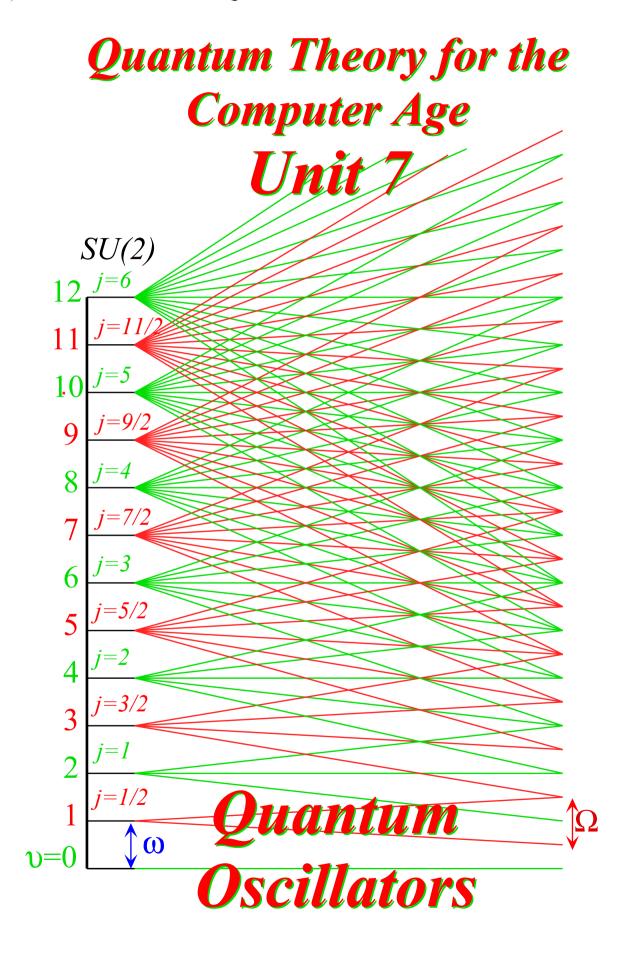
Harter And—LearnIt Unit 7 Quantum Oscillators 20 - 1



## **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†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.

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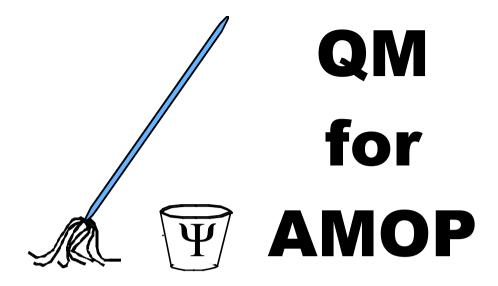
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# **Chapter 20**

## **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.

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## 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  $\omega$  totally independent of amplitude A.

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

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

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

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.

$$V(x) = \int_{0}^{x} k x' dx' = \frac{1}{2} kx^{2} = \frac{1}{2} m\omega^{2} x^{2}$$
 (20.1.4)

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

$$E = H(x, p) = \frac{1}{2m}p^2 + \frac{1}{2}m\omega^2 x^2$$
 (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  $\mathbf{x}$  and  $\mathbf{p}$ , something a five-year-old could do!

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

However, we need to decide how to represent those thick-headed operators  $\mathbf{x}$  and  $\mathbf{p}$ , and right away we notice something unique about this Hamiltonian. Apart from scale factors I/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  $\mathbf{X}$  and momentum  $\mathbf{P}$  (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  $V(x) = M\omega^2 x^2/2$ .

$$i\hbar \left\langle x \middle| \frac{\partial}{\partial t} \middle| \Psi \right\rangle = \left\langle x \middle| \mathbf{H} \middle| \Psi \right\rangle = \left\langle x \middle| \frac{\mathbf{p^2}}{2M} + \frac{M\omega^2 \mathbf{x^2}}{2} \middle| \Psi \right\rangle ,$$

$$i\hbar \frac{\partial \Psi(x,t)}{\partial t} = \frac{-\hbar^2}{2M} \frac{\partial^2 \Psi(x,t)}{\partial x^2} + \frac{M\omega^2 x^2}{2} \Psi(x,t)$$
(20.1.7a)

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

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

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

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

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

$$\psi_{E_n}(x) = \langle x | E_n \rangle = \langle x | n \rangle,$$
 (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*.

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

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

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

yield the following solution of (20.1.8)

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

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

$$\alpha = \frac{M\omega}{2\hbar}$$
, and:  $E = \frac{\hbar^2}{2M}\varepsilon = \frac{\hbar\omega}{2}$  (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

4

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

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

$$(20.1.8). \qquad s \cdot \phi'' + 2s' \cdot \phi' + \left(s'' + \varepsilon s - \alpha x^2 s\right) \phi = 0 = e^{-\alpha x^2} \left[\phi'' - 4\alpha x \phi' + \left(-2\alpha + 4\alpha^2 x^2 + \varepsilon - \alpha x^2\right)\phi\right]$$

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

$$K \cdot \phi = \phi'' - 4\alpha x \phi' + (\varepsilon - 2\alpha)\phi = 0 \tag{20.1.11}$$

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

$$\Psi(x) = s(x)\Phi(x) = e^{-\alpha x^2} \text{ (const.)}$$
 (20.1.12)

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

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

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

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

$$H(x,p) = P^2 + X^2 = (X-iP)(X+iP)/2 + (X+iP)(X-iP)/2$$

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

$$\mathbf{H}(\mathbf{x},\mathbf{p}) = \mathbf{p}^2/_{2M} + M\omega^2 \mathbf{x}^2/_2 = \hbar\omega (\mathbf{a}^{\dagger}\mathbf{a} + \mathbf{a}\mathbf{a}^{\dagger})/2$$
 (20.2.1b)

The resulting operator factors include the following destruction operator a

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

and the conjugate factor is called a *creation operator* **a**<sup>†</sup>. This naming will make sense shortly.

