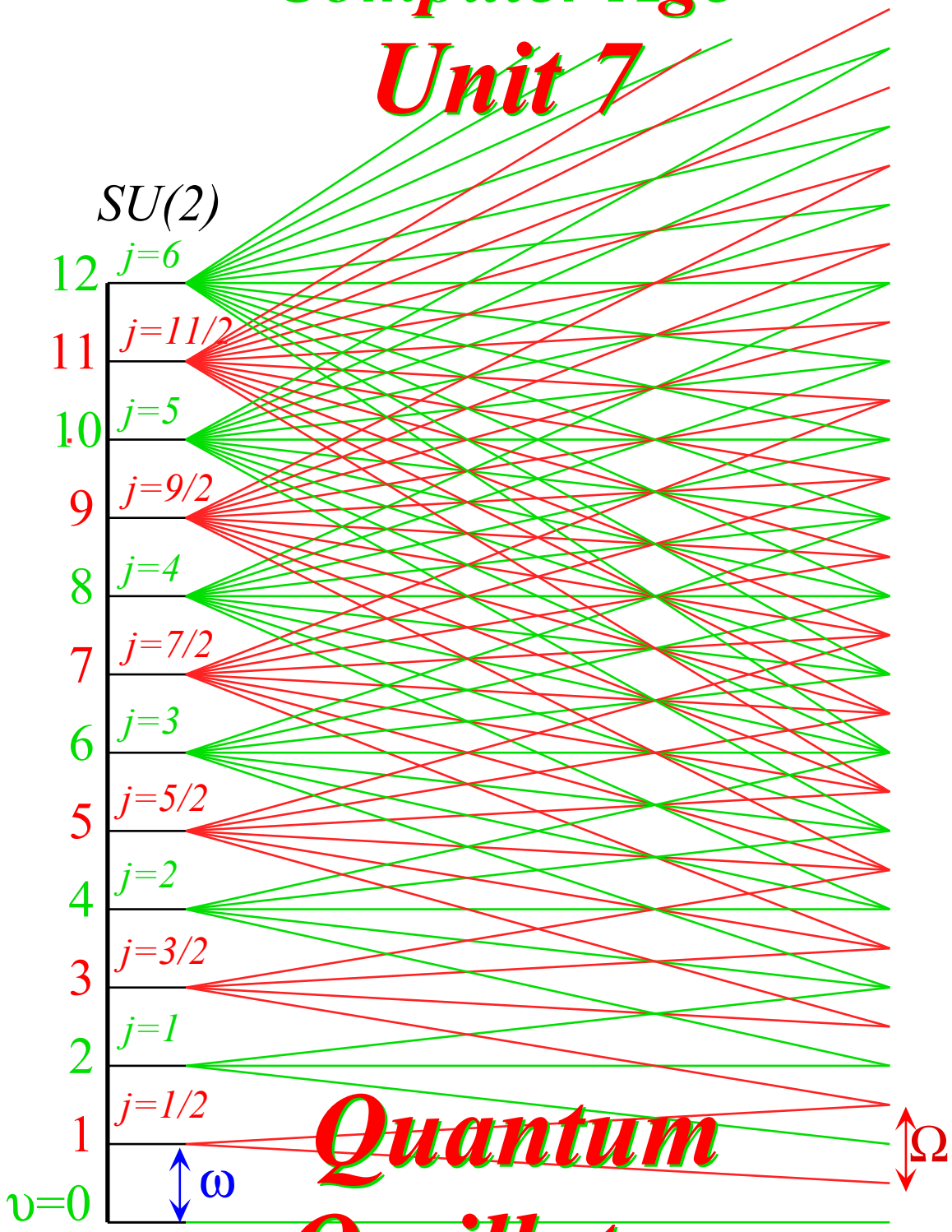
# Quantum Theory for the Computer Age

# Unit 7




# Quantum Oscillators

# Unit 7 Quantum Oscillators

Harmonic oscillation is the end-all and be-all of quantum theory. Planck's oscillation hypothesis begins it, and it's nothing but oscillation and resonance from there on. This unit begins the analysis of 1D oscillation in the non-relativistic Schrodinger context and then develops the creation-destruction ($a^\dagger a$) operator technology for multi-dimensional oscillators. Particular attention is paid to 2D oscillators that served as classical ABCD spin-and 2-state analogs in Chapter 10 of Unit 3. The quantum versions of the ABCD oscillator further elucidate the elegant U(2) quantum mechanics of Schwinger used in the next unit to finesse angular momentum theory. It also begins the elementary quantum radiation ("photon") theory that is sometimes mistakenly referred to as "2nd quantization" if dimensions and "particles" get confused. Similar techniques are used to define "phonon" excitations for mechanical waves in solds, liquids, molecules, or molecular clusters.

**W. G. Harter**

**Department of Physics**

**University of Arkansas**

**Fayetteville**

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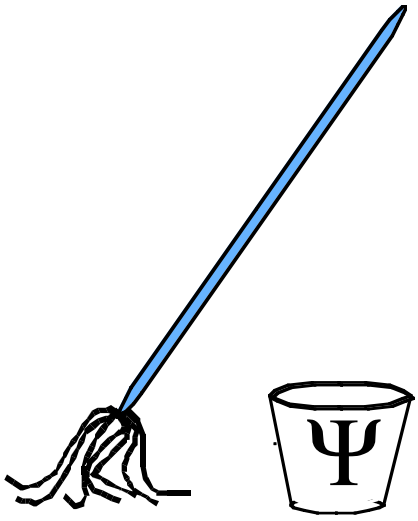

# QM for AMOP

# Chapter 20

# One-Dimensional Oscillator States and Dynamics

W. G. Harter

Every continuous potential may be expanded in a Taylor polynomial about a minimum point so that the first variable term is quadratic: $V(x-x_{min})=V_{min}+{}^1/_2k(x-x_{min})^2$... This is just one of about a million reasons that harmonic oscillator analysis is useful in physics. The harmonic oscillator potential $V(x)={}^1/_2kx^2$ gives a most symmetric non-relativistic Hamiltonian with the (rescaled) form: $H=P^2+X^2$. Because of this symmetry, its eigensoultion analysis and application is extraordinarily convenient. We plan to take advantage of this here in Chapter 20 and in many of the later Chapters, as well.

## CHAPTER 20. 1D-HARMONIC OSCILLATOR STATES AND DYNAMICS .....1



## CHAPTER 21. 2D-HARMONIC OSCILLATOR STATES AND DYNAMICS .....1

# Chapter 20. 1D-Harmonic Oscillator States and Dynamics

## *20.1 Harmonic Oscillator Equations*

### (a) Classical harmonic oscillator equations

To be *harmonic*, an oscillating body must return to a given initial position and velocity with the same frequency for a wide range of amplitudes. A sufficient (but not necessary) condition for this is that the body has a *linear* restoring force, that is, a Hooke's law force with a fixed *spring constant k*.

$$F = -kx \tag{20.1.1}$$

Then, and only then, will the classical motion of a body of mass $M$ be purely sinusoidal with a single angular frequency ω totally independent of amplitude $A$.

$$x(t) = A\sin(\omega t + \alpha)\ , \quad \text{where:} \quad \omega = \sqrt{\frac{k}{m}} \tag{20.1.2}$$

The acceleration, and hence, by Newton II, the force is always proportional to the displacement $x(t)$,

$$\frac{d^2x}{dt^2} = \ddot{x}(t) = -\omega^2 A\sin(\omega t - \alpha) = -\omega^2 x(t)\,, \tag{20.1.3a}$$

or

$$m\ddot{x}(t) = -\omega^2 A\sin(\omega t - \alpha) = -m\omega^2 x(t) = -k\,x(t)\,. \tag{20.1.3b}$$

Given the proportionality or linearity between force and displacement, it follows that the work or potential energy associated with a Hooke-spring type force must be a *quadratic* potential.

$$V(x) = \int_0^x k\,x'dx' = \frac{1}{2}kx^2 = \frac{1}{2}m\omega^2 x^2 \tag{20.1.4}$$

From this follows the classical total energy or *Hamiltonian function* of the 1D harmonic oscillator.

$$E = H(x,p) = \frac{1}{2m}p^2 + \frac{1}{2}m\omega^2 x^2 \tag{20.1.5a}$$

Here the classical momentum is

$$p = m\frac{dx}{dt} = m\dot{x} \tag{20.1.5b}$$

It should be noted that the oscillator equations apply to a good deal more than a glob of lead on a coiled spring or pendulum. As pointed out in Chapter 10, harmonic oscillator equations of motion apply to any independent oscillator system such as a normal mode of vibration or a classical electromagnetic wave introduced in Chapter 4 or an electromagnetic mode such as we touched on in Chapter 6 (Sec. 6.3(d)) or for the classical electromagnetic Hamiltonian developed in Chapter 17.

It is these more complicated systems, primarily electromagnetic oscillation, that really make use of the oscillator quantum mechanics we are about to develop. However, just to get started, we can think of a (very small) blob of lead bouncing up and down on a (frictionless) spring as in Fig. 10.1.1 or a pendulum swinging back and forth at the end of a string as sketched in Fig. 16.1.1(a).

## (b) Quantum harmonic oscillator equations

Converting the classical Hamiltonian $H$ to a quantum Hamiltonian **H**-operator is done in the same way for the oscillator as it was for a general potential $V(x)$ in equations (11.4.5). The first step is to convert all the coordinates and momenta to operators. At first, this just means just writing $x$ and $p$ with a thick pen to give **x** and **p**, something a five-year-old could do!

$$\mathbf{H}(\mathbf{x},\mathbf{p}) = \mathbf{p}^2/2M + V(\mathbf{x}) = \mathbf{p}^2/2M + M\omega^2\mathbf{x}^2/2 \qquad (20.1.6)$$

However, we need to decide how to represent those thick-headed operators **x** and **p**, and right away we notice something unique about this Hamiltonian. Apart from scale factors $1/2M$ or $M\omega^2/2$, this Hamiltonian has a form $(\mathbf{P}^2 + \mathbf{X}^2)/2$ which is symmetric to interchange of position **X** and momentum **P** (or DeBroglie wavevector $\hbar\mathbf{k}$). It isn't going to make much difference whether we represent this problem in position $x$-space $\{..|x\rangle ..\}$ or in momentum (Fourier wavevector) $k$-space $\{..|k\rangle ..\}$.

So which do we use? The best answer turns out to be neither and both! We will solve this system's Schrodinger equations using discrete abstract algebra, but first, tie this to a standard historical approach to the harmonic oscillator that uses the calculus of continuous differential equations.

*(1) Schrodinger oscillator equation*

The commonly stated form of Schrodinger's equation is in the position $x$-space basis $\{..|x\rangle..\}$ for which the representation of the Hamiltonian is that given by (11.4.5c) with potential $V(x) = M\omega^2\boldsymbol{x}^2/2$.

$$\begin{aligned} i\hbar\left\langle x\left|\frac{\partial}{\partial t}\right|\Psi\right\rangle &= \left\langle x\left|\mathbf{H}\right|\Psi\right\rangle = \left\langle x\left|\frac{\mathbf{p}^2}{2M} + \frac{M\omega^2\mathbf{x}^2}{2}\right|\Psi\right\rangle , \\ i\hbar\frac{\partial\Psi(x,t)}{\partial t} &= \frac{-\hbar^2}{2M}\frac{\partial^2\Psi(x,t)}{\partial x^2} + \frac{M\omega^2x^2}{2}\Psi(x,t) \end{aligned} \qquad (20.1.7a)$$

The time dependent equation describes all the possible motion of a quantum oscillator, but first, we have to solve the time independent oscillator Schrodinger equation, that is, its *energy eigenvalue equations*,

$$\left\langle x\left|\mathbf{H}\right|E\right\rangle = E\left\langle x\left|E\right.\right\rangle , \quad \text{or:} \quad \frac{-\hbar^2}{2M}\frac{\partial^2\psi_E(x)}{\partial x^2} + \frac{M\omega^2x^2}{2}\psi_E(x) = E\psi_E(x) \qquad (20.1.7b)$$

where the latter follow from a simple substitution of a special time-dependent wavefunction

$$\Psi_{special}(x,t) = e^{-i\omega t}\psi_E(x) = e^{-iEt/\hbar}\psi_E(x) \qquad (20.1.7c)$$

into (20.1.7a). Once we get the allowed energy (or frequency) eigenvalues $E=E_n$ and eigenfunctions

$$\psi_{E_n}(x) = \left\langle x\left|E_n\right.\right\rangle = \left\langle x\left|n\right.\right\rangle , \qquad (20.1.7c)$$

then oscillator time behavior depends on linear combinations $\Psi_{general}(x,t)$ of eigenfunctions.

$$\Psi_{general}(x,t) = \sum_n a_n e^{-i\omega_n t}\psi_{E_n}(x) = \sum_n a_n e^{-iE_n t/\hbar}\psi_{E_n}(x), \qquad (20.1.7d)$$

Each eigenfunction oscillates at its own (eigen) frequency and contributes to a Fourier time function.

The "special" wavefunctions $\Psi_{special}(x,t)$ or eigenfunctions $\psi_E(x)$ represent *stationary states*. Their probability distributions are motionless, that is, dead as a doornail.

$$\frac{d}{dt}\left(\Psi^*_{special}\Psi_{special}\right)=\frac{d\left|\psi_E(x)\right|^2}{dt}=0 \ .$$

Motion and life as we know it comes only from a general wavefunction $\Psi_{general}(x,t)$ that is a combination of at least two such eigenfunctions with different (eigen)frequencies. Remember, the fundamental quantum time principle: "It takes two to Tango!" which was shown in Sec.4.4(a), 9.4(a), 10.2 (b) and 12.1(b).

*(2) Hermite equations: Gaussians and zero point energy*

The resulting eigenfunction differential equation is the Hermitian form of *Hermite's equation*.

$$H\cdot\psi_E(x)=\frac{d^2\psi_E(x)}{dx^2}+\left(\varepsilon-ax^2\right)\psi_E(x)=0 \quad \text{where: } a=\frac{M^2\omega^2}{\hbar^2} \quad \text{and: } \varepsilon=\frac{2ME}{\hbar^2} \qquad (20.1.8)$$

Historically, this is significant since Hermite's name appears on both this special equation and the concept of Hermitian (self-conjugate) operators $(H^\dagger=H)$ which satisfy the Sturm-Liouville requirements discussed in Ch. 11 in equations (11.2.20) to (11.2.23). Gauss's name is significant, too, because it was known that a Guassian function $e^{-\alpha x^2}$ is one very important solution to this equation as seen here. The derivatives

$$\frac{d}{dx}e^{-\alpha x^2}=-2\alpha x e^{-\alpha x^2}, \qquad \frac{d^2}{dx^2}e^{-\alpha x^2}=-2\alpha e^{-\alpha x^2}+4\alpha^2x^2e^{-\alpha x^2} \qquad (20.1.9)$$

yield the following solution of (20.1.8)

$$\frac{d^2\psi_E(x)}{dx^2}+\left(\varepsilon-ax^2\right)\psi_E(x)=0 \quad \text{where: } \psi_E(x)=\frac{e^{-\alpha x^2}}{norm} \ , \ a=4\alpha^2 \quad \text{and: } \varepsilon=2\alpha \qquad (20.1.10a)$$

This gives the following Guassian decay constant $\alpha$ and energy eigenvalue $E$.

$$\alpha=\frac{M\omega}{2\hbar} \ , \quad \text{and:} \quad E=\frac{\hbar^2}{2M}\varepsilon=\frac{\hbar\omega}{2} \qquad (20.1.10b)$$

The energy value $E=\hbar\omega/2$ is the ground state energy of a harmonic oscillator. It is called the *vacuum zero point energy* $E_0=\hbar\omega/2$, and it has tremendous physical significance. It is related to the great "roar of the vacuum" at absolute zero temperature. It is the electromagnetic energy that remains after all "photons" and other excitation energies are as gone as is possible.

In spite of the overwhelming presence and significance of the zero-point wave, it is regarded as a nuisance for the treatment of differential equations. So the Gaussian is factored out by making it a scaling function $s(x)=e^{-\alpha x^2}$ such that the differential operator for a rescaled function $\psi(x)=s(x)\phi(x)$ is easier to

solve in polynomial form. Derivatives of a rescaled wavefunction convert the Hermite equation

$$\psi = s\cdot\phi \quad , \qquad \psi' = s'\cdot\phi + s\cdot\phi' \quad , \qquad \psi'' = s''\cdot\phi + 2s'\cdot\phi' + s\cdot\phi''$$

(20.1.8).

$$s\cdot\phi'' + 2s'\cdot\phi' + \left(s'' + \varepsilon s - ax^2 s\right)\phi = 0 = e^{-\alpha x^2}\left[\phi'' - 4\alpha x\phi' + \left(-2\alpha + 4\alpha^2 x^2 + \varepsilon - ax^2\right)\phi\right]$$

The rescaled equation is a standard form of Hermites's equation. Here we use $a=4\alpha^2$ from (20.1.10a).

$$K\cdot\phi = \phi'' - 4\alpha x\phi' + \left(\varepsilon - 2\alpha\right)\phi = 0 \qquad (20.1.11)$$

Putting in the ground state energy $\varepsilon=2\alpha$ from (20.1.10a) gives two solutions: $\phi=const.$ and $\phi=\int dx e^{2\alpha x^2}$ .

Only the first solution is of interest here, but it just gives back the Guassian wavefunction

$$\psi(x)=s(x)\phi(x) = e^{-\alpha x^2} \ (const.) \qquad (20.1.12)$$

which was known (for centuries) before. The second solution blows up.

$$\psi(x)=s(x)\phi(x) = e^{-\alpha x^2}\int dx e^{2\alpha x^2}\to\infty \text{ as } x\to\infty \qquad (20.1.13)$$

This "blow-up" solution is not wrong. It is the manifestation of the non-resonant eigenchannel wave or the "wrong" local-symmetry wavefunction discussed before in Sec. 14.1(c) (Fig. 14.1.13) and Sec.15.4(c). These waves are only needed if we plan to make "global" waves that flow in and out of the harmonic oscillator potential well. Since we are only dealing with local wavefunctions, this type of wave solution will not be considered in this section. The same applies to solution of (20.1.11) for other values of $\varepsilon$ including other eigenvalues. (Only "quantized" eigenvalues give localized solutions.)

