Quantum Motion in a Paul Trap

Lowell S. Brown[a]
Department of Physics, Columbia University, New York, New York 10027
(Received 8 November 1990)

Quasienergy eigenstates are constructed for a quantum harmonic oscillator with a periodic, time-dependent "spring constant." This is done by a sequence of canonical transformations. The wave function in the new variables is that of an ordinary oscillator.

PACS numbers: 03.65.Ge, 32.80.Pj, 33.80.Ps, 42.50.Vk

The Paul trap is a device which enables extraordinary experiments to be performed.[1] The trap provides an oscillating quadrupole potential with the resulting motion of an ion described by a one-dimensional Hamiltonian of the form

$$H=(1/2m)p^2+\tfrac{1}{2}k(t)q^2 \tag{1}$$

for each of the three rectangular coordinates.[2] The effective spring constant is a periodic function of the time, $k(t+\tau)=k(t)$. In the experiments,

$$k(t)=a+b\cos(2\pi t/\tau)\,, \tag{2}$$

but our work will apply to any $k(t)$ which is periodic with period τ. The Hamiltonian (1) yields the equation of motion

$$m\ddot{q}(t)+k(t)q(t)=0 \tag{3}$$

for the Heisenberg operator $q(t)$. We shall show that the quantum-mechanical problem[3] may be solved entirely in terms of a suitably defined classical solution $f(t)$ to Eq. (3). We shall construct quasienergy eigenstates whose wave functions $\psi_n(q',t)$ are quasiperiodic; they acquire an overall phase factor when the time is advanced by the period τ.

Let us first review the character of the two linearly independent classical solutions to the equation of motion (3). Since the equation is periodic, an independent solution at time $t+\tau$ is a linear combination of the two solutions at time t. Linear combinations of the two solutions may be found which diagonalize this relationship. Thus solutions $f_\pm(t)$ exist which obey $f_\pm(t+\tau)=\lambda_\pm f_\pm(t)$, where $\lambda_\pm$ are constants. We shall consider only the case in which the classical motion is bounded for arbitrary initial conditions. This imposes restrictions on the functional form of $k(t)$ and requires that $|\lambda_+|\le 1$ and $|\lambda_-|\le 1$. Since the Wronskian $\dot{f}_+(t)f_-(t)-f_+(t)\dot{f}_-(t)$ is time independent, the constants obey $\lambda_+\lambda_-=1$. In conjunction with the bounded-motion requirement, this implies that $|\lambda_\pm|=1$ and $\lambda_\pm=e^{\pm i\theta}$. We shall adopt the convention that the phase θ is positive, $\theta>0$, and denote the corresponding solution by $f(t)$, with

$$f(t+\tau)=e^{i\theta}f(t)\,. \tag{4}$$

The other independent solution is the complex conjugate $f^*(t)$. We shall write the Wronskian of these two solutions as

$$\dot{f}(t)f^*(t)-f(t)\dot{f}^*(t)=2iW\,, \tag{5}$$

where W is real. We shall assume that W is positive, $W>0$, which is the case for the Mathieu-function solution[4] for the "spring constant" (2).

The quantum-mechanical problem may be solved by making canonical transformations which are implemented by unitary operators U, $U^\dagger=U^{-1}$. We work in the Heisenberg picture so that basis states and operators are transformed according to $\langle q',t|U(t)=\langle\bar{q}',t|$, $\bar{q}(t)=U^{-1}(t)q(t)U(t)$, $\bar{p}(t)=U^{-1}(t)p(t)U(t)$. The form of the time evolution $i\partial\langle q',t|/\partial t=\langle q',t|H$ is preserved if the Hamiltonian in the new representation is given by

$$\bar{H}=H+U^{-1}i\frac{\partial U}{\partial t}\,. \tag{6}$$

Here the partial time derivative acts only on the time dependence of the parameters which appear in $U(t)$, not on the time-dependent operators that it contains. We first perform a canonical transformation with

$$U_1=\exp[-i\chi(t)q^2(t)]\,, \tag{7}$$

where

$$\chi=\frac{m}{4}\left(\frac{\dot{f}}{f}+\frac{\dot{f}^*}{f^*}\right). \tag{8}$$

