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Aspects of two-level systems under external time-dependent fields

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Abstract

The dynamics of two-level systems in time-dependent backgrounds is under consideration. We present some new exact solutions in special backgrounds decaying in time. On the other hand, following ideas of Feynman *et al*, we discuss in detail the possibility of reducing the quantum dynamics to a classical Hamiltonian system. This, in particular, opens the possibility of directly applying powerful methods of classical mechanics (e.g. KAM methods) to study the quantum system. Following such an approach, we draw conclusions of relevance for 'quantum chaos' when the external background is periodic or quasi-periodic in time.

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1. Introduction

Models of quantum two-level systems in time-dependent backgrounds are widely used in different physical problems, with applications ranging from condensed matter physics to quantum optics, particularly in the semiclassical theory of the laser [1]. They may, for instance, represent the behaviour of a (frozen in space) spin $1/2$ in a time-dependent magnetic field. In such a case, the corresponding Schrödinger equation can be treated as the reduction of the Pauli equation to the $0+1$-dimensional case. It takes the form (for simplicity we adopt $\hbar = 1$)

$$\mathrm{i}\partial_t \Psi = H(t)\Psi \tag{1.1}$$

where $\Psi = \Psi(t) = \binom{\psi_1(t)}{\psi_2(t)}$, with the quantum Hamiltonian $H(t)$ given by

$$H(t) = -\frac{1}{2}\vec{B}(t)\cdot\vec{\sigma} = -\frac{1}{2}\begin{pmatrix} B_z(t) & B_x(t) - \mathrm{i}B_y(t) \\ B_x(t) + \mathrm{i}B_y(t) & -B_z(t) \end{pmatrix} \tag{1.2}$$

$\vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ being the Pauli matrices and $\vec{B}(t) = (B_x(t), B_y(t), B_z(t))$.

Equation (1.1) and its solutions have been widely studied. Our contribution in this paper is threefold: we present a formulation of (1.1) in terms of *classical* Hamiltonian systems in section 2, and in section 3 we present several new exact solutions for (1.1) in time-dependent backgrounds which are switched off at the time infinity. These new exact solutions can be useful in solving scattering-like problems. Finally, in section 4 we further develop the classical Hamiltonian formulation of section 2 to discuss how qualitative methods of analysis of classical Hamiltonian systems, such as the KAM method, can be used to shed some light on properties related to 'quantum chaos' of two-level systems under periodic or quasi-periodic time-dependent interactions [6]. Section 4 has left several open problems which, together with the applications of section 3, will be left to further publications. In sections 3 and 4 we will consider the special case

$$B_x(t) = -2\epsilon \qquad B_y(t) = 0 \qquad B_z(t) = -2f(t) \tag{1.3}$$

where ϵ is a constant and f (possibly after addition of a suitable constant) decays in time. The Schrödinger equation (1.1) then reads $\mathrm{i}\dot{\psi}_{1,2} = \pm f(t)\psi_{1,2} + \epsilon\psi_{2,1}$. One of the basic facts we use in section 3 is that the Schrödinger equation above may be shown to be equivalent to the pair of independent second-order equations

$$\ddot{\psi}_{1,2} + (\pm\mathrm{i}\dot{f} + f^2 + \epsilon^2)\psi_{1,2} = 0. \tag{1.4}$$

The particular Schrödinger equation for (1.3) describes two-level systems with unperturbed energy levels $\pm\epsilon$ ($f \equiv 0$) subject to an external time-dependent interaction $f(t)$ inducing a transition between the unperturbed eigenstates. Alternatively, it describes a spin $1/2$ subject to a constant magnetic field -2ϵ in direction 'x' and a time-dependent magnetic field $2f(t)$ in direction 'z' produced, for instance, by a linearly (in direction 'z') polarized plane wave field propagating in direction 'x'. This system has been analysed by many authors in various approximations. For historical references, see [9, 11, 12].

2. Classical Hamiltonian formulation for two-level systems

It is known that a classical description for spinning systems is usually related to the limit $S \to \infty, \hbar \to 0$ (with $\hbar S = 1$), where S is the spin value. Thus, there is a common belief that a spin-$1/2$ system is a purely quantum object. The possibility of a pseudo-classical description of such a system does not contradict that fact [17–21]. However, as first remarked by Feynman *et al* [5], there is a correspondence between equation (1.1) and a classical Hamiltonian system, and solutions of this mechanical system can be used to obtain solutions of (1.1). Moreover, this allows us to directly apply non-perturbative methods of classical Hamiltonian systems, such as the KAM methods, to the analysis of our time-dependent two-level systems. In section 4 we will discuss the significance of this fact to properties of two-level system in extremal (i.e. in weak or strong coupling regime) conditions, drawing conclusions of relevance for 'quantum chaos' when the field is periodic or quasi-periodic.

