} = \mathrm{i}[H, \hat{q}] = \mathrm{i}[h_0(\hat{p}, \hat{q}), \hat{q}].$$

Thus, we see that it is not possible to satisfy the last two required equations, namely $\dot{\hat{p}} = -\omega\hat{q}$ and $\dot{\hat{q}} = \omega\hat{p} - \gamma\omega_0\omega^{-1}S_y$, except for the trivial case $\gamma = 0$. In conclusion we may say that, in the special case of spin-$\frac{1}{2}$ (two-level atom), the equations of Milonni *et al* may not be derived from a quantum Hamiltonian as mentioned in the introduction.

Remark. Equation (3.4) may also be replaced by $\dot{q} = \omega p$ and

$$\dot{p} = -\omega q + \frac{\gamma}{\omega^2}\ddot{x} = -\omega q - \frac{\gamma\omega_0^2}{\omega^2}x + \frac{\gamma^2\omega_0}{\omega^2}qz$$

instead of (3.5). The same reasoning as above applies and we arrive at the same conclusions for this case.

Finally we point out that our last conclusion is indeed inherent to spin-$\frac{1}{2}$. This is explicitly seen in the form (3.8). As mentioned in the introduction, our final result is that the Milonni *et al* equations may be derived from a quantum Hamiltonian for any spin quantum number $s > \frac{1}{2}$. This is seen by quantising the Hamiltonian (3.6) (with $[\hat{q}', \hat{p}'] = \mathrm{i}$) in order to get

$$H' = \tfrac{1}{2}\omega(\hat{p}'^2 + \hat{q}'^2) + \gamma\hat{q}' S_x + \frac{\gamma^2}{2\omega}S_x^2 + \omega_0 S_z.$$

For $s = \frac{1}{2}$ we have $S_x^2 = \mathbb{1}/4$; then the term involving S_x^2 in H is, of course, irrelevant and the Hamiltonian is equivalent to (2.1). On the other hand, for $s >_2$ this term is non-trivial and provides an additional contribution to the Heisenberg equations, allowing us to obtain (3.7) (considering again expectation values and factorising expectation values for products).

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