This gives $\bar{q}=q$, $\bar{p}=p-2\chi q$. Writing the Hamiltonian in terms of the new coordinates, using $\ddot{f}=-kf$ and the Wronskian (5), a little algebra shows that the new Hamiltonian (6) is given by

$$\bar{H}=\frac{1}{2m}\bar{p}^2+\frac{\chi}{m}(\bar{p}\bar{q}+\bar{q}\bar{p})+\frac{mW^2}{|f|^4}\bar{q}^2\,. \tag{9}$$

The cross term involving $\chi(t)$ in Eq. (9) is removed by a final transformation U_2. Noting that $\chi=(m/4)(d/dt)\times\ln|f|^2$, Eq. (6) shows that this is done with

$$U_2=\exp[\tfrac{1}{4}i(\bar{p}\bar{q}+\bar{q}\bar{p})\ln|f|^2]\,. \tag{10}$$

This is a scale transformation which defines the final set of variables,

$$Q=U_2^{-1}\bar{q}U_2=\frac{1}{|f|}\bar{q}=\frac{1}{|f|}q\,, \tag{11}$$

and

$$P=U_2^{-1}\bar{p}U_2=|f|\bar{p}=|f|(p-2\chi q)\,. \tag{12}$$

In terms of these operators

$$\tilde{H}=\frac{1}{|f(t)|^2}\left[\frac{1}{2m}P^2(t)+\tfrac{1}{2}mW^2Q^2(t)\right]. \tag{13}$$

Except for an overall, time-dependent factor, Eq. (13) defines a simple-harmonic-oscillator Hamiltonian which is resolved in terms of the annihilation operator $A=\sqrt{mW/2}Q+i\sqrt{1/2mW}P$ and the creation operator $A^\dagger$. These operators have the commutator $[A,A^\dagger]=1$ and express

$$\tilde{H}=\frac{W}{|f(t)|^2}[A^\dagger(t)A(t)+\tfrac{1}{2}]\,. \tag{14}$$

The equation of motion for the annihilation operator is

$$\frac{d}{dt}A=i[\tilde{H},A]=-i\frac{W}{|f|^2}A\,. \tag{15}$$

To solve it, we define the phase ϕ by

$$\exp[2i\phi(t)]=f(t)/f^*(t)\,. \tag{16}$$

The Wronskian (5) shows that $\dot{\phi}=W/|f|^2$ and thus the solution of Eq. (15) is given by

$$A(t)=\exp\{-i[\phi(t)-\phi(t_0)]\}A(t_0)\,. \tag{17}$$

In view of Eqs. (4) and (16), $\phi(t+\tau)=\phi(t)+\theta$, and so the solution is quasiperiodic, $A(t+\tau)=e^{i\theta}A(t)$.

As in the ordinary harmonic oscillator, the ground state $|0\rangle$ is defined by $A|0\rangle=0$ with the unit norm condition $\langle 0|0\rangle=1$. The zero-point term involving the factor of $\frac{1}{2}$ in the transformed Hamiltonian (14) is of no consequence, and we shall omit it. This term contributes an irrelevant overall phase to the quantum amplitudes. With this omission, $H|0\rangle=0$, and the ground state $|0\rangle$ is time independent. Quasienergy eigenstates are then built upon the ground state in the usual way,

$$|n,t_0\rangle=(1/\sqrt{n!})[A^\dagger(t_0)]^n|0\rangle\,, \tag{18}$$

with the corresponding wave functions in the new Q representation being given by

$$\Psi_{n,t_0}(Q',t)=\langle Q',t|n,t_0\rangle\,. \tag{19}$$

The Hermitian adjoint of the $A(t)$ time evolution (17) now yields

$$\Psi_{n,t_0}(Q',t)=\exp\{-in[\phi(t)-\phi(t_0)]\}\langle Q',t|(1/\sqrt{n!})[A^\dagger(t)]^n|0\rangle\,. \tag{20}$$

