Time-evolution operator and propagator for quadratic Hamiltonians

1988 J. Phys. A: Math. Gen. 21 1357

(http://iopscience.iop.org/0305-4470/21/6/012)

J. Phys. A: Math. Gen. **21** (1988) 1357-1359. Printed in the UK

Time-evolution operator and propagator for quadratic Hamiltonians

Francisco M Fernández

Instituto de Investigaciones Fisicoquímicas Teóricas y Aplicadas (INIFTA), División Química Teórica, Sucursal 4, Casilla de Correo 16, 1900 La Plata, Argentina

Received 15 July 1987, in final form 7 October 1987

Abstract. The time-evolution operator and the propagator for a general one-dimensional quadratic Hamiltonian are obtained. The method is based on the equations of motion for the coordinate and momentum in the Heisenberg representation and the problem is reduced to solving the classical equations of motion.

1. Introduction

The harmonic oscillator with linear and bilinear terms in coordinates and momenta proves to be a useful model for a number of physical phenomena (Gazdy and Micha 1985, Braum 1985, Um *et al* 1987 and references therein). The exact form of the time-evolution operator and propagator for the one-dimensional case has already been obtained (Pechukas and Light 1966, Gazdy and Micha 1985, Fernández and Castro 1987a, Landovitz *et al* 1983, Um *et al* 1987). Although the time-evolution operator for the general multidimensional quadratic Hamiltonian has also been obtained (Fernández and Castro 1987b) the calculation of physical properties does not appear to be an easy task.

The purpose of this paper is to present an alternative method that yields both the time-evolution operator and propagator simultaneously. Because of its simplicity, the procedure may in principle be generalised to handle more than one degree of freedom.

2. Equations of motion

A general one-dimensional quadratic Hamiltonian can be written (units are chosen so that $\hbar = 1$)

$$H = \sum_{j=1}^{5} f_j(t) x_j \tag{1}$$

where $f_j(t)$, $j = 1, 2, \ldots, 5$, are real continuous functions of time, $x_1 = \frac{1}{2}q^2$, $x_2 = \frac{1}{2}(qp + pq)$, $x_3 = \frac{1}{2}p^2$, $x_4 = q$, $x_5 = p$ and $p = -\mathrm{i}\,\mathrm{d}/\mathrm{d}q$. The time-evolution operator $U(t, t_0)$ is a solution of the Schrödinger equation $\mathrm{d}U/\mathrm{d}t = -\mathrm{i}HU$ with the initial condition $U(t_0, t_0) = I$, where I is the identity operator. Both the time-evolution operator and the propagator $K(q, t; q_0, t_0)$ can be simultaneously determined because they are related by (Pechukas and Light 1966) $K(q, t; q_0, t_0) = U(t, t_0)\delta(q - q_0)$ where δ is the Dirac delta function.

The present method is based on the equations of motion for the coordinate and momentum operators in the Heisenberg representation, $q_t = U^+ qU$ and $p_t = U^+ pU$, respectively, that obey $\mathrm{d}O_t = \mathrm{i}U^+(HO - OH)U$, where $O = q, p$. Therefore, they can be written (Fernández and Castro 1987a, b) $q_t = Q_0(t) + Q_1(t)q + Q_2(t)p$ and $p_t = P_0(t) + P_1(t)q + P_2(t)p$, where the functions Q_j and P_j are solutions of the classical equations of motion

$$\begin{aligned} \dot{Q}_j &= f_2 Q_j + f_3 P_j + f_5 \delta_{j0} \\ \dot{P}_j &= -f_1 Q_j - f_2 P_j - f_4 \delta_{j0} \end{aligned} \qquad j = 0, 1, 2 \tag{2}$$

with the initial conditions $Q_0 = P_0 = Q_2 = P_1 = 0$ and $Q_1 = P_2 = 1$ at $t = t_0$. Since $q_t p_t - p_t q_t = \mathrm{i}$ we have $Q_1 P_2 - Q_2 P_1 = 1$ for all t values.

It is worth noticing that it is not necessary to know the form of the wavefunction in order to calculate matrix elements or expectation values at $t = t$ (Um *et al* 1987) since they are simply obtained from their values at $t = t_0$. In other words, the dynamics of the quantum mechanical system is determined by the classical equations of motion. In fact, if $W(p, q, t)$ satisfy $W_t = W(p_t, q_t, t)$, then $\langle \psi_n(t) | W \psi_m(t) \rangle = \langle \psi_n(t_0) | W(p_t, q_t, t) \psi_m(t_0) \rangle$.