As mentioned, the possibility to formulate (1.1) in terms of a classical Hamiltonian system has its roots in the work of Feynman *et al* [5], who introduced an approach which is instrumental in the semiclassical theory of the laser [1]. Consider the Schrödinger equation (1.1) and let

$$\rho(t) := |\Psi(t)\rangle\langle\Psi(t)| = \begin{pmatrix} \psi_1(t) \\ \psi_2(t) \end{pmatrix} (\psi_1^*(t) \quad \psi_2^*(t)) = \begin{pmatrix} |\psi_1|^2 & \psi_1\psi_2^* \\ \psi_2\psi_1^* & |\psi_2|^2 \end{pmatrix} \tag{2.1}$$

denote the density matrix. Then ρ satisfies the equation $\mathrm{i}\dot{\rho} = [H(t), \rho]$. Writing

$$\rho(t) = \frac{1}{2}(Q_0\,\mathbb{I} + \vec{Q}\cdot\vec{\sigma}) = \frac{1}{2}\begin{pmatrix} Q_0 + Q_3 & Q_1 - \mathrm{i}Q_2 \\ Q_1 + \mathrm{i}Q_2 & Q_0 - Q_3 \end{pmatrix} \tag{2.2}$$

we have, by comparison of (2.1) and (2.2):

$$Q_0 = |\psi_1|^2 + |\psi_2|^2 = \mathrm{Tr}\,\rho = 1 \qquad Q_1 = \psi_1\psi_2^* + \psi_2\psi_1^*$$
$$Q_2 = \mathrm{i}(\psi_1\psi_2^* - \psi_2\psi_1^*) \qquad Q_3 = |\psi_1|^2 - |\psi_2|^2$$

The equation of motion $\mathrm{i}\dot{\rho} = [H(t), \rho]$ yields [1, 5]

$$\dot{\vec{Q}} := \frac{\mathrm{d}}{\mathrm{d}t}\vec{Q} = -\vec{\Omega} \wedge \vec{Q} \qquad \vec{\Omega} \equiv (B_x(t), B_y(t), B_z(t)) \tag{2.3}$$

and the condition $\rho^2 = \rho$, which expresses that ρ is a pure state, yields

$$Q_1^2 + Q_2^2 + Q_3^2 = \vec{Q}^2 = Q_0^2 = 1. \tag{2.4}$$

Henceforth the overdot denotes a derivative with respect to time and $\wedge$ denotes the vector product.

Equations (2.3) and (2.4) determine the wavefunction completely in that ψ_1 and ψ_2 are two complex numbers, and the phase of Ψ is irrelevant. So three numbers — i.e. the vector $\vec{Q}$—suffice. They are the basis of a simple geometric picture of quantum spin-1/2 (or two-level) systems: the unit vector $\vec{Q}(t)$ precesses around the vector $\vec{\Omega}(t)$ just like a *classical* gyromagnet precesses in a magnetic field [1, 5].

This observation suggests that (2.3) and (2.4) are associated with a classical Hamiltonian system. Let us further develop this idea. Let us consider the unit sphere $\mathcal{S}^2$ with the usual angular coordinates $0 \leqslant \theta \leqslant \pi$, $0 \leqslant \varphi < 2\pi$, and let

$$\vec{\mathscr{S}} = (\mathscr{S}_x, \mathscr{S}_y, \mathscr{S}_z) = (\sin\theta\cos\varphi, \sin\theta\sin\varphi, \cos\theta) \tag{2.5}$$

define the coordinates of a unit vector on $\mathcal{S}^2$. Introducing

$$p = \cos\theta \qquad q = \varphi \tag{2.6}$$

as canonically conjugate variables, we may write

$$\mathscr{S}_x = \sqrt{1-p^2}\cos q \qquad \mathscr{S}_y = \sqrt{1-p^2}\sin q \qquad \text{and} \qquad \mathscr{S}_z = p \tag{2.7}$$

with the usual Poisson brackets

$$\{\mathscr{S}_x, \mathscr{S}_y\} = \frac{\partial\mathscr{S}_x}{\partial q}\frac{\partial\mathscr{S}_y}{\partial p} - \frac{\partial\mathscr{S}_x}{\partial p}\frac{\partial\mathscr{S}_y}{\partial q} = p = \mathscr{S}_z \tag{2.8}$$

plus cyclic permutations. From (2.5), of course, $(\mathscr{S}_x)^2 + (\mathscr{S}_y)^2 + (\mathscr{S}_z)^2 = 1$.

Let us now define in $\mathcal{S}^2$ the classical Hamiltonian

$$\mathscr{H}^{(1)}(t) := -\vec{B}(t)\cdot\vec{\mathscr{S}}. \tag{2.9}$$

This describes the interaction of a classical gyromagnet with an extremal time-dependent magnetic field $\vec{B}(t)$. By (2.9) and (2.7) we may write

$$\mathscr{H}^{(1)}(t) = -[B_x(t)\cos q + B_y(t)\sin q]\sqrt{1-p^2} - B_z(t)p. \tag{2.10}$$

From (2.9) and (2.8) one sees immediately

$$\dot{\vec{\mathscr{S}}} = \{\vec{\mathscr{S}}, \mathscr{H}^{(1)}\} = -\vec{B}(t) \wedge \vec{\mathscr{S}}. \tag{2.11}$$

Equation (2.11) leads to the following picture: under the time evolution defined by $\mathscr{H}^{(1)}$ the unit vector $\vec{\mathscr{S}}(t)$ simply precesses around the magnetic field vector $\vec{B}(t)$.

