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Exact solutions to operator differential equations

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This paper considers the Heisenberg equations of motion $\dot{q}=-i[q,H],\dot{p}=-i[p,H]$, for the quantum-mechanical Hamiltonian $H(p,q)$ having one degree of freedom. It is a commonly held belief that such operator differential equations are intractable. However, a technique is presented here that allows one to obtain exact, closed-form solutions for huge classes of Hamiltonians. This technique, which is a generalization of the classical action-angle-variable methods, allows us to solve, albeit formally and implicitly, the operator differential equations of the anharmonic oscillator whose Hamiltonian is $H=p^2/2+q^4/4$.

The classical Hamiltonian $H(p,q)$ describes a dynamical system that evolves according to the time-evolution equations

$$\dot{q}=\frac{\partial H}{\partial p}\,,\quad \dot{p}=-\frac{\partial H}{\partial q}\,, \tag{1}$$

and satisfies the initial conditions $p(0)=p_0$, $q(0)=q_0$. Although (1) is equivalent to a single second-order differential equation, it is often possible to find a closed-form solution because the Hamiltonian H is a constant of the motion. Thus, in principle we can use the algebraic equation $H(p,q)=E$ to solve for and eliminate one of the variables $p(t)$ or $q(t)$ in (1) and then to solve the resulting *first-order* differential equation for $q(t)$ or $p(t)$. For example, consider the Hamiltonian $H=p^2/2+V(q)$, for which Eq. (1) takes the form

$$\dot{q}=p\,,\quad \dot{p}=-V'(q)\,. \tag{2}$$

Now, solving $H(p,q)=E$ for $p(t)$ and using the first equation of (2) gives $\dot{q}=\{2[E-V(q)]\}^{1/2}$. This is a first-order separable equation whose implicit solution satisfying $q(0)=q_0$ is

$$F[q(t)]=t+F(q_0)\,, \tag{3}$$

where

$$F(q)=\int^q \frac{dx}{\sqrt{2[E-V(x)]}}\,. \tag{4}$$

The quantum equations of motion for the Hamiltonian $H(p,q)$ are

$$\dot{q}=-i[q,H]\,,\quad \dot{p}=-i[p,H]\,, \tag{5}$$

where the operators $q(t)$ and $p(t)$ satisfy the equal-time commutation relation $[q(t),p(t)]=i$. It is the noncommutivity of $q(t)$ and $p(t)$ that makes (5) difficult to solve if it is a nonlinear system. Only the special case of the harmonic oscillator $H=p^2/2+q^2/2$ gives rise to the easily solvable linear equations $\dot{q}=p$, $\dot{p}=-q$, whose exact solution is

$$q(t)=q_0\cos t+p_0\sin t\,, \tag{6}$$

$$p(t)=p_0\cos t-q_0\sin t\,. \tag{7}$$

We propose to solve operator equations that are nonlinear by constructing a quantum analogy to Eq. (3). Specifically, we will attempt to obtain a function of $F(p,q)$ of the operators $p(t)$ and $q(t)$ that satisfies

$$-i[F(p,q),H(p,q)]=\frac{d}{dt}F(p,q)=1\,. \tag{8}$$

[Note that F is not unique: $\bar{F}=F+\phi(H)$, where ϕ is an arbitrary function of the Hamiltonian, satisfies (8).] If such a function F can be found then of course the solution to (8),

$$F(p(t),q(t))=t+F(p_0,q_0)\,, \tag{9}$$

together with

$$H(p(t),q(t))=H(p_0,q_0)\,, \tag{10}$$

constitutes an exact *implicit* solution to the operator equations of motion (5). If we can then solve (9) and (10) simultaneously for $p(t)$ and $q(t)$ as functions of p_0, q_0, and t, we have an *explicit* solution to the equations of motion. Here are some simple examples.

Example 1. $H=(pe^q+e^qp)/2$. The operator equation of motion for q, $\dot{q}=e^q$, immediately suggests that $F(p,q)$ in (8) is actually a function of q only: $F(p,q)=-e^{-q(t)}$. The *explicit* solution to the operator equations of motion is

$$q(t)=-\ln(e^{-q_0}-t)\,,\quad p(t)=p_0-t(p_0e^{q_0}+e^{q_0}p_0)/2\,.$$

Example 2. $H=pe^{aq}p$, where a is a constant. For this Hamiltonian, a function F satisfying (5) is

$$F=-\frac{1}{a}\frac{1}{\sqrt{H}}p(t)\frac{1}{\sqrt{H}}\,.$$

The *explicit* solution to the operator equations of motion is

$$p(t) = -aH(p_0,q_0)t + p_0 ,$$
$$q(t) = -\frac{1}{a}\ln[e^{aq_0} - 2p_0 t + a^2 H(p_0,q_0)t^2] .$$