All local wavefunctions have an over-riding Gaussian envelope $e^{-\alpha x^2}$ with the constant $\alpha= M\omega/2\hbar$ proportional to mass $M$ and natural frequency $\omega$. The Gaussian width or "uncertainty" is proportional to the inverse square-root $1/\sqrt{\alpha}$ of this constant. (Just remember that $e^{-3}=5\%$ so the wave is down by $95\%$ in a distance $x_{5\%}$ such that $\alpha(x_{5\%})^2 = 3$ or $x_{5\%} = \sqrt{(3/\alpha)}$ .) So the quantum uncertainty fringe of the evanescent wave decreases exponentially with increasing mass or natural frequency.

The resulting standard Hermite equation (20.1.11) has some disadvantages over (20.1.8). The differential operator $K$ is not Hermitian, that is, ($\mathbf{K}^\dagger\neq\mathbf{K}$). For these (and other) reasons we will go back to modern algebraic methods which deal with Hermitian Hamiltonian equations and unitary evolution operators. From time to time we will check our results with the differential equation (20.1.11).

## 20.2 Harmonic Oscillator Eigensolutions

### (a) Creation and destruction operators

The key to the quantum oscillator eigensolutions is almost as simple as the factoring $a^2-b^2$ into $(a+b)(a-b)$. Actually, it involves factoring $\mathbf{P}^2+\mathbf{X}^2$ into $(\mathbf{X}+i\mathbf{P})(\mathbf{X}-i\mathbf{P})$ where operators

$$\mathbf{X} = \sqrt{M\omega}\,\mathbf{x}/\sqrt{2} \qquad \text{and} \qquad \mathbf{P} = \mathbf{p}/\sqrt{(2M)} \tag{20.2.1a}$$

are scaled position **x** and momentum **p** operators that square and sum to make the oscillator Hamiltonian (20.1.6). Since **x** and **p** do not commute the factorization is done symmetrically.

$$\mathbf{H}(\mathbf{x},\mathbf{p}) = \mathbf{P}^2+\mathbf{X}^2 = (\mathbf{X}-i\mathbf{P})(\mathbf{X}+i\mathbf{P})/2 + (\mathbf{X}+i\mathbf{P})(\mathbf{X}-i\mathbf{P})/2$$

Also, Planck's quantum oscillator energy $\hbar\omega$ is factored out as well.

$$\mathbf{H}(\mathbf{x},\mathbf{p}) = \mathbf{p}^2/2M + M\omega^2\mathbf{x}^2/2 = \hbar\omega\,(\mathbf{a}^\dagger\mathbf{a} + \mathbf{a}\mathbf{a}^\dagger)/2 \tag{20.2.1b}$$

The resulting operator factors include the following *destruction operator* **a**

$$\mathbf{a} = \frac{(\mathbf{X}+i\mathbf{P})}{\sqrt{\hbar\omega}} = \frac{\left(\sqrt{M\omega}\,\mathbf{x} + i\mathbf{p}/\sqrt{M\omega}\right)}{\sqrt{2\hbar}}, \tag{20.2.1c}$$

and the conjugate factor is called a *creation operator* $\mathbf{a}^\dagger$. This naming will make sense shortly.

$$\mathbf{a}^\dagger = \frac{(\mathbf{X}-i\mathbf{P})}{\sqrt{\hbar\omega}} = \frac{\left(\sqrt{M\omega}\,\mathbf{x} - i\mathbf{p}/\sqrt{M\omega}\right)}{\sqrt{2\hbar}} \tag{20.2.1d}$$

Recall from (11.3.10) and (11.3.11) that position **x** and momentum **p** are Hermitian operators.

$$\mathbf{x}^\dagger = \mathbf{x} \qquad\qquad \mathbf{p}^\dagger = \mathbf{p} = \hbar\mathbf{k}$$

So the **a** and $\mathbf{a}^\dagger$ operators differ only by the sign of the imaginary $i$. Why the operator holding the dagger † should be called a creation operator is like a murder mystery that will be revealed in due time!

The classical equivalent of the **a**-operators are the *phasor coordinates* introduced in Ch. 10. The phasor coordinates $a_1=x_1+ip_1$ and $a_2=x_2+ip_2$ defined in (10.1.1c) related the classical phase space of a two-dimensional oscillator to the wave amplitudes of a 2-state quantum system. Later, we will discuss quantum oscillation of dimension-two, too, to do *SU(2)* quantum theory using two independent sets of **a** and $\mathbf{a}^\dagger$ operators $\{\mathbf{a}_1=\mathbf{X}_1 + i\mathbf{P}_1\,,\ \mathbf{a}_1^\dagger=\mathbf{X}_1 - i\mathbf{P}_1\}$ and $\{\mathbf{a}_2=\mathbf{X}_2 + i\mathbf{P}_2,\ \mathbf{a}_2^\dagger=\mathbf{X}_2 - i\mathbf{P}_2\}$.

*(1) Operator commutation relations*

Operator algebra invariably involves questions of commutation or lack thereof. Here it starts with finding the basic commutation difference **xp-px** of position and momentum called a *commutator* $[\mathbf{x}\,,\,\mathbf{p}]$. One way to do this appeals to coordinate representations (11.3.10) and (11.3.11).

$$\langle x|\mathbf{xp}-\mathbf{px}|\psi\rangle = \frac{\hbar}{i}\left(x\frac{\partial}{\partial x}\psi(x) - \frac{\partial}{\partial x}x\psi(x)\right) = \frac{\hbar}{i}\left(x\frac{\partial}{\partial x}\psi(x) - x\frac{\partial}{\partial x}\psi(x) - \frac{\partial x}{\partial x}\psi(x)\right)$$

$$= \langle x|[\mathbf{x},\mathbf{p}]|\psi\rangle = -\frac{\hbar}{i}\psi(x) = \hbar i\psi(x)$$

In abstract operator notation this is written simply as a *commutator* $[\mathbf{x}\,,\,\mathbf{p}]$ *relation*.

$$[\mathbf{x},\mathbf{p}] \equiv \mathbf{xp}-\mathbf{px} = \hbar i\,\mathbf{1} \tag{20.2.2}$$

Oscillator quantum mechanics involves commutation relations with $\mathbf{a}$ and $\mathbf{a}^\dagger$.

$$\left[\mathbf{a},\mathbf{a}^\dagger\right]\equiv \mathbf{a}\mathbf{a}^\dagger - \mathbf{a}^\dagger\mathbf{a}$$

$$=\frac{1}{2\hbar}\left(\sqrt{M\omega}\,\mathbf{x}+i\mathbf{p}/\sqrt{M\omega}\right)\left(\sqrt{M\omega}\,\mathbf{x}-i\mathbf{p}/\sqrt{M\omega}\right)-\left(\sqrt{M\omega}\,\mathbf{x}-i\mathbf{p}/\sqrt{M\omega}\right)\left(\sqrt{M\omega}\,\mathbf{x}+i\mathbf{p}/\sqrt{M\omega}\right)$$

This is nicely simplified using (20.2.2) to give

$$\left[\mathbf{a},\mathbf{a}^\dagger\right]=\frac{2i}{2\hbar}\left(\mathbf{p}\mathbf{x}-\mathbf{x}\mathbf{p}\right)=\frac{-i}{\hbar}\left[\mathbf{x},\mathbf{p}\right]=\mathbf{1} \qquad (20.2.3a)$$

or $$\mathbf{a}\,\mathbf{a}^\dagger=\mathbf{a}^\dagger\mathbf{a}+\mathbf{1} \qquad (20.2.3b)$$

Just this simple relation by itself lets us simplify the Hamiltonian (20.2.1b) and expose the zero-point energy $E_0 = \hbar\omega/2$ first seen in (20.1.10b).

$$\mathbf{H}(\mathbf{x},\mathbf{p}) = \hbar\omega\,(\mathbf{a}^\dagger\mathbf{a} + \mathbf{a}\mathbf{a}^\dagger)/2 = \hbar\omega\,(\mathbf{a}^\dagger\mathbf{a} + \mathbf{a}^\dagger\mathbf{a} + \mathbf{1})/2$$
$$= \hbar\omega\,\mathbf{a}^\dagger\mathbf{a} + \mathbf{1}\hbar\omega/2 \qquad (20.2.4)$$

*(2) Eigenstate creationism (and destruction)*

Let us define the *ground state* $|0\rangle$ as the eigenstate of $\mathbf{H}(\mathbf{x},\mathbf{p})$ with the zero point eigenvalue $E_0$.

$$\mathbf{H}(\mathbf{x},\mathbf{p})\,|0\rangle = \hbar\omega/2\,|0\rangle \qquad \langle 0|\,\mathbf{H}(\mathbf{x},\mathbf{p}) = \hbar\omega/2\,\langle 0| \qquad (20.2.5a)$$

From (20.2.4) action by $\mathbf{a}$ on the ground ket $|0\rangle$ (or $\mathbf{a}^\dagger$ on ground bra $\langle 0|$) gives *nothing* (zero vectors).

$$\mathbf{a}\,|0\rangle = \boldsymbol{0} \qquad \langle 0|\,\mathbf{a}^\dagger = \boldsymbol{0} \qquad (20.2.5b)$$

However, $\mathbf{a}^\dagger$ acting on the ground ket gives a non-zero vector whose eigenvalue is $\hbar\omega$ greater than $E_0$.

$$\mathbf{H}(\mathbf{x},\mathbf{p})\,\mathbf{a}^\dagger|0\rangle = \hbar\omega\,\mathbf{a}^\dagger\mathbf{a}\,\mathbf{a}^\dagger|0\rangle + \hbar\omega/2\,\mathbf{a}^\dagger|0\rangle$$

Commutation (20.2.3b) gives the following since $\mathbf{a}\,|0\rangle = \boldsymbol{0}$ by (20.2.5b).

$$\mathbf{H}(\mathbf{x},\mathbf{p})\,\mathbf{a}^\dagger|0\rangle = \hbar\omega\,\mathbf{a}^\dagger(\mathbf{a}^\dagger\mathbf{a} + \mathbf{1})|0\rangle + \hbar\omega/2\,\mathbf{a}^\dagger|0\rangle$$
$$= (\hbar\omega + \hbar\omega/2)\,\mathbf{a}^\dagger|0\rangle \qquad (20.2.5c)$$

This is the *one-quantum* or *first excited eigenket* $|1\rangle$ and *eigenbra* $\langle 1|$ defined as follows.

$$|1\rangle = \mathbf{a}^\dagger|0\rangle \qquad \langle 0|\,\mathbf{a} = \langle 1| \qquad (20.2.5d)$$

For kets, $\mathbf{a}^\dagger$ is a creation operator since it creates higher level kets while $\mathbf{a}$ does the reverse.

$$\mathbf{a}|1\rangle = \mathbf{a}\mathbf{a}^\dagger|0\rangle = (\mathbf{a}^\dagger\mathbf{a} + \mathbf{1})|0\rangle = |0\rangle \qquad (20.2.5d)$$

Perhaps, the † that $\mathbf{a}^\dagger$ carries shouldn't be thought of as a dagger but more like a magic wand. But, beware of its dark side. For bras, $\mathbf{a}^\dagger$ is the destructor, and it is $\mathbf{a}$ that does the creation in "bra-space."

A semi-infinite sequence $\{|0\rangle, |1\rangle, \}|2\rangle, |3\rangle, |4\rangle, ...|n\rangle, ...\}$ of eigenkets with $n=0, 1, 2, 3, ...$ quanta can be built this way using repeated applications of this magic creation operator $\mathbf{a}^\dagger$. Before we do this, we need to check that this more than just formalistic posturing. It remains to be shown whether the operator algebra can yield wavefunctions and solutions to the old-fashioned differential equations (20.1.10) of yore.

*(3) Wavefunction creationism*

The coordinate representation of the "nothing" equation (20.2.5b) is as follows.

$$\langle x\,|\,\mathbf{a}\,|0\rangle = \boldsymbol{0} \tag{20.2.6}$$

Expanding the destruction operator using (20.2.1c) gives

$$\left\langle x\middle|\mathbf{a}\middle|0\right\rangle = \frac{1}{\sqrt{2\hbar}}\left(\sqrt{M\omega}\,\left\langle x\middle|\mathbf{x}\middle|0\right\rangle + i\left\langle x\middle|\mathbf{p}\middle|0\right\rangle/\sqrt{M\omega}\right) = 0 \tag{20.2.7a}$$

The operator coordinate representations turn this into a simple differential equation for ground state wavefunction $\psi_0(x) = \langle x\,|0\rangle$.

$$\sqrt{M\omega}\,x\psi_0(x) + i\frac{\hbar}{i}\frac{\partial\psi_0(x)}{\partial x}/\sqrt{M\omega} = 0 \tag{20.2.7b}$$

$$\psi_0'(x) = \frac{M\omega}{\hbar}\,x\psi_0(x) \tag{20.2.7c}$$

Integrating this gives the familiar Gaussian wave mentioned before (20.1.9) and (20.1.10).

$$\int\frac{d\psi}{\psi} = \int\frac{M\omega}{\hbar}\,x dx\,,\quad \ln\psi + \ln const. = \frac{-M\omega}{\hbar}\,\frac{x^2}{2},\quad \psi = \frac{e^{-M\omega x^2/2\hbar}}{const.} \tag{20.2.7d}$$

The normalization *const.* is evaluated using a standard Gaussian integral $\int_{-\infty}^{\infty} dx\, e^{-\alpha x^2} = \sqrt{\frac{\pi}{\alpha}}$ .

$$\left\langle\psi_0\middle|\psi_0\right\rangle = 1 = \int_{-\infty}^{\infty} dx\,\frac{e^{-M\omega x^2/\hbar}}{const.^2} = \sqrt{\frac{\pi\hbar}{M\omega}}/const.^2 \Rightarrow const. = \left(\frac{\pi\hbar}{M\omega}\right)^{1/4} \tag{20.2.7e}$$

The first excited state wavefunction $\psi_1(x) = \langle x\,|1\rangle$ is derived using a representation of (20.2.5d).

$$\langle x\,|\,\mathbf{a}^\dagger|0\rangle = \langle x\,|1\rangle = \psi_1(x) \tag{20.2.8a}$$

Expanding the creation operator using (20.2.1d) gives

$$\left\langle x\middle|\mathsf{a}^\dagger\middle|0\right\rangle = \frac{1}{\sqrt{2\hbar}}\left(\sqrt{M\omega}\,\left\langle x\middle|\mathsf{x}\middle|0\right\rangle - i\left\langle x\middle|\mathsf{p}\middle|0\right\rangle/\sqrt{M\omega}\right) = \left\langle x\middle|1\right\rangle = \psi_1(x)\,. \tag{20.2.8b}$$

The operator coordinate representations generate the first excited state wavefunction.

$$\begin{aligned}
\left\langle x\middle|1\right\rangle = \psi_1(x) &= \frac{1}{\sqrt{2\hbar}}\left(\sqrt{M\omega}\,x\psi_0(x) - i\frac{\hbar}{i}\frac{\partial\psi_0(x)}{\partial x}/\sqrt{M\omega}\right)\\
&= \frac{1}{\sqrt{2\hbar}}\left(\sqrt{M\omega}\,x\frac{e^{-M\omega x^2/2\hbar}}{const.} - i\frac{\hbar}{i}\frac{\partial}{\partial x}\frac{e^{-M\omega x^2/2\hbar}}{const.}/\sqrt{M\omega}\right)\\
&= \frac{1}{\sqrt{2\hbar}}\frac{e^{-M\omega x^2/2\hbar}}{const.}\left(\sqrt{M\omega}\,x + i\frac{\hbar}{i}\frac{M\omega x}{\hbar}/\sqrt{M\omega}\right)\\
&= \frac{\sqrt{M\omega}}{\sqrt{2\hbar}}\frac{e^{-M\omega x^2/2\hbar}}{const.}(2x) = \left(\frac{M\omega}{\pi\hbar}\right)^{3/4}\sqrt{2\pi}\left(x\,e^{-M\omega x^2/2\hbar}\right)
\end{aligned} \tag{20.2.8c}$$

Plots of wavefunctions (20.2.7d) and (20.2.8c) are shown in Fig. 20.2.1a and Fig. 20.2.1b, respectively. (These were constructed using an *N=1* well of *P=24*-pendulum model of Bloch waves as described in Sec. 3.8.) Note the even and odd symmetry, respectively, of the $\psi_0(x)$ and $\psi_1(x)$ waves.