The important remark is that equations (2.3) with the parametrization

$$\vec{Q} = (\sin\theta\,\cos\varphi, \sin\theta\,\sin\varphi, \cos\theta) \tag{2.12}$$

can be written in *classical* Hamiltonian form

$$\dot{q} = \left\{q, \mathscr{H}^{(1)}\right\} = \frac{\partial\mathscr{H}^{(1)}}{\partial p} \qquad \dot{p} = \left\{p, \mathscr{H}^{(1)}\right\} = -\frac{\partial\mathscr{H}^{(1)}}{\partial q} \tag{2.13}$$

with $q = \varphi$, $0 \leqslant \varphi < 2\pi$ and $p = \cos\theta$, $0 \leqslant \theta \leqslant \pi$ and $\mathscr{H}^{(1)}$ the classical Hamiltonian (2.10). This is immediate by comparing (2.11) with (2.3) and the parametrizations (2.5) and (2.12).

In section 4 we shall also deal with another equivalent Hamiltonian, by the classical canonical transformation $q_1 = -p = -\cos\theta$, $p_1 = q = \varphi$, with $0 \leqslant \theta \leqslant \pi$ and $0 \leqslant \varphi \leqslant 2\pi$. We again write $q_1 = q$ and $p_1 = p$, so as to keep the notation simple, and put

$$\mathscr{H}^{(2)}(t) = -[B_x(t)\cos p + B_y(t)\sin p]\sqrt{1-q^2} + B_z(t)q. \tag{2.14}$$

The spin variables (2.7) become

$$\mathscr{S}_x^{(2)} = \sqrt{1-q^2}\,\cos p \qquad \mathscr{S}_y^{(2)} = \sqrt{1-q^2}\,\sin p \qquad \text{and} \qquad \mathscr{S}_z^{(2)} = -q. \tag{2.15}$$

Since $\mathscr{H}^{(2)} = -\vec{B}(t)\cdot\vec{\mathscr{S}}^{(2)}$, equation (2.11) reads now

$$\dot{\vec{\mathscr{S}}}^{(2)} = \{\vec{\mathscr{S}}^{(2)}, \mathscr{H}^{(2)}\} = -\vec{B}(t)\wedge\vec{\mathscr{S}}^{(2)} \tag{2.16}$$

again with $\left(\mathscr{S}_x^{(2)}\right)^2 + \left(\mathscr{S}_y^{(2)}\right)^2 + \left(\mathscr{S}_z^{(2)}\right)^2 = 1$. With the parametrizations $p = \varphi$ and $q = -\cos\,\theta$, $0 \leqslant \varphi < 2\pi$ and $0 \leqslant \theta \leqslant \pi$, equation (2.15) becomes (as (2.5)) the usual angular representation of the unit vector $\vec{\mathscr{S}}^{(2)}$ on the unit sphere: $\vec{\mathscr{S}}^{(2)} = (\sin\theta\,\cos\varphi, \sin\theta\,\sin\varphi, \cos\theta)$.

In spite of being conceptually enlightening as discussed above, the connection between the quantum equations (2.3) and the classical Hamiltonian system of (2.13) does not seem to have been applied to some of the most exciting recent developments associated with the Hamiltonian (1.2) for spin-1/2 systems in external periodic and quasi-periodic fields [6], both in weak coupling [7] and strong coupling [8, 9]. This will be done in section 4. There we show that the geometric approach provides very interesting insights into several aspects of 'quantum chaos' associated with two-level systems [6].

What can we say if the external field is not periodic or quasi-periodic? In this case some *exact* solutions may be found, and in section 3 we show how the geometric picture helps to find them, having as a basis the solution for constant field. More precisely, we consider the special case (1.3) where ε is a constant and f (possibly after addition of a suitable constant) decays in time.

2.1. Remarks on the semiclassical limit of spin systems

The theory of one spin (of spin quantum number S) or, alternatively, a $N = 2S + 1$-level system, interacting with an external time-dependent magnetic (or electric) field has always been the object of intense study in quantum optics and in the statistical mechanics of quantum spin systems.

In the classical limit, $S \to \infty$, $\hbar \to 0$ with $\hbar S = 1$ the spin operators $\vec{S} = (S_x, S_y, S_z)$ satisfying the $su(2)$ commutation relations $[S_x, S_y] = \mathrm{i}\hbar S_z$, plus cyclic permutations, converge [2, 3] to the classical canonically conjugate variables of a gyromagnet. More precisely

$$\frac{S_x}{S} \to \mathscr{S}_x := \sin\theta\,\cos\varphi \qquad \frac{S_y}{S} \to \mathscr{S}_y := \sin\theta\,\sin\varphi \qquad \frac{S_z}{S} \to \mathscr{S}_z := \cos\theta \tag{2.17}$$

with $0 < \theta < \pi$, $0 \leqslant \varphi < 2\pi$, the usual angles on the unit sphere.

Consider now this spin in an extremal time-dependent magnetic field $\vec{B}(t)$. The corresponding Hamiltonian

$$H(\vec{S}, t) = -\vec{B}(t) \cdot \vec{S} \tag{2.18}$$

satisfies, by (2.17)

$$\frac{H(\vec{S}, t)}{S} \to -\vec{B}(t) \cdot \vec{\mathscr{S}} \equiv \mathscr{H}^{(1)}(t) \tag{2.19}$$

showing that the classical Hamiltonian $\mathscr{H}^{(1)}(t)$ is relevant *both* for $S \to \infty$ *and* $S = 1/2$.