Example 3. $H = p^\alpha q^{2\beta} p^\alpha$. For this Hamiltonian it is easy to see that a function F satisfying (5) is

$$F(p,q) = \frac{1}{4\alpha - 4\beta}\frac{1}{\sqrt{H}}(pq+qp)\frac{1}{\sqrt{H}} . \tag{11}$$

Note that (11) ceases to exist when $\alpha = \beta$. However, the special case $\alpha = \beta$ gives what we call an *Euler* Hamiltonian. [By an Euler Hamiltonian, we mean one in which the operator $p(t)$ is always accompanied by a multiple of $q(t)$; that is, $H = H(pq)$.] In general, the operator equations for Euler Hamiltonians can always be solved explicitly and in closed form.[1] Solving $F(p,q) = t + F(p_0,q_0)$ simultaneously with $H(p,q) = H(p_0,q_0)$ can be complicated. However, a relatively simple case arises when $\alpha = 1$ and $\beta = N/2$. Now the explicit solution is

$$q(t) = \{[p_0 q_0 + (2-N)p_0 q_0^N p_0 t]^{-1} p_0 q_0^N \times p_0 [q_0 p_0 + (2-N)p_0 q_0^N p_0 t]^{-1}\}^{1/(N-2)} ,$$
$$p(t) = \{[q(t)]^{-N/2} p_0 q_0^N p_0 [q(t)]^{-N/2} - \tfrac{1}{4}N(N-2)[q(t)]^{-2}\}^{1/2} .$$

Example 4. $H = \alpha p^\gamma + \beta q^{-\gamma}$. Here, the form of $F(p,q)$ is similar to that in example 3:

$$F(p,q) = \frac{1}{2\gamma}\frac{1}{\sqrt{H}}(pq+qp)\frac{1}{\sqrt{H}} .$$

Our objective is now to describe a general procedure for obtaining an operator $F(p,q)$ that satisfies (8). To do so we introduce an operator basis. Our basis elements $T_{m,n}$ are defined as the sum of all possible terms containing m factors of p and n factors of q multiplied by $m!n!/(m+n)!$. $T_{m,n}$ is thus a totally symmetric Hermitian object containing $(m+n)!/(m!n!)$ individual terms. For example,

$$T_{0,0} = 1 ,$$
$$T_{0,3} = q^3 ,$$
$$T_{1,1} = (pq+qp)/2 ,$$
$$T_{2,1} = (p^2 q + pqp + qp^2)/3 ,$$
$$T_{2,2} = (p^2q^2 + q^2p^2 + pqpq + qpqp + pq^2p + qp^2q)/6 .$$

For two reasons, this seems to be a natural basis with which to express operators. First, $T_{m,n}$ contains positive powers of p and q, so it should be useful for constructing Taylor-type expansions of operators. Note that we can expand operators, regardless of whether they are symmetric. For example,

$$p^2 q^3 = T_{2,3} - 3iT_{1,2} - 3T_{0,1}/2 .$$

Second, $T_{m,n}$ satisfies an extremely useful set of commutation and anticommutation relations. Commuting with p or q has the effect of a lowering operator:

$$[T_{m,n},p] = inT_{m,n-1} ,$$
$$[T_{m,n},q] = -imT_{m-1,n} . \tag{12}$$

Anticommuting with p or q is analogous to applying a raising operator:

$$[T_{m,n},p]_+ = 2T_{m+1,n} ,$$
$$[T_{m,n},q]_+ = 2T_{m,n+1} . \tag{13}$$

Shortly, we will make use of the property that the totally symmetric operator $T_{m,n}$ can be completely reorganized using the commutation relation $[q,p] = i$ and recast in Weyl-ordered form

$$T_{m,n} = \frac{1}{2^m}\sum_{j=0}^{\infty}\binom{m}{j} p^j q^n p^{m-j} = \frac{1}{2^n}\sum_{k=0}^{\infty}\binom{n}{k} q^k p^m q^{n-k} . \tag{14}$$

The operators $T_{m,n}$ have many more remarkable properties and have played a central role in previous studies involving finite-element lattice approximations,[2] operator ordering,[3] and Hahn polynomials.[4]

