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Harmonic Oscillator Wave Functions

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A harmonic oscillator wave packet which oscillates sinusoidally without change in shape has been described by Schrödinger and others. It is shown in the present note that there are an infinite number of such wave packets—of which the above is a special one—having the shapes of the various eigenfunctions of the harmonic oscillator Hamiltonian. The relation of these wave packets to the classical oscillator is discussed.

DUE to the importance which the one-dimensional harmonic oscillator problem has in quantum theory, its wave functions have been given considerable attention. Several authors[1–3] have shown that there is a particular harmonic oscillator wave function in the form of a wave packet, the center of which oscillates sinusoidally about the origin and the shape of which remains constant in time. The purpose of the present note is to show that there are an infinite number of such wave packets.

The most general expression for a complex function of q and t, the absolute value of which remains constant in shape, is given by

$$\psi(q,t)=f(q-q_0(t))e^{i\varphi(q,t)}, \tag{1}$$

where f, q_0, and φ are real, arbitrary functions. Inserting (1) into Schrödinger's equation for the harmonic oscillator,

$$i\hbar\frac{\partial\psi}{\partial t}=-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial q^2}+\frac{m\omega^2}{2}q^2\psi,$$

and equating real and imaginary parts separately, we obtain

$$-\frac{\hbar^2}{2m}\frac{\partial^2 f}{\partial q^2}+\frac{m\omega^2}{2}q^2 f+\left[\frac{\hbar^2}{2m}\left(\frac{\partial\varphi}{\partial q}\right)^2+\hbar\frac{\partial\varphi}{\partial t}\right]f=0, \tag{2}$$

and

$$-\frac{\partial f}{\partial q}\dot{q}_0+\frac{\hbar}{m}\frac{\partial f}{\partial q}\frac{\partial\varphi}{\partial q}+\frac{\hbar}{2m}f\frac{\partial^2\varphi}{\partial q^2}=0. \tag{3}$$

Equation (3) can easily be transformed into

$$\frac{\partial}{\partial q}\left(-\dot{q}_0+\frac{\hbar}{m}\frac{\partial\varphi}{\partial q}\right)f^2=0,$$

which yields, as the solution,

$$\left(-\dot{q}_0+\frac{\hbar}{m}\frac{\partial\varphi}{\partial q}\right)f^2=\text{constant}.$$

Now, if $\psi(q,t)$ is to be normalizable, f must vanish at infinity. The constant is therefore equal to zero, and we have

$$\varphi(q,t)=(m/\hbar)q\dot{q}_0+S(t), \tag{4}$$

where S is an arbitrary function of the time only. Substituting this expression into Eq. (2) and completing the square involving q, we obtain

$$-\frac{\hbar^2}{2m}\frac{\partial^2 f}{\partial q^2}+\frac{m\omega^2}{2}\left(q+\frac{1}{\omega^2}\ddot{q}_0\right)^2 f+\left(\hbar\frac{dS}{dt}+\frac{m}{2}\dot{q}_0^2-\frac{m}{2\omega^2}\ddot{q}_0^2\right)f=0. \tag{5}$$

This is a differential equation for f. Since we have taken f to be a function of $q-q_0$, the coefficients in this equation must be functions of $q-q_0$. We must therefore

[1] E. Schrödinger, Naturwiss. 14, 664 (1926).
[2] L. I. Schiff, *Quantum Mechanics* (McGraw-Hill Book Company, Inc., New York, 1949), Sec. 13.
[3] D. Bohm, *Quantum Theory* (Prentice-Hall, Inc., New York, 1951), Chap. 13.