Classical considerations play an important role in condensed matter physics, in particular in the theory of magnetism. There they are even applied to the extreme quantum limit, namely, spin 1/2, often with remarkably good results. In order to give just one striking example, the quantum mechanical ground-state energy per spin, in the thermodynamic limit, computed by linear spin-wave theory around the classical ground state[3], is off the exact value by only 3% [4]. The above features may be justified by the fact that (2.17) is also applicable to spin 1/2, as we saw. This may be surprising, because in the spin-1/2 case the error committed by replacing $\vec{S}/S$ by the rhs of (2.17) is very large, but it may explain some of the striking successes of classical considerations for spin $S = 1/2$ systems mentioned above.

3. Exact solutions

In section 4 we will learn how classical KAM methods can be used to shed some light on the properties of some quantum systems, such as spin-1/2 or two-level systems under the action of an external periodic or quasi-periodic field f. The situation where f is non-periodic or non-quasi-periodic may be, in general, more subtle. A surprising fact, however, is that in some situations exact solutions can be found. Besides being interesting for their own sake, they may be of relevance for the study of physical properties of the quantum systems described, such as the computation of asymptotic transition probabilities and its large-time corrections.

In the present section we are going to present some exact solutions of the equation (2.3) or equivalently to equations (1.4). In this connection, one ought to remark that the first component $\psi_1(t)$ in equations (1.4) is a solution of the stationary one-dimensional Schrödinger equation $\ddot{\psi}_1 + V\psi_1 = 0$ with a complex potential V related to the function f by a differential equation of the first order: $V = (\mathrm{i}\dot{f} + f^2 + \epsilon^2)$. In this case, by the Schrödinger equation $\mathrm{i}\dot{\psi}_{1,2} = \pm f(l)\psi_{1,2} + \epsilon\psi_{2,1}$, the second component $\psi_2(t)$ can be restored from ψ_1 through

$$\psi_2 = \epsilon^{-1}(\mathrm{i}\partial_t - f(t))\psi_1. \tag{3.1}$$

Solutions of the one-dimensional Schrödinger equation are discussed in [16], whose results and considerations can be used to find concrete functions f that admit exact solutions of the equations (2.3) and the respective explicit solutions. Below we present two physically interesting exact solutions of the equations under consideration. Convergent perturbative solutions for periodic f can be found in [11, 12].

3.1. An auxiliary solution

One can find a solution of the equations (2.3) for $f = \text{const}$. The vector $\mathbf{\Omega}$, given in (2.3), is, by (1.3)

$$\begin{aligned} \mathbf{\Omega} &= -2(\epsilon, 0, f) = -2\omega(\sin 2\gamma, 0, \cos 2\gamma) \\ \omega &= \sqrt{\epsilon^2 + f^2} \qquad \epsilon = \omega \sin 2\gamma \qquad f = \omega\cos 2\gamma. \end{aligned} \tag{3.2}$$

[3] For the classical spin-wave theory in the ferromagnetic case, see Straumann [4].

In the general case $0 \leqslant \gamma \leqslant 2\pi$, but if we restrict ourselves to positive $\epsilon > 0$, then $0 \leqslant \gamma \leqslant \pi/2$. The general solution of the equations under consideration has the form

$$\begin{aligned} \psi_1(t) &= +p \sin\gamma \exp(\mathrm{i}\omega t) + q\cos\gamma \exp(-\mathrm{i}\omega t) \\ \psi_2(t) &= -p\cos\gamma \exp(\mathrm{i}\omega t) + q \sin\gamma \exp(-\mathrm{i}\omega t). \end{aligned} \tag{3.3}$$

Here p, q are two complex constants. Let us introduce two angles φ_0 and ψ by the relations

$$pq^* = |pq| \exp(2\mathrm{i}\varphi_0) \qquad \psi = \omega t + \varphi_0. \tag{3.4}$$

Then we find

$$\begin{aligned} &Q_0 = R^2 = |p|^2 + |q|^2 \qquad Q_1 = (|q|^2 - |p|^2)\sin 2\gamma - 2|pq|\cos 2\gamma\ \cos 2\psi \\ &Q_2 = 2|pq|\sin 2\psi \qquad Q_3 = (|q|^2 - |p|^2)\cos 2\gamma + 2|pq|\sin 2\gamma\ \cos 2\psi \\ &|\psi_1|^2 = |p|^2 \sin^2\gamma + |q|^2\cos^2\gamma + |pq|\sin 2\gamma\ \cos 2\psi \\ &|\psi_2|^2 = |p|^2\cos^2\gamma + |q|^2 \sin^2\gamma - |pq|\sin 2\gamma\ \cos 2\psi. \end{aligned} \tag{3.5}$$

3.2. The first exact solution

The function f of the form

$$f = f_0 \tanh\tau + f_1 \qquad \tau = \frac{t}{T} \tag{3.6}$$

admits an exact solution as will be demonstrated below. Here f_0 and f_1 are two arbitrary real constants. It is obvious that $\lim_{t\to\pm\infty} f(t) = f_\pm = f_1 \pm f_0$. Thus, at large $|t|$, the solution has to coincide with those obtained above for constant $f_\pm$. Let us introduce a new variable z,

$$z = \tfrac{1}{2}(1 + \tanh\tau) \qquad 0 < z < 1 \tag{3.7}$$

and dimensionless constants

$$a = Tf_0 \qquad b = Tf_1 \qquad E = \epsilon T \qquad \omega_\pm = \sqrt{E^2 + (a \pm b)^2}. \tag{3.8}$$