Now we return to the problem of obtaining a solution to (8). We represent $F(p,q)$ as an arbitrary sum of operator basis elements:

$$F(p,q) = \sum_{m,n} \alpha_{m,n} T_{m,n} , \tag{15}$$

where $\alpha_{m,n}$ are constants to be determined from the requirement in (8) that $-i[F(p,q),H(p,q)] = 1$. To illustrate, we begin by finding $F(p,q)$ for the harmonic-oscillator Hamiltonian $H(p,q) = p^2/2 + q^2/2$. Equations (12) and (13) make the computation very easy:

$$\frac{1}{i}[T_{m,n},\tfrac{1}{2}p^2] = \frac{1}{2i}(p[T_{m,n},p] + [T_{m,n},p]p) = \frac{n}{2}[p,T_{m,n-1}]_+ = nT_{m+1,n-1} . \tag{16}$$

Similarly,

$$\frac{1}{i}[T_{m,n},\tfrac{1}{2}q^2] = -mT_{m-1,n+1} . \tag{17}$$

Combining (15)–(17), we see that the commutation relation in (8) takes the form

$$\sum_{m,n}\alpha_{m,n}(nT_{m+1,n-1} - mT_{m-1,n+1}) = T_{0,0} . \tag{18}$$

Hence, assuming completeness, we determine that the coefficients $\alpha_{m,n}$ satisfy the linear partial difference equation

$$(n+1)\alpha_{m-1,n+1} - (m+1)\alpha_{m+1,n-1} = \delta_{m,0}\delta_{n,0} . \tag{19}$$

As we pointed out earlier, F is *not* uniquely determined. We are free to take the simplest particular solution $\alpha_{m,n}$ that satisfies (19). We choose the solution

$$\alpha_{-2m-1,2m+1} = (-1)^m/(2m+1) , \quad m = 0,1,2,3,\ldots ,$$

and $\alpha_{m,n} = 0$ for other values of m,n. Thus, the formula for $F(p,q)$ in (15) becomes

$$F(p,q)=\sum_{m=0}^{\infty}\frac{(-1)^m}{2m+1}T_{-2m-1,2m+1}\,. \tag{20}$$

Observe that we are forced to generalize our initial assumption that, by analogy with Taylor series, our basis $T_{m,n}$ has $m,n\geq 0$. Apparently, a more accurate analogy is with Laurent series in which powers may be positive or negative. Fortunately, the formulas in (14) allows us to define $T_{m,n}$ when $m\geq 0$ and $n<0$ and when $n\geq 0$ and $m<0$. Moreover, the commutation and anticommutation relations in (12) and (13) continue to hold in this extended and singular basis.

In order to understand the formal series in (20) we return to the exact solution to the harmonic oscillator in (6) and (7). We divide (6) by (7) and let $Z(t)=q(t)\times[p(t)]^{-1}$:

$$\begin{aligned}Z(t)&=(q_0\cos t+p_0\sin t)(p_0\cos t-q_0\sin t)^{-1}\\&=(q_0\cos t+p_0\sin t)p_0^{-1}p_0(p_0\cos t-q_0\sin t)^{-1}\\&=(Z_0\cos t+\sin t)[(p_0\cos t-q_0\sin t)p_0^{-1}]^{-1}\\&=\frac{Z_0+\tan t}{1-Z_0\tan t}\,.\end{aligned} \tag{21}$$

Since $Z(t)$ is a function of Z_0, $Z(t)$ must commute with Z_0. Thus, we can treat (21) as a c-number algebraic equation and solve for $\tan t$: $\tan t=[Z(t)-Z_0]/[1+Z(t)Z_0]$. Finally, taking the inverse tangent of this equation, we obtain

$$\arctan Z(t)=t+\arctan Z_0\,. \tag{22}$$

This equation is an instance of (9), so we identify

$$F(p,q)=\arctan\{q(t)[p(t)]^{-1}\}\,. \tag{23}$$

Compare (20) and (23). Note that the coefficients a in (20) correspond exactly with the Taylor expansion of

$$\arctan x=\sum_{n=0}^{\infty}\frac{(-1)^n}{2n+1}x^{2n+1}\,.$$

Even more important, the physical meaning of $F(p,q)$ is now more evident: Classically, the harmonic oscillator describes an orbit in phase space which is a circle of radius $p_0^2+q_0^2$. The singular quantity $\arctan[q(t)/p(t)]$ is the *angle* θ of a point on this circle. Apparently, (20) is the generalization of the angle coordinate from a classical (c-number) theory to a quantum (operator) theory.