Since the ground-state ket is time independent and the bra and operators appear at the same time, the matrix element in Eq. (20) is time independent. Since $A^\dagger$ and A obey the usual rules of the creation and annihilation operators of the ordinary harmonic oscillator, this matrix element is just the familiar oscillator wave function involving Hermite polynomials,

$$\langle Q',t|\frac{1}{\sqrt{n!}}[A^\dagger(t)]^n|0\rangle=\langle Q'|\frac{1}{\sqrt{n!}}(A^\dagger)^n|0\rangle=\frac{1}{(2^n n!)^{1/2}}\left(\frac{mW}{\pi}\right)^{1/4}H_n(\sqrt{mW}Q')\exp(-\tfrac{1}{2}mWQ'^2)\,. \tag{21}$$

To transform back to the original variables, we first note that since U_2 performs the scale change $Q=\bar{q}/|f|$, the states are related by[5]

$$\langle Q',t|=\langle\bar{q}',t|U_2(t)=\sqrt{|f(t)|}\langle\bar{q}'=|f(t)|Q',t|\,. \tag{22}$$

It follows directly from Eq. (7) that

$$\langle\bar{q}',t|=\langle q',t|U_1(t)=\exp[-i\chi(t)q'^2]\langle q',t|\,. \tag{23}$$

Hence the wave functions in the original and transformed coordinates are related by

$$\psi_{n,t_0}(q',t)=\Psi_{n,t_0}(q'/|f(t)|,t)|f(t)|^{-1/2}\times\exp[i\chi(t)q'^2]\,. \tag{24}$$

The functions $|f(t)|$ and $\chi(t)$ are strictly periodic; they are not changed when the time is advanced by a period, $t\to t+\tau$. Only the phase prefactor in Eq. (20) is altered when the time is so advanced,

$$\psi_{n,t_0}(q',t+\tau)=e^{-in\theta}\psi_{n,t_0}(q',t)\,. \tag{25}$$

The states $|n,t_0\rangle$ are quasienergy eigenstates in the sense that the wave functions acquire only an altered phase when the time is advanced by a period τ. To bring this out, we define

$$\omega=\theta/\tau,\quad E_n=n\omega\,, \tag{26}$$

and write

$$\psi_{n,t_0}(q',t)=e^{-iE_nt}\tilde{\psi}_{n,t_0}(q',t)\,, \tag{27}$$

in which $\tilde{\psi}_{n,t_0}(q',t)$ is strictly periodic. The situation here is akin to the Bloch waves in a periodic crystal, but with space and time interchanged and the crystal momentum replaced by the quasienergy E_n. Although in general $\tilde{\psi}_{n,t_0}(q',t)$ is time dependent, experiments are often performed where $\tilde{\psi}_{n,t_0}(q',t)$ is nearly time independent. This can be the case for the "spring constant" (2) with $a=0$. Writing $\omega_0=2\pi/\tau$, this is the case if

$b/m\omega_0^2 \ll 1$, and

$$f(t) = e^{i\omega t}[1 + (b/m\omega_0^2)\cos\omega_0 t] \tag{28}$$

is a good approximation to the solution. In this case, $\omega^2/\omega_0^2 \simeq \frac{1}{2}(b/m\omega_0^2)^2 \ll 1$, the Wronskian $W \simeq \omega$, and $\bar{\psi}_{n,t_0}(q',t)$ is approximated by the wave function of a simple harmonic oscillator of frequency ω.

We have described the wave function in some detail since it gives a clear description of the nature of our system. However, actual calculations are most simply performed by using the transformation to the creation and annihilation operators $A^\dagger, A$. To give an example of the utility of this method and also to illustrate the periodic nature of the system, we consider the perturbation of the oscillator resulting from its interaction with an external electromagnetic field. This we do in the dipole approximation with the interaction Hamiltonian $H_1(t) = -eE(t)q(t)$. Using

$$q(t) = \frac{|f(t)|}{\sqrt{2mW}}[A(t) + A^\dagger(t)], \tag{29}$$

the usual oscillator rules imply that first-order transitions take place only from an initial state n to a final state n' with $n' = n \pm 1$. Moreover, using Eqs. (16) and (17), it is easy to check that the first-order transition amplitude is given by[6]

$$T_{n'n} = -i\int_{-\infty}^{\infty} dt \langle n', +\infty | H_1(t) | n, -\infty \rangle$$

$$= \frac{ie}{\sqrt{2mW}} \int_{-\infty}^{\infty} dt\, E(t)[f^*(t)\sqrt{n}\,\delta_{n',n-1} + f(t)\sqrt{n+1}\,\delta_{n',n+1}]\,. \tag{30}$$

