Exact Quantum Dynamical Solutions for Oscillator-Like Systems*

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The solution of the quantum dynamical equation $i\hbar dT/dt = HT$, for the time-displacement operator T, is given, when the Hamiltonian H is a polynomial of the second degree in canonically conjugate variables, with arbitrary time-dependent coefficients. Heisenberg's equations of motion are then solved, and the general integral of Schrödinger's equation in coordinate space is expressed by the Green's function corresponding to T. An example is given.

INTRODUCTION

HERE are very few cases in which the exact solutions of the quantum-mechanical equations of motion are known. For a certain class, however, it is possible to obtain explicit solutions, or rather to express the quantum-mechanical solutions in terms of the classical ones. This class consists of systems whose Hamiltonians are polynomials of the second degree in canonically conjugate dynamical variables (i.e., "oscillator-like"). As these systems play a rather important role in quantum theory, it seems worth while to present briefly an exact treatment of their dynamics.

In order to study the variation with time of the state or, of the dynamical variables, of a system, it is convenient to introduce the unitary time-displacement operator T, which satisfies¹

$$ihdT/dt = HT, T(0) = 1.$$
 (1)

The solution of Heisenberg's equation of motion for a given dynamical variable v(p,q) is then expressed by

$$v_t(p,q) = T^{\dagger}v(p,q)T = v(p_t,q_t). \tag{2}$$

The solution of Schrödinger's equation of motion for the state $|t\rangle$, when the initial state $|0\rangle$ at t=0 is known, is given by

$$|t\rangle = T|0\rangle. \tag{3}$$

In this paper we first present (without proof) an explicit expression for the operator T, for the case in which the Hamiltonian has the following form:

$$H = \frac{1}{2}A_{ij}p_{i}p_{j} + a_{i}p_{i} + \frac{1}{2}B_{ij}q_{i}q_{j} + b_{i}q_{i} + \frac{1}{2}C_{ij}(p_{i}q_{j} + q_{j}p_{i})$$

= $\frac{1}{2}\mathbf{p}\cdot\mathbf{A}\cdot\mathbf{p} + \mathbf{a}\cdot\mathbf{p} + \frac{1}{2}\mathbf{q}\cdot\mathbf{B}\cdot\mathbf{q} + \mathbf{b}\cdot\mathbf{q}$
+ $\frac{1}{2}(\mathbf{p}\cdot\mathbf{C}\cdot\mathbf{q} + \mathbf{q}\cdot\mathbf{C}^{T}\cdot\mathbf{p}).$ (4)

The upper limit of the summation, say n, is unspecified. The *n*-dimensional vectors **a**,**b** and tensors (dyadics) $A = A^{T}[(A^{T})_{ij} \equiv A_{ji}], B = B^{T}, C$ are arbitrary functions of the time. Their components are c-numbers. The dynamical variables p and q have commutators

$$[p_m,q_n] = -i\hbar\delta_{mn}$$

* The main results in this paper were presented at the Meetings of the Norwegian Physical Society held in Bergen 1953 and in Oslo 1955. A more extensive paper with proofs and applications will be published elsewhere.

By means of this T operator, the explicit form of the moving operators \mathbf{p}_t and \mathbf{q}_t will be given. The timedependent state function in coordinate space is then expressed by an integral operation on the initial state function, and the corresponding kernel is given. Finally the formulas are applied to a typical case, viz., a 3-dimensional harmonic oscillator in a time-dependent homogeneous magnetic field and the corresponding (induced) circular electric field. In order to cover a greater variety of special cases, we add an extra homogeneous time-dependent field.