Finally, we consider the anharmonic oscillator whose Hamiltonian is given by $H=p^2/2+q^4/4$. To find $F(p,q)$ we first evaluate the commutator

$$\begin{aligned}i[T_{m,n},q^4]&=-m(q^3T_{m-1,n}+q^2T_{m-1,n}q+qT_{m-1,n}q^2+T_{m-1,n}q^3)\\&=-2m(q^2T_{m-1,n+1}+T_{m-1,n+1}q^2)\\&=-m(q[q,T_{m-1,n+1}]_++[T_{m-1,n+1},q]_+q+q[q,T_{m-1,n+1}]+[T_{m-1,n+1},q]q)\\&=-m(2[q,T_{m-1,n+2}]_++(m-1)i[q,T_{m-2,n+1}])\\&=-4mT_{m-1,n+3}+m(m-1)(m-2)T_{m-3,n+1}\,.\end{aligned} \tag{24}$$

Combining the result in (16) with that in (24), and assuming that the operators $T_{m,n}$ form a complete basis gives a recursion relation for $a_{m,n}$ in (15):

$$(n+1)a_{m-1,n+1}-(m+1)a_{m+1,n-3}+(m+3)(m+2)(m+1)a_{m+3,n-1}/4=\delta_{m,0}\delta_{n,0}\,. \tag{25}$$

Note that the solution to this recursion relation has nonzero coefficients for positive and negative values of both m and n. Thus, we must further generalize the operator basis $T_{m,n}$ to negative values of both m and n. We do this by expressing the binomial coefficients in (14) in terms of gamma functions. The representation for $T_{m,n}$ now becomes an *infinite* series when $n,m<0$. For example,

$$T_{-1,-1}=2\sum_{j=-\infty}^{\infty}(-1)^j p^j q^{-1}p^{-1-j}\,.$$

The singular operators $T_{m,n}$ continue to obey formally the algebraic relations in (12) and (13) even when both m and n are negative.

To solve (25) we let $m=2k$, $n=2l$, and $a_{2k+1,2l+1}=\gamma_{k,l}\Gamma(\frac{1}{2})/\Gamma(k+\frac{3}{2})$. Then $\gamma_{k,l}$ satisfies

$$(2l+1)\gamma_{k-1,l}-2\gamma_{k,l-2}+(2k+2)\gamma_{k+1,l-1}=\delta_{k,0}\delta_{l,0}\,,$$

which we solve by introducing the generating function

$$g(x,y)=\sum_{k,l}x^k y^l\gamma_{k,l}\,.$$

The function $g(x,y)$ satisfies the first-order linear partial differential equation

$$2xyg_y+2yg_x+(x-2y^2)g=1\,. \tag{26}$$

We solve (26) by making the change of variables $r=y+x^2/2$, $s=y-x^2/2$, $g(x,y)=h(r,s)$. Now, h satisfies the ordinary differential equation

$$h_r+\left[\frac{1}{2(r+s)}-\frac{r+s}{4\sqrt{r-s}}\right]h=\frac{1}{2(r+s)\sqrt{r-s}}\,,$$

whose integrating factor is $(r+s)^{1/2}\exp[-s(r-s)^{1/2}-(r-s)^{3/2}/6]$. Thus, we can express the solution to (26) in quadrature form in terms of the integral

$$\int^r dx\frac{\exp[-s\sqrt{x-s}-(x-s)^{3/2}/6]}{2\sqrt{x^2-s^2}}\,,$$

which simplifies to $\int dz\, e^{-a(z+z^3/3)}/(z^2+1)^{1/2}$, where a is a constant. This is the solution, albeit extremely singular, formal, and implicit, to the anharmonic oscillator.

The progress we have reported here is formal because the operator $F(p,q)$ can be extremely singular as it contains in many cases arbitrary powers of $1/p(t)$ and/or $1/q(t)$. If $F(p,q)$ did exist as an operator in a Hilbert space, then by virtue of (8), $U \equiv \exp[i\lambda F(p,q)]$ would be an energy raising operator. That is, if $H|E\rangle = E|E\rangle$, then $H(U|E\rangle) = (E+\lambda)(U|E\rangle)$. Clearly, for Hamiltonians with discrete spectra, U must map states out of the Hilbert space except for special discrete values of λ. A natural direction for future research is to find a way to identify these special values of λ and thereby to use the operator solution to a quantum theory to compute such quantities as eigenvalues and also unequal-time commutation relations. One should also consider applying the ideas presented here to systems having more than one degree of freedom and especially to models that exhibit quantum chaos. It was our sole intention here to point out that operator differential equations are not inaccessible to exact analytic methods and that in many cases they can actually be solved in closed form.

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