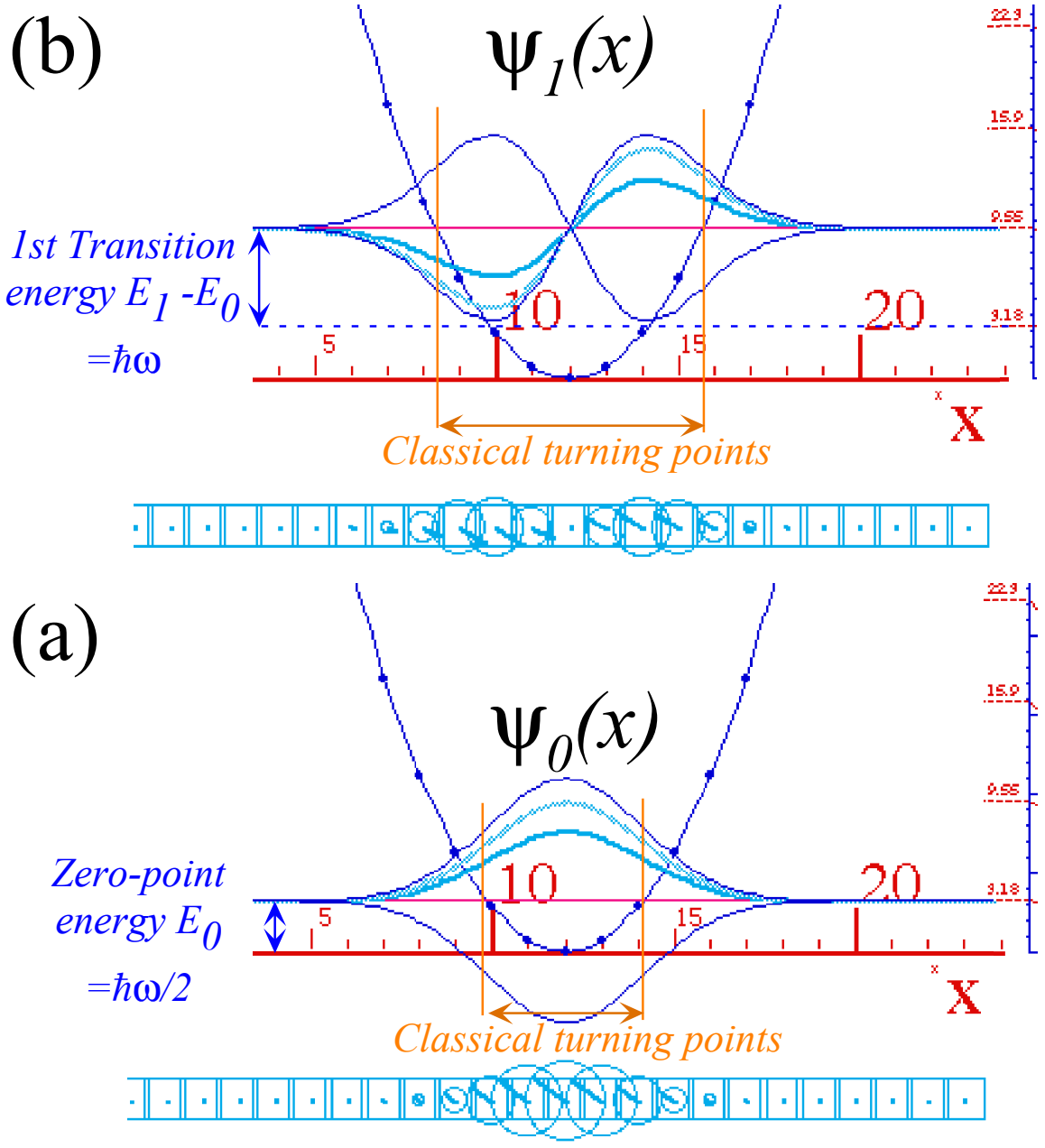


*Fig. 20.2.1 Harmonic oscillator wavefunctions (a) Ground state, (a) First excited state.*

Fig. 20.2.1 shows the points where the total energy equals the potential *(V=E)* and kinetic energy is zero. These are the *classical turning points* of an energy eigenstate. Beyond these points the wave becomes evanescent like a dying exponential. In this case it is a dying Gaussian $e^{-\alpha x^2}$ that dies even faster than $e^{-\alpha x}$. By Schrodinger's equation $\psi'' + \frac{2\hbar^2}{M}[E - V(x)]\psi = 0$, eigenfunction curvature $\psi_n''$ is zero at turning points where *E-V=0*. Turning points of square wells are *fixed* walls. Here our "walls" vary with *E*.

### (b) Matrix and normalization calculations

The main advantage of the algebraic approach is that bra-ket calculations of matrix components like $\langle m|\mathbf{x}^k|n\rangle$ or $\langle m|\mathbf{a}^k|n\rangle$ generally do not have to involve coordinate (or momentum) integration. To facilitate the algebra of $\mathbf{a}$ and $\mathbf{a}^\dagger$ matrices it helps to reorder them using commutator identity $\mathbf{AB} = [\mathbf{A}, \mathbf{B}] + \mathbf{BA}$. In a matrix such as follows, it helps to move destructive $\mathbf{a}$ operators to the right so they zero out.

$$\langle 0|f(\mathbf{a})g(\mathbf{a}^\dagger)|0\rangle = \langle 0|\,[f(\mathbf{a}),\, g(\mathbf{a}^\dagger)]\,|0\rangle + \langle 0|\,g(\mathbf{a}^\dagger)\,f(\mathbf{a})\,|0\rangle$$

Then only the commutator matrix $\langle 0|\,[f(\mathbf{a}),\, g(\mathbf{a}^\dagger)]\,|0\rangle$ needs to be evaluated.

For example, the following generalizations of the basic (20.3.3) relation $[\mathbf{a}, \mathbf{a}^\dagger] = \mathbf{1}$ are useful.

$$\left[\mathbf{a},\mathbf{a}^{\dagger 2}\right] = 2\mathbf{a}^\dagger\ ,\quad \left[\mathbf{a},\mathbf{a}^{\dagger 3}\right] = 3\mathbf{a}^{2\dagger},\ \cdots\ ,\quad ,\quad \left[\mathbf{a},\mathbf{a}^{\dagger n}\right] = n\mathbf{a}^{\dagger n-1} \qquad (20.2.9a)$$

These are special cases of applying what might be called the *commutator derivative identity*.

$$[\mathbf{A}, \mathbf{BC}] = \mathbf{ABC} - \mathbf{BCA} = [\mathbf{A}, \mathbf{B}]\mathbf{C} + \mathbf{BAC} - \mathbf{BCA}$$
$$= [\mathbf{A}, \mathbf{B}]\mathbf{C} + \mathbf{B}[\mathbf{A}, \mathbf{C}] \qquad (20.2.9b)$$

The name recognizes the similarity between these relations and power-law derivatives. It goes either way.

$$[\mathbf{AB}, \mathbf{C}] = -[\mathbf{C}, \mathbf{AB}] = -[\mathbf{C}, \mathbf{A}]\mathbf{B} - \mathbf{A}[\mathbf{C}, \mathbf{B}]$$
$$= [\mathbf{A}, \mathbf{C}]\mathbf{B} + \mathbf{A}[\mathbf{B}, \mathbf{C}] \qquad (20.2.9c)$$

Using (20.2.9a) we can commute arbitrary powers to get something that resembles binomial expansions.

$$\mathbf{a}\mathbf{a}^{\dagger n} = n\mathbf{a}^{\dagger n-1} + \mathbf{a}^{\dagger n}\mathbf{a}$$
$$\mathbf{a}^2\mathbf{a}^{\dagger n} = n\mathbf{a}\mathbf{a}^{\dagger n-1} + \mathbf{a}\mathbf{a}^{\dagger n}\mathbf{a}$$
$$= n(n-1)\mathbf{a}^{\dagger n-2} + n\mathbf{a}^{\dagger n-1}\mathbf{a} + n\mathbf{a}^{\dagger n-1}\mathbf{a} + \mathbf{a}^{\dagger n}\mathbf{a}^2$$
$$= n(n-1)\mathbf{a}^{\dagger n-2} + 2n\mathbf{a}^{\dagger n-1}\mathbf{a} + \mathbf{a}^{\dagger n}\mathbf{a}^2$$
$$\mathbf{a}^3\mathbf{a}^{\dagger n} = n(n-1)\mathbf{a}\mathbf{a}^{\dagger n-2} + 2n\mathbf{a}\mathbf{a}^{\dagger n-1}\mathbf{a} + \mathbf{a}\mathbf{a}^{\dagger n}\mathbf{a}^2$$
$$= n(n-1)(n-2)\mathbf{a}^{\dagger n-3} + n(n-1)\mathbf{a}^{\dagger n-2}\mathbf{a} + 2n(n-1)\mathbf{a}^{\dagger n-2}\mathbf{a} + 2n\mathbf{a}^{\dagger n-1}\mathbf{a}^2 + n\mathbf{a}^{\dagger n-1}\mathbf{a}^2 + \mathbf{a}^{\dagger n}\mathbf{a}^3$$
$$= n(n-1)(n-2)\mathbf{a}^{\dagger n-3} + 3n(n-1)\mathbf{a}^{\dagger n-2}\mathbf{a} + 3n\mathbf{a}^{\dagger n-1}\mathbf{a}^2 + \mathbf{a}^{\dagger n}\mathbf{a}^3$$

Using binomial coefficients $\binom{m}{r} = \dfrac{m!}{r!(m-r)!}$ this becomes a formula for any power $m$=..3,4..

$$\mathbf{a}^3\mathbf{a}^{\dagger n} = \binom{3}{0}\frac{n!}{(n-3)!}\mathbf{a}^{\dagger n-3} + \binom{3}{1}\frac{n!}{(n-2)!}\mathbf{a}^{\dagger n-2}\mathbf{a} + \binom{3}{2}\frac{n!}{(n-1)!}\mathbf{a}^{\dagger n-1}\mathbf{a}^2 + \binom{3}{3}\frac{n!}{(n-0)!}\mathbf{a}^{\dagger n}\mathbf{a}^3$$

The general $\mathbf{a}..\mathbf{a}^\dagger$ *to* $\mathbf{a}^\dagger..\mathbf{a}$ *power shuffle formula* is the result we want.

$$\mathbf{a}^m\mathbf{a}^{\dagger n} = \sum_{r=0}^{m}\binom{m}{r}\frac{n!}{(n-m+r)!}\mathbf{a}^{\dagger n-m+r}\mathbf{a}^r = \sum_{r=0}^{m}\frac{m!}{r!(m-r)!}\frac{n!}{(n-m+r)!}\mathbf{a}^{\dagger n-m+r}\mathbf{a}^r \qquad (20.2.10a)$$

Normalization requires a special case of this formula with $m$=$n$.

$$\mathbf{a}^n\mathbf{a}^{\dagger n} = \sum_{r=0}^{n}\binom{n}{r}\frac{n!}{r!}\mathbf{a}^{\dagger r}\mathbf{a}^r = n!\left(\mathbf{1} + n\mathbf{a}^\dagger\mathbf{a} + \frac{n(n-1)}{2!\,2!}\mathbf{a}^{\dagger 2}\mathbf{a}^2 + \frac{n(n-1)(n-3)}{3!\,3!}\mathbf{a}^{\dagger 3}\mathbf{a}^3 + \ldots\right) \qquad (20.2.10b)$$

*(1) Normalization and ladder operations*

To create quantum states $|n\rangle$ with $n$ greater than *0* or *1*, it is necessary to derive the normalization constant as a function of $n$ for a state obtained by applying the $\mathbf{a}^\dagger$ operator $n$-times.

$$|n\rangle = \frac{\mathbf{a}^{\dagger n}|0\rangle}{const.}, \quad \text{where:} \quad 1 = \langle n|n\rangle = \frac{\langle 0|\mathbf{a}^n\mathbf{a}^{\dagger n}|0\rangle}{(const.)^2} = n!\frac{\langle 0|\mathbf{1}+n\mathbf{a}^\dagger\mathbf{a}+..|0\rangle}{(const.)^2} = \frac{n!}{(const.)^2}.$$

The result is root-factorial normalization: $$|n\rangle = \frac{\mathbf{a}^{\dagger n}|0\rangle}{\sqrt{n!}} \qquad (20.2.11)$$

Note that for $n$ equal to *0* or *1*, the normalization is unity. (Yes, it is conventional to define *0! = 1 = 1!* ) Clearly, we need to generalize the *n = 0* or *1* creation and destruction formulas (20.2.5) to higher $n$-quanta.

Applying a creation operator $\mathbf{a}^\dagger$ to an $n$-quantum state (20.10.11) gives the following.

$$\mathbf{a}^\dagger|n\rangle = \frac{\mathbf{a}^{\dagger n+1}|0\rangle}{\sqrt{n!}} = \sqrt{n+1}\,\frac{\mathbf{a}^{\dagger n+1}|0\rangle}{\sqrt{(n+1)!}} \qquad (20.2.12a)$$

Applying a destruction operator $\mathbf{a}$ to an $n$-quantum state using (20.2.10) gives the following.

$$\mathbf{a}|n\rangle = \frac{\mathbf{a}\mathbf{a}^{\dagger n}|0\rangle}{\sqrt{n!}} = \frac{(n\mathbf{a}^{\dagger n-1}+\mathbf{a}^{\dagger n}\mathbf{a})|0\rangle}{\sqrt{n!}} = \sqrt{n}\,\frac{\mathbf{a}^{\dagger n-1}|0\rangle}{\sqrt{(n-1)!}} \qquad (20.2.12b)$$

These can be summarized by the following oscillator ladder relations.

$$\mathbf{a}^\dagger|n\rangle = \sqrt{n+1}\,|n+1\rangle \quad (20.10.13a) \qquad \mathbf{a}|n\rangle = \sqrt{n}\,|n-1\rangle \quad (20.2.13b)$$

A mnemonic rule: Always put the larger of the two quanta under the radical factor for either case. The creation and destruction operators are represented in the $\{|0\rangle, |1\rangle, \}|2\rangle,...\}$ basis by semi-infinite matrices.

$$\langle \mathbf{a}^\dagger \rangle = \begin{pmatrix} \cdot & & & & & \\ 1 & \cdot & & & & \\ & \sqrt{2} & \cdot & & & \\ & & \sqrt{3} & \cdot & & \\ & & & \sqrt{4} & \cdot & \\ & & & & \ddots & \cdot \end{pmatrix} \quad (20.2.13c) \qquad \langle \mathtt{a} \rangle = \begin{pmatrix} \cdot & 1 & & & & \\ & \cdot & \sqrt{2} & & & \\ & & \cdot & \sqrt{3} & & \\ & & & \cdot & \sqrt{4} & \\ & & & & \cdot & \ddots \\ & & & & & \cdot \end{pmatrix} \quad (20.2.13d)$$

*(2) Number operator*

The Hamiltonian (20.2.4) contains the operator $\hbar\omega\,\mathbf{a}^\dagger\mathbf{a}$ plus the zero-point energy $\mathbf{1}\hbar\omega/2$ . It is important to understand the operator $\mathbf{a}^\dagger\mathbf{a}$. Its effect on a quantum state follows using (20.2.10).

$$\mathbf{a}^\dagger\mathbf{a}|n\rangle = \frac{\mathbf{a}^\dagger\mathbf{a}\mathbf{a}^{\dagger n}|0\rangle}{\sqrt{n!}} = n\frac{\mathbf{a}^\dagger\mathbf{a}^{\dagger n-1}|0\rangle}{\sqrt{n!}} = n\frac{\mathbf{a}^{\dagger n}|0\rangle}{\sqrt{n!}} = n|n\rangle \qquad (20.2.14)$$

It counts quanta and hence it is called the *number operator* $\mathbf{a}^\dagger\mathbf{a}$. This is proof that $|n\rangle$ are $\mathbf{H}$ eigenstates.

$$\mathbf{H}\,|n\rangle = \hbar\omega\,\mathbf{a}^\dagger\mathbf{a}\,|n\rangle + \hbar\omega/2\mathbf{1}\,|n\rangle = (\hbar\omega\, n + \hbar\omega/2)\,|n\rangle \qquad (20.2.15a)$$

$$\langle \mathtt{H} \rangle = \hbar\omega\langle \mathtt{a}^\dagger\mathtt{a} \rangle + \frac{\hbar\omega}{2}\langle \mathtt{1} \rangle = \hbar\omega \begin{pmatrix} 0 & & & \\ & 1 & & \\ & & 2 & \\ & & & 3 \\ & & & & \ddots \end{pmatrix} + \hbar\omega \begin{pmatrix} 1/2 & & & \\ & 1/2 & & \\ & & 1/2 & \\ & & & 1/2 \\ & & & & \ddots \end{pmatrix} \qquad (20.2.15b)$$

*(3) Expectation values and uncertainty*

The **a**-algebra helps to find expectation values of operators besides the Hamiltonian **H**. Consider position **x** and momentum **p**. Solving (20.2.1) gives **x** and **p** in terms of **a** and $\mathbf{a}^\dagger$ .

$$\sqrt{\frac{M\omega}{2\hbar}}\mathbf{x} = \frac{\mathbf{a}+\mathbf{a}^\dagger}{2} \quad , \qquad \sqrt{\frac{1}{2\hbar M\omega}}\,\mathbf{p} = \frac{\mathbf{a}-\mathbf{a}^\dagger}{2i} \tag{20.2.16}$$

The eigenstates expectation values of **x** and **p** for are zero because $\langle n|\mathbf{a}|n\rangle = 0 = \langle n|\mathbf{a}^\dagger|n\rangle$ .

$$\bar{\mathbf{x}}\,|_n = \langle n|\mathbf{x}|n\rangle = \sqrt{\frac{\hbar}{2M\omega}}\langle n|\left(\mathbf{a}+\mathbf{a}^\dagger\right)|n\rangle = 0 \tag{20.2.17a}$$

$$\bar{\mathbf{p}}\,|_n = \langle n|\mathbf{p}|n\rangle = i\sqrt{\frac{\hbar M\omega}{2}}\langle n|\left(\mathbf{a}^\dagger-\mathbf{a}\right)|n\rangle = 0 \tag{20.2.17b}$$

The zeros can also be seen to be a result of the symmetry of the potential and its eigenfunctions such as were shown in Fig. 20.2.1. However, the mean squares or $\mathbf{x}^2$ and $\mathbf{p}^2$ expectations are non-zero.

$$\overline{\mathbf{x}^2}\,|_n = \langle n|\mathbf{x}^2|n\rangle = \frac{\hbar}{2M\omega}\langle n|\left(\mathbf{a}+\mathbf{a}^\dagger\right)^2|n\rangle$$
$$= \frac{\hbar}{2M\omega}\langle n|\left(\mathbf{a}^2+\mathbf{a}^\dagger\mathbf{a}+\mathbf{a}\mathbf{a}^\dagger+\mathbf{a}^{\dagger 2}\right)|n\rangle$$
$$= \frac{\hbar}{2M\omega}\quad (2n+1) \tag{20.2.18a}$$

$$\overline{\mathbf{p}^2}\,|_n = \langle n|\mathbf{p}^2|n\rangle = i^2\frac{\hbar M\omega}{2}\langle n|\left(\mathbf{a}^\dagger-\mathbf{a}\right)^2|n\rangle$$
$$= -\frac{\hbar M\omega}{2}\langle n|\left(\mathbf{a}^{\dagger 2}-\mathbf{a}^\dagger\mathbf{a}-\mathbf{a}\mathbf{a}^\dagger+\mathbf{a}^2\right)|n\rangle$$
$$= \frac{\hbar M\omega}{2}\quad (2n+1) \tag{20.2.18b}$$

The basic commutation $\mathbf{a}\mathbf{a}^\dagger = \mathbf{a}^\dagger\mathbf{a} + \mathbf{1}$ (20.2.3) and number value (20.2.14) was used. This lets us estimate the mean or expected kinetic and potential energies.

$$\overline{PE}\,|_n = \frac{1}{2}M\omega^2\,\overline{\mathbf{x}^2}\,|_n = \frac{1}{2}M\omega^2\,\frac{\hbar(2n+1)}{2M\omega}$$
$$= \frac{1}{2}\hbar\omega\left(n+\frac{1}{2}\right) \tag{20.2.19a}$$

$$\overline{KE}\,|_n = \frac{1}{2M}\overline{\mathbf{p}^2}\,|_n = \frac{1}{2M}\frac{\hbar M\omega}{2}(2n+1)$$
$$= \frac{1}{2}\hbar\omega\left(n+\frac{1}{2}\right) \tag{20.2.19b}$$

The fact that they are equal is peculiar to the harmonic oscillator's phase space or $X \leftrightarrow P$ symmetry.