We consider a sinusoidal drive, $E(t) = E_0\cos(\omega_d t)$, and write $f(t) = e^{i\omega t}F(t)$, with $F(t)$ strictly periodic. Exploiting the periodicity shows that the time integration in Eq. (30) involves

$$\int_{-\infty}^{\infty} dt\, e^{\pm i\omega_d t} f(t) = \sum_{l=-\infty}^{\infty} e^{i(\omega \pm \omega_d)l\tau} \int_0^\tau dt\, e^{i(\omega \pm \omega_d)t} F(t)$$

$$= \sum_{l=-\infty}^{\infty} 2\pi\delta\left(\omega \pm \omega_d + \frac{2\pi l}{\tau}\right) \frac{1}{\tau}\int_0^\tau dt \exp\left(-\frac{2\pi i l}{\tau}t\right) F(t)\,. \tag{31}$$

The $l=0$ member of the sum corresponds to photon emission or absorption at the resonant frequency $\omega_d = \omega = \theta/\tau = E_{n+1} - E_n$. The other terms in the sum correspond to these processes occurring at higher harmonic or overtone frequencies. The final integral in Eq. (31) defines the lth Fourier component of the periodic function $F(t)$, and so the transition probability is proportional to the absolute square of this Fourier amplitude of the classical motion.

I should like to acknowledge the hospitality of the Physics Department of Columbia University and the kindness of G. Feinberg and E. Weinberg.

---

[a]Permanent address: Physics Department, FM-15, University of Washington, Seattle, WA 98195.

[1]The physics done with a Paul trap is reviewed in two recent Nobel Prize Lectures: Hans Dehmelt, Rev. Mod. Phys. **62**, 525 (1990); and Wolfgang Paul, Rev. Mod. Phys. **62**, 531 (1990), and references therein.

[2]Previous work on this system has been done by R. J. Cook, D. G. Shankland, and A. L. Wells, Phys. Rev. A **31**, 564 (1985); and by M. Combescure, Ann. Inst. Henri Poincaré **44**, 293 (1986). Cook, Shankland, and Wells provide an approximate treatment of the quantum motion by perturbing about a harmonic oscillator solution for a time-independent, effective potential. Combescure obtained the wave given below in Eq. (24) by a roundabout procedure rather than the simple, direct, canonical transformation method used here. Our method makes the calculation of other important quantities easy, such as the transition amplitude evaluated in Eqs. (30) and (31) below. Moreover, our method applies to any oscillator with a periodic "spring constant," not only the sinusoidal form [our Eq. (2)] used by Combescure.

[3]The need for a completely quantum-mechanical treatment is shown by the experiment of F. Diedrich, J. C. Bergquist, W. M. Itano, and D. J. Wineland, Phys. Rev. Lett. **62**, 403 (1989), which places a single ion in the quantum ground state of its motion in a Paul trap.

[4]Proof: In the limit $b=0$, $f(t) = \exp(it\sqrt{a/m})$ and hence $W>0$. With $b \neq 0$, continuity demands that W remain positive since it cannot vanish because in the parameter space (a,b) of stable solutions, $\theta \neq 0$ which implies that $f(t)$ and $f^*(t)$ are linearly independent.

[5]The prefactor $\sqrt{|f(t)|}$ appears since both sets of states are properly normalized, $\langle Q',t|Q'',t\rangle = \delta(Q'-Q'')$ and $\langle \bar{q}',t|\bar{q}'',t\rangle = \delta(\bar{q}'-\bar{q}'')$ while $|f(t)|\delta(|f(t)|(Q'-Q'')) = \delta(Q'-Q'')$.

[6]The overall phase associated with the initial and final states is omitted in the second equality.