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

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

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

So the **a** and  $\mathbf{a}^{\dagger}$  operators differ only by the sign of the imaginary *i*. Why the operator holding the dagger  $\dagger$  should be called a <u>creation</u> 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  $\mathbf{xp-px}$  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).

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

In abstract operator notation this is written simply as a *commutator* [x, p] *relation*.

$$[\mathbf{x}, \mathbf{p}] \equiv \mathbf{x} \mathbf{p} - \mathbf{p} \mathbf{x} = \hbar i \mathbf{1}$$
 (20.2.2)

Oscillator quantum mechanics involves commutation relations with **a** and **a**<sup>†</sup>.

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

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

This is nicely simplified using (20.2.2) to give

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

or

$$a a^{\dagger} = a^{\dagger} a + 1$$
 (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).

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

## (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  $E_0$ .

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

$$\langle 0 | \mathbf{H}(\mathbf{x}, \mathbf{p}) = \hbar \omega /_2 \langle 0 |$$

(20.2.5a)

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

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

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 **a**  $|0\rangle = 0$  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.

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

For kets, **a**<sup>†</sup> is a creation operator since it creates higher level kets while **a** does the reverse.

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

Perhaps, the † that **a**† carries shouldn't be thought of as a dagger but more like a magic wand. But, beware of its dark side. For bras, **a**† is the destructor, and it is **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.

$$\langle x \mid \mathbf{a} \mid 0 \rangle = \mathbf{0} \tag{20.2.6}$$

Expanding the destruction operator using (20.2.1c) gives

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

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

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

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

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

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

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

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

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

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

Expanding the creation operator using (20.2.1d) gives

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

The operator coordinate representations generate the first excited state wavefunction.

$$\langle x|1\rangle = \psi_{1}(x) = \frac{1}{\sqrt{2\hbar}} \left( \sqrt{M\omega} x \psi_{0}(x) - i\frac{\hbar}{i} \frac{\partial \psi_{0}(x)}{\partial x} / \sqrt{M\omega} \right)$$

$$= \frac{1}{\sqrt{2\hbar}} \left( \sqrt{M\omega} x \frac{e^{-M\omega x^{2}/2\hbar}}{const.} - i\frac{\hbar}{i} \frac{\partial}{\partial x} \frac{e^{-M\omega x^{2}/2\hbar}}{const.} / \sqrt{M\omega} \right)$$

$$= \frac{1}{\sqrt{2\hbar}} \frac{e^{-M\omega x^{2}/2\hbar}}{const.} \left( \sqrt{M\omega} x + i\frac{\hbar}{i} \frac{M\omega x}{\hbar} / \sqrt{M\omega} \right)$$

$$= \frac{\sqrt{M\omega}}{\sqrt{2\hbar}} \frac{e^{-M\omega x^{2}/2\hbar}}{const.} (2x) = \left( \frac{M\omega}{\pi\hbar} \right)^{3/4} \sqrt{2\pi} \left( x e^{-M\omega x^{2}/2\hbar} \right)$$

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.

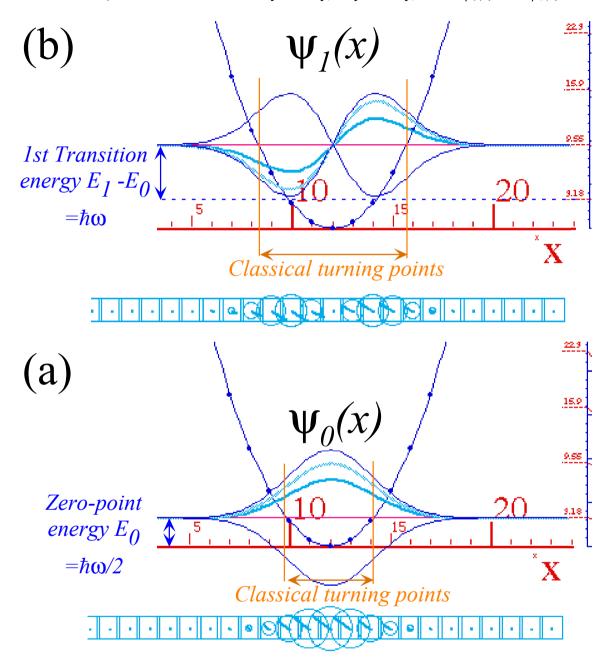


Fig. 20.2.1 Harmonic oscillator wavefunctions (a) Ground state, (a) First excited state.