*Uncertainty* or *standard deviation* $\Delta q$ of a statistical quantity $q$ is its root mean-square difference.

$$(\Delta q)^2 = \overline{(q-\bar{q})^2} \;\;,, \quad \text{or:} \quad \Delta q = \sqrt{\overline{(q-\bar{q})^2}} \tag{20.2.20a}$$

Harmonic oscillator coordinate and momentum uncertainty follow from (20.2.17) and (20.2.18).

$$\Delta x = \sqrt{\overline{\mathbf{x}^2}} = \sqrt{\frac{\hbar(2n+1)}{2M\omega}} \tag{20.2.20b}$$

$$\Delta p = \sqrt{\overline{\mathbf{p}^2}} = \sqrt{\frac{\hbar M\omega(2n+1)}{2}} \tag{20.2.20c}$$

The *Heisenberg uncertainty product* for the $n$-quantum eigenstate is

$$\Delta x\cdot\Delta p\,|_n = \sqrt{\overline{\mathbf{x}^2}}\sqrt{\overline{\mathbf{p}^2}}\,|_n = \sqrt{\frac{\hbar(2n+1)}{2M\omega}}\sqrt{\frac{\hbar M\omega(2n+1)}{2}} = \hbar\left(n+\frac{1}{2}\right) \tag{20.2.20d}$$

The *Heisenberg minimum uncertainty product* occurs for the *0*-quantum (ground) eigenstate.

$$\Delta x\cdot\Delta p\,|_0 = \frac{\hbar}{2} \tag{20.2.20e}$$

*(4) Uncertainty approximation for anharmonic spectra*

The preceding harmonic oscillator uncertainty relations are the simplest ones we've seen so far. They are a great deal simpler than the $\Delta p$ or $\Delta x$ functions for most anharmonic oscillator power-law potentials $V(x) = Ax^P$ with powers other than $P=2$.

While relation (20.2.20d) is only exact for $P=2$ potentials, it may be used to approximate the spectra of other potentials, too. The idea that an $n$-quantum state occupies $n\hbar$ units of phase space is related to the classical Liouville phase-space-incompressibility theorem and applies to any potential.

The trick is to set *root-mean-square (rms)* values $x = \Delta x$ and $p = \Delta p$ in the Hamiltonian $H$ and minimize $H=E$ with respect to $\Delta x$ subject to the constraint (20.2.20d) of phase-space-incompressibility.

$$E_\upsilon = MIN\left( \frac{p^2}{2M} + Ax^P = \frac{(\Delta p)^2}{2M} + A(\Delta x)^P \right) \text{ subject to: } \Delta x \cdot \Delta p = x \cdot p = \upsilon = (n+\frac{1}{2})\hbar \quad (20.2.21a)$$

By putting $p = \Delta p = \upsilon/\Delta x = \upsilon/x$ into an energy function and zeroing the $x$-derivative we find $\Delta x = x_{min}$.

$$\frac{d}{dx}\left( \frac{p^2}{2M} + Ax^P \right) = \frac{d}{dx}\left( \frac{\upsilon^2}{2Mx^2} + Ax^P \right) = \frac{-2\upsilon^2}{2Mx^3} + APx^{P-1} = 0 = \frac{-\upsilon^2}{M} + APx^{P+2}$$

$$\Delta x = x_{\min} = \left( \frac{\upsilon^2}{MAP} \right)^{\frac{1}{P+2}}, \qquad \Delta p = p_{\min} = \frac{\upsilon}{x_{\min}} = \upsilon\left( \frac{\upsilon^2}{MAP} \right)^{\frac{-1}{P+2}} \quad (20.2.21b)$$

For the harmonic oscillator PE power $P=2$ and spring constant $A = k/2 = 1/2 M\omega^2$, the values (20.2.21) equal the exact results (20.2.20) and minimum energy subject to constant $\Delta x\, \Delta p$.

Quantum $\upsilon$-number dependence factors out of the resulting general minimum energy.

$$E_\upsilon = \frac{\upsilon^2}{2M}\left( \frac{\upsilon^2}{MAP} \right)^{\frac{-2}{P+2}} + A\left( \frac{\upsilon^2}{MAP} \right)^{\frac{P}{P+2}} = \upsilon^{\frac{2P}{P+2}}\left( \frac{1}{2M^{\frac{P}{P+2}}A^{\frac{-2}{P+2}}P^{\frac{-2}{P+2}}} + \frac{1}{M^{\frac{P}{P+2}}A^{\frac{-2}{P+2}}P^{\frac{P}{P+2}}} \right) \quad (20.2.22a)$$

Then the kinetic $(KE = p^2/2M)$ and the potential $(PE = Ax^P)$ parts simplify, too.

$$E_\upsilon = \upsilon^{\frac{2P}{P+2}} \frac{A^{\frac{2}{P+2}}}{M^{\frac{P}{P+2}}}\left[ \frac{1}{2P^{\frac{-2}{P+2}}} + \frac{1}{P^{\frac{P}{P+2}}} \right] = \upsilon^{\frac{2P}{P+2}} \frac{A^{\frac{2}{P+2}}}{(MP)^{\frac{P}{P+2}}}\left[ \frac{P+2}{2} \right] \quad (20.2.22b)$$

Again, the oscillator parameters $P=2$ and $A = k/2 = 1/2 M\omega^2$ reduce this to the exact energy $E_\upsilon = \upsilon\omega = \hbar\omega(n+1/2)$.

However, this approximation works pretty well for other power-laws. First, it gives the *Virial ratio P:2* between KE and PE that was derived in (18.3.10). Then a uniform force field (like terrestrial gravity) with $P=1$ has a spectrum shown in Fig. 20.4.2 that goes as $\upsilon^{2/3}$. A square-well corresponds to a large power $P\to\infty$. Then, (20.2.22b) correctly predicts the quantum dependence $\upsilon^{2P/P+2}$ approaches $\upsilon^2$. At the opposite extreme, a Coulomb potential $k/r$ has $P=-1$. According to (20.2.22b), it has an inverse power $\upsilon^{-2}$-spectrum. As we will see in Chapter 26, this result is exactly true. (Note that (20.2.21) gives the Bohr radius discussed back in (5.4.3a) and the momentum (20.2.21b) agrees with (5.4.3b).)

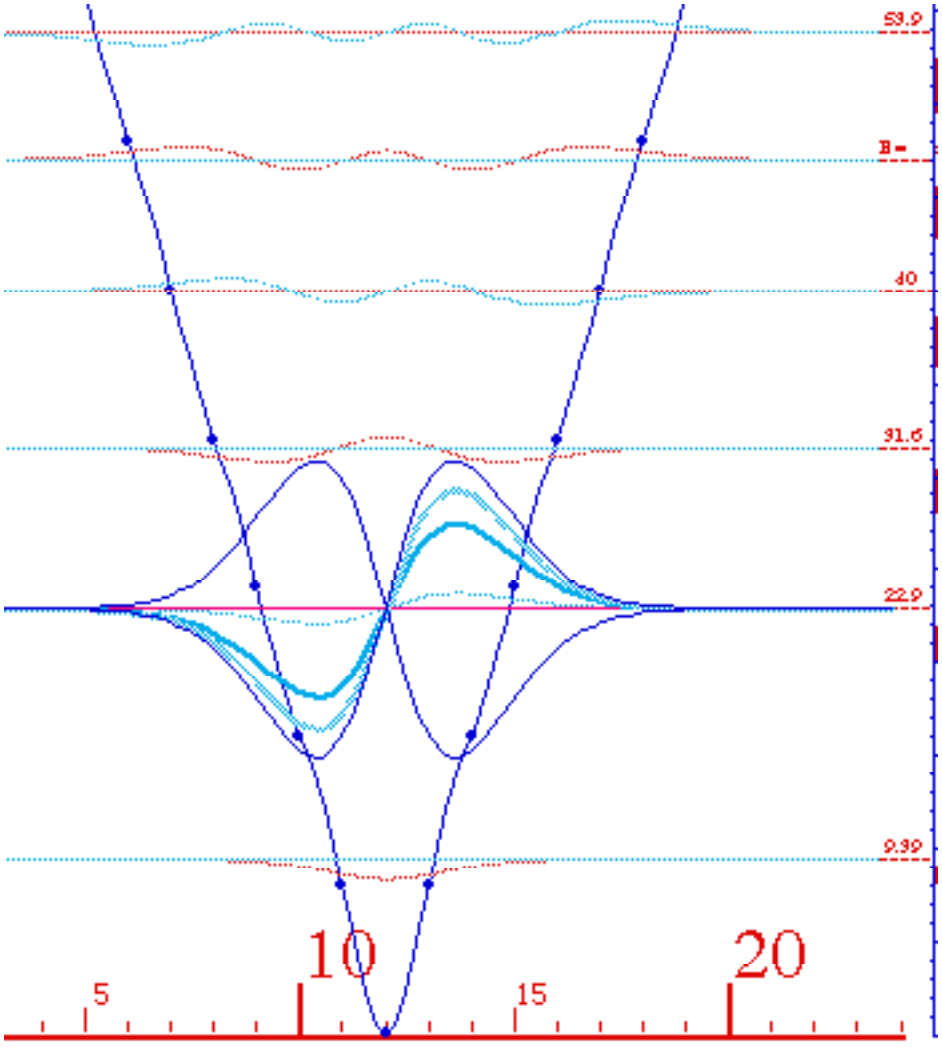


*Fig. 20.2.2 First excited state wavefunction of linear potential V(y)=mg|y|. (V=98 Bu for N=24 )*

A *24*-pendulum model in Fig. 20.2.2 provides a wavefunction and energy spectrum for a linear potential $V(x)=V|x|$ and clearly shows the decreasing energy level spacing as energy increases. The linear potential wavefunctions $\psi_\mu(x)$ have a superficial resemblance to the corresponding Hermite oscillator wavefunctions shown in Fig. 20.2.1. However, their algebraic properties are quite different. First of all, the zero-point energy is a larger fraction 0.69 of the first transition energy than the 0.5 obtained for the harmonic oscillator. The fraction $\mu_0$ in quantum phase space area $\hbar\omega(n + \mu_0)$ is called *Maslov's index*.

The linear potential wavefunctions are called *Airy functions*. If you keep only odd-*n* anti-symmetric Airy wavefunctions such as the $\psi_1(x)$ shown and $\psi_3(x), \psi_5(x), \psi_7(x), ...$ and discard the even-*n* $\psi_0(x), \psi_2(x), \psi_4(x), ...$ waves, then you will have a complete set of *bouncing-ball eigensolutions* due to an infinite potential wall at the origin (and symmetry axis) of Fig. 20.2.2. These are discussed in an article by Julio Geo-Benacloche. (AJP September 1999)

### (c) High quantum oscillator states

The repeated application of the creation operator to the ground state yields higher and higher quantum numbers and eigenstates and more and more complicated wavefunctions. An example with *n=20* is shown in Fig. 20.2.3.

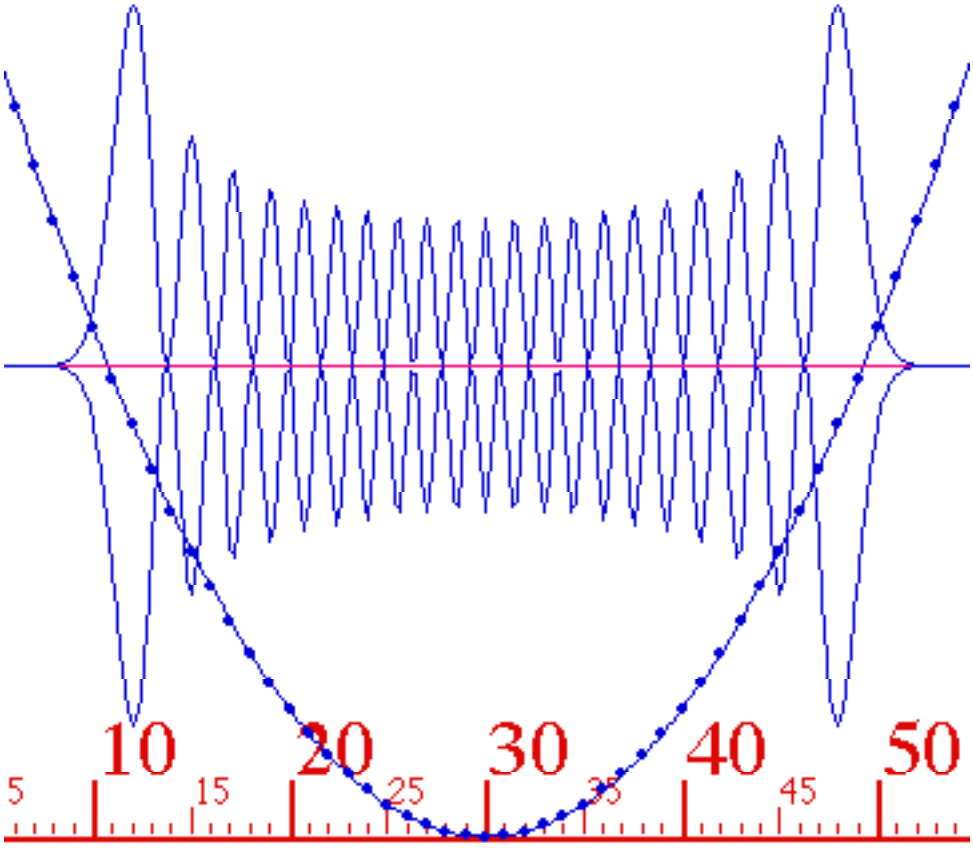


*Fig. 20.2.3 n=20 probability for harmonic oscillator potential* $V(x)=Vx^2$*.(V=100 Bu for P=60 )*

This is still a long way from a classical energy value of *1 Joule*; for a *1 Hz* oscillator that would take a quantum number of roughly $n= 100,000,000,000,000,000,000,000,000,000,000,000,000=10^{35}$ which is to say the least, beyond the capability of current computers to simulate. (How big would the number *P* of pendulums be?)

However, even this relatively low quantum excitation is showing some visible classical properties. The envelope of the probability distribution is beginning to look like an inverse cosine function which is the classical probability distribution of a sinusoidally oscillating particle.

## 20.3 Harmonic Oscillator Dynamics and Coherent States

### (a) Oscillator quantum beats

So far, our study of oscillator eigenstates has been lifeless; eigenstates, by themselves, appear to be dead since the absolute square kills Planck phase oscillation ($\psi_\mu(x,t) = e^{-i\omega_\mu t}\psi_\mu(x)$) of each eigenstate.

$$|\psi_0(x,t)|^2 = |e^{-i\omega_0 t}\langle x|0\rangle|^2 = |\psi_0(x)|^2\ , \quad |\psi_1(x,t)|^2 = |e^{-i\omega_1 t}\langle x|1\rangle|^2 = |\psi_1(x)|^2\ ,... \qquad (20.3.1)$$

Planck's oscillation of a quantum phasor is observable only relative to another phasor which has a different frequency and when the two phasors can interfere with each other. Then their combined probability distribution wobbles or "beats" at a frequency that is the difference between their Planck rates.