MATHEMATICAL PROCEDURE

Our method consists mainly in using unitary transformations, i.e. $(S^{\dagger} = S)$

$$\xi_{tr} = \exp(iS/\hbar)\xi \exp(-iS/\hbar) = \xi + (i/\hbar)[S,\xi] + \frac{1}{2}(i/\hbar)^2[S,[S,\xi]] + \cdots,$$

of the following kinds²:

$$S = f(\mathbf{p}), \qquad \mathbf{q}_{tr} = \mathbf{q} + \frac{\partial f}{\partial \mathbf{p}}, \qquad \mathbf{p}_{tr} = \mathbf{p},$$

$$S = g(\mathbf{q}), \qquad \mathbf{q}_{tr} = \mathbf{q}, \qquad \mathbf{p}_{tr} = \mathbf{p} - \frac{\partial g}{\partial \mathbf{q}},$$

$$S = \frac{1}{2} (\mathbf{p} \cdot \Gamma \cdot \mathbf{q} + \mathbf{q} \cdot \Gamma^T \cdot \mathbf{p}),$$

$$\mathbf{q}_{tr} = e^{\Gamma} \cdot \mathbf{q}, \qquad \mathbf{p}_{tr} = \mathbf{p} \cdot e^{-\Gamma} \cdot \mathbf{p},^3$$

where Γ^{T} (and e^{Γ}) are tensors. In addition, we utilize a formula, which we present without derivation²:

$$i\hbar(\partial/\partial t) \exp\left[-\frac{1}{2}i\hbar^{-1}(\mathbf{p}\cdot\Gamma\cdot\mathbf{q}+\mathbf{q}\cdot\Gamma^{T}\cdot\mathbf{p})\right]$$

=\frac{1}{2}(\mbox{p}\cdot \mbox{C}\cdot \mbox{q}+\mbox{q}\cdot \mbox{C}^{T}\cdot \mbox{p}) \exp[-\frac{1}{2}i\hbar^{-1}(\mbox{p}\cdot \mbox{r}\cdot \mbox{q}+\mbox{q}\cdot \mbox{\Gamma}^{T}\cdot \mbox{p})],

where

$$(\partial/\partial t)e^{\Gamma} = \mathbf{C} \cdot e^{\Gamma}.$$

The "deformation" tensor e^{Γ} can be factorized into a rotation part e^{Φ} and a dilatation part e^{Δ} :

$$e^{\Gamma} = e^{\Phi} \cdot e^{\Delta}, \quad \Phi^{T} = -\Phi, \quad \Delta^{T} = \Delta,$$

where

$$e^{\Delta} = [(e^{\Gamma})^T \cdot e^{\Gamma}]^{\frac{1}{2}}, \quad e^{\Phi} = e^{\Gamma} \cdot [(e^{\Gamma})^T \cdot e^{\Gamma}]^{-\frac{1}{2}}$$

If we introduce the principal axes of Δ as coordinate

¹ P. A. M. Dirac, *The Principles of Quantum Mechanics* (Clarendon Press, Oxford, 1947), third edition, p. 110.

² They can be proved directly by series expansion.
³ A special form of this unitary operator has also been used by J. Plebanski, Phys. Rev. 101, 1825 (1956).

axes, the dilatation tensor has the component matrix

$$\begin{bmatrix} e^{\Delta} \end{bmatrix} = \begin{pmatrix} e^{\Delta'} & 0 & \cdots \\ 0 & e^{\Delta''} & \cdots \\ \cdots & \cdots & \cdots \end{pmatrix}.$$

The transformation $e^{\Delta} \cdot \mathbf{q}$ thus consists of multiplying each component of \mathbf{q} along the principal axes of e^{Δ} by the corresponding eigenvalue of e^{Δ} .