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 [ $\mathbf{a}$ ,  $\mathbf{a}^{\dagger}$ ] = 1 are useful.

$$\begin{bmatrix} \mathbf{a}, \mathbf{a}^{\dagger 2} \end{bmatrix} = 2\mathbf{a}^{\dagger}, \quad \begin{bmatrix} \mathbf{a}, \mathbf{a}^{\dagger 3} \end{bmatrix} = 3\mathbf{a}^{2\dagger}, \quad \cdots, \quad , \quad \begin{bmatrix} \mathbf{a}, \mathbf{a}^{\dagger n} \end{bmatrix} = n\mathbf{a}^{\dagger n-1}$$
 (20.2.9a)

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

$$[A, BC] = ABC - BCA = [A, B]C + BAC - BCA$$
  
=  $[A, B]C + B[A, C]$  (20.2.9b)

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

$$[AB, C] = -[C, AB] = -[C, A]B - A[C, B]$$
  
=  $[A, C]B + A[B, C]$  (20.2.9c)

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

$$\mathbf{a}\mathbf{a}^{\dagger n} = n\mathbf{a}^{\dagger n-1} + \mathbf{a}^{\dagger n}\mathbf{a}$$

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

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

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

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

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

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

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

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

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

The general **a**..**a**<sup>†</sup> to **a**<sup>†</sup>..**a** power shuffle formula is the result we want.

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

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

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

#### (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.

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

The result is root-factorial normalization:

$$|n\rangle = \frac{\mathbf{a}^{\dagger n}|0\rangle}{\sqrt{n!}} \tag{20.2.11}$$

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.

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

Applying a destruction operator **a** to an n-quantum state using (20.2.10) gives the following.

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

These can be summarized by the following oscillator ladder relations.

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

A mnemonic rule: Always put the <u>larger</u> 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.

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

#### (2) Number operator

The Hamiltonian (20.2.4) contains the operator  $\hbar\omega$  **a**<sup>†</sup>**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).

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

$$\mathbf{H} |n\rangle = \hbar \omega \, \mathbf{a}^{\dagger} \mathbf{a} |n\rangle + \hbar \omega /_2 \mathbf{1} |n\rangle = (\hbar \omega \, n + \hbar \omega /_2) |n\rangle \qquad (20.2.15a)$$

$$\langle \mathbf{H} \rangle = \hbar \omega \langle \mathbf{a}^{\dagger} \mathbf{a} \rangle + \frac{\hbar \omega}{2} \langle \mathbf{1} \rangle = \hbar \omega \begin{pmatrix} 0 & & & \\ & 1 & & \\ & & 2 & \\ & & & 3 & \\ & & & \ddots \end{pmatrix} + \hbar \omega \begin{pmatrix} 1/2 & & & \\ & 1/2 & & \\ & & & 1/2 & \\ & & & & 1/2 & \\ & & & & \ddots \end{pmatrix}$$
(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  $\mathbf{a}^{\dagger}$ .

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

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

$$\overline{\mathbf{x}} \mid_{n} = \langle n \mid \mathbf{x} \mid n \rangle = \sqrt{\frac{\hbar}{2M\omega}} \langle n \mid \left( \mathbf{a} + \mathbf{a}^{\dagger} \right) \mid n \rangle = 0 \qquad \qquad \overline{\mathbf{p}} \mid_{n} = \langle n \mid \mathbf{p} \mid n \rangle = i\sqrt{\frac{\hbar M\omega}{2}} \langle n \mid \left( \mathbf{a}^{\dagger} - \mathbf{a} \right) \mid n \rangle = 0$$

$$(20.2.17a) \qquad (20.2.17b)$$

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.

$$\overline{\mathbf{x}^{2}} \mid_{n} = \langle n \mid \mathbf{x}^{2} \mid n \rangle = \frac{\hbar}{2M\omega} \langle n \mid (\mathbf{a} + \mathbf{a}^{\dagger})^{2} \mid n \rangle \qquad \overline{\mathbf{p}^{2}} \mid_{n} = \langle n \mid \mathbf{p}^{2} \mid n \rangle = i^{2} \frac{\hbar M \omega}{2} \langle n \mid (\mathbf{a}^{\dagger} - \mathbf{a})^{2} \mid n \rangle 
= \frac{\hbar}{2M\omega} \langle n \mid (\mathbf{a}^{2} + \mathbf{a}^{\dagger} \mathbf{a} + \mathbf{a} \mathbf{a}^{\dagger} + \mathbf{a}^{\dagger 2}) \mid n \rangle \qquad = \frac{\hbar M \omega}{2} \langle n \mid (\mathbf{a}^{\dagger 2} - \mathbf{a}^{\dagger} \mathbf{a} - \mathbf{a} \mathbf{a}^{\dagger} + \mathbf{a}^{2}) \mid n \rangle 
= \frac{\hbar M \omega}{2} (2n+1) \qquad (20.2.18b)$$

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.

$$\overline{PE} \mid_{n} = \frac{1}{2} M \omega^{2} \overline{\mathbf{x}^{2}} \mid_{n} = \frac{1}{2} M \omega^{2} \frac{\hbar (2n+1)}{2M \omega} \qquad \overline{KE} \mid_{n} = \frac{1}{2M} \overline{\mathbf{p}^{2}} \mid_{n} = \frac{1}{2M} \frac{\hbar M \omega}{2} (2n+1)$$

$$= \frac{1}{2} \hbar \omega \left( n + \frac{1}{2} \right) \qquad \qquad = \frac{1}{2} \hbar \omega \left( n + \frac{1}{2} \right)$$

$$(20.2.19a) \qquad (20.2.19b)$$

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.

$$(\Delta q)^2 = \overline{(q - \overline{q})^2}$$
,, or:  $\Delta q = \sqrt{\overline{(q - \overline{q})^2}}$  (20.2.20a)

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

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

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

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

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

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

$$\Delta x \cdot \Delta p \mid_0 = \frac{\hbar}{2} \tag{20.2.20e}$$

## (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.

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

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

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

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

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

Quantum v-number dependence factors out of the resulting general minimum energy.