have

$$\frac{1}{\omega^2}\ddot{q}_0=-q_0, \tag{6}$$

and

$$\hbar\frac{dS}{dt}+\frac{m}{2}\dot{q}_0^2-\frac{m}{2\omega^2}\ddot{q}_0^2=-E, \tag{7}$$

where E is a constant independent of the time. Equation (5) can now be written as

$$-\frac{\hbar^2}{2m}\frac{\partial^2 f}{\partial Q^2}+\frac{m\omega^2}{2}Q^2 f=Ef, \tag{8}$$

where we have put $q-q_0(t)=Q$. But Eq. (8) is just the time-reduced Schrödinger equation for the harmonic oscillator. Its solutions are the well-known harmonic oscillator eigenfunctions,[2]

$$f_n(Q)=\left(\frac{\alpha}{\pi^{\frac{1}{2}}2^n n!}\right)^{\frac{1}{2}}H_n(\alpha Q)\exp(-\tfrac{1}{2}\alpha^2Q^2), \tag{9}$$

corresponding to the eigenvalues $E_n=(n+\frac{1}{2})\hbar\omega$, where $\alpha^2=m\omega/\hbar$, H_n is the nth Hermite polynomial, and n is any non-negative integer. The solutions of Eqs. (6) and (7) can be written down immediately. These are

$$q_0=A\cos(\omega t+\theta), \tag{10}$$

and

$$S=-\frac{E_n}{\hbar}t-\frac{1}{\hbar}\int(\tfrac{1}{2}m\dot{q}_0^2-\tfrac{1}{2}m\omega^2q_0^2)dt, \tag{11}$$

where A and θ are arbitrary constants.

We see, thus, that there are an infinite number of harmonic oscillator wave packets defined by Eqs. (1), (4), (9), (10), and (11), for each of which the absolute value remains constant in shape while oscillating sinusoidally about the origin. The wave packet described in references 1–3 is obtained by setting n in Eq. (9) and θ in Eq. (10) equal to zero.

It is interesting to note that if q_0, which, in view of Eq. (9), is the expectation value of q, be regarded as the coordinate of a classical particle, then the integral in Eq. (11) is Hamilton's principle function for that particle. The energy of this classical particle, however, has no direct connection with the eigenvalue E_n, since it depends on the arbitrary constant A.

It is also interesting to obtain the expectation value of the energy of our oscillating wave packets. We have

$$\langle H\rangle=i\hbar\int_{-\infty}^{\infty}\psi^*\frac{\partial\psi}{\partial t}dq$$
$$=i\hbar\dot{q}_0\int_{-\infty}^{\infty}ff'dq-\hbar\int_{-\infty}^{\infty}f^2\frac{\partial\varphi}{\partial t}dq.$$

The first integral vanishes, since the limit of f is zero as q becomes infinite either positively or negatively. We thus have

$$\langle H\rangle=-\hbar\int_{-\infty}^{\infty}f^2\frac{\partial\varphi}{\partial t}dq$$
$$=-m\ddot{q}_0\int_{-\infty}^{\infty}Qf^2(Q)dQ$$
$$+[E_n+(\tfrac{1}{2}m\dot{q}_0^2+\tfrac{1}{2}m\omega^2q_0^2)]\int_{-\infty}^{\infty}f^2(Q)dQ$$
$$=E_n+(\tfrac{1}{2}m\dot{q}_0^2+\tfrac{1}{2}m\omega^2q_0^2), \tag{12}$$

where use has been made of Eq. (6), of the normalization of $f(Q)$, and the symmetry of $f^2(Q)$. It is seen, therefore, that the expectation value of the energy is just the sum of the quantum-mechanical energy of the wave packet when it is stationary and the classical energy of the particle with coordinate $q_0(t)$. Equation (12) can be written as

$$\langle H\rangle=m\omega^2(\langle Q^2\rangle+\langle q_0^2\rangle_{\text{Av}}),$$

where the average of q_0^2 is the time average. It is evident, then, that if the amplitude of oscillation is large compared to the width of the wave packet, the energy is predominantly of classical origin, while if the amplitude of oscillation is small compared to the width of the wave packet, the energy is predominantly of quantum-mechanical origin.

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