The rotation tensor e^{Φ} may, in the 3-dimensional case, be expressed in the following way:

$$\Phi = \phi \epsilon \times I, \quad e^{\Phi} = \epsilon \epsilon + (I - \epsilon \epsilon) \cos \phi + \epsilon \times I \sin \phi$$

(I=unit tensor, $\varepsilon =$ unit vector). In an orthogonal coordinate system ε_1 , ε_2 , $\varepsilon_3 = \varepsilon$, the rotation tensor e^{Φ} has the component matrix

$$\begin{bmatrix} e^{\Phi} \end{bmatrix} = \begin{bmatrix} \cos\phi & -\sin\phi & 0 \\ \sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{bmatrix}.$$

The tensor $\exp(\phi \times I)$ thus brings about a rotation by an angle ϕ about the axis ϕ . This corresponds to

$$S = \frac{1}{2} (\mathbf{p} \cdot \mathbf{\Phi} \cdot \mathbf{r} + \mathbf{r} \cdot \mathbf{\Phi}^T \cdot \mathbf{p}) = \boldsymbol{\phi} \cdot (\mathbf{r} \times \mathbf{p})$$

In passing, we note that if⁴

$$[\Gamma; [\Gamma; \Gamma^T]] = 0,$$

it can be shown that

$$\Phi = \frac{1}{2} (\Gamma - \Gamma^{T}), \quad \Delta = \frac{1}{2} (\Gamma + \Gamma^{T}) + \frac{1}{4} [\Gamma^{T}; \Gamma],$$

$$\Gamma = \Phi + \Delta + \frac{1}{2} [\Phi; \Delta].$$

TIME-DISPLACEMENT OPERATOR

The solution of Eqs. (1) and (4) can be given in the following form:

$$T = \exp[-i\hbar^{-1}(\frac{1}{2}\mathbf{q}\cdot\mathbf{G}\cdot\mathbf{q}+\boldsymbol{\beta}\cdot\mathbf{q}+\boldsymbol{\sigma})] \\ \times \exp[-i\hbar^{-1}\frac{1}{2}(\mathbf{p}\cdot\Gamma\cdot\mathbf{q}+\mathbf{q}\cdot\Gamma^{T}\cdot\mathbf{p})] \\ \times \exp[-i\hbar^{-1}(\frac{1}{2}\mathbf{p}\cdot\mathbf{G}\cdot\mathbf{p}+\boldsymbol{\alpha}\cdot\mathbf{p})], \quad (5)$$

where the tensors $\alpha = \alpha^T$, $\beta = \beta^T$, Γ , the vectors α , β and the scalar σ are functions of time given by

$$d\mathfrak{B}/dt + \mathfrak{B} \cdot \mathbb{C} + \mathbb{C}^T \cdot \mathfrak{B} - \mathfrak{B} \cdot \mathbb{A} \cdot \mathfrak{B} = \mathbb{B}, \quad \mathfrak{B}(0) = 0,$$

$$e^{\Gamma} \equiv \mathbb{C}, \quad d\mathbb{C}/dt = (\mathbb{C} - \mathbb{A} \cdot \mathbb{B}) \cdot \mathbb{C}, \quad \Gamma(0) = 0, \quad \mathbb{C}(0) = \mathbb{I},$$

$$\mathbb{Q} = \int_{0}^{t} \mathbb{C}^{-1} \cdot \mathbb{A} \cdot (\mathbb{C}^{T})^{-1} dt,$$

$$\mathfrak{g} = (\mathbb{C}^{T})^{-1} \cdot \int_{0}^{t} \mathbb{C}^{T} \cdot (\mathbf{b} - \mathbb{B} \cdot \mathbf{a}) dt,$$

$$\alpha = \int_{0}^{t} \mathbb{C}^{-1} \cdot (\mathbf{a} - \mathbb{A} \cdot \mathfrak{g}) dt,$$

$$\sigma = \int_{0}^{t} (\frac{1}{2} \mathfrak{g} \cdot \mathbb{A} \cdot \mathfrak{g} - \mathbf{a} \cdot \mathfrak{g}) dt.$$
(6)

 $[A; B] = A \cdot B - B \cdot A$.

It is possible to give other explicit forms of T, for example

$$T = T_1 \exp\left[-i\hbar^{-1}\tau(t)H_0\right],$$

where H_0 is some time-independent part of H. This form is clearly convenient when the initial state is an eigenstate of H_0 .