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

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

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

Again, the oscillator parameters P=2 and  $A=k/2=1/2M\omega^2$  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  $v^{2/3}$ . A square-well corresponds to a large power  $P\to\infty$ . Then, (20.2.22b) correctly predicts the quantum dependence  $v^{2P/P+2}$  approaches  $v^2$ . At the opposite extreme, a Coulomb potential k/r has P=-1. According to (20.2.22b), it has an inverse power  $v^{-2}$ -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).)

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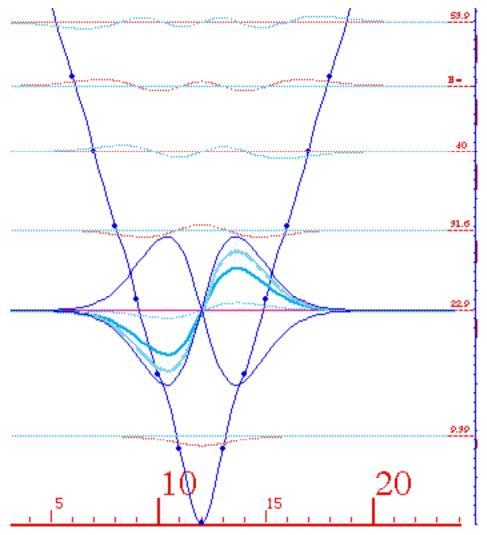


Fig. 20.2.2 First excited state wavefunction of linear potential V(y)=mg|y|. (V=98 Bu for N=24)

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  $\mu_{\theta}$  in quantum phase space area  $\hbar\omega(n + \mu_{\theta})$  is called *Maslov's index*.

The linear potential wavefunctions are called *Airy functions*. If you keep only odd-*n* antisymmetric 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.

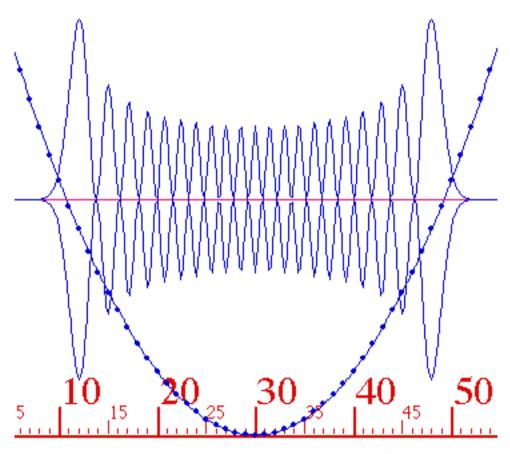


Fig. 20.2.3 n=20 probability for harmonic oscillator potential  $V(x)=Vx^2$ . (V=100 Bu for P=60)

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.

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## 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.

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

Planck's oscillation of a quantum phasor is observable only <u>relative</u> to another phasor which has a <u>different</u> 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 <u>difference</u> 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  $|\psi_0(x)\rangle = \langle x|0\rangle$  and  $|\psi_1(x)\rangle = \langle x|1\rangle$  shown in Fig. 20.2.1, gives the following state.

$$|\Psi\rangle = |0\rangle\langle 0|\Psi\rangle + |1\rangle\langle 1|\Psi\rangle = |0\rangle\Psi_0 + |1\rangle\Psi_1 \tag{20.3.2a}$$

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

$$\Psi(x) = \langle x | \Psi \rangle = \langle x | 0 \rangle \langle 0 | \Psi \rangle + \langle x | 1 \rangle \langle 1 | \Psi \rangle = \psi_0(x) \Psi_0 + \psi_1(x) \Psi_1 \tag{20.3.2b}$$

The greatest oscillation occurs with 50-50 mixing coefficients

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

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

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

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

$$|\Psi(x,t)| = \sqrt{\Psi^* \Psi} = \sqrt{\left(e^{-i\omega_0 t} \psi_0(x) + e^{-i\omega_1 t} \psi_1(x)\right)^* \left(e^{-i\omega_0 t} \psi_0(x) + e^{-i\omega_1 t} \psi_1(x)\right)/2}$$

$$= \sqrt{\left(\left|\psi_0(x)\right|^2 + \left|\psi_1(x)\right|^2 + \psi_0(x)\psi_1(x)\left(e^{i(\omega_1 - \omega_0)t} + e^{-i(\omega_1 - \omega_0)t}\right)\right)/2}$$

$$= \sqrt{\left(\left|\psi_0(x)\right|^2 + \left|\psi_1(x)\right|^2 + 2\psi_0(x)\psi_1(x)\cos(\omega_1 - \omega_0)t\right)/2}$$

$$= \sqrt{\left(\left|\psi_0(x)\right|^2 + \left|\psi_1(x)\right|^2 + 2\psi_0(x)\psi_1(x)\cos(\omega_1 - \omega_0)t\right)/2}$$
(20.3.5a)

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  $\omega_I - \omega_0 = 2\pi/\tau_{beat}$ . The general 2-state quantum probability beat wavefunction is

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

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

$$A_0(x) A_1(x) = |A_0(x) A_1(x)| e^{i\Theta_{01}(x)}$$
 (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

$$\omega_{beat} = \omega_1 - \omega_0 = \omega \,, \tag{20.3.5d}$$

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

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

Here  $\Delta E$  is the energy difference between the first excited level  $E_I = \hbar \omega_I$  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  $\omega$ .

