# Quantum Action-Angle Variables for the Harmonic Oscillator

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Operators conjugate to the Hamiltonian are constructed explicitly for the quantum harmonic oscillator by two approaches in the space spanned by the eigenstates of $q$ and the eigenstates of $p$. The operators are quantum analogs of a classical angle variable divided by the oscillator frequency. Matrix elements have been evaluated in the coherent state representation. Either conjugate operator can be used to construct an explicitly time-dependent operator invariant. It can be used as the starting point in a new perturbative procedure for constructing invariant operators for nonlinear, nonautonomous Hamiltonians. [S0031-9007(96)01905-9]

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The asymmetry between space and time in quantum theory runs deeper in quantum mechanics than in classical mechanics. Time is simply a parameter in both cases, but position coordinates are operators in quantum mechanics. For any autonomous classical Hamiltonian $H(q,p)$, time along the phase-space trajectory that represents a solution of Hamilton's equations can be expressed in terms of the canonical variables $(q,p)$. That "time function" is canonically conjugate to the Hamiltonian [1]. (See Appendices B and C of Ref. [1].) In connection with a consideration of the role of time and the energy-time uncertainty relation in quantum theory, Aharonov and Bohm [2] used the operator that is analogous to the classical time function for a free particle. The present paper concerns an operator analog of the classical time function for the case of a quantum harmonic oscillator. (The time function for the harmonic oscillator is $\pi/2$ minus the frequently discussed phase function divided by the oscillator frequency.)

Much work has been carried out in pursuit of appropriate quantum operators analogous to the classical time function for the harmonic oscillator, particularly in regard to its relevance to the quantum treatment of the electromagnetic field. A recent review has been published by Lynch [3]. The focus of the work has been on the existence and definition of a quantum time operator defined in the Hilbert space of energy eigenstates of the oscillator. Susskind and Glogower [4] showed that the quantum time operator does not exist in this Hilbert space, and they proposed the use of a pair of alternate operators. There have been proposals to enlarge the Hilbert space of energy eigenstates in order to remedy the nonexistence of the time operator in that space; an analysis of these approaches has been given by Luis and Sánchez-Soto [5].

We consider the quantum harmonic oscillator, described by the Hamiltonian

$$H = \frac{1}{2m}p^2 + \frac{1}{2}m\omega^2 q^2, \qquad [q,p] = i\hbar, \tag{1}$$

in the space spanned by the eigenstates of $q$ and the eigenstates of $p$. The Hilbert space of energy eigenstates is a subspace. In the larger space we derive two Hermitian quantum time operators in analogy to the classical time function; the two operators differ by at most a function of the Hamiltonian. From either time operator we derive a Hermitian invariant operator in addition to the Hamiltonian. The Hamiltonian along with this invariant operator constitutes a pair of quantum action-angle variables for the harmonic oscillator.

The motivation for seeking a quantum action-angle representation was to provide the required starting point for the extension to quantum systems of a new classical time-dependent perturbation theory for the construction of invariants of Hamiltonian systems [6]. The quantum perturbation theory [7], which is based on the Heisenberg picture of quantum mechanics, determines operator invariants perturbatively, the eigenstates and eigenvalues of which can be used according to the general theory of Lewis and Riesenfeld [8] to construct the solution of the time dependent Schrödinger equation explicitly. This general theory has been used to construct exact invariants for time-dependent Hamiltonian systems [8,9]. The introduction of canonically conjugate angular momentum and angle variables, which are in some respects analogous to the action-angle variables considered here, has proven useful [see Eqs. (105) and (106) of Ref. [8]].