This is how a quantum harmonic oscillator can actually oscillate like a classical pendulum. The simplest example of this is had by mixing the first two eigenstates, the ground and excited states $|0\rangle$ and $|1\rangle$ with wave functions $\psi_0(x) = \langle x|0\rangle$ and $\psi_1(x) = \langle x|1\rangle$ shown in Fig. 20.2.1, gives the following state .

$$|\Psi\rangle = |0\rangle\langle 0|\Psi\rangle + |1\rangle\langle 1|\Psi\rangle = |0\rangle\Psi_0 + |1\rangle\Psi_1 \qquad (20.3.2a)$$

Eigenfunctions $\psi_0(x) = \langle x|0\rangle$ and $\psi_1(x) = \langle x|1\rangle$ (shown in Fig. 20.2.1) are mixed to give

$$\Psi(x) = \langle x|\Psi\rangle = \langle x|0\rangle\langle 0|\Psi\rangle + \langle x|1\rangle\langle 1|\Psi\rangle = \psi_0(x)\,\Psi_0 + \psi_1(x)\,\Psi_1 \qquad (20.3.2b)$$

The greatest oscillation occurs with *50-50* mixing coefficients

$$\Psi_0 = \langle 0|\Psi\rangle = 1/\sqrt{2}\ , \qquad \Psi_1 = \langle 1|\Psi\rangle = 1/\sqrt{2} \qquad (20.3.3)$$

The time dependence $\Psi(x,t)$ of the mixed wave is then

$$\Psi(x,t) = \psi_0(x)\,e^{-i\omega_0 t}\Psi_0 + \psi_1(x)\,e^{-i\omega_1 t}\Psi_1 = (\psi_0(x)\,e^{-i\omega_0 t} + \psi_1(x)\,e^{-i\omega_1 t})/\sqrt{2} \qquad (20.3.4)$$

and probability amplitude $|\Psi(x,t)|$ envelope beats back and forth according to

$$\begin{aligned}|\Psi(x,t)| &= \sqrt{\Psi^*\Psi} = \sqrt{\left(e^{-i\omega_0 t}\psi_0(x) + e^{-i\omega_1 t}\psi_1(x)\right)^*\left(e^{-i\omega_0 t}\psi_0(x) + e^{-i\omega_1 t}\psi_1(x)\right)/2} \\ &= \sqrt{\left(|\psi_0(x)|^2 + |\psi_1(x)|^2 + \psi_0(x)\psi_1(x)\left(e^{i(\omega_1-\omega_0)t} + e^{-i(\omega_1-\omega_0)t}\right)\right)/2} \qquad (20.3.5a) \\ &= \sqrt{\left(|\psi_0(x)|^2 + |\psi_1(x)|^2 + 2\psi_0(x)\psi_1(x)\cos(\omega_1-\omega_0)t\right)/2}\end{aligned}$$

This oscillation of $\Psi(x,t)$ and $|\Psi(x,t)|$ is shown in Fig. 20.3.1 for a single beat period $\tau_{beat}$. It is strong wherever *wave overlap* $\psi_0(x)\psi_1(x)$ is large and occurs at the angular beat frequency $\omega_1 - \omega_0 = 2\pi/\tau_{beat}$.

The general 2-state quantum probability beat wavefunction is

$$\Psi(x,t)^*\Psi(x,t) = |A_0(x)|^2 + |A_1(x)|^2 + 2|A_0(x)\,A_1(x)|\cos(\theta_{01}(x) + (\omega_1-\omega_0)t)\ , \qquad (20.3.5b)$$

Here individual mixed-wave amplitudes are $A_0(x) = \psi_0(x)\Psi_0$ and $A_1(x) = \psi_1(x)\Psi_1$ and wave overlap

$$A_0(x)\,A_1(x) = |A_0(x)\,A_1(x)|\,e^{i\theta_{01}(x)} \qquad (20.3.5c)$$

may be complex with a phase $\theta_{01}$ that varies with $x$. In (20.3.4) both $A_0(x)$ and $A_1(x)$ are real and $\theta_{01} = 0$. The beat frequency is the eigenfrequency difference

$$\omega_{beat} = \omega_1 - \omega_0 = \omega\ , \qquad (20.3.5d)$$

which also happens to be the classical oscillator's natural frequency $\omega$. So, this is the first example of a quantum oscillator behaving like a classical oscillator or pendulum.

Frequency $\omega_{beat}$ is called a *transition frequency* since it is $(1/\hbar)$ times a *transition energy*

$$\Delta E = E_{1\leftarrow 0\ transition} = E_1 - E_0 = \hbar\omega \qquad (20.3.6)$$

Here $\Delta E$ is the energy difference between the first excited level $E_1 = \hbar\omega_1$ and ground level $E_0 = \hbar\omega_0$. However, for a harmonic oscillator all neighboring pairs of levels have the same transition frequency $\omega$. Furthermore, all pairs of levels will beat at a frequency that is an integral harmonic of $\omega$.

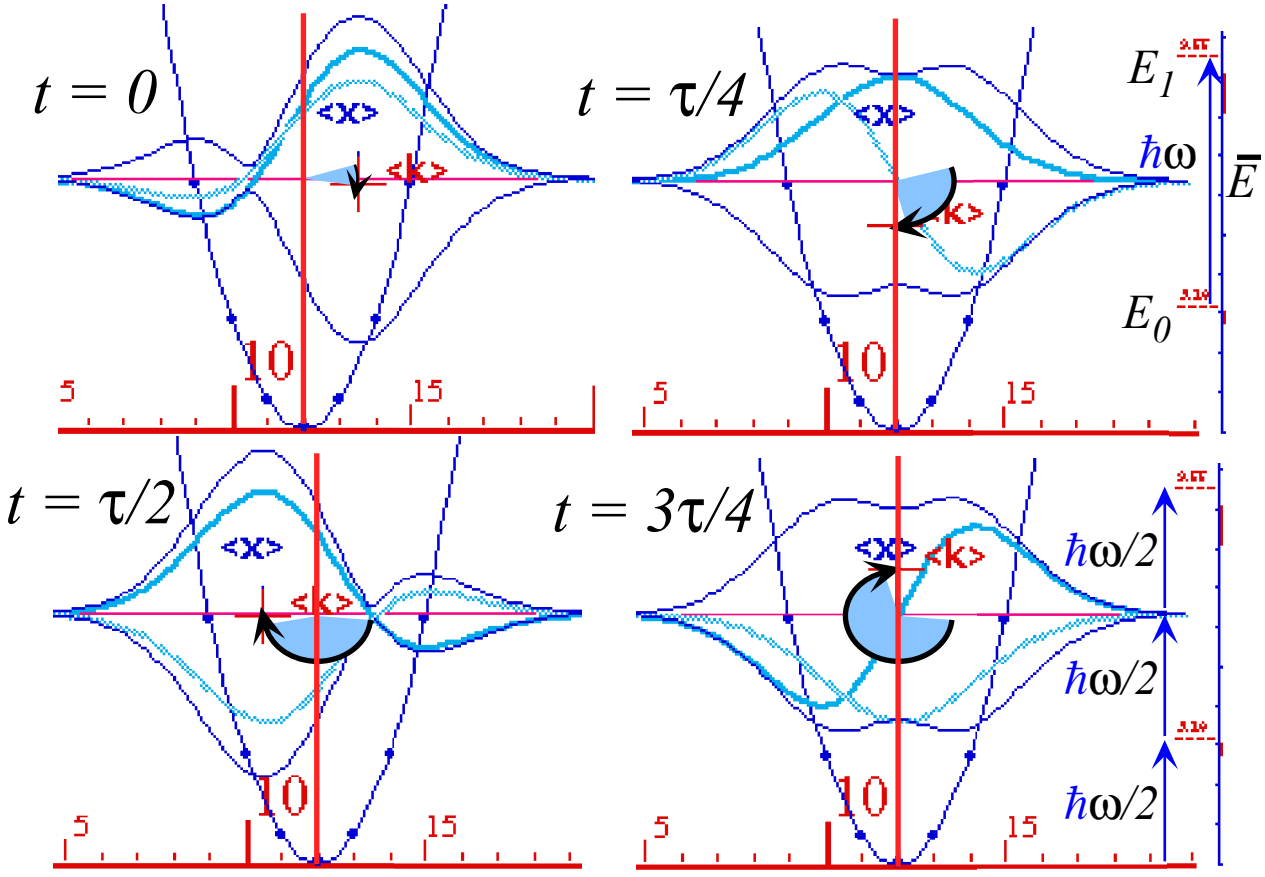


*Fig. 20.3.1 Beat oscillation for mixed 01-state of harmonic oscillator showing x and k expectation.*

*(1) Energy expectation value*

The energy expectation value or mean energy was given in Sec. 12.1(c) as the matrix sum (12.1.8) over energy eigenvalues $E_n$ times the probability $|\Psi_n|^2$ for each of the eigenstates.

$$\bar{E} = \langle\Psi|\mathbf{H}|\Psi\rangle = \langle 0|\mathbf{H}|0\rangle|\langle 0|\Psi\rangle|^2 + \langle 1|\mathbf{H}|1\rangle|\langle 1|\Psi\rangle|^2 + \ldots$$
$$= E_0\ |\Psi_0|^2 + E_1\ |\Psi_1|^2 + \ldots \qquad (20.3.7a)$$

For a *50-50* combination example (20.4.3) pictured in Fig. 20.3.1 the expected or mean energy is $\hbar\omega$, too.

$$\bar{E} = E_0\ 1/2 + E_1\ 1/2 = (\hbar\omega/2)\ 1/2 + (3\hbar\omega/2)\ 1/2 = \hbar\omega \qquad (20.3.7b)$$

(Mean $(E_0+E_1)/2$ of oscillator $E$-values $E_0$ and $E_1$ just happens to equal their transition energy $E_0$-$E_1$.)

*(2) Position expectation values*

The position expectation involves a double matrix sum over eigenstates since the **x**-operator is not diagonal in the energy basis. The Ch. 12 equation (12.1.11) treats the general case.

$$\bar{x}\,|_{\Psi} = \langle\Psi|\mathbf{x}|\Psi\rangle = \Sigma_{m=1}^{\infty}\ \Sigma_{n=1}^{\infty}\ \langle\Psi|m\rangle\langle m|\mathbf{x}|n\rangle\langle n|\Psi\rangle \qquad (20.3.8a)$$

Here the *dipole matrix elements* $\langle m|\mathbf{x}|n\rangle$ are easily derived using **a**-algebra. Generalizing (20.2.17a) gives

$$\begin{aligned}\langle m|\mathrm{x}|n\rangle &= \sqrt{\frac{\hbar}{2M\omega}}\langle m|\left(\mathrm{a}+\mathrm{a}^{\dagger}\right)|n\rangle = \sqrt{\frac{\hbar}{2M\omega}}\left(\sqrt{n}\,\langle m|n-1\rangle + \sqrt{n+1}\,\langle m|n+1\rangle\right)\\ &= \left(x_0/\sqrt{2}\right)\left(\sqrt{n}\delta_{m,n-1} + \sqrt{n+1}\delta_{m,n+1}\right)\end{aligned} \qquad (20.3.8b)$$

where $x_0$ is the *zero-point classical turning point* $x_0$ is where $E_0 = {}^1/_2 M\omega^2 x_0{}^2 = \hbar\omega/2$.

$$x_0 = [\hbar/M\omega]^{1/2} \qquad (20.3.8c)$$

The off-diagonal **x**-matrix means the **x**-expectation value is not constant for a general state.

$$|\Psi(t)\rangle = |0\rangle e^{-i\omega_0 t}\Psi_0 + |1\rangle e^{-i\omega_1 t}\Psi_1 + \ldots \qquad (20.3.9)$$

The matrix form of (20.3.8) is, perhaps, easier to compute and more revealing.

$$\begin{aligned}\langle \mathrm{x}\rangle = \bar{x}\,|_{\Psi(t)} &= \langle\Psi(t)|\mathbf{x}|\Psi(t)\rangle\\ &= \sqrt{\frac{\hbar}{2M\omega}}\begin{pmatrix}\Psi_0^*(t) & \Psi_1^*(t) & \Psi_2^*(t) & \cdots\end{pmatrix}\begin{pmatrix}\cdot & \sqrt{1} & \cdot & \cdots\\ \sqrt{1} & \cdot & \sqrt{2} & \cdots\\ \cdot & \sqrt{2} & \cdot & \sqrt{3}\\ \vdots & \vdots & \sqrt{3} & \ddots\end{pmatrix}\begin{pmatrix}\Psi_0(t)\\ \Psi_1(t)\\ \Psi_2(t)\\ \vdots\end{pmatrix}\\ &= \left(x_0/\sqrt{2}\right)\begin{pmatrix}\Psi_0^* e^{i\omega_0 t} & \Psi_1^* e^{i\omega_1 t} & \Psi_2^* e^{i\omega_2 t} & \cdots\end{pmatrix}\begin{pmatrix}\cdot & \sqrt{1} & \cdot & \cdots\\ \sqrt{1} & \cdot & \sqrt{2} & \cdots\\ \cdot & \sqrt{2} & \cdot & \sqrt{3}\\ \vdots & \vdots & \sqrt{3} & \ddots\end{pmatrix}\begin{pmatrix}\Psi_0 e^{-i\omega_0 t}\\ \Psi_1 e^{-i\omega_1 t}\\ \Psi_2 e^{-i\omega_2 t}\\ \vdots\end{pmatrix}\\ &= \left(x_0/\sqrt{2}\right)\begin{pmatrix}\Psi_0^* e^{i\omega_0 t} & \Psi_1^* e^{i\omega_1 t} & \Psi_2^* e^{i\omega_2 t} & \cdots\end{pmatrix}\begin{pmatrix}\sqrt{1}\Psi_1 e^{-i\omega_1 t}\\ \sqrt{1}\Psi_0 e^{-i\omega_0 t} + \sqrt{2}\Psi_2 e^{-i\omega_2 t}\\ \sqrt{2}\Psi_1 e^{-i\omega_1 t} + \sqrt{3}\Psi_3 e^{-i\omega_3 t}\\ \vdots\end{pmatrix}\end{aligned} \qquad (20.3.10a)$$

If only the first two levels have non-zero amplitude then $\langle x\rangle$ beats at frequency $\omega_{10} = \omega_1 - \omega_0$.

$$\begin{aligned}\langle \mathrm{x}\rangle = \bar{x}\,|_{\Psi(t)} &= \left(x_0/\sqrt{2}\right)\left(\Psi_0^* e^{i\omega_0 t}\sqrt{1}\Psi_1 e^{-i\omega_1 t} + \Psi_1^* e^{i\omega_1 t}\sqrt{1}\Psi_0 e^{-i\omega_0 t}\right)\\ &= \left(x_0/\sqrt{2}\right)\left|\Psi_1^*\Psi_0\right|\left(e^{i(\omega_{10}t+\theta_{10})} + e^{-i(\omega_{10}t+\theta_{10})}\right) where: \omega_{10} = \omega_1 - \omega_0\end{aligned} \qquad (20.3.10b)$$

The *amplitude overlap product* is $\Psi_1^*\Psi_0 = \left|\Psi_1^*\Psi_0\right| e^{i\theta_{10}}$ (20.3.10c)

This product is *(1/√2)(1/√2)=1/2* for a *50-50* combination state (20.3.3) giving the following *x*-oscillation.

$$\langle \mathrm{x(t)}\rangle = \bar{x}\,|_{\Psi(t)} = \left(x_0/\sqrt{2}\right)\cos\left(\omega_1 - \omega_0\right)t = \left(x_{01}/2\right)\cos\omega t \qquad (20.3.10d)$$

Oscillation amplitude $\langle x\rangle$ is $\sqrt{1/2}$ of $x_0$ or *1/2* of the classical turning point $x_{01}$ at mean energy $\bar{E} = \hbar\omega$ of a 50-50 combination of $E_0$ and $E_1$ states given by (20.3.7b). $x_{01}$ is also the dipole matrix element $\langle 0|\mathbf{x}|1\rangle$.

The range of expectation $\langle x\rangle$ is plotted numerically with the expectation $\langle k\rangle$ of momentum in Fig. 20.3.1. It is larger than the 18% achieved by poor prisoner *M* in the square well $\langle x\rangle$ of (12.1.15). This is because the harmonic oscillator is a "softer" prison than an infinite square well, and it allows a significant fraction of the low-*n* waves to evanesce into walls. The widening potential at higher *E* increases their uncertainty range $\Delta x$, but high-*n* waves meet steeper walls with more momentum. So, the fraction of evanescent wave goes down as *n* goes up as seen in the *n=20* example of Fig. 20.2.3.

*(3) Momentum expectation values*

For a *50-50* combination state (20.3.3) the mean or expected momentum is

$$\langle p(t)\rangle = \bar{p}\,|_{\Psi(t)} = -\left(M\omega x_0/\sqrt{2}\right)\sin\left(\omega_1-\omega_0\right)t = \left(p_{01}/2\right)\sin\omega t \qquad (20.3.11)$$

(The derivation is left as an exercise.) The expected momentum $\langle p\rangle$ or Fourier transform wavevector component $\langle k\rangle$ is plotted vertically versus $\langle x\rangle$ for four *1/4*-periods of the oscillator in Fig. 20.3.1. The resulting path resembles a classical phase space ellipse, or if $\langle p\rangle$ is rescaled by $M\omega$, a phasor circle.

This shows some essential classical dynamics of the oscillator being reproduced by a *50-50* mixing of the lowest two quantum states, $|0\rangle$ and $|1\rangle$, of the quantum oscillator. Uneven mixtures *40-60*, *30-70*, and so forth, will oscillate on similar phase paths but with reduced amplitude according to the value of the overlap product (20.3.10c). However, even the maximum amplitude achieved with a *50-50* mixture is still only a fraction of the corresponding classical oscillation of the same energy. This fraction gradually increases for mixtures of quantum states $|n\rangle$ and $|n+1\rangle$ for larger and larger *n*. Again, this is related to the decreasing fraction of the evanescent parts of higher quantum states. Now we see ways to involve many eigenstates in making more effective or "coherent" wave packet dynamics.

### (b) Oscillator coherent states ("Shoved" and "kicked" states)

Most who study quantum mechanics have a desire to see classical manifestations of classical dynamics in quantum systems. The harmonic oscillator is one of few systems that can indulge our desire for a return to our classical birthplace. The oscillator has a nearly perfect classical-imitation-state having an almost child-like simplicity. This state is called a harmonic oscillator *coherent state*.