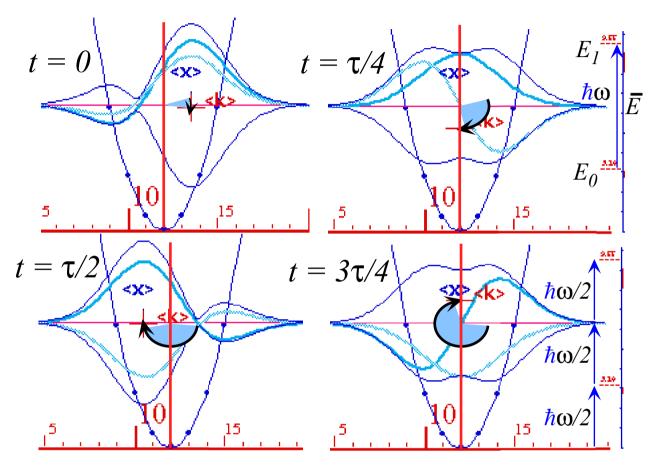


Fig. 20.3.1 Beat oscillation for mixed 01-state of harmonic oscillator showing x and k expectation.

#### (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.

$$\overline{E} = \langle \Psi | \mathbf{H} | \Psi \rangle = \langle 0 | \mathbf{H} | 0 \rangle | \langle 0 | \Psi \rangle |^2 + \langle 1 | \mathbf{H} | 1 \rangle | \langle 1 | \Psi \rangle |^2 + \dots$$

$$= E_0 |\Psi_0|^2 + E_1 |\Psi_1|^2 + \dots \tag{20.3.7a}$$

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

$$\overline{E} = E_0 \ 1/2 + E_1 \ 1/2 = (\hbar \omega/2) \ 1/2 + (3\hbar \omega/2) \ 1/2 = \hbar \omega$$
 (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  $\mathbf{x}$ -operator is not diagonal in the energy basis. The Ch. 12 equation (12.1.11) treats the general case.

$$\overline{x} \mid_{\Psi} = \langle \Psi | \mathbf{x} | \Psi \rangle = \sum_{m=1}^{\infty} \sum_{n=1}^{\infty} \langle \Psi | m \rangle \langle m | \mathbf{x} | n \rangle \langle n | \Psi \rangle$$
(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

$$\langle m|\mathbf{x}|n\rangle = \sqrt{\frac{\hbar}{2M\omega}} \langle m|\left(\mathbf{a} + \mathbf{a}^{\dagger}\right)|n\rangle = \sqrt{\frac{\hbar}{2M\omega}} \left(\sqrt{n} \langle m|n-1\rangle + \sqrt{n+1} \langle m|n+1\rangle\right)$$

$$= \left(x_0 / \sqrt{2}\right) \left(\sqrt{n}\delta_{m,n-1} + \sqrt{n+1}\delta_{m,n+1}\right)$$
(20.3.8b)

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

$$x_0 = \left[\hbar/M\omega\right]^{1/2} \tag{20.3.8c}$$

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

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

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

$$\langle \mathbf{x} \rangle = \overline{\mathbf{x}} |_{\Psi(t)} = \qquad \qquad \langle \Psi(t) | \mathbf{x} | \Psi(t) \rangle$$

$$= \sqrt{\frac{\hbar}{2M\omega}} \left( \begin{array}{cccc} \Psi_0^*(t) & \Psi_1^*(t) & \Psi_2^*(t) & \cdots \\ \end{array} \right) \begin{pmatrix} \vdots & \sqrt{1} & \vdots & \cdots \\ \sqrt{1} & \sqrt{2} & \cdots \\ \vdots & \vdots & \sqrt{3} & \ddots \\ \end{array} \right) \begin{pmatrix} \Psi_0(t) \\ \Psi_1(t) \\ \Psi_2(t) \\ \vdots \\ \end{array}$$

$$= \left( x_0 / \sqrt{2} \right) \left( \begin{array}{cccc} \Psi_0^* e^{i\omega_0 t} & \Psi_1^* e^{i\omega_1 t} & \Psi_2^* e^{i\omega_2 t} & \cdots \\ \end{array} \right) \begin{pmatrix} \vdots & \sqrt{1} & \vdots & \cdots \\ \sqrt{1} & \sqrt{2} & \cdots & \sqrt{3} \\ \vdots & \vdots & \sqrt{3} & \ddots \\ \end{array} \right) \begin{pmatrix} \Psi_0 e^{-i\omega_0 t} \\ \Psi_1 e^{-i\omega_1 t} \\ \Psi_2 e^{-i\omega_2 t} \\ \vdots \\ \end{array} \right)$$

