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Pseudo-nonlinear quantum mechanical Hamiltonians for dissipation and other physical phenomena

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Abstract. I investigate the equations of motion for a class of apparently nonlinear Hamiltonian operators with applications to dissipation and other physical phenomena. Under certain conditions one obtains linear dynamical equations which in some cases can be solved exactly. A multidimensional harmonic oscillator with a damping potential depending on the expectation values of the coordinates and momenta is explicitly treated as an illustrative example.

1. Introduction

Dissipation phenomena are of great importance in chemistry and physics. The correct quantization of dissipative forces is a difficult problem because quantum mechanics is based on a Hamiltonian formulation. Many approaches have been suggested to the treatment of quantum mechanical damping (for reviews on the subject see [1, 2]). Here I am interested in model Hamiltonians that depend on the state of the system, in particular when such a dependence occurs via the expectation values of quantum mechanical observables [1–5].

Quantum mechanical dissipation occurs in a variety of physical phenomena, such as fission, heavy-ion experiments, and giant resonances [1], among others [2]. Nonlinear time-dependent Hamiltonians also appear in the local harmonic approximation [6, 7] and other approaches [8] to dynamical systems. A nonlinear quantal Hamiltonian for dissipation has recently been discussed in the context of information theory [9]. The time-evolution equations for expectation values of operators spanning a Lie algebra were found to be nonlinear and integrated numerically [9]. Later I showed that this problem can be reduced to a set of exactly solvable first-order linear differential equations obtained by the introduction of a formal time-evolution operator and the use of properties of the Lie algebras [10]. It is worth mentioning here that another set of linear dynamical equations for such a nonlinear Hamiltonian had been obtained before (see, for example, [2]).

The purpose of this paper is to investigate the conditions under which one expects to obtain linear equations of motion for dynamical systems governed by nonlinear Hamiltonians. In particular I concentrate on such problems that can be formulated in terms of Lie algebras and justify the use of a formal time-evolution operator [10]. A general dynamical model of this kind is considered in section 2 and a multidimensional nonlinear oscillator [5] is discussed in section 3 as an illustrative example. Further comments and conclusions are found in section 4.

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2. Equations of motion for nonlinear Hamiltonians

In the treatment of dissipative systems one can consider wavepackets that move along classical damped trajectories [1, 3–5]. However, for the sake of generality I assume that the system may not be in a pure state so that one has to consider the time-evolution of the density operator $\rho(t)$:

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho(t)=\frac{\mathrm{i}}{\hbar}[\rho(t), H]. \tag{1}$$

The expectation value of an operator $O(t)$, $\langle 0\rangle=\mathrm{tr}[\rho(t)O(t)]$, propagates in time according to

$$\frac{\mathrm{d}}{\mathrm{d}t}O(t)=\frac{\mathrm{i}}{\hbar}\langle[H, O(t)]\rangle+\left\langle\frac{\partial O(t)}{\partial t}\right\rangle. \tag{2}$$

In this paper I confine attention to the case that there is a set of time-independent Hermitian operators $\{L_1, L_2, \ldots, L_N\}$ satisfying

$$[H, L_j]=\sum_{k=1}^{N}\mathbb{H}_{jk}L_k \qquad j=1, 2, \ldots N. \tag{3}$$

This situation is commonly found in many models for quantum mechanical friction [1–5, 9, 10] and other phenomena [6, 7]. In these particular cases the nonlinear Hamiltonian is written as a linear combination of operators that span a finite-dimensional Lie algebra.

For the sake of simplicity I define the column matrix $\mathbf{L}$, and the square matrix $\mathbf{S}$ with elements

$$\mathbf{L}_j=\langle L_j\rangle \qquad \mathbf{S}_{jk}=\tfrac{1}{2}\langle L_jL_k+L_kL_j\rangle \qquad j, k=1, 2, \ldots, N \tag{4}$$

respectively. The mean-square deviation and correlations of the expectation values $\mathbf{L}$ are defined as the diagonal and off-diagonal elements, respectively, of the matrix

$$\mathbf{\Delta}=\mathbf{S}-\mathbf{L}\mathbf{L}^{\mathrm{T}} \tag{5}$$

in which T denotes transpose.