The points $z = 1, 0$ correspond to $t = \pm\infty$ respectively, and

$$\frac{\mathrm{d}}{\mathrm{d}t} = \frac{2}{T} z(1-z)\frac{\mathrm{d}}{\mathrm{d}z} \qquad \frac{\mathrm{d}^2}{\mathrm{d}t^2} = \frac{4}{T^2}\left[z^2(1-z)^2\frac{\mathrm{d}^2}{\mathrm{d}z^2} + z(1-z)(1-2z)\frac{\mathrm{d}}{\mathrm{d}z}\right].$$

We search for a solution of the first equation in (1.4) of the form

$$\psi_1(t) = z^\mu (1-z)^\nu F(z). \tag{3.9}$$

Taking into account that $f = \frac{1}{T}(2az + b - a)$ and $\dot{f} = \frac{4a}{T^2} z(1-z)$ we obtain the following equation for the function $F(z)$:

$$z^2(1-z)^2 \frac{\mathrm{d}^2}{\mathrm{d}z^2} F + z(1-z)[1 + 2\mu - 2(\mu+\nu+1)z]\frac{\mathrm{d}}{\mathrm{d}z} F + \Phi(z)F = 0 \tag{3.10}$$

where

$$\Phi(z) = \mu^2 + \frac{\omega_-^2}{4} + \left(\nu^2 + \frac{\omega_+^2}{4} - \mu^2 - \frac{\omega_-^2}{4}\right) z - (\mu+\nu+1+\mathrm{i}a)(\mu+\nu-\mathrm{i}a)z(1-z).$$

Selecting $2\mu = \mathrm{i}\omega_-$ and $2\nu = \mathrm{i}\omega_+$ we arrive at the hypergeometric equation for the function F (see [22] equation (9.151)). Then the general solution for the function $\psi_1(t)$ has the form

$$\psi_1(t) = c_1\varphi(\mu, \nu; z) + c_2\varphi(-\mu, \nu; z) \tag{3.11}$$

where c_1 and c_2 are some complex constants and

$$\varphi(\mu, \nu; z) = (1-z)^\nu z^\mu F(\mu+\nu+1+\mathrm{i}a,\ \mu+\nu-\mathrm{i}a; 1+2\mu; z). \tag{3.12}$$

Here $F(\alpha, \beta; \gamma; z)$ is the hypergeometric function (see [22] equation (9.100)).

Taking into account (3.7), we may write

$$z = \frac{e^{2\tau}}{1 + e^{2\tau}} \qquad \tau = \frac{t}{T}. \tag{3.13}$$

Thus, $\lim_{t\to-\infty} z = 0$. Besides,

$$F(\alpha, \beta; \gamma; z = 0) = 1. \tag{3.14}$$

Then one can find the asymptote as $t \to -\infty$,

$$\psi_1(t) \approx c_1 e^{i\omega_- \tau} + c_2 e^{-i\omega_- \tau}. \tag{3.15}$$

This matches with (3.3) if we set

$$c_1 = p \sin\gamma_- \qquad c_2 = q \cos\gamma_-. \tag{3.16}$$

The angle γ_- is defined from the relations $T\epsilon = E = \omega_- \sin 2\gamma_-$ and $Tf_- = \omega_- \cos 2\gamma_-$.

Searching for another asymptote as $t \to \infty$ (which corresponds to $z \to 1$), one has to take into account that $z = 1$ is the bifurcation point of $F(\alpha, \beta; \gamma; z)$. Thus, to use the relation (3.14) one has to make the transformation $F(z) \to F(1 - z)$. That can be done by using the relation (9.131.2) of [22]. Then we get

$$\varphi(\mu, \nu; z) = \bar{\varphi}(\mu, \nu; z) + \bar{\varphi}(\mu, -\nu; z) \tag{3.17}$$

where

$$\bar{\varphi}(\mu, \nu; z) = \frac{\Gamma(1 + 2\mu)\Gamma(-2\nu)\, z^{\mu}(1 - z)^{\nu}}{\Gamma(1 + \mu - \nu + ia)\Gamma(\mu - \nu - ia)}.$$

It follows from (3.13) that $\lim_{t\to\infty}(1 - z) = 0$. Taking this into account we find the asymptote (as $t \to \infty$) from (3.17),

$$\varphi(\mu, \nu; z) \approx \frac{\Gamma(1 + 2\mu)\Gamma(-2\nu)e^{i\omega_+\tau}}{\Gamma(1 + \mu - \nu + ia)\Gamma(\mu - \nu - ia)} + \frac{\Gamma(1 + 2\mu)\Gamma(2\nu)e^{-i\omega_+\tau}}{\Gamma(1 + \mu + \nu + ia)\Gamma(\mu + \nu - ia)}.$$