There is hardly a child (or healthy adult) alive who, when seeing a pendulum, spring and mass, or other oscillator, can resist the urge to swing it or ring it. The more gentle of us might just pull it off center and release it, while a more impatient provocateur might just kick it. A true physicist will only be satisfied after repeatedly dealing the poor oscillator both kinds of punishment. Here we consider quantum operators that perform these child-like acts on wave functions and quantum states in general, and we will see how such actions affect oscillators in particular.

The usual coherent state is the result of applying such operations to an oscillator ground state $|0\rangle$, but more general sorts of states are possible as we will see. Quantum states have infinitely more freedom and variety than classical states, but now we just want it to reproduce a tiny piece of a classical world.

Coherent states are made by translation and boost (shove and kick) operators just like the ones discussed in Chapter 17.1(d). The Geoppert-Mayer-Snyder-Richards gauge transformation (17.1.16b) is the boost or "kick" operator derived in (20.3.20) below. But, first we derive the "shove" operator.

*(1) Translation operators and generators: (A "shove")*

Suppose there exists an operator $\mathbf{T}(a)$ which does nothing more than translate *x*-wavefunctions.

$$\mathbf{T}(a)\cdot\psi(x) = \psi(x-a) = \langle x|\mathbf{T}(a)|\psi\rangle = \langle x-a\,|\psi\rangle \qquad (20.3.12a)$$

Such an operator is called a *translation operator* **T***(a)* (Good name, don't you think?) Its effect is to move the function *a* units to the right (positively). (Or, its dual moves the *x*-space *a* units negatively to the left.)

$$\langle x|\mathbf{T}(a) = \langle x\text{-}a| \ , \text{ or: } \ \mathbf{T}^\dagger(a)|x\rangle = |x\text{-}a\rangle \ , \text{ or since } \mathbf{T}^\dagger(a) = \mathbf{T}(\text{-}a): \ \mathbf{T}(a)|x\rangle = |x+a\rangle. \quad (20.3.12b)$$

For very small translations $a \to da$ such an operation becomes nearly the identity operation **1** with a small add-on operator **G***da* which is linear in, or proportional to, the tiny (infinitesimal) translation $\delta a$.

$$\mathbf{T}(\delta a) = \mathbf{1} + \mathbf{G}\delta a \quad (20.3.13a)$$

The tiny-translation operator is called an *infinitesimal translation operator* **T***(da)* and the add-on operator is called a *generator* **G** *of translations*. If **T***(a)* is a continuous function of *a* then the generator is the first-derivative part of a Taylor series.

$$\mathbf{G} = \left.\frac{\partial \mathbf{T}}{\partial a}\right|_{a=0} \quad (20.3.13b)$$

Tiny translations on an arbitrary continuous function $\psi(x)$ gives a single-term Taylor series, too.

$$\mathbf{T}(da)\cdot\psi(x) = \psi(x-da) = \psi(x) - \frac{\partial}{\partial x}\psi(x)da \quad (20.3.14a)$$

Comparing this to the effect of (20.3.13) gives

$$\mathbf{T}(da)\cdot\psi(x) = \left(\mathbf{1} + \mathbf{G}da\right)\cdot\psi(x) = \psi(x) + \mathbf{G}\cdot\psi(x)da \quad (20.3.14b)$$

Solving (20.3.13b) and (20.3.14) yields an abstract operator exponential expression for finite **T***(a)* ,

$$\mathbf{T}\left(a\right) = \mathbf{T}\left(0\right)\cdot e^{a\mathbf{G}} = e^{a\mathbf{G}} \quad (20.3.15a)$$

and a coordinate *x*-space representation of the generator **G** ,

$$\mathbf{G}\cdot\psi(x) = -\frac{\partial}{\partial x}\psi(x) = \left\langle x\middle|\mathbf{G}\middle|\psi\right\rangle \quad (20.3.15b)$$

and the *x*-representation of the finite translation of a function.

$$\begin{aligned}\mathbf{T}(a)\cdot\psi(x) = e^{a\mathbf{G}}\cdot\psi(x) &= e^{-a\frac{\partial}{\partial x}}\cdot\psi(x) \\ &= \psi(x) - a\frac{\partial\psi(x)}{\partial x} + \frac{a^2}{2!}\frac{\partial^2\psi(x)}{\partial x^2} - \frac{a^3}{2!}\frac{\partial^3\psi(x)}{\partial x^3} + \ldots\end{aligned} \quad (20.3.15c)$$

Note the relation between the translation generator **G** and the momentum operator $\mathbf{p} \to \frac{\hbar}{i}\frac{\partial}{\partial x} = -i\hbar\frac{\partial}{\partial x}$

$$\mathbf{G} = -\frac{i}{\hbar}\mathbf{p} \quad (20.3.15d)$$

In terms of **a**-operators the finite translation has a useful form.

$$\mathbf{T}(a) = e^{-ia\mathbf{p}/\hbar} = e^{a\left(\mathbf{a}^\dagger - \mathbf{a}\right)\sqrt{M\omega/2\hbar}} \quad (20.3.15e)$$

To check ±signs of a **T***(a)* operator try it out on a plane-wave function using the DeBroglie relation $p=\hbar k$.

$$\mathbf{T}(a)e^{ikx} = e^{-ia\mathbf{p}/\hbar}e^{ikx} = e^{-iak}e^{ikx} = e^{ik(x-a)} \quad (20.3.16)$$

*(2) Boost operators and generators: (A "kick")*

There also exists an operator **B***(b)* which "translates" momentum *p*-wavefunctions.

$$\mathbf{B}(b)\cdot\psi(p) = \psi(p-b) = \langle x|\mathbf{B}(b)|\psi\rangle = \langle p-b\,|\psi\rangle \qquad (20.3.17a)$$

Such an operator is called a *boost operator* **B***(b)* and it increases the momentum of any ket-state by *b* units. (Or, its dual moves the *p*-space *b* units negatively or to the left.)

$$\langle p\,|\mathbf{B}(b) = \langle p-b|\ \text{, or: }\ \mathbf{B}^\dagger(b)|p\,\rangle = |p-b\rangle\ \text{, or: }\ \mathbf{B}(b)|p\,\rangle = |p+b\rangle\ . \qquad (20.3.17b)$$

For very small boosts $b\to db$ such an operation becomes nearly the identity operation **1** with a small add-on operator **K***db* linear in, or proportional to, the tiny (infinitesimal) boost *db*.

$$\mathbf{B}(db) = \mathbf{1}+\mathbf{K}db \qquad (20.3.18a)$$

If **B***(b)* is a continuous function of *b* then **K***db* is the first- derivative part of a Taylor series.

$$\mathbf{K} = \left.\frac{\partial\mathbf{B}}{\partial b}\right|_{b=0} \qquad (20.3.18b)$$

Tiny boosts of a momentum function ψ*(p)* give a single-term Taylor series.

$$\mathbf{B}(db)\cdot\psi(p) = \psi(p-db) = \psi(p) - \frac{\partial}{\partial p}\psi(p)db \qquad (20.3.19a)$$

Comparing this to the effect of (20.3.18) gives

$$\mathbf{B}(db)\cdot\psi(p) = \left(\mathbf{1}+\mathbf{K}db\right)\cdot\psi(p) = \psi(p) + \mathbf{K}\cdot\psi(p)db \qquad (20.3.19b)$$

Solving (20.3.18b) and (20.3.19) yields an abstract operator exponential expression for finite **B***(b)*,

$$\mathbf{B}\left(b\right) = \mathbf{B}\left(0\right)\cdot e^{b\mathbf{K}} = e^{b\mathbf{K}} \qquad (20.3.20a)$$

and a momentum *p*-space representation of the boost generator **K**,

$$\mathbf{K}\cdot\psi(p) = -\frac{\partial}{\partial p}\psi(p) = \left\langle p\middle|\mathbf{K}\middle|\psi\right\rangle \qquad (20.3.20b)$$

and the *p*-representation of the finite boost.

$$\begin{aligned}\mathbf{B}\left(b\right)\cdot\psi(p) = e^{b\mathbf{K}}\cdot\psi(p) &= e^{-b\frac{\partial}{\partial p}}\cdot\psi(p)\\ &= \psi(p) - b\frac{\partial\psi(p)}{\partial p} + \frac{b^2}{2!}\frac{\partial^2\psi(p)}{\partial p^2} - \frac{b^3}{2!}\frac{\partial^3\psi(p)}{\partial p^3} + \ldots\end{aligned} \qquad (20.3.20c)$$

Note a relation between the boost generator **K** and the position operator $\mathbf{x}\to\hbar i\frac{\partial}{\partial p} = i\frac{\partial}{\partial k}$

$$\mathbf{K} = \frac{i}{\hbar}\mathbf{x} \to -\frac{\partial}{\partial p} = \frac{-1}{\hbar}\frac{\partial}{\partial k} \qquad (20.3.20d)$$

In terms of **a**-operators the finite boost has a form analogous to the form (20.3.15e) for **T***(a)*.

$$\mathbf{B}\left(b\right) = e^{ib\mathbf{x}/\hbar} = e^{ib\left(\mathbf{a}^\dagger+\mathbf{a}\right)/\sqrt{2\hbar M\omega}} \qquad (20.3.20e)$$

To check ±signs of a **B***(b)* operator try it out on a plane-wave function using the deBroglie relation $p=\hbar k$.

$$\mathbf{B}\left(b\right)e^{ikx} = e^{ib\mathbf{x}/\hbar}e^{ikx} = e^{ibx/\hbar}e^{ikx} = e^{i\left(k+b/\hbar\right)x} \qquad (20.3.21)$$

*(3) Applying boost-translation combinations*

The **T***(a)* and **B***(b)* operations do not commute. The question arises: "Which should come first?" Again, neither and both seems a fair settlement! A *combined boost-translation operation* is defined.

$$\mathbf{C}(a,b) = e^{i(b\mathbf{x}-a\mathbf{p})/\hbar} \tag{20.3.22}$$

This choice is like a Darboux rotation operator $e^{-i\Omega t/\hbar}$. Euler operations, on the other hand, consist of three factors $e^{-i\mathbf{J}_z\alpha/\hbar}e^{-i\mathbf{J}_y\beta/\hbar}e^{-i\mathbf{J}_z\gamma/\hbar}$ in a special order. These operators are related in Appendix. 10.A.

The **C***(a,b)* combination is easier to disentangle, however, using the following operator identity.

$$e^{\mathbf{A}+\mathbf{B}} = e^{\mathbf{A}}e^{\mathbf{B}}e^{-[\mathbf{A},\mathbf{B}]/2} = e^{\mathbf{B}}e^{\mathbf{A}}e^{[\mathbf{A},\mathbf{B}]/2} \ , \text{ where: } \big[\mathbf{A},[\mathbf{A},\mathbf{B}]\big] = \mathbf{0} = \big[\mathbf{B},[\mathbf{A},\mathbf{B}]\big] \tag{20.3.23}$$

This is known as the *Baker-Campbell-Hausdorf identity* and is left as an exercise. Since $[\mathbf{x},\mathbf{p}]=i\hbar\mathbf{1}$, the double commutations $[[\mathbf{x},\mathbf{p}],\mathbf{x}]$ and $[[\mathbf{x},\mathbf{p}],\mathbf{p}]$ are zero as required and **C***(a,b)* factors either way.

$$\begin{aligned}\mathbf{C}(a,b) &= e^{i(b\mathbf{x}-a\mathbf{p})/\hbar} = e^{ib\mathbf{x}/\hbar}e^{-ia\mathbf{p}/\hbar}e^{-ab[\mathbf{x},\mathbf{p}]/2\hbar^2} = e^{ib\mathbf{x}/\hbar}e^{-ia\mathbf{p}/\hbar}e^{-iab/2\hbar} \\ &= \mathbf{B}(b)\mathbf{T}(a)e^{-iab/2\hbar} = \mathbf{T}(a)\mathbf{B}(b)e^{iab/2\hbar}\end{aligned} \tag{20.3.24a}$$

Reordering only affects the overall phase. The same applies to an **a**-operator expression for **C***(a,b)*.

$$\begin{aligned}\mathbf{C}(a,b) &= e^{i(b\mathbf{x}-a\mathbf{p})/\hbar} = e^{ib\left(\mathbf{a}^\dagger+\mathbf{a}\right)/\sqrt{2\hbar M\omega}+a\left(\mathbf{a}^\dagger-\mathbf{a}\right)\sqrt{M\omega/2\hbar}} \\ &= e^{\alpha\mathbf{a}^\dagger-\alpha^*\mathbf{a}} = e^{-|\alpha|^2/2}e^{\alpha\mathbf{a}^\dagger}e^{-\alpha^*\mathbf{a}} = e^{|\alpha|^2/2}e^{-\alpha^*\mathbf{a}}e^{\alpha\mathbf{a}^\dagger}\end{aligned} \tag{20.3.24b}$$

Here the complex *phasor-space position coordinate* $\alpha(a,b)$ is defined by

$$\alpha(a,b) = a\sqrt{M\omega/2\hbar} + ib/\sqrt{2\hbar M\omega} = \left[a + i\frac{b}{M\omega}\right]\sqrt{M\omega/2\hbar} \ . \tag{20.3.24c}$$

Applying the combination operator $\mathbf{C}(x_0,p_0)$ to the ground state $|0\rangle$ simple picks up the ground state Gaussian and plunks it down at phase space position $(x_0,p_0)$ with an overall factor $e^{-|\alpha|^2}$. This is called a *coherent wavepacket state* $|\alpha(x_0,p_0)\rangle$. It turns out to have expected position $x_0$ and momentum $p_0$.

$$\begin{aligned}\big|\alpha_0(x_0,p_0)\big\rangle &= \mathbf{C}(x_0,p_0)|0\rangle = e^{i(x_0\mathbf{x}-p_0\mathbf{p})/\hbar}|0\rangle \\ &= e^{-|\alpha_0|^2/2}e^{\alpha_0\mathbf{a}^\dagger}e^{-\alpha_0{}^*\mathbf{a}}|0\rangle \\ &= e^{-|\alpha_0|^2/2}e^{\alpha_0\mathbf{a}^\dagger}|0\rangle \\ &= e^{-|\alpha_0|^2/2}\sum_{n=0}^{\infty}\left(\alpha_0\mathbf{a}^\dagger\right)^n|0\rangle/n! \\ &= e^{-|\alpha_0|^2/2}\sum_{n=0}^{\infty}\frac{(\alpha_0)^n}{\sqrt{n!}}|n\rangle \ , \quad \text{where: } |n\rangle = \frac{\mathbf{a}^{\dagger n}|0\rangle}{\sqrt{n!}}\end{aligned} \tag{20.3.25a}$$

What's neat about a coherent $|\alpha(x_0,p_0)\rangle$ state is that it is an eigenvector of the destruction operator.

$$\begin{aligned}\mathbf{a}\big|\alpha_0(x_0,p_0)\big\rangle &= e^{-|\alpha_0|^2/2}\sum_{n=0}^{\infty}\frac{(\alpha_0)^n}{\sqrt{n!}}\mathbf{a}|n\rangle = e^{-|\alpha_0|^2/2}\sum_{n=0}^{\infty}\frac{(\alpha_0)^n}{\sqrt{n!}}\sqrt{n}\,|n-1\rangle \\ &= \alpha_0\big|\alpha_0(x_0,p_0)\big\rangle\end{aligned} \tag{20.3.25b}$$

And the left-pointing coherent bra is an eigenvector of the creation operator. *(Quelle apropos'!)*

$$\big\langle\alpha_0(x_0,p_0)\big|\mathbf{a}^\dagger = \big\langle\alpha_0(x_0,p_0)\big|\alpha_0{}^* \tag{20.3.25c}$$

This makes calculation of position and momentum expectation operators quite easy.

$$\begin{aligned}\left\langle \alpha_0(x_0,p_0)\right|\mathsf{x}\left|\alpha_0(x_0,p_0)\right\rangle &= \sqrt{\frac{\hbar}{2M\omega}}\left\langle \alpha_0(x_0,p_0)\right|\left(\mathsf{a}+\mathsf{a}^\dagger\right)\left|\alpha_0(x_0,p_0)\right\rangle \\ &= \sqrt{\frac{\hbar}{2M\omega}}\left(\alpha_0+\alpha_0{}^*\right)=x_0\end{aligned} \tag{20.3.25d}$$

$$\begin{aligned}\left\langle \alpha_0(x_0,p_0)\right|\mathbf{p}\left|\alpha_0(x_0,p_0)\right\rangle &= i\sqrt{\frac{M\omega\hbar}{2}}\left\langle \alpha_0(x_0,p_0)\right|\left(\mathbf{a}^\dagger-\mathbf{a}\right)\left|\alpha_0(x_0,p_0)\right\rangle \\ &= i\sqrt{\frac{M\omega\hbar}{2}}\left(\alpha_0{}^*-\alpha_0\right)=p_0\end{aligned} \tag{20.3.25e}$$

The expected position and momentum is, well, exactly what we would expect classically.