DYNAMICAL VARIABLES

From (2) and (5) we obtain the following expressions for the moving (Heisenberg) coordinates and momenta:

$$\mathbf{q}_{t} = T^{\dagger} \mathbf{q} T = \mathbf{C} \cdot \mathbf{q} + \mathbf{C} \cdot \mathbf{\alpha} \cdot \mathbf{p} + \mathbf{C} \cdot \mathbf{\alpha},$$

$$\mathbf{p}_{t} = T^{\dagger} \mathbf{p} T = ((\mathbf{C}^{T})^{-1} - \mathbf{G} \cdot \mathbf{C} \cdot \mathbf{\alpha}) \cdot \mathbf{p} - \mathbf{G} \cdot \mathbf{C} \cdot \mathbf{q} \qquad (7)$$

$$- (\mathbf{g} + \mathbf{G} \cdot \mathbf{C} \cdot \mathbf{\alpha}).$$

These operator functions \mathbf{q}_t and \mathbf{p}_t are formally the same as the classical solutions, say $\mathbf{q}(t)$ and $\mathbf{p}(t)$, of Hamilton's equations

$$\frac{d\mathbf{q}(t)}{dt} = \frac{\partial H}{\partial \mathbf{p}(t)} = \mathbf{A} \cdot \mathbf{p}(t) + \mathbf{C} \cdot \mathbf{q}(t) + \mathbf{a},$$
$$\frac{d\mathbf{p}(t)}{dt} = -\frac{\partial H}{\partial \mathbf{q}(t)} = -\mathbf{B} \cdot \mathbf{q}(t) - \mathbf{C}^{T} \cdot \mathbf{p}(t) - \mathbf{b}.$$

The initial operators \mathbf{q} and \mathbf{p} correspond to the classical constants of integration $\mathbf{q}(0)$ and $\mathbf{p}(0)$. The agreement is of course a general property of the Heisenberg operators in a classical-like system, apart from the symmetrized form of operator products. Because, however, \mathbf{q}_t and \mathbf{p}_t are *linear* functions of the operators \mathbf{q} and \mathbf{p} , the expectation values $\langle \mathbf{q}_t \rangle$ and $\langle \mathbf{p}_t \rangle$ will also agree with the classical solutions. Different states just imply different values of the initial constants $\langle \mathbf{q} \rangle = \mathbf{q}(0)$ and $\langle \mathbf{p} \rangle = \mathbf{p}(0)$.

As an application of (7) we shall find the connection between the movement of the "center" and the variation of the "width" of an arbitrary wave packet in coordinate space.^{3,5} This connection is demonstrated by comparing $\langle \mathbf{q}_l \rangle$ with the mean square deviation in position

$$egin{aligned} &\langle \mathbf{q}_t^2
angle - \langle \mathbf{q}_t \mathcal{D}^2 \cdot \mathbf{q}
angle - \langle \mathbf{q}
angle \cdot \mathcal{D}^2 \cdot \langle \mathbf{q}
angle \ &+ \langle \mathbf{p} \cdot \mathbf{\alpha} \cdot \mathcal{D}^2 \cdot \mathbf{\alpha} \cdot \mathbf{p}
angle - \langle \mathbf{p}
angle \cdot \mathbf{\alpha} \cdot \mathcal{D}^2 \cdot \mathbf{\alpha} \cdot \langle \mathbf{p}
angle \ &+ \langle \mathbf{q} \cdot \mathcal{D}^2 \cdot \mathbf{\alpha} \cdot \mathbf{p}
angle + \langle \mathbf{p} \cdot \mathbf{\alpha} \cdot \mathcal{D}^2 \cdot \mathbf{q}
angle \ &- \langle \mathbf{q}
angle \cdot \mathcal{D}^2 \cdot \mathbf{\alpha} \cdot \langle \mathbf{p}
angle - \langle \mathbf{q}
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angle - \langle \mathbf{q}
angle \cdot \mathcal{D}^2 \cdot \mathbf{\alpha} \cdot \langle \mathbf{p}
angle - \langle \mathbf{p}
angle \cdot \mathbf{\alpha} \cdot \mathcal{D}^2 \cdot \langle \mathbf{q}
angle \end{aligned}$$