The corresponding asymptote for $\psi_1(t)$ reads

$$\begin{aligned}\psi_1(t) \approx{}& \left[\frac{\Gamma(1 + 2\mu)c_1}{\Gamma(1 + \mu + \nu + ia)\Gamma(\mu + \nu - ia)} + \frac{\Gamma(1 - 2\mu)c_2}{\Gamma(1 - \mu + \nu + ia)\Gamma(-\mu + \nu - ia)}\right] e^{i\omega_+\tau} \\ &+ \left[\frac{\Gamma(1 + 2\mu)c_1}{\Gamma(1 + \mu - \nu + ia)\Gamma(\mu - \nu - ia)} + \frac{\Gamma(1 - 2\mu)c_2}{\Gamma(1 - \mu - \nu + ia)\Gamma(-\mu - \nu - ia)}\right] e^{-i\omega_+\tau}.\end{aligned}$$

They correspond to solutions (3.3) with the frequency ω_+ in the final state, if $c_{1,2}$ obey (3.16). Thus, the scattering problem is solved completely without calculating the function $\psi_2(t)$. However, the latter function can be recovered from the function $\psi_1(t)$ using the second equation in (1.4) and the formulae (9.137) of [22] for the hypergeometric functions.

3.3. Second exact solution

The function f of the form

$$f = \frac{f_0}{\cosh\tau} \qquad \tau = \frac{t}{T} \tag{3.18}$$

admits another exact solution. Here f_0 is an arbitrary real constant. Since $f \to 0$ at $|t| \to \infty$, the corresponding asymptotic at $\gamma = \pi/4$ has the form (3.3). Introducing the variable z,

$$z = \frac{2}{1 - i\sinh\tau} \tag{3.19}$$

we find

$$\frac{\mathrm{d}}{\mathrm{d}t} = \frac{z}{T}\sqrt{1-z}\frac{\mathrm{d}}{\mathrm{d}z} \qquad \frac{\mathrm{d}^2}{\mathrm{d}t^2} = \frac{z^2(1-z)}{T^2}\frac{\mathrm{d}^2}{\mathrm{d}z^2} + \frac{z}{2T^2}(2-3z)\frac{\mathrm{d}}{\mathrm{d}z}.$$

We search for a solution of the first equation in (1.4) in the form (3.9) at $\mu = \mathrm{i}\epsilon T$ and $2\nu = -Tf_0$. Thus, we find

$$\psi_1(t) = c_1\varphi(\mu, \nu; z) + c_2\varphi(-\mu, \nu; z)$$
$$\varphi(\mu, \nu; z) = (1-z)^{\nu} z^{\mu} F\left(\mu, \tfrac{1}{2} + 2\nu - \mu; 1 + 2\mu; z\right). \tag{3.20}$$

As one can see, $z \to 0$ as $|t| \to \infty$. However, one has to be careful and consider asymptotes at $t \to \infty$ and $t \to -\infty$ separately. Indeed, it follows from (3.19) that $1 - z = (\sinh\tau - \mathrm{i})/(\sinh\tau + \mathrm{i})$, and

$$z|_{t\to-\infty} \approx -4\mathrm{i}\mathrm{e}^{\tau} = \exp\left(\tau - \mathrm{i}\frac{\pi}{2} + \ln 4\right)$$
$$z|_{t\to\infty} \approx 4\mathrm{i}\mathrm{e}^{-\tau} = \exp\left(-\tau + \mathrm{i}\frac{\pi}{2} + \ln 4\right). \tag{3.21}$$

Let us put $\exp\tau = \tan\frac{\varphi}{4}$, $0 < \varphi < 2\pi$ and $1 - z = \exp\varphi$. Then, $t \to -\infty \Longrightarrow \varphi \to 0$; $t \to \infty \Longrightarrow \varphi \to 2\pi$, and we have $\lim_{t\to-\infty}\arg(1-z) = 0$ and $\lim_{t\to\infty}\arg(1-z) = 2\pi$. Taking this into account and remembering (3.14), (3.21), we get as $t \to -\infty$

$$\psi_1(t) \approx c_1\exp(\chi_1) + c_2\exp(-\chi_1) \qquad \chi_1 = \mathrm{i}\epsilon t + \tfrac{\pi}{2}\epsilon T + \mathrm{i}\epsilon T\ln 4. \tag{3.22}$$

The corresponding asymptote as $t \to \infty$ has the form

$$\psi_1(t) \approx \mathrm{e}^{-\mathrm{i}\pi f_0 T}[c_1\exp(-\chi_2) + c_2\exp(\chi_2)] \qquad \chi_2 = \mathrm{i}\epsilon t + \tfrac{\pi}{2}\epsilon T - \mathrm{i}\epsilon T\ln 4 \tag{3.23}$$

which has a complete correspondence with (3.3). At $t \to \infty$ we may observe an exchange of the coefficients and an additional phase appears.

4. 'Quantum chaos' in two-level systems

The problem of 'quantum chaos' has attracted a lot of attention in recent times (see [6] and references quoted therein). We will now focus on it from the point of view of the classical Hamiltonian system provided by (2.13) for the Hamiltonian (2.14), describing the two-level systems discussed above with periodic or quasi-periodic time-dependent interactions.