$$= \left( x_0 / \sqrt{2} \right) \left( \begin{array}{cccc} \Psi_0^* e^{i\omega_0 t} & \Psi_1^* e^{i\omega_1 t} & \Psi_2^* e^{i\omega_2 t} & \cdots \\ \end{array} \right) \begin{pmatrix} \sqrt{1} \Psi_1 e^{-i\omega_1 t} \\ \sqrt{1} \Psi_0 e^{-i\omega_0 t} + \sqrt{2} \Psi_2 e^{-i\omega_2 t} \\ \vdots \\ \sqrt{2} \Psi_1 e^{-i\omega_1 t} + \sqrt{3} \Psi_3 e^{-i\omega_3 t} \\ \vdots \\ \end{array} \right)$$

$$= \left( x_0 / \sqrt{2} \right) \left( \begin{array}{cccc} \Psi_0^* e^{i\omega_0 t} & \Psi_1^* e^{i\omega_1 t} & \Psi_2^* e^{i\omega_2 t} & \cdots \\ \end{array} \right) \begin{pmatrix} \sqrt{1} \Psi_0 e^{-i\omega_0 t} + \sqrt{2} \Psi_2 e^{-i\omega_2 t} \\ \sqrt{2} \Psi_1 e^{-i\omega_1 t} + \sqrt{3} \Psi_3 e^{-i\omega_3 t} \\ \vdots & \vdots & \cdots \\ \end{array} \right)$$

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

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

The amplitude overlap product is  $\Psi_1^* \Psi_0 = |\Psi_1^* \Psi_0| e^{i\theta_{10}}$ 

$$\Psi_1^* \Psi_0 = \left| \Psi_1^* \Psi_0 \right| e^{i\theta_{10}} \tag{20.3.10c}$$

This product is  $(1/\sqrt{2})(1/\sqrt{2})=1/2$  for a 50-50 combination state (20.3.3) giving the following x-oscillation.

$$\langle \mathbf{x}(t) \rangle = \overline{x} \mid_{\Psi(t)} = \left( x_0 / \sqrt{2} \right) \cos\left( \omega_1 - \omega_0 \right) t = \left( x_{0I} / 2 \right) \cos \omega t \tag{20.3.10d}$$

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  $\overline{E} = \hbar \omega$  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

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

(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 T(a) which does nothing more than translate x-wavefunctions.

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

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.)

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

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

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

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

$$\mathbf{G} = \frac{\partial \mathbf{T}}{\partial a}\Big|_{a=0} \tag{20.3.13b}$$

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

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

Comparing this to the effect of (20.3.13) gives

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

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

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

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

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

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

$$\mathbf{T}(a) \cdot \psi(x) = e^{a\mathbf{G}} \cdot \psi(x) = e^{-a\frac{\partial}{\partial x}} \cdot \psi(x)$$

$$= \psi(x) - a\frac{\partial \psi(x)}{\partial x} + \frac{a^2}{2!} \frac{\partial^2 \psi(x)}{\partial x^2} - \frac{a^3}{2!} \frac{\partial^3 \psi(x)}{\partial x^3} + \dots$$
(20.3.15c)

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

$$\mathbf{G} = -\frac{i}{\hbar}\mathbf{p} \tag{20.3.15d}$$

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

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

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

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

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

There also exists an operator  $\mathbf{B}(b)$  which "translates" momentum p-wavefunctions.

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

Such an operator is called a *boost operator*  $\mathbf{B}(b)$  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.)

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

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

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

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

$$\mathbf{K} = \frac{\partial \mathbf{B}}{\partial b} \bigg|_{b=0} \tag{20.3.18b}$$

Tiny boosts of a momentum function  $\psi(p)$  give a single-term Taylor series.

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

Comparing this to the effect of (20.3.18) gives

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

Solving (20.3.18b) and (20.3.19) yields an abstract operator exponential expression for finite  $\mathbf{B}(b)$ ,

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

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

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

and the p-representation of the finite boost.

$$\mathbf{B}(b) \cdot \psi(p) = e^{b\mathbf{K}} \cdot \psi(p) = e^{-b\frac{\partial}{\partial p}} \cdot \psi(p)$$

$$= \psi(p) - b\frac{\partial \psi(p)}{\partial p} + \frac{b^2}{2!} \frac{\partial^2 \psi(p)}{\partial p^2} - \frac{b^3}{2!} \frac{\partial^3 \psi(p)}{\partial p^3} + \dots$$
(20.3.20c)

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

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

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

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

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

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

$$\mathbf{C}(a,b) = e^{i(b\mathbf{x} - a\mathbf{p})/\hbar}$$
(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  $e^{-i\mathbf{J}_z\alpha/\hbar}e^{-i\mathbf{J}_z\gamma/\hbar}e^{-i\mathbf{J}_z\gamma/\hbar}$  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.

$$e^{\mathbf{A}+\mathbf{B}} = e^{\mathbf{A}}e^{\mathbf{B}}e^{-[\mathbf{A},\mathbf{B}]/2} = e^{\mathbf{B}}e^{\mathbf{A}}e^{[\mathbf{A},\mathbf{B}]/2}$$
, where:  $[\mathbf{A},[\mathbf{A},\mathbf{B}]] = \mathbf{0} = [\mathbf{B},[\mathbf{A},\mathbf{B}]]$  (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  $\mathbf{C}(a,b)$  factors either way.