3. The time-evolution operator and propagator

Since the operators x_j $(j = 1, 2, \ldots, 5)$ and $x_6 = I$ span a six-dimensional Lie algebra the time-evolution operator can be written (Wei and Norman 1963)

$$U = \prod_{j=1}^{6} U_j \qquad U_j = \exp\{\mathrm{i}a_j(t) x_j\} \tag{3}$$

where $a_j(t)$, $j = 1, 2, \ldots, 6$, are real functions of time that vanish at $t = t_0$. The trivial phase factor $\exp(\mathrm{i}a_6)$ is disregarded from now on.

It seems to be necessary to distinguish two levels of 'solvability'. First, whenever H can be written as a linear combination of operators spanning a finite-dimensional Lie algebra, the form of U is exactly known (Wei and Norman 1963) (equation (3) is merely an example). However, the analytical dependence of U on t can only be determined provided certain differential equations, such as the classical equations of motion (2) or those discussed by Wei and Norman (1963), are solved by quadrature. Some particular cases are discussed by Landovitz *et al* (1979) and Um *et al* (1987).

In order to obtain the propagator one can use the representation

$$\delta(q - q_0) = (2\pi)^{-1} \int_{-\infty}^{\infty} u_k \, \mathrm{d}k \tag{4}$$

where $u_k = \exp[\mathrm{i}k(q - q_0)]$. Since u_k is an eigenfunction of p with eigenvalue k it follows immediately that

$$v_k = U u_k = b_2^{1/2} \exp\{\mathrm{i}[k(b_2 q - q_0 + a_5) + a_4 b_2 q + \tfrac{1}{2} a_3 (k + a_4)^2 + \tfrac{1}{2} a_1 q^2]\} \tag{5}$$

where $b_2 = \exp(a_2)$. Besides, v_k satisfies

$$U^+ p v_k = p_t u_k \tag{6a}$$

$$\frac{\partial}{\partial k} u_k = \mathrm{i}(q - q_0) u_k = U^+ \frac{\partial}{\partial k} v_k = \mathrm{i}[b_2 q_t - q_0 + a_5 + a_3(k + a_4)] u_k. \tag{6b}$$

A straightforward algebraic manipulation of these last equations yields

$$a_1 = P_1/Q_1 \qquad a_2 = -\ln Q_1 \qquad a_3 = -Q_2/Q_1$$
$$a_4 = Q_1P_0 - Q_0P_1 \qquad a_5 = Q_2P_0 - Q_0P_2. \tag{7}$$

Clearly, the functions a_j (except a_6), and thereby U, are obtained from the classical equations of motion.

Finally, the propagator is given by

$$K = (2\pi)^{-1} \int_{-\infty}^{\infty} v_k \, \mathrm{d}k \tag{8}$$

which, except for a phase factor, leads to

$$K = (2\pi Q_2)^{-1/2} \exp[\mathrm{i}(2Q_2)^{-1}(P_2q^2 - 2qq_0 + 2a_5q + Q_1q_0^2 + 2Q_0q_0)] \tag{9}$$

in agreement with the result obtained by Landovitz *et al* (1983). The main advantage of the present procedure is, in addition to its simplicity, that it yields both U and K simultaneously and avoids the tiresome calculation of commutators characteristic of the algebraic methods. The general multidimensional problem will be investigated in a forthcoming paper.

Note added in proof. The time-evolution operator and propagator for the general multidimensional model was obtained some time ago by M Kolsrud (1956 *Phys. Rev.* **104** 1186). I am most grateful to Professor S T Epstein (University of Wisconsin-Madison) for having called my attention to this paper.

References

Braun E 1985 *Physica* **129A** 262
Fernández F M and Castro E A 1987a *Int. J. Quantum Chem.* **32** 591
—— 1987b *Phys. Lett.* A in press
Gazdy B and Micha D A 1985 *J. Chem. Phys.* **82** 4926
Landovitz L F, Levine A M, Ozizmir E and Schreiber W M 1983 *J. Chem. Phys.* **78** 291
Landovitz L F, Levine A M and Schreiber W M 1979 *Phys. Rev.* A **20** 1162
Pechukas P and Light J C 1966 *J. Chem. Phys.* **44** 3897
Um C I, Yeon K H and Kahng W H 1987 *J. Phys. A: Math. Gen.* **20** 611
Wei J and Norman E 1963 *J. Math. Phys.* **4** 575