Let us consider the situation where

$$B_x(t) = 2f(t) \qquad B_y(t) = 0 \qquad B_z(t) = -2\epsilon \tag{4.1}$$

we get from (1.2) the quantum Hamiltonian

$$H^{(1)}(t) = \epsilon\sigma_z - f(t)\sigma_x. \tag{4.2}$$

This is the most usual form of the Hamiltonian of a time-dependent two-level system: ϵ is the energy difference of the (unperturbed) levels in a two-level atomic system, and $-f(t)\sigma_x$ is the interaction with an external electromagnetic field in a two-level approximation [1]. By (2.14), the corresponding classical Hamiltonian is

$$\mathcal{H}_1 = -2f(t)\sqrt{1-q^2}\cos p - 2\epsilon q. \tag{4.3}$$

Rotation of $\pi/2$ around the y-axis leads from (4.2) to

$$H^{(2)}(t) = \epsilon\sigma_x + f(t)\sigma_z \tag{4.4}$$

which corresponds to

$$B_x(t) = -2\epsilon \qquad B_y(t) = 0 \qquad B_z(t) = -2f(t) \tag{4.5}$$

in (1.2). The classical Hamiltonian (2.14) becomes

$$\mathcal{H}_2 = 2\epsilon\sqrt{1-q^2}\cos p - 2f(t)q. \tag{4.6}$$

In both cases, the situation where ϵ is 'small' is called the strong-coupling case [8, 9] and the situation where f is 'small' is called the weak-coupling case. We will analyse both separately. We will consider (4.6) for the strong-coupling regime and (4.3) for the weak-coupling regime.

We now consider f periodic with frequency ω:

$$f = f(\omega t). \tag{4.7}$$

We are led, by Howland's method in classical mechanics (see [6] or [10], chapter 7.4), to consider the autonomous Hamiltonians corresponding to (4.3) and (4.6). Roughly speaking, this method allows a non-autonomous Hamiltonian $H(q, p, \omega t)$ to be transformed into an autonomous Hamiltonian by treating ωt as a coordinate θ with a corresponding canonically conjugate momentum I. The associated autonomous Hamiltonian is $K(q, p, \theta, I) = H(q, p, \theta) + \omega I$ and one easily checks the equivalence of the Hamilton equations for both.

Let us denote by $\mathcal{K}_1$ and $\mathcal{K}_2$ the autonomous Hamiltonians corresponding to (4.3) and (4.6), respectively. For (4.3) we get

$$\mathcal{K}_1 = \mathcal{H}_1^0 + \epsilon\mathcal{V}_1 \quad \text{where} \quad \mathcal{H}_1^0 = -2f(\theta)\sqrt{1-q^2}\cos p + \omega I \quad \text{and} \quad \mathcal{V}_1 = -2q \tag{4.8}$$

defined on the Cartesian product phase space $\Pi_1 \times \Pi_2$, where

$$\Pi_1 = \{(q, p); -1 \leqslant q \leqslant 1; 0 \leqslant p < 2\pi \text{ with } 2\pi \text{ and } 0 \text{ identified}\}$$
$$\Pi_2 = \{(\theta, I); 0 \leqslant \theta < 2\pi \text{ with } 2\pi \text{ and } 0 \text{ identified}; -\infty < I < \infty\}.$$

Above, I is the variable canonically conjugate to the angle θ, with $\dot\theta = \frac{\partial\mathcal{K}_1}{\partial I} = \omega$. On the other hand, for (4.6) we get

$$\mathcal{K}_2 = \mathcal{H}_2^0 + \epsilon\mathcal{V}_2 \quad \text{where} \quad \mathcal{H}_2^0 = -2f(\theta)q + \omega I \quad \text{and} \quad \mathcal{V}_2 = 2\sqrt{1-q^2}\cos p. \tag{4.9}$$

Again, I is the variable canonically conjugate to the angle θ, with $\dot\theta = \frac{\partial\mathcal{K}_2}{\partial I} = \omega$.

The important observation now is that $\mathcal{H}_2^0$ is integrable. In fact, $\mathcal{H}_2^0$ and q are two independent constants of motion in involution. $\mathcal{K}_2$ is, however, not integrable and for ϵ 'small' $\mathcal{K}_2$ is, by (4.9), a small perturbation about an integrable Hamiltonian. Hence, KAM methods are applicable [6] to the analysis of the Hamiltonian system associated with $\mathcal{K}_2$ and to the corresponding quantum spin-1/2 or two-level system. Before we discuss the consequences of this fact below let us look at the situation for the weak-coupling regime.

For weak coupling it is more natural to write $\epsilon \equiv \omega_0$ and $f \equiv \tilde\epsilon\,\tilde f$ for $\tilde\epsilon$ 'small'. Equations (4.2) and (4.4) become $\tilde H^{(1)} = \omega_0\sigma_z - \tilde\epsilon\,\tilde f(t)\sigma_x$ and $\tilde H^{(2)}(t) = \omega_0\sigma_x + \tilde\epsilon\,\tilde f(t)\sigma_z$, respectively. The classical autonomous Hamiltonians $\mathcal{K}_1$ and $\mathcal{K}_2$ become

$$\tilde{\mathcal{K}}_1 = \tilde{\mathcal{H}}_1^0 + \tilde\epsilon\,\tilde{\mathcal{V}}_1 \quad \text{where} \quad \tilde{\mathcal{H}}_1^0 = -2\omega_0 q + \omega I \quad \text{and} \quad \tilde{\mathcal{V}}_1 = -2\tilde f(\theta)\sqrt{1-q^2}\cos p \tag{4.10}$$

and

$$\tilde{\mathcal{K}}_2 = \tilde{\mathcal{H}}_2^0 + \tilde\epsilon\,\tilde{\mathcal{V}}_2 \quad \text{where} \quad \tilde{\mathcal{H}}_2^0 = 2\omega_0\sqrt{1-q^2}\cos p + \omega I \quad \text{and} \quad \tilde{\mathcal{V}}_2 = -2\tilde f(\theta)q. \tag{4.11}$$