$$\mathbf{C}(a,b) = e^{i(b\mathbf{x} - a\mathbf{p})/\hbar} = e^{ib\mathbf{x}/\hbar} e^{-ia\mathbf{p}/\hbar} e^{-ab[\mathbf{x},\mathbf{p}]/2\hbar^2} = e^{ib\mathbf{x}/\hbar} e^{-ia\mathbf{p}/\hbar} e^{-iab/2\hbar}$$

$$= \mathbf{B}(b)\mathbf{T}(a)e^{-iab/2\hbar} = \mathbf{T}(a)\mathbf{B}(b)e^{iab/2\hbar}$$
(20.3.24a)

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

$$\mathbf{C}(a,b) = e^{i(b\mathbf{x} - a\mathbf{p})/\hbar} = e^{ib(\mathbf{a}^{\dagger} + \mathbf{a})/\sqrt{2\hbar M\omega} + a(\mathbf{a}^{\dagger} - \mathbf{a})\sqrt{M\omega/2\hbar}}$$

$$= e^{\alpha \mathbf{a}^{\dagger} - \alpha * \mathbf{a}} = e^{-|\alpha|^{2}/2} e^{\alpha \mathbf{a}^{\dagger}} e^{-\alpha * \mathbf{a}} = e^{|\alpha|^{2}/2} e^{-\alpha * \mathbf{a}} e^{\alpha \mathbf{a}^{\dagger}}$$
(20.3.24b)

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

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

Applying the combination operator  $\mathbb{C}(x_0,p_0)$  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  $p_0$ .

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

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

$$\mathbf{a} |\alpha_{0}(x_{0}, p_{0})\rangle = e^{-|\alpha_{0}|^{2}/2} \sum_{n=0}^{\infty} \frac{(\alpha_{0})^{n}}{\sqrt{n!}} \mathbf{a} |n\rangle = e^{-|\alpha_{0}|^{2}/2} \sum_{n=0}^{\infty} \frac{(\alpha_{0})^{n}}{\sqrt{n!}} \sqrt{n} |n-1\rangle$$

$$= \alpha_{0} |\alpha_{0}(x_{0}, p_{0})\rangle$$
(20.3.25b)

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

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

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

$$\begin{split} \left\langle \alpha_{0}\left(x_{0},p_{0}\right)\middle|\mathbf{x}\middle|\alpha_{0}\left(x_{0},p_{0}\right)\right\rangle &=\sqrt{\frac{\hbar}{2M\omega}}\left\langle \alpha_{0}\left(x_{0},p_{0}\right)\middle|\left(\mathbf{a}+\mathbf{a}^{\dagger}\right)\middle|\alpha_{0}\left(x_{0},p_{0}\right)\right\rangle \\ &=\sqrt{\frac{\hbar}{2M\omega}}\left(\alpha_{0}+\alpha_{0}^{\phantom{0}*}\right) = x_{0} \end{split} \tag{20.3.25d}$$

$$\langle \alpha_0(x_0, p_0) | \mathbf{p} | \alpha_0(x_0, p_0) \rangle = i \sqrt{\frac{M\omega\hbar}{2}} \langle \alpha_0(x_0, p_0) | (\mathbf{a}^{\dagger} - \mathbf{a}) | \alpha_0(x_0, p_0) \rangle$$

$$= i \sqrt{\frac{M\omega\hbar}{2}} (\alpha_0^* - \alpha_0^*) = p_0$$
(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

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

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

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

The coherent state evolution uses this result.

$$\begin{split} \mathbf{U}(t,0) \Big| \alpha_{0}(x_{0},p_{0}) \Big\rangle &= e^{-|\alpha_{0}|^{2}/2} \sum_{n=0}^{\infty} \frac{(\alpha_{0})^{n}}{\sqrt{n!}} \mathbf{U}(t,0) \Big| n \Big\rangle = e^{-|\alpha_{0}|^{2}/2} \sum_{n=0}^{\infty} \frac{(\alpha_{0})^{n}}{\sqrt{n!}} e^{-i(n+1/2)\omega t} \Big| n \Big\rangle \\ &= e^{-i\omega t/2} e^{-|\alpha_{0}|^{2}/2} \sum_{n=0}^{\infty} \frac{(\alpha_{0}e^{-i\omega t})^{n}}{\sqrt{n!}} \Big| n \Big\rangle \end{split}$$

This simplifies to a variable coherent state

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

with a time dependent phasor coordinate (20.3.24c)

$$\alpha_{t}(x_{t}, p_{t}) = e^{-i\omega t} \alpha_{0}(x_{0}, p_{0})$$

$$\left[x_{t} + i\frac{p_{t}}{M\omega}\right] = e^{-i\omega t} \left[x_{0} + i\frac{p_{0}}{M\omega}\right],$$
(20.3.29a)

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

$$x_{t} = x_{0} \cos \omega t + \frac{p_{0}}{M\omega} \sin \omega t$$

$$\frac{p_{t}}{M\omega} = -x_{0} \sin \omega t + \frac{p_{0}}{M\omega} \cos \omega t$$
(20.3.29b)