The time-evolution of the matrices defined above is easily obtained by straightforward application of (2):

$$\mathrm{d}\mathbf{L}/\mathrm{d}t=\mathbb{A}\mathbf{L} \tag{6a}$$

$$\mathrm{d}\mathbf{S}/\mathrm{d}t=\mathbb{A}\mathbf{S}+\mathbf{S}\mathbb{A}^{\mathrm{T}} \tag{6b}$$

$$\mathrm{d}\mathbf{\Delta}=\mathbb{A}\mathbf{\Delta}+\mathbf{\Delta}\mathbb{A}^{\mathrm{T}} \tag{6c}$$

where $\mathbb{A}=\mathrm{i}\mathbb{H}/\hbar$. The initial conditions are $\mathbf{L}(t_0)=\mathbf{L}^0$, $\mathbf{S}(t_0)=\mathbf{S}^0$, and $\mathbf{\Delta}(t_0)=\mathbf{\Delta}^0$.

There are many approaches to quantum mechanical friction [1, 2], some of which are based on Hamiltonian operators depending on the state of the system [1–5]. Here I assume that H depends on $\mathbf{L}$ thus obtaining a generalization of the model discussed by Albrecht [3] and Hasse [1, 4, 5]. Under such a condition equations (6) are nonlinear. However, after solving (6a) one obtains $\mathbf{L}(t)$ and thereby $\mathbb{A}(t)$ which will depend on $\mathbf{L}^0$. Therefore, for each set of initial conditions $\mathbf{L}^0$, $\mathbf{L}(t)$ can be written $\mathbf{U}(t)\mathbf{L}^0$ where the matrix $\mathbf{U}(t)$ is obtained from

$$\mathrm{d}\mathbf{U}(t)/\mathrm{d}t=\mathbb{A}(t)\mathbf{U}(t) \qquad \mathbf{U}(t_0)=\mathbf{I} \tag{7}$$

I being the $N \times N$ identity matrix. The remaining matrices **S** and **Δ** are also expressed in terms of $\mathbf{U}(t)$:

$$\mathbf{S}(t) = \mathbf{U}(t)\mathbf{S}^0\mathbf{U}(t)^{\mathrm{T}} \qquad \mathbf{\Delta}(t) = \mathbf{U}(t)\mathbf{\Delta}^0\mathbf{U}(t)^{\mathrm{T}}. \tag{8}$$

If the operators L_j, $j = 1, 2, \ldots, N$, span an N-dimensional Lie algebra, one may define a formal time-evolution operator $U(t, t_0)$, $U(t_0, t_0)$ being the identity operator $\hat{1}$, in terms of the matrix elements U_{jk} of **U** as follows:

$$U(t, t_0)^{\dagger} L_j U(t, t_0) = \sum_{k=1}^{N} U_{jk} L_k \tag{9}$$

in which † stands for adjoint. This is not a true time-evolution operator because it depends on the state of the sytem. Rather, $U(t, t_0)$ is a unitary operator that can be obtained from the solution of

$$\mathrm{i}\hbar \frac{\mathrm{d}}{\mathrm{d}t} U(t, t_0) = \mathscr{H} U(t, t_0) \tag{10}$$

where $\mathscr{H}$ belongs to the Lie algebra and satisfies $[\mathscr{H}, L_j] = [H, L_j]$ for all j values. Such a mathematical artifact was used to transform the nonlinear equations of motion satisfied by certain observables of a system composed of a harmonic oscillator with a nonlinear damping perturbation [9] into linear differential equations for the elements U_{jk} [10]. The previous argument is aimed to throw light on the meaning of the formal time-evolution operator $U(t, t_0)$ and to explain when one can use it.

In what follows I discuss particular conditions under which the dynamical equations (6) are linear. First, notice that if $L_1 = \hat{1}$ then $\mathbb{H}_{1j}$, Δ_{1j}, and Δ_{j1} vanish for all j values and one can reduce the dimension of the differential equations from N to $N-1$. To this end I define $(N-1)\times(N-1)$ matrices $\mathbb{A}'$, $\mathbf{\Delta}'$, and $\mathbf{U}'$ by removal of the first row and column from $\mathbb{A}$, **Δ**, and **U**, respectively. The mean-square deviations and correlations for the relevant operators L_j, $j = 2, 3, \ldots, N$, are then given by

$$\mathbf{\Delta}'(t) = \mathbf{U}'(t)\mathbf{\Delta}'^0\mathbf{U}'(t)^{\mathrm{T}} \tag{11}$$

in which $\mathbf{U}'(t)$ is the solution of

$$\mathrm{d}\mathbf{U}'(t)/\mathrm{d}t = \mathbb{A}'(t)\mathbf{U}(t) \qquad \mathbf{U}'(t_0) = \mathbf{I}' \tag{12}$$