Here we have introduced the dilatation tensor $\mathfrak{D} \equiv e^{\Delta} = (\mathfrak{C}^T \cdot \mathfrak{C})^{\frac{1}{2}}$. We notice that the variation with time of the width is closely connected with the homogeneous solution

$$\langle (\mathbf{q}_t)_{\mathrm{hom}} \rangle = e^{\Phi} \cdot \mathfrak{D} \cdot \langle \mathbf{q} \rangle + e^{\Phi} \cdot \mathfrak{D} \cdot \mathfrak{a} \cdot \langle \mathbf{p} \rangle$$

for the movement of the wave packet (i.e., independent of a and b).

⁵ I. R. Senitzky, Phys. Rev. 95, 1115 (1954).

STATE FUNCTION

The coordinate representation of (3) is

$$\psi(\mathbf{q},t) = T(\mathbf{q}, -i\hbar\partial/\partial\mathbf{q}, t)\psi(\mathbf{q},0).$$

This differential operation on the initial state $\psi(\mathbf{q},0)$ can be expressed by an integral operation in the n-dimensional \mathbf{q} space:

$$\psi(\mathbf{q},t) = \int d_n \mathbf{q}' K(\mathbf{q}',\mathbf{q},t) \psi(\mathbf{q}',0).$$

We obtain the kernel

$$\begin{split} K(\mathbf{q}',\mathbf{q},t) &= \left[(i\hbar)^n \exp\left(\sum \Gamma_{ii}\right) \det \alpha \right]^{-\frac{1}{2}} \\ \times \exp\left[-i\hbar^{-1} \left(\frac{1}{2}\mathbf{q} \cdot \mathfrak{G} \cdot \mathbf{q} + \boldsymbol{\mathfrak{g}} \cdot \mathbf{q} + \sigma\right) \right] \\ \times \exp\left[i\hbar^{-1} \left[\left(\mathbf{q}' + \boldsymbol{\alpha} - \mathfrak{C}^{-1} \cdot \mathbf{q}\right) \right] \\ \cdot \mathfrak{C}^{-1} \cdot \left(\mathbf{q}' + \boldsymbol{\alpha} - \mathfrak{C}^{-1} \cdot \mathbf{q}\right) \right] \end{split}$$

EXAMPLE

As a typical example we choose the Hamiltonian

$$H = (1/2m) \{ \mathbf{p} - (e/c)\mathbf{A} \}^2 + \frac{1}{2}m\omega_0^2 \mathbf{r}^2 - \mathbf{F} \cdot \mathbf{r},$$

where

$$\mathbf{A} = \frac{1}{2}H(t)\mathbf{k} \times \mathbf{r}, \quad \mathbf{F} = \mathbf{F}(t).$$

The classical equation of motion is, accordingly

$$m\frac{d^{2}\mathbf{r}}{dt^{2}} = -m\omega_{0}\mathbf{r} - \left(\frac{e}{2c}\right)\frac{d\mathbf{H}}{dt} \times \mathbf{r} + \left(\frac{e}{c}\right)\frac{d\mathbf{r}}{dt} \times \mathbf{H} + \mathbf{F}.$$