The definition of the time operator $\chi$ is that it be conjugate to the Hamiltonian:

$$[\chi, H] = i\hbar, \tag{2}$$

where $\chi = \tilde{\chi}(q,p)$ is explicitly time independent with respect to the operators $(q,p)$. That $\chi$ is appropriately called a time operator is seen as follows. The total time derivative of any operator $X(q,p,t)$ with respect to the operators $(q,p)$ is

$$\frac{dX}{dt} = \frac{\partial X}{\partial t} + \frac{1}{i\hbar}[X,H]. \tag{3}$$

Thus

$$\frac{d\chi}{dt} = 1 \rightarrow \tilde{\chi}[q(t),p(t)] - \tilde{\chi}[q(0),p(0)] = t\mathbf{1}, \tag{4}$$

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where **1** is the identity operator. From the conjugate operator $\chi$, we can construct an operator invariant $\alpha$, which is defined by

$$\alpha = \tilde{\alpha}(q,p,t) = -t\mathbf{1} + \tilde{\chi}(q,p). \tag{5}$$

From (3) if follows immediately that the operator $\alpha$ is an invariant operator; that is, its total time derivative vanishes. For the classical harmonic oscillator, the function analogous to $\tilde{\chi}(q,p)$ is $\omega^{-1}\tan^{-1}(m\omega q/p)$; when evaluated along a solution trajectory of Hamilton's equations, it equals the time elapsed since $q$ assumed the value zero.

In order to derive the action-angle representation for the quantum oscillator, we will postulate in Sec. 2 that the angle operator $\chi$ be a function of some *single* operator $Q$: $\chi = F(Q)$. Then we will choose $Q$ and the function $F$ such that $[\chi, H] = i\hbar$. This will require a formulation in which the commutator $[\chi, H]$ can be evaluated explicitly before the function $F(Q)$ is specified. We will achieve this in analogy to a simple and elegant way of obtaining the corresponding Poisson bracket result ($[F(Q), H]_{\mathrm{PB}} = 1$) for the classical oscillator. In Sec. 1 we explain the classical procedure; and we extend it to the quantum case in Sec. 2. That approach may allow generalization to more complicated quantum systems than the harmonic oscillator. In Sec. 3 we present a derivation of a time operator for the harmonic oscillator in terms of annihilation and creation operators, and we give the matrix elements of the operator in the coherent state representation.

*1. The classical case.*—Consider the classical harmonic oscillator described by the Hamiltonian

$$H = \frac{1}{2m}p^2 + \frac{1}{2}m\omega^2 q^2, \qquad [q,p]_{\mathrm{PB}} = 1. \tag{6}$$

We seek to represent $\chi$ as a function $F(Q)$ of a new generalized coordinate $Q = \tilde{Q}(q,p)$:

$$[\chi, H]_{\mathrm{PB}} = [F(Q), H]_{\mathrm{PB}} = 1. \tag{7}$$

We choose

$$Q = q/p, \tag{8}$$

which we know to be appropriate in the classical case. With this choice we can derive $F(Q)$ by a simple procedure that is directly generalizable to the quantum case, despite the noncommutability of the operators $q$ and $p$. Take the new generalized momentum to be

$$P = \tfrac{1}{2}p^2 \Rightarrow [Q,P]_{\mathrm{PB}} = 1. \tag{9}$$

Written in terms of $(Q,P)$, the Hamiltonian is a linear function of $P$,

$$H = m^{-1}P(1 + m^2\omega^2 Q^2), \tag{10}$$

and its Poisson bracket with $F(Q)$ is easily evaluated:

$$\begin{aligned}[F(Q), H]_{\mathrm{PB}} &= F'(Q)[Q,P]_{\mathrm{PB}} m^{-1}(1 + m^2\omega^2 Q^2) \\ &= F'(Q) m^{-1}(1 + m^2\omega^2 Q^2).\end{aligned} \tag{11}$$

Thus the solution of (7) is

$$F(Q) = \omega^{-1}\tan^{-1}(m\omega Q), \tag{12}$$

which is the correct classical result. The functions $H$ and $\chi = F(Q)$ are a pair of action-angle variables for the classical oscillator. The crucial point in this derivation of $F(Q)$ is that the Hamiltonian expressed as a function of $(Q,P)$ is a linear function of $P$.