I′ being the $(N-1)\times(N-1)$ unit matrix. A further simplification occurs when $\mathbb{A}$ only depends on **L** through the elements $\mathbb{A}_{j1}$ which are of the form

$$\mathbb{A}_{j1} = \sum_{m=1}^{N} C_{jm}\mathbf{L}_m \qquad j = 2, 3, \ldots, N \tag{13}$$

where **C** does not depend on **L**. Under these conditions one can define a new $N \times N$ matrix **Â**, independent of **L**, according to

$$\sum_{k=1}^{N} \mathbb{A}_{jk}\mathbf{L}_k = \sum_{k=1}^{N} C_{jk}\mathbf{L}_k + \sum_{k=2}^{N} \mathbb{A}_{jk}\mathbf{L}_k = \sum_{k=1}^{N} A_{jk}\mathbf{L}_k \qquad j = 2, 3, \ldots, N. \tag{14}$$

It follows from (6*a*) and (14) that the column matrix **L** is also a solution of

$$\mathrm{d}\mathbf{L}(t)/\mathrm{d}t = \mathbf{A}\mathbf{L}(t) \qquad \mathbf{L}(t_0) = \mathbf{L}^0 \tag{15}$$

where $A_{1j} = 0$ for all j values. In this last equation there is a fictitious variable: $L_1 = \langle L_1 \rangle = 1$, which is kept only to make the differential equations look more compact. According to (15) one can write $\mathbf{L}(t) = \mathbf{U}''(t)\mathbf{L}^0$, in which

$$\mathrm{d}\mathbf{U}''(t)/\mathrm{d}t = \mathbf{A}(t)\mathbf{U}''(t) \qquad \mathbf{U}''(t_0) = \mathbf{I}. \tag{16}$$

It is worth noticing that because of the conditions above the time-evolution equation for $\mathbf{\Delta}'$ is linear although the one for $\mathbf{S}$ is not. As a particular example of this result compare equations (3.10) of [9] with equations (2.15)-(2.17) of [2]. The former equations were transformed into linear differential equations by means of the above-mentioned formal time-evolution operator [10]. Of course, this trick is unnecessary as one can use the exact solutions for $\langle x\rangle$, $\langle p\rangle$, σ_{pp}, σ_{px}, and σ_{xx} to derive those for $\langle p^2\rangle$, $\langle x^2\rangle$, and $\langle px+xp\rangle$ [10].

The solutions to the general dynamical equations discussed before can be obtained in closed form in certain cases. For instance, if the matrices $\mathbb{A}'$ and $\mathbf{A}$ are time independent then

$$\mathbf{U}'(t)=\exp[(t-t_0)\mathbb{A}'] \qquad \mathbf{U}''(t)=\exp[(t-t_0)\mathbf{A}] \tag{17a}$$

$$\mathbf{L}(t)=\mathbf{U}''(t)\mathbf{L}^0 \qquad \Delta'(t)=\mathbf{U}'(t)\mathbf{\Delta}'^0\mathbf{U}'(t)^{\mathrm{T}} \tag{17b}$$

$$\mathbf{S}(t)=\mathbf{U}'(t)\mathbf{\Delta}'^0\mathbf{U}'(t)^{\mathrm{T}}-\mathbf{L}'(t)\mathbf{L}'(t)^{\mathrm{T}} \tag{17c}$$

where $\mathbf{L}'(t)$ is obtained by removing $\langle L_1\rangle=1$ from $\mathbf{L}(t)$. The nonlinear Hamiltonians discussed by Albrecht [3] and Hasse [1, 4, 5] (see also [2]) belong to such a class of systems as shown in the next section.

3. A pseudo-nonlinear frictional Hamiltonian in many dimensions

It is not the purpose of this paper to discuss the advantages and disadvantages of the various quantal frictional models. Rather, I will consider the multidimensional model proposed by Hasse [5] to illustrate the application of the quite general results developed in the previous section to a concrete case. The Hamiltonian operator is written [5]

$$H=\tfrac{1}{2}\boldsymbol{p}^{\mathrm{T}}\boldsymbol{n}\boldsymbol{p}+\tfrac{1}{2}\boldsymbol{x}^{\mathrm{T}}\boldsymbol{K}\boldsymbol{x}+\boldsymbol{g}^{\mathrm{T}}\boldsymbol{m}\boldsymbol{x}+\langle\boldsymbol{p}\rangle\boldsymbol{\gamma}(\boldsymbol{x}-\langle\boldsymbol{x}\rangle)$$
$$+\tfrac{1}{2}c[(\boldsymbol{x}-\langle\boldsymbol{x}\rangle)^{\mathrm{T}}\boldsymbol{\gamma}(\boldsymbol{p}-\langle\boldsymbol{p}\rangle)+(\boldsymbol{p}-\langle\boldsymbol{p}\rangle)^{\mathrm{T}}\boldsymbol{\gamma}(\boldsymbol{x}-\langle\boldsymbol{x}\rangle)] \tag{18}$$