Now, $\tilde{\mathcal{H}}_1^0$ is integrable, since q and I or q and $\tilde{\mathcal{H}}_1^0$ are independent constants of the motion in involution. $\tilde K_1$, however, is not integrable, and again, by (4.10), is a small perturbation about an integrable Hamiltonian. Therefore, KAM methods are again applicable. Note that in (4.10), with $q = \mathscr{S}_z = I_1$ and $I = I_2$, one has $\tilde{\mathcal{H}}_1^0 = \tilde{\mathcal{H}}_1^0(I_1, I_2)$ which is the standard form of integrable $\tilde{\mathcal{H}}_1^0$.

Several remarks already follow from this description. Firstly $\mathcal{K}_2$ and $\tilde{\mathcal{K}}_1$ are non-integrable even in the periodic case, which lends further insight into the nontrivial character of the (quantum) perturbation theory developed in [11, 12]. Secondly, the complete equivalence of the classical dynamics described by (4.9) or (4.10) to the quantum evolution throws further light onto properties of the quantum system, as we now discuss briefly.

In the periodic case (4.7), $\mathcal{K}_2$ and $\tilde{\mathcal{K}}_1$ (given by (4.9) and (4.10), respectively) are Hamiltonians of a system of two degrees of freedom. They are thus expected to exhibit an Aubry–Mather transition [6], at a certain critical ϵ_c, which may correspond to the first avoided crossing. The ingenious method of [13], which combines the KAM transformation with a specific treatment of resonances and pushes the convergence radius of the classical perturbation expansion up to $|\epsilon| = \epsilon_c$ (or $|\tilde{\epsilon}| = \epsilon_c$) may, if applicable to the present classical model, be translated exactly to the quantum case, with interesting implications for a modified Rayleigh–Schrödinger perturbation theory for the Floquet eigenvalues of the quantum system.

As a final interesting insight provided by the classical description, consider the case of quasi-periodic $f(t) = f(\omega_1 t, \omega_2 t)$ with two incommensurate frequencies [6, 9]. In cases (4.9) and (4.10) we are led to three-degrees-of-freedom Hamiltonians

$$\mathcal{K}_2 = \mathcal{H}_2^0 + \epsilon\mathcal{V}_2 \quad \text{where} \quad \mathcal{H}_2^0 = -2f(\vec{\theta})q + \vec{\omega}\cdot\vec{I} \quad \text{and} \quad \mathcal{V}_2 = 2\sqrt{1-q^2}\cos p \tag{4.12}$$

and

$$\tilde{\mathcal{K}}_1 = \tilde{\mathcal{H}}_1^0 + \tilde{\epsilon}\tilde{\mathcal{V}}_1 \quad \text{where} \quad \tilde{\mathcal{H}}_1^0 = -2\omega_0 q + \vec{\omega}\cdot\vec{I} \quad \text{and} \quad \tilde{\mathcal{V}}_1 = -2\tilde{f}(\vec{\theta})\sqrt{1-q^2}\cos p \tag{4.13}$$

respectively, with $\vec{\theta} := (\theta_1, \theta_2)$, $\vec{I} := (I_1, I_2)$, $\vec{\omega} := (\omega_1, \omega_2)$. It has, in general, quite different critical properties from the two-degrees-of-freedom case [14]!. This may be a clue to the nature of the differences between the periodic and the quasi-periodic cases. Although the quasi-energy spectra are dense pure point in both cases [6, 15], there are basic differences in the nature of the perturbative series (without secular terms [9, 11, 12]) in the coupling constant ϵ: in contrast to the periodic case, in the quasi-periodic case the series is not, for reasons explained in [9], expected to define an analytic function in any circle $|\epsilon| \leqslant \epsilon_0$ (for ϵ_0 however small) for any values of the frequencies and coefficients of the Fourier expansion of f (which are supposed to be O(1) with respect to ϵ).

5. Some final remarks

For certain Hamiltonians which are at most quadratic in coordinates and momenta obeying the Heisenberg–Weyl algebra (flat phase space), there exist different explicit expressions for the basic quantum mechanical quantities in terms of classical solutions [23]. As an example, we mention the well-known expression of the transition amplitude via the van-Vleck determinant [24].

In the case of compact phase space considered in this paper, there are two semiclassical approaches: the WKB theory for spin, due to van Hemmen and Sütő [25], and the path integral formalism (see [26], chapter 23 and references given there), but the connection with classical dynamics is not established for any spin quantum number, but only in the classical limit $\hbar \to 0$, $S \to \infty$ with $\hbar S = 1$.

The phase space path integral for spin has also been employed, notably in [27], which uses the Villain approximation. In this context, but along different lines, we have shown that the classical Hamiltonian (2.10) (or (2.14)) is relevant to both the classical and extreme quantum (spin 1/2) limits of the Hamiltonian of a quantum spin in an external magnetic field, one of whose components is a time-dependent function f.

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