The total time derivative of any classical function $X(q,p,t)$ with respect to the phase-space variables $(q,p)$ is

$$\frac{dX}{dt} = \frac{\partial X}{\partial t} + [X,H]_{\mathrm{PB}}. \tag{13}$$

The Hamiltonian $H$ is obviously an invariant; it does not depend explicitly on $t$ and its Poisson bracket with itself vanishes. A second invariant is

$$\alpha = \tilde{\alpha}(q,p,t) = -t + F(Q) = -t + F[\tilde{Q}(q,p)]. \tag{14}$$

*2. The quantum case.*—We now consider the quantum Hamiltonian (1) and the canonical transformation $(q,p) \rightarrow (Q,P)$ defined by

$$Q = A + \zeta(P), \qquad P = \tfrac{1}{2}p^2, \tag{15}$$

where

$$A = \tfrac{1}{2}(p^{-1}q + qp^{-1}) \tag{16}$$

is the symmetrized version of (8). (It will turn out that $A$ could have been taken to be $p^{-1}q$ or $qp^{-1}$, but that would not have been the intuitively natural choice at this point.) The operators $Q$ and $P$ satisfy $[Q,P] = i\hbar$ for any function $\zeta(P)$. That function can be chosen such that the Hamiltonian expressed as a function of $(Q,P)$ is a linear function of $P$. In order to do that, we can first use

$$\begin{aligned}A^2 &= \tfrac{1}{4}(p^{-1}qp^{-1}q + p^{-1}q^2p^{-1} + qp^{-2}q \\ &\quad + qp^{-1}qp^{-1}) = p^{-1}q^2p^{-1} + \tfrac{3}{4}\hbar^2 p^{-4}\end{aligned} \tag{17}$$

to evaluate $Q^2$ as

$$Q^2 = p^{-1}q^2p^{-1} + \tfrac{3}{4}\hbar^2p^{-4} + (\zeta A + A\zeta) + \zeta^2, \tag{18}$$

then use this expression and

$$[A, f(p)] = i\hbar p^{-1}f'(p), \tag{19}$$

where $f(p)$ is any function of $p$, to write

$$\begin{aligned}PQ^2 &= \tfrac{1}{2}q^2 - i\hbar qp^{-1} + \tfrac{3}{8}\hbar^2p^{-2} + p^2\zeta A \\ &\quad + \tfrac{1}{2}p^2[A,\zeta] + \tfrac{1}{2}p^2\zeta^2,\end{aligned} \tag{20}$$

$$\begin{aligned}Q^2P &= \tfrac{1}{2}q^2 + i\hbar p^{-1}q + \tfrac{3}{8}\hbar^2p^{-2} + A\zeta p^2 \\ &\quad + \tfrac{1}{2}[\zeta, A]p^2 + \tfrac{1}{2}p^2\zeta^2,\end{aligned} \tag{21}$$

and obtain

$$\begin{aligned}PQ^2 + Q^2P &= q^2 - \tfrac{1}{4}\hbar^2p^{-2} + (p^2\zeta A + A\zeta p^2) \\ &\quad + p^2\zeta^2 \\ &= q^2 - \tfrac{1}{4}\hbar^2p^{-2} + p^2\zeta(Q - \zeta) \\ &\quad + (Q - \zeta)p^2\zeta + p^2\zeta^2.\end{aligned} \tag{22}$$

From (22) we see that $q^2$, expressed in terms of $(Q,P)$, will be a linear function of $P$ if $\zeta(P)$ is chosen as

$$\zeta(P) = \pm i\,\frac{\hbar}{2}\,p^{-2} = \pm i\,\frac{\hbar}{4}\,P^{-1}, \tag{23}$$

in which case the Hamiltonian will also be a linear function of $P$:

$$H = \frac{1}{m}P + \frac{m\omega^2}{2}[(PQ^2 + Q^2P) \mp i\hbar Q]. \tag{24}$$

It is now easy to find an operator $\chi = F(Q)$ that is conjugate to $H$. The condition $i\hbar = [\chi, H]$ reduces to