in which $\boldsymbol{x}$, $\boldsymbol{p}$, and $\boldsymbol{g}$ are column matrices for the coordinate, momenta and constant acceleration vector, respectively, $\boldsymbol{K}$, $\boldsymbol{m}$, and $\boldsymbol{\gamma}$ are the stiffness, inertia, and friction symmetric matrices, respectively, and $\boldsymbol{n}=\boldsymbol{m}^{-1}$. Here, the set of operators $\{L_1, L_2, \ldots, L_N\}$ is given by $\{\hat{1}, x_j, p_j, j=1, 2, \ldots, M\}$. It follows from the commutation relations

$$\mathrm{i}[H, \boldsymbol{x}]/\hbar=-c\boldsymbol{\gamma}\langle\boldsymbol{x}\rangle+c\boldsymbol{\gamma}\boldsymbol{x}+\boldsymbol{n}\boldsymbol{p} \tag{19a}$$

$$\mathrm{i}[H, \boldsymbol{p}]/\hbar=-\boldsymbol{g}^{\mathrm{T}}\boldsymbol{m}+(c-1)\boldsymbol{\gamma}\langle\boldsymbol{p}\rangle-\boldsymbol{K}\boldsymbol{x}-c\boldsymbol{\gamma}\boldsymbol{p} \tag{19b}$$

that

$$\mathbb{A}'=\begin{bmatrix}\boldsymbol{\gamma}' & \boldsymbol{n}\\ -\boldsymbol{K} & -\boldsymbol{\gamma}'\end{bmatrix} \qquad \mathbf{C}=\begin{bmatrix}0 & \mathbf{0}^{\mathrm{T}} & \mathbf{0}^{\mathrm{T}}\\ \mathbf{0} & -\boldsymbol{\gamma}' & \mathbf{0}\\ -\boldsymbol{g}^{\mathrm{T}}\boldsymbol{m} & \mathbf{0} & \boldsymbol{\gamma}'-\boldsymbol{\gamma}\end{bmatrix}$$
$$\mathbf{A}=\begin{bmatrix}0 & \mathbf{0}^{\mathrm{T}} & \mathbf{0}^{\mathrm{T}}\\ \mathbf{0} & \mathbf{0} & \boldsymbol{n}\\ -\boldsymbol{g}^{\mathrm{T}}\boldsymbol{m} & -\boldsymbol{K} & -\boldsymbol{\gamma}\end{bmatrix} \tag{20}$$

where $\boldsymbol{\gamma}'=c\boldsymbol{\gamma}$ and $\mathbf{0}$ is an $M\times 1$ column matrix of zeros. If the eigenvalues of $\mathbb{A}'$ and $\mathbf{A}$ are known one can easily express $\mathbf{U}'(t)$ and $\mathbf{U}''(t)$ as polynomial functions of $\mathbb{A}'$ and

A. This is not a difficult task because the number of collective degrees of freedom in frictional models is small [1]. It is therefore concluded that the equations of motion for the frictional model (18) can be easily solved in a more general case than that in which $\boldsymbol{m}$, $\boldsymbol{K}$ and γ are diagonal [5].

4. Further comments and conclusions

In this paper I discuss the solutions of the equations of motion for pseudo-nonlinear Hamiltonians. The general results of section 2 apply to a wide class of quantum mechanical problems in addition to the frictional models considered above. As an example I mention the local harmonic approximation to dynamical phenomena which is based on the expansion of the potential surface around the trajectory of the wavepacket so that the resulting Hamiltonian depends on the expectation values of the coordinates [6]. Commonly it is not considered to be nonlinear because the expectation values of the coordinates and momenta satisfy classical equations of motion and appear in the model potential merely as functions of time. However, the Hamiltonian actually depends on the initial position of the wavepacket and thereby on the dynamical state. One can reduce the number of differential equations to be solved by writing them in such an apparent nonlinear way [7].

In section 2 I considered that the system may not be in a pure state. However, in the case of the model treated in section 3 one can assume that the solutions of the equations of motion yield the position widths and other parameters of a wavepacket [1, 3–5].

The advantage of introducing abstract operators in section 2 is that the results apply to a wider class of problems. One can treat, for instance, degrees of freedom which have no classical analogue.

It has been argued that the frictional model in section 3 can be improved by allowing c to depend on time in a prescribed way [3]. Equations (11), (12), (15) and (16) also apply in this more general case, although one cannot expect to solve equations (12) and (16) exactly for an arbitrary $c(t)$. However, numerical solutions may be obtained quite easily.

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