*(4) Time evolution of coherent states*

Time evolution is calculated using the time evolution operator whose general form is

$$\mathbf{U}(t,0)=\mathrm{e}^{-\mathrm{i}\mathbf{H}t/\hbar} \quad , \tag{20.3.26}$$

according to (2.8.10e). Oscillator eigenstate time evolution is simply determined by harmonic phases.

$$\mathbf{U}(t,0)\left|n\right\rangle = e^{-i\mathbf{H}t/\hbar}\left|n\right\rangle = e^{-i(n+1/2)\omega t}\left|n\right\rangle \tag{20.3.27}$$

The coherent state evolution uses this result.

$$\begin{aligned}\mathbf{U}(t,0)\left|\alpha_0(x_0,p_0)\right\rangle &= e^{-|\alpha_0|^2/2}\sum_{n=0}^{\infty}\frac{(\alpha_0)^n}{\sqrt{n!}}\mathbf{U}(t,0)\left|n\right\rangle = e^{-|\alpha_0|^2/2}\sum_{n=0}^{\infty}\frac{(\alpha_0)^n}{\sqrt{n!}}e^{-i(n+1/2)\omega t}\left|n\right\rangle \\ &= e^{-i\omega t/2}e^{-|\alpha_0|^2/2}\sum_{n=0}^{\infty}\frac{\left(\alpha_0 e^{-i\omega t}\right)^n}{\sqrt{n!}}\left|n\right\rangle\end{aligned}$$

This simplifies to a variable coherent state

$$\mathbf{U}(t,0)\left|\alpha_0(x_0,p_0)\right\rangle = e^{-i\omega t/2}\left|\alpha_t(x_t,p_t)\right\rangle \tag{20.3.28}$$

with a time dependent phasor coordinate (20.3.24c)

$$\begin{aligned}&\alpha_t(x_t,p_t) = e^{-i\omega t}\alpha_0(x_0,p_0) \\ &\left[x_t+i\frac{p_t}{M\omega}\right] = e^{-i\omega t}\left[x_0+i\frac{p_0}{M\omega}\right],\end{aligned} \tag{20.3.29a}$$

whose real and imaginary parts (the expected $x_t$ and $p_t/M\omega$) go clockwise around the phasor circle.

$$\begin{aligned}x_t &= x_0\cos\omega t+\frac{p_0}{M\omega}\sin\omega t \\ \frac{p_t}{M\omega} &= -x_0\sin\omega t+\frac{p_0}{M\omega}\cos\omega t\end{aligned} \tag{20.3.29b}$$

The $(x_t,p_t)$ mimic perfectly a classical oscillator. Evolution of $|\alpha_t(x_t,p_t)\rangle$ is shown in Fig. 20.3.2.

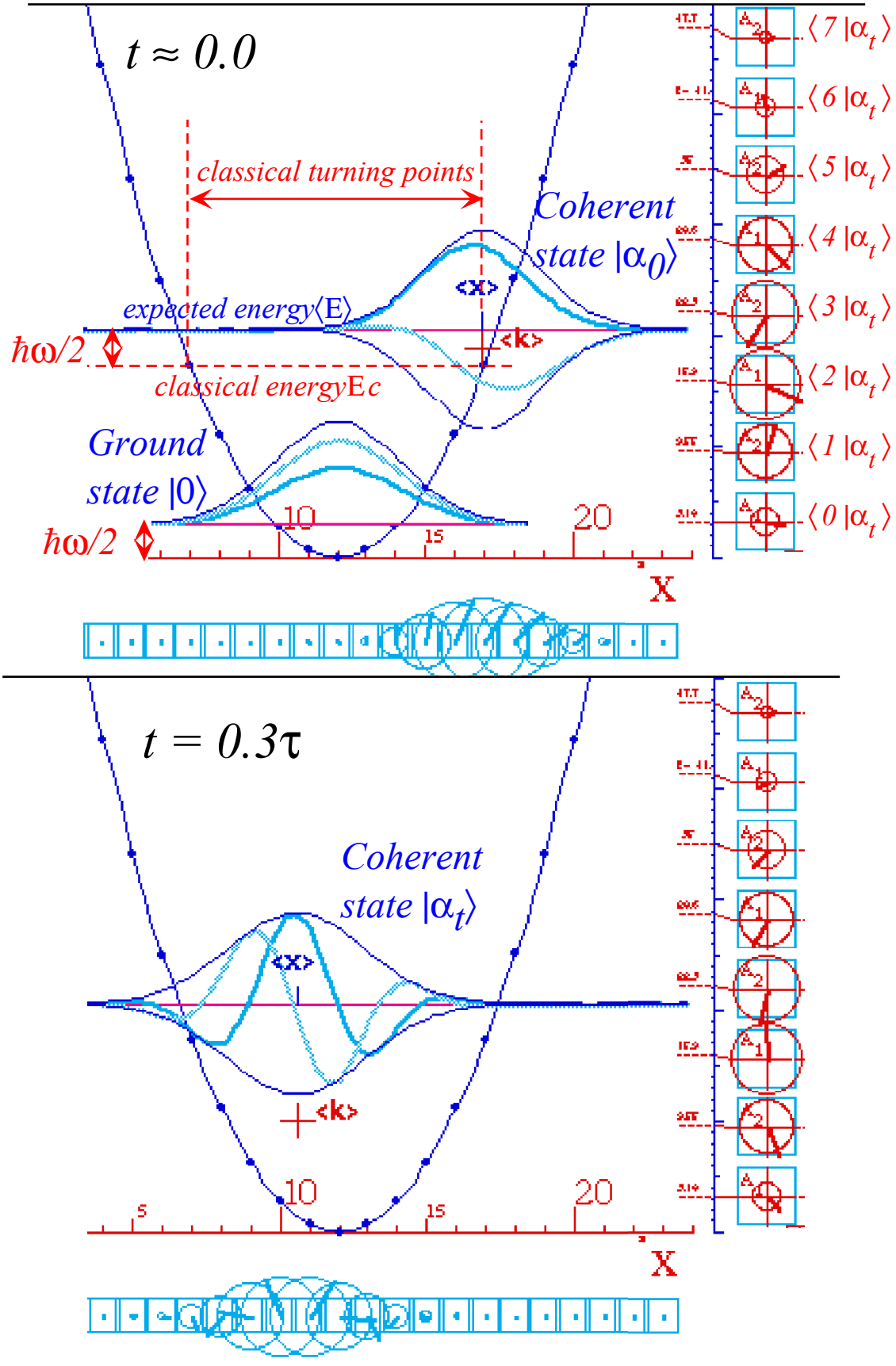


*Fig. 20.3.2 Coherent state oscillation for harmonic oscillator showing E, x and k expectation.*

At last, it appears that the goal of recovering perfect classical correspondence of a quantum system has been achieved! Well, almost. There are still some issues that we will discuss shortly. But, at least Fig. 20.3.2 is a big improvement over the wobbly wave beating that appeared in Fig. 20.3.1. The coherent wave envelope $|\langle x|\psi\rangle| = |\langle x|\alpha_t(x_t,p_t)\rangle|$ and the $\langle x\rangle$ expectation march rigidly in lock step from one side of the well to the other and back again without the envelope distorting even the slightest from the Gaussian shape of the ground state wave. Recall that the $\langle x\rangle$ expectation of the wave in Fig. 20.3.1 only beats itself half way to the classical turning point corresponding to its expected energy.

Closer examination of Fig. 20.3.2 reveals that the coherent wave also fails to reach the classical turning points corresponding to its expected energy. Its expected quantum energy is

$$\begin{aligned}\langle E\rangle\big|_{\alpha_0} &= \langle\alpha_0(x_0,p_0)|\mathsf{H}|\alpha_0(x_0,p_0)\rangle = \langle\alpha_0(x_0,p_0)|\left(\hbar\omega\mathsf{a}^\dagger\mathsf{a}+\frac{\hbar\omega}{2}\mathsf{1}\right)|\alpha_0(x_0,p_0)\rangle \\ &= \hbar\omega\alpha_0^*\alpha_0+\frac{\hbar\omega}{2}\end{aligned} \tag{20.3.30a}$$

This has two parts. The first term is the classical energy using the phasor coordinate (20.3.24c).

$$\begin{aligned}E_{classical} = \hbar\omega\alpha_0^*\alpha_0 &= \hbar\omega\left|\left[x_0+i\frac{p_0}{M\omega}\right]\sqrt{M\omega/2\hbar}\right|^2 \\ &= \frac{1}{2}M\omega x_0^2+\frac{p_0^2}{2M}\end{aligned} \tag{20.3.30b}$$

The second term is the zero-point energy $E_0$ that is part of the quantum result.

$$\begin{aligned}\langle E\rangle\big|_{\alpha_0} = E_{classical}+E_0 &= \hbar\omega\alpha_0^*\alpha_0+\frac{\hbar\omega}{2} \\ &= \frac{1}{2}M\omega x_0^2+\frac{p_0^2}{2M}+\frac{\hbar\omega}{2}\end{aligned} \tag{20.3.30c}$$

Fig. 20.3.2 shows both the quantum expectation and classical energy levels. It is seen that the expectation values oscillate between the intersections of the classical energy ($E_{classical}$) level with the potential $V(x) = 1/2M\omega x^2$ parabola. The classical level lies $\hbar\omega/2$ below the true total energy (20.3.30c) of the coherent wave state. The turning points associated with the true quantum energy are not reached by the $x$-expectation value. So quantum mechanics gets the last word even in this, a nearly perfect of example of classical correspondence. And, well that it should.

The distribution of quantum eigenstates needed to make a coherent wave are given by (20.3.25c).

$$\langle n|\alpha_0(x_0,p_0)\rangle = e^{-|\alpha_0|^2/2}\frac{(\alpha_0)^n}{\sqrt{n!}}\ , \qquad |\langle n|\alpha_0(x_0,p_0)\rangle|^2 = e^{-|\alpha_0|^2}\frac{|\alpha_0|^{2n}}{n!} \tag{20.3.31}$$

This $a^{2n}\,e^{-a^2}/_{n!}$ probability distribution is called a *Poissonian distribution*. The corresponding amplitude distribution is evident in the varying size of eigenphasors on the extreme right hand side of Fig. 20.3.2. The peak and mean of the distribution occurs near the expected energy levels. (See exercises.)

## (c) Classical and quantum dynamics of wavepackets

The coherent state wavefunction follows from its abstract state definition (20.3.25a). To get the coordinate wavefunction we just clothe (20.3.25a) with an $\langle x|$-bra.

$$\begin{aligned}\langle x|\alpha_0(x_0,p_0)\rangle &= \langle x|\mathbf{C}(x_0,p_0)|0\rangle = \langle x|e^{i(x_0\mathbf{x}-p_0\mathbf{p})/\hbar}|0\rangle \\ &= e^{-|\alpha_0|^2/2}\sum_{n=0}^{\infty}\frac{(\alpha_0)^n}{\sqrt{n!}}\langle x|n\rangle\end{aligned} \tag{20.3.32}$$

Starting with (20.3.24a) the first line uses boost function (20.3.20e) and translation axiom (20.3.12).

$$\begin{aligned}\langle x|\alpha_0(x_0,p_0)\rangle &= \langle x|\mathbf{C}(x_0,p_0)|0\rangle = \langle x|\mathbf{B}(p_0)\mathbf{T}(x_0)|0\rangle e^{-ix_0p_0/2\hbar} \\ &= \langle x|e^{ip_0\mathbf{x}/\hbar}\mathbf{T}(x_0)|0\rangle e^{-ix_0p_0/2\hbar} \\ &= e^{ip_0x/\hbar}\langle x|\mathbf{T}(x_0)|0\rangle e^{-ix_0p_0/2\hbar} \\ &= e^{ip_0x/\hbar}\langle x-x_0|0\rangle e^{-ix_0p_0/2\hbar}\end{aligned} \tag{20.3.33}$$

Let us change Dirac notation back to $\psi(x)$-notation using ground state wavefunction from (20.2.7).

$$\langle x|\psi_0\rangle = \psi_0(x) = e^{-M\omega x^2/2\hbar}(M\omega/\pi\hbar)^{1/4} \tag{20.3.34a}$$

Rearrangement turns the coherent wave into a *complex Gaussian wavepacket* $e^{-A(z-\alpha)^2}$.

$$\begin{aligned}\Psi_{\alpha_0}(x) = \langle x|\alpha_0(x_0,p_0)\rangle &= e^{ip_0x/\hbar}e^{-M\omega(x-x_0)^2/2\hbar}e^{-ix_0p_0/2\hbar}\left(\frac{M\omega}{\pi\hbar}\right)^{1/4} \\ &= e^{ip_0x_0/2\hbar}e^{-M\omega(x-x_0)^2/2\hbar+ip_0(x-x_0)/\hbar}\left(\frac{M\omega}{\pi\hbar}\right)^{1/4}\end{aligned} \tag{20.3.34b}$$

The peak of the complex Gaussian $\langle x|\alpha_0\rangle$ is located in the complex $z$-plane or phasor space at $z=\alpha_t$

$$\alpha_t(x_t,p_t) = e^{-i\omega t}\alpha_0(x_0,p_0) = \left[x_t + i\frac{p_t}{M\omega}\right] = e^{-i\omega t}\left[x_0 + i\frac{p_0}{M\omega}\right], \tag{20.3.34c}$$

according to (20.3.29). Its time behavior is obtained from (20.3.28).

$$\Psi_{\alpha_t}(x) = \langle x|\alpha_t(x_t,p_t)\rangle = e^{ip_tx_t/2\hbar - i\omega t/2\hbar}\left[e^{-M\omega(x-x_t)^2/2\hbar+ip_t(x-x_t)/\hbar}\left(\frac{M\omega}{\pi\hbar}\right)^{1/4}\right] \tag{20.3.34d}$$

The phase factor outside the complex Gaussian in the braces ([ ]) is known as the *semi-classical action phase* or *eikonal phase factor*. Its theory has a wonderful history. We give a brief sketch of parts of the theory. We first discussed action and phase back in Section 5.3(a).

*(1) Classical action and phase*

Dirac and Feynman are generally credited with fully realizing the significance and utility of the classical action, but many of the creators of quantum mechanics beginning with Bohr, Einstein, Keller, Jordan, Wentzels, Kramers, Born (of the *JWKB* method) and others have developed the ideas which continue to grow in modern physics.

The beginnings of these ideas go back even to Newton who started the classical mechanics which Lagrange, Legendre, Poincare, Hamilton, and Jacobi developed to such a high level that they almost discovered quantum theory using logical deduction alone. (Or, so it might appear using 20-20 hindsight!) There are four or five related classical developments of classical mechanics which foreshadow quantum theory and experienced a later renaissance.

These are, in order of their appearance, the *Lagrangian function L=T-V* which for the oscillator is

$$L = T - V = \frac{M\dot{x}^2}{2} - \frac{M\omega^2 x^2}{2} = \frac{p^2}{2M} - \frac{M\omega^2 x^2}{2}\,, \qquad (20.3.35a)$$

the *Hamiltonian function H=T+V* which for the oscillator has the form (preferred format first)

$$H = T + V = \frac{p^2}{2M} + \frac{M\omega^2 x^2}{2} = \frac{M\dot{x}^2}{2} + \frac{M\omega^2 x^2}{2}\,, \qquad (20.3.35b)$$

and the *Poincare invariant dS* or *Legendre transformation generator* relation between $H$ and $L$

$$dS = L\,dt = p\,dx - H\,dt\,, \qquad (20.3.35c)$$

whose integral is the *Hamilton's Principle action integral* $S_P$

$$S_P = \int dS = \int L\,dt = \int p\,dx - \int H\,dt\,, \qquad (20.3.35d)$$

which includes *Hamilton's Characteristic action integral* $S_H$ also known as *"reduced" action*

$$S_H = \int p\,dx\,, \qquad (20.3.35e)$$

The word *"Principle"* (not "Principal") may be capitalized since it refers to *Hamilton's Minimum Principle* , that is, that $S_P$ is minimum for classical paths. So is the word *"Characteristic"* since it refers to the *Method of Characteristics* used to solve partial differential wave equations by integrating along their ray trajectories. The partial differential equations being solved in those days were (among others) the *Hamilton Jacobi equations* which follow directly from (20.3.35c)

$$dS = L\,dt = \frac{\partial S}{\partial x}dx + \frac{\partial S}{\partial t}dt \quad , \qquad (20.3.35f)$$

where:
$$p = \frac{\partial S}{\partial x} \quad , \qquad H = -\frac{\partial S}{\partial t} \qquad (20.3.35g)$$

determine *S-eikonal* wavefronts normal to the classical momentum. ($\mathbf{p} = \nabla S$ in 2 or 3-dimensions.)

Dirac and Feynman developed the idea that the quantum wave function correspond to the $S$-wavefronts and that a wavefunction such as (20.3.34d) has the form

$$\Psi = e^{iS/\hbar}\phi = e^{i\int L\,dt/\hbar}\phi\,. \qquad (20.3.36)$$

It certainly works well when both $p$ and $H=E$ are constant since then (20.3.35d) reduces to the form

$$S_P/\hbar = (p\,x - H\,t)/\hbar = k\,x - \omega\,t\,, \qquad (20.3.37)$$

of the relativistically invariant plane wave phase angle of the plane wave $e^{i(kx-\omega t)}$.

However, the idea applies to the oscillator wavefunction and many other problems as well. For the oscillator the reduced action comes out as follows.

$$S_H = \int_0^t p_t dx_t = \int_0^t \sqrt{2M\left(E_c - \frac{M\omega^2}{2}x_t^2\right)}dx_t = S_P + E_c t$$
$$= \frac{x_t p_t}{2}\Big|_0^t + \frac{E_c}{\omega}\arcsin\left(\frac{M\omega}{\sqrt{2ME_c}}x_t\right)\Big|_0^t = \frac{x_t p_t - x_0 p_0}{2} + E_c t \qquad (20.3.38a)$$

So, (20.3.36) is consistent with the oscillator wavepacket (20.3.34d)

$$\Psi = e^{iS/\hbar}\phi = e^{i(x_t p_t - x_0 p_0)/2\hbar - i\omega t/2}\phi\,, \qquad (20.3.38b)$$

if the zero-point energy difference (20.3.30c) between classical and quantum-expectation energies is accounted for.