By writing

$$H = (1/2m)(p_x^2 + p_y^2 + p_z^2) + \frac{1}{2}m\{(\omega_0^2 + \omega^2)(x^2 + y^2) + \omega_0^2 z^2\} + \omega(xp_y - yp_x) - (F_x x + F_y y + F_z z),$$

where

$$\omega \equiv -eH(t)/2mc$$
,
we see that

$$\begin{bmatrix} A \end{bmatrix} = \frac{1}{m} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \begin{bmatrix} B \end{bmatrix} = m \begin{pmatrix} \omega_0^2 + \omega^2 & 0 & 0 \\ 0 & \omega_0^2 + \omega^2 & 0 \\ 0 & 0 & \omega_0^2 \end{pmatrix},$$
$$\begin{bmatrix} C \end{bmatrix} = \omega \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \mathbf{a} = 0, \quad \mathbf{b} = -\mathbf{F}.$$

From Eqs. (6) we get the following expressions (the tensors are given by the matrices of their components):

$$\begin{bmatrix} (3) \end{bmatrix} = -m \begin{bmatrix} \dot{\delta}\delta^{-1} & 0 & 0 \\ 0 & \dot{\delta}\delta^{-1} & 0 \\ 0 & 0 & \dot{\delta}_{0}\delta_{0}^{-1} \end{bmatrix}, \quad \delta_{0} = \cos\omega_{0}t,$$

$$d^{2}\delta/dt^{2} + (\omega_{0}^{2} + \omega^{2})\delta = 0, \quad \delta(0) = 1, \quad \dot{\delta}(0) = 0,$$

$$\begin{bmatrix} \Gamma \end{bmatrix} = \begin{bmatrix} \Phi \end{bmatrix} + \begin{bmatrix} \Delta \end{bmatrix}$$

$$= \phi \begin{bmatrix} 0 & -1 & -0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} + \begin{bmatrix} \ln\delta & 0 & 0 \\ 0 & \ln\delta & 0 \\ 0 & 0 & \ln\delta_{0} \end{bmatrix}, \quad \phi = \int_{0}^{t} \omega dt,$$

$$\begin{bmatrix} C \end{bmatrix} = \begin{bmatrix} e^{\Phi} \end{bmatrix} \cdot \begin{bmatrix} e^{\Delta} \end{bmatrix} = \begin{bmatrix} \cos\phi & -\sin\phi & 0 \\ \sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{bmatrix} \cdot \begin{bmatrix} \delta & 0 & 0 \\ 0 & \delta & 0 \\ 0 & 0 & \delta_{0} \end{bmatrix},$$

(notice that $\begin{bmatrix} \Phi; \Delta \end{bmatrix} = 0, \text{ or } [\Gamma; \Gamma^{T}] = 0),$
$$\begin{bmatrix} C \end{bmatrix} = \frac{1}{m} \int_{0}^{t} \begin{bmatrix} \delta^{-2} & 0 & 0 \\ 0 & \delta^{-2} & 0 \\ 0 & 0 & \delta_{0}^{-2} \end{bmatrix} dt, \quad \alpha_{zz} = \frac{1}{m\omega_{0}} \tan\omega_{0}t,$$

 $m\omega_0$

$$\boldsymbol{\beta} = -e^{-\Delta} \cdot e^{\Phi} \cdot \int_{0}^{t} e^{-\Phi} \cdot e^{\Delta} \cdot \mathbf{F} dt,$$
$$\boldsymbol{\beta}_{z} = -\frac{1}{\cos\omega_{0}t} \int_{0}^{t} \cos\omega_{0}t' F_{z}(t') dt',$$

$$\alpha = \int_{0}^{t} \left[\alpha(t) - \alpha(t') \right] \cdot e^{-\Phi(t')} \cdot e^{\Delta(t')} \cdot \mathbf{F}(t') dt',$$
$$\alpha_{z} = \frac{1}{m\omega_{0} \cos\omega_{0}t} \int_{0}^{t} \sin\omega_{0}(t-t') F_{z}(t') dt',$$
$$\sigma = \frac{1}{m\omega_{0}} \int_{0}^{t} \beta^{2} dt,$$

$$\sigma = \frac{1}{2m} \int_0^t \mathcal{G}^2 dt.$$