$$i\hbar = \frac{1}{m}[\chi, P] + \frac{m\omega^2}{2}\{[\chi,P]Q^2 + Q^2[\chi,P]\}$$
$$= i\hbar F'(Q)\,\frac{1}{m}(1 + m^2\omega^2Q^2), \tag{25}$$

where $F'(Q)$ is the derivative of $F$ with respect to its argument. The solution of (25) is

$$F(Q) = \omega^{-1}\tan^{-1}(m\omega Q), \tag{26}$$

exactly as in the classical case. The two choices of sign in (23) give results for $F'(Q)$ that are Hermitian conjugates of one another. Therefore a Hermitian operator $\chi$ can be constructed by taking the average:

$$\chi = \frac{1}{2\omega}\tan^{-1}\left\{m\omega\left[\frac{1}{2}(p^{-1}q + qp^{-1}) + i\,\frac{\hbar}{2}\,p^{-2}\right]\right\} + \frac{1}{2\omega}\tan^{-1}\left\{m\omega\left[\frac{1}{2}(p^{-1}q + qp^{-1}) - i\,\frac{\hbar}{2}\,p^{-2}\right]\right\}. \tag{27}$$

It is interesting to note that the arguments of the arctangent functions are simply expressed in terms of the unsymmetrized versions of the classical $q/p$:

$$\chi = \frac{1}{2\omega}\tan^{-1}(m\omega p^{-1}q) + \frac{1}{2\omega}\tan^{-1}(m\omega qp^{-1}). \tag{28}$$

The operators $H$ and $\chi = F(Q)$ are quantum analogs of the corresponding action-angle variables for the classical oscillator. The invariant operator $\alpha$ is given by (5).

*3. An angle variable as a function of a and $a^\dagger$.*—Making the transformation to the usual annihilation and creation operators $a$ and $a^\dagger$,

$$a = \sqrt{\frac{m\omega}{2\hbar}}\left(q + i\,\frac{p}{m\omega}\right), \qquad [a, a^\dagger] = 1, \tag{29}$$

we can rewrite the Hamiltonian (1) as

$$H = \hbar\omega(a^\dagger a + \tfrac{1}{2}). \tag{30}$$

When $H$ is written in this way, it is common to speak of a phase operator $\phi$ that satisfies the commutation relation

$$[N, \phi] = [a^\dagger a, \phi] = i \tag{31}$$

with the number operator $N = a^\dagger a$. The time operator is related to the phase operator by

$$\omega\chi = \frac{\pi}{2}\mathbf{1} - \phi + G(H), \tag{32}$$

where $G(H)$ is some function of the Hamiltonian. A solution of (31) can be found with the simple ansatz that $\phi$ is some function of $a$ by using the relation

$$[f(a), a^\dagger] = f'(a), \tag{33}$$

where $f'$ is the derivative with respect to its argument of any function $f$. A solution is

$$\phi = \frac{1}{2i}(\ln a - \ln a^\dagger). \tag{34}$$

Because this operator is a function of $a$ plus a function of $a^\dagger$, its coherent state representation may be evaluated easily. Coherent states are defined by

$$a|\beta\rangle = \beta|\beta\rangle. \tag{35}$$

If we write the eigenvalue as $\beta = \rho e^{i\varphi}$, where $\rho$ and $\varphi$ are real, then the matrix elements of $\phi$ can be expressed as

$$\langle\beta'|\phi|\beta\rangle = \langle\rho' e^{i\varphi'}|\phi|\rho e^{i\varphi}\rangle$$
$$= \frac{1}{2}\left\{(\varphi + \varphi') + i\ln\left(\frac{\rho'}{\rho}\right)\right\} \times \frac{\exp(\beta'^*\beta)}{\exp[(|\beta'|^2 + |\beta|^2)/2]}. \tag{36}$$

Thus the expectation value of $\phi$ in the coherent state $|\beta\rangle$ is just arg $\beta$:

$$\langle\beta|\phi|\beta\rangle = \varphi. \tag{37}$$


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