*(2) Quantum generating functions*

The coherent wavepacket with zero momentum ($p_0=0$) from (20.3.32) and (20.3.34b) is

$$\Psi_{x_0}(x) = e^{-M\omega|x_0|^2/4\hbar}\sum_{n=0}^{\infty}\left(\frac{M\omega}{2\hbar}\right)^{n/2}\frac{(x_0)^n}{\sqrt{n!}}\psi_n(x) = e^{-M\omega(x-x_0)^2/2\hbar}\left(\frac{M\omega}{\pi\hbar}\right)^{1/4} \qquad (20.3.39)$$

This yields *eigenwave generating functions*.

$$\sum_{n=0}^{\infty}\left(\frac{M\omega}{2\hbar}\right)^{n/2}\frac{(x_0)^n}{\sqrt{n!}}\psi_n(x) = e^{-\frac{M\omega x^2}{2\hbar}}\,e^{-\frac{M\omega}{2\hbar}\left(\frac{x_0^2}{2}-2xx_0\right)}\left(\frac{M\omega}{\pi\hbar}\right)^{1/4} \qquad (20.3.40a)$$

We redefine $\psi_n$ and write coordinate $x$ in units $y$ of zero-point classical turning point. ($x_0^{CTP}=[\hbar/M\omega]^{1/2}$)

$$\psi_n(x) = \left(\frac{\pi\hbar}{M\omega}\right)^{1/4}\frac{2^{n/2}H_n(y)e^{-y^2/2}}{\sqrt{n!}} \quad \text{and:}\quad x=\sqrt{\frac{\hbar}{M\omega}}\,y\,,\ x_0=\sqrt{\frac{\hbar}{M\omega}}\,y_0 \qquad (20.3.40c)$$

This simplifies the generating expansion.

$$\sum_{n=0}^{\infty}\frac{(y_0)^n}{n!}H_n(y) = H_0(y) + y_0H_1(y) + \frac{y_0^{\,2}}{2!}H_2(y) + \ldots = e^{-\left(y_0^2/4 - yy_0\right)} \qquad (20.3.40b)$$

(20.3.40b) gives successive *Hermite polynomials $H_n(y)$* which multiply the Gaussian $e^{-y^2/2}$.

$$H_0(y) = e^{-\frac{y_0^2}{4}+yy_0}\Big|_{y_0=0} = 1\,, \qquad H_1(y) = \frac{d}{dy_0}e^{-\frac{y_0^2}{4}+yy_0}\Big|_{y_0=0} = y$$
$$H_2(y) = \frac{d^2}{dy_0^{\,2}}e^{-\frac{y_0^2}{4}+yy_0}\Big|_{y_0=0} = y^2 - \frac{1}{2}\,, \qquad H_3(y) = \frac{d^3}{dy_0^{\,3}}e^{-\frac{y_0^2}{4}+yy_0}\Big|_{y_0=0} = y^3 - \frac{3}{2}y \qquad (20.3.40d)$$

In many texts, the Hermite polynomials $H_n(y)$ are defined as the above multiplied by $2^n$. (Let: $y_0 \to 2y_0$.) When using that convention, move the $2^n$-factor of (20.3.40c) down to the denominator.

### (d) Shaped packet states ("Squeezed" states)

Coherent state motion in Fig. 20.3.3(a) results if a ground state (or "vacuum" state) Gaussian wave function $e^{-y^2/\Delta^2}$ a translated by $e^{-ia\mathsf{p}} = e^{-a\partial/\partial y}$ or boosted by $e^{ib\mathsf{x}} = e^{iby}$. We may generalize this to include exponentials of polynomials of generators $-i\mathsf{p}$ and $i\mathsf{x}$. Perhaps, the simplest is the squared or quadratic generator $(i\mathsf{x})^2 = -y^2$ in an operator $e^{-s\mathsf{x}^2} = e^{-sy^2}$ that gives a state called a *squeezed state* whose wave function $\psi_s(y) = e^{-sy^2}e^{-y^2/\Delta^2} = e^{-y^2/\Delta'^2}$ is a Gaussian whose width $\Delta$ is altered to $\Delta' = 1/\sqrt{s+1/\Delta^2}$, that is, either *expanded*, if squeezing parameter $s$ is negative, or else *squeezed* if $s$ is positive.

The time behavior of such a squeezed wave is shown in Fig. 20.3.3(b). As expected it returns to its "natural" width, but then overshoots to become an expanded Gaussian. The result is a "breathing" motion of expansion and squeezing at *twice* natural frequency ω. (This is called "squeezed vacuum" oscillation.)

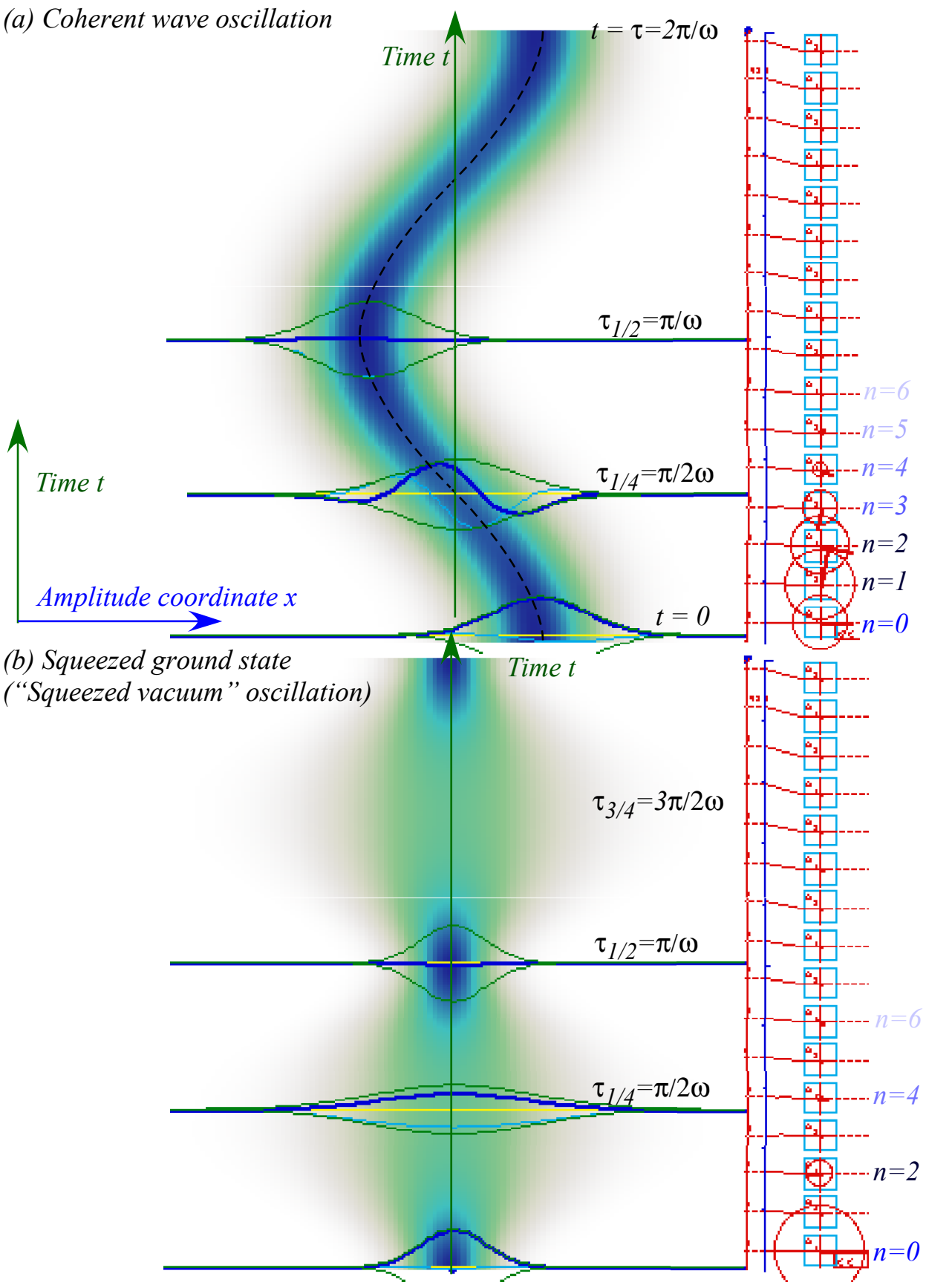


*Fig. 20.3.3 (a) Elementary coherent wave. (b) Elementary squeezed ground state wave*

Notice that the squeezed vacuum "breathing" is symmetric since it involves only even quantum states *n=0, 2, 4,...* in its $|n\rangle$ expansion. This accounts for its double-frequency $(2\omega)$ of oscillation that starts with a fraction $f = 0.5$ of zero-point uncertainty $\Delta x_0 = \sqrt{\hbar / 2M\omega}$, "inhales" and expands to a maximum value $\Delta x_0 / f = 2 \cdot \Delta x_0$ in a quarter period $\tau_{1/4} = \frac{1}{4}(2\pi / \omega)$, then "exhales" back to the minimum value $f \cdot \Delta x_0 = 0.5 \cdot \Delta x_0$ at half period $\tau_{1/2}$, and takes another breath between $\tau_{1/2}$ and $\tau$ in Fig. 20.3.3(b).

Compare this to the elementary coherent oscillation in Fig. 20.3.3(a) that combines both odd and even states *n=0, 1, 2, 3, 4,...* in its $|n\rangle$ expansion (20.3.25), and so its center of intensity $\langle \mathbf{x} \rangle = \bar{x}$ oscillates at the fundamental frequency $\omega$, in fact, it follows a classical $\bar{x} = x_0 \cos \omega t$ time trajectory clearly visible in the figure and consistent with (20.3.29b) in the case that initial expected momentum is zero $(p_0 = 0)$.

By combining the elementary coherent $\langle \mathbf{x} \rangle$ oscillation in Fig. 20.3.3(a) with the coherent $\langle \mathbf{x^2} \rangle$ "breathing" oscillation in Fig. 20.3.3(b) it is possible to sharpen the precision of either amplitude or phase of a coherent oscillation. If we simply combine the two distributions in Fig. 20.3.3(a-b), then a squeezed amplitude wave results with sharpened uncertainty at each of the $\frac{1}{4}$-period times of maximum (or minimum) amplitude as shown in Fig. 20.3.4(a). The price we pay for more precise or *certain* amplitude position is more *un*certain momentum, and this translates into more uncertain location at the times when the amplitude crosses the zero point. That is, more *certain amplitude* implies more *uncertain phase*.

To have a more *certain phase* we need to adjust zero-crossing time to coincide with moments of *x*-inhalation as shown in Fig. 20.3.4(b), but this gives a state with more *uncertain amplitude*. It should not be surprising that phase and amplitude behave like conjugate variables of position and momentum. Phase angle $\Phi$ and amplitude $A$ obey a generalized Heisenberg uncertainty relation analogous to (20.2.20d-e).

$$\Delta\Phi \cdot \Delta A \geq \frac{\hbar}{2A}$$

Since the product $c = A \cdot \Phi$ is the circumferential arc length orthogonal to the radial amplitude distance $A$, this relation is really identical to (20.2.20e) and to one for angular momentum to be derived later. Note that angular uncertainty is inversely proportional to the product $A \cdot \Delta A$. This is responsible for the tremendous phase precision of high-amplitude lasers.

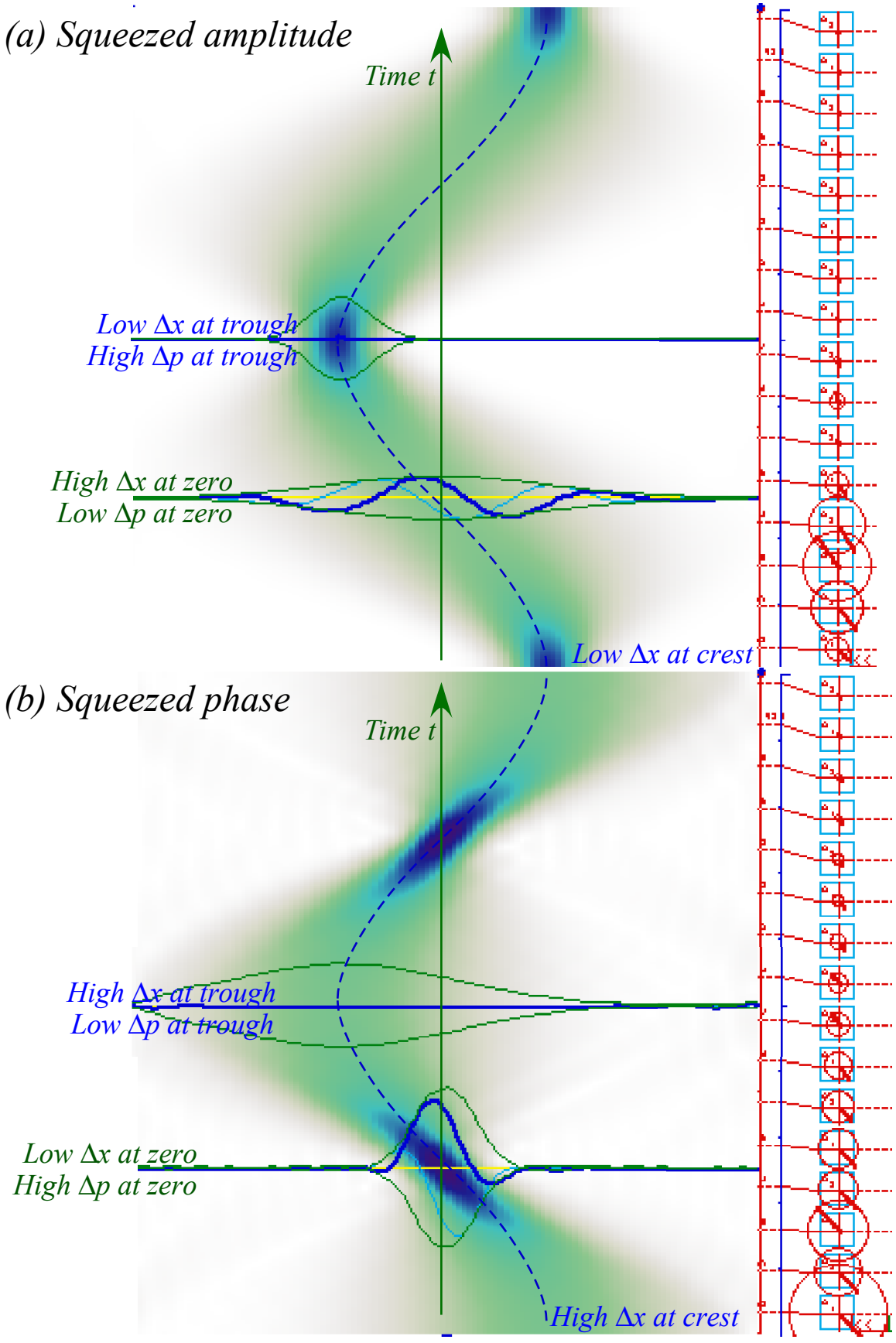


*Fig. 20.3.4 (a) Squeezed amplitude. (b) Squeezed phase zeros.*

## *Problems for Chapter 20*

*Uncertain Quantum Viriality*

1. First: verify equations (20.2.21) to (20.2.22).

(a) With: $\mathsf{H}=\mathsf{p}^2/2M+V(\mathsf{x})$.show that $[\mathsf{H}\,,\,\mathsf{x}] = \hbar\,\mathsf{p}/Mi$ .

(b) With: $\mathsf{H}|j\rangle=\hbar\omega_j|j\rangle$ and $\Omega_{j1}=\omega_j-\omega_1$ show that $\langle j|\,\mathsf{p}|\,1\rangle = Mi\,\Omega_{j1}\,\langle j|\,\mathsf{x}|\,1\rangle$.

(c) Use (a-b) to show $\langle k|\,\mathsf{xp}|k\rangle=\hbar i/2=-\langle k|\,\mathsf{px}|k\rangle$ for any eigenstate $|\Psi\rangle=|\,k\rangle$ .

(d) Show: $\partial/\partial t\,\langle k|\,\mathsf{xp}|k\rangle =0 = i/\hbar\langle k|\,[\mathsf{H}\,,\,\mathsf{xp}]|k\rangle$ .

(e) Compare uncertainty calculation for Coulomb $(P=-1)$ potential to the Bohr radius and $\Delta p$ in (5.4.3).

(f) For $V(x)=Ax^P$ show that: $\langle k|\mathsf{KE}|k\rangle=\langle k|\,\mathsf{p}^2/2M|k\rangle=\langle k||\mathsf{PE}|k\rangle P/2$ (A *virial theorem*)

(g) Derive energy spectrum and the KE/PE ratio for a hyper-power Hamiltonian $\mathsf{p}^Q/2M + Ax^P$ .

*The Beats Go On*

2. Consider quantum beats between saturated (50-50) pairs of harmonic oscillator states.

(a) Derive expected momentum $\overline{p}$ as a function of time for a 50-50 combination state of the ground $|0\rangle$ and first excited state $|1\rangle$. Compare to the expected position. Does $m\dot{\overline{x}} = \overline{p}$ ?

(b) Derive the expected position-squared $\left\langle x^2 \right\rangle$ and momentum-squared $\left\langle p^2 \right\rangle$ for the same combination state as (a). Discuss their relations.

(c) Derive the expected position and momentum as a function of time for a 50-50 combination state of the ground $|0\rangle$ and second excited state $|2\rangle$. Compare. Does $m\dot{\overline{x}} = \overline{p}$ ?

*Coherent Deviation*

3. Here we consider the mean and standard deviation (20.2.20a) or "width" of coherent state distributions for physical quantities.

(a) Derive a (simple) formula for the coherent state norm $\langle\alpha|\alpha\rangle$.

(b) Derive formulas for the position-squared and momentum-squared expectation values in a coherent state $|\alpha\rangle$.

(c) Use (b) to derive the standard deviation of position and momentum distributions.

(d) Derive a formula for the mean value $\overline{n}$ of $n$ in the Poisson distribution (20.3.25b).

(d) Approximate a formula for the width of the Poisson distribution around mean value $\overline{n}$ .

*Coherent Derivation*

4. Use the coherent wave generating function to derive analytic formula for oscillator eigenfunctions $\langle x|n\rangle$ and write out the first three. Derive the momentum wavefunctions $\langle p|n\rangle$, too. (Should be an easy symmetry task.)