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

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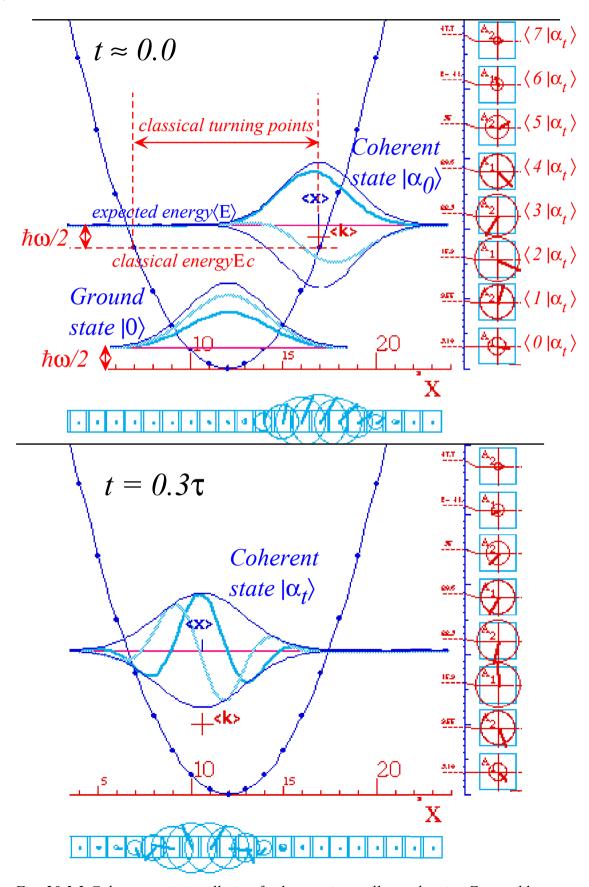


Fig. 20.3.2 Coherent state oscillation for harmonic oscillator showing E, x and k expectation.

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

$$\begin{split} \left\langle E \right\rangle \Big|_{\alpha_{0}} &= \left\langle \alpha_{0} \left( x_{0}, p_{0} \right) \middle| \mathsf{H} \middle| \alpha_{0} \left( x_{0}, p_{0} \right) \right\rangle = \left\langle \alpha_{0} \left( x_{0}, p_{0} \right) \middle| \left( \hbar \omega \mathsf{a}^{\dagger} \mathsf{a} + \frac{\hbar \omega}{2} \mathsf{1} \right) \middle| \alpha_{0} \left( x_{0}, p_{0} \right) \right\rangle \\ &= \hbar \omega \alpha_{0}^{*} \alpha_{0} + \frac{\hbar \omega}{2} \end{split} \tag{20.3.30a}$$

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

$$E_{classical} = \hbar \omega \alpha_0^* \alpha_0 = \hbar \omega \left[ x_0 + i \frac{p_0}{M \omega} \right] \sqrt{M \omega / 2\hbar}^2$$

$$= \frac{1}{2} M \omega x_0^2 + \frac{p_0^2}{2M}$$
(20.3.30b)

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

$$\langle E \rangle \Big|_{\alpha_0} = E_{classical} + E_0 = \hbar \omega \alpha_0^* \alpha_0 + \frac{\hbar \omega}{2}$$

$$= \frac{1}{2} M \omega x_0^2 + \frac{p_0^2}{2M} + \frac{\hbar \omega}{2}$$
(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 <u>classical</u> 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 xexpectation 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).

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

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## (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.

$$\langle x | \alpha_0 (x_0, p_0) \rangle = \langle x | \mathbf{C}(x_0, p_0) | 0 \rangle = \langle x | e^{i(x_0 \mathbf{x} - p_0 \mathbf{p})/\hbar} | 0 \rangle$$

$$= e^{-|\alpha_0|^2/2} \sum_{n=0}^{\infty} \frac{(\alpha_0)^n}{\sqrt{n!}} \langle x | n \rangle$$
(20.3.32)

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

$$\langle x | \alpha_{0}(x_{0}, p_{0}) \rangle = \langle x | \mathbf{C}(x_{0}, p_{0}) | 0 \rangle = \langle x | \mathbf{B}(p_{0}) \mathbf{T}(x_{0}) | 0 \rangle e^{-ix_{0}p_{0}/2\hbar}$$

$$= \langle x | e^{ip_{0}\mathbf{x}/\hbar} \mathbf{T}(x_{0}) | 0 \rangle e^{-ix_{0}p_{0}/2\hbar}$$

$$= e^{ip_{0}x/\hbar} \langle x | \mathbf{T}(x_{0}) | 0 \rangle e^{-ix_{0}p_{0}/2\hbar}$$

$$= e^{ip_{0}x/\hbar} \langle x - x_{0} | 0 \rangle e^{-ix_{0}p_{0}/2\hbar}$$

$$(20.3.33)$$

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

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

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

$$\Psi_{\alpha_{0}}(x) = \langle x | \alpha_{0}(x_{0}, p_{0}) \rangle = e^{ip_{0}x/\hbar} e^{-M\omega(x-x_{0})^{2}/2\hbar} e^{-ix_{0}p_{0}/2\hbar} \left(\frac{M\omega}{\pi\hbar}\right)^{1/4} \\
= e^{ip_{0}x_{0}/2\hbar} e^{-M\omega(x-x_{0})^{2}/2\hbar + ip_{0}(x-x_{0})/\hbar} \left(\frac{M\omega}{\pi\hbar}\right)^{1/4} \tag{20.3.34b}$$

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

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

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

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

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

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

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

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

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

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

whose integral is the *Hamilton's Principle action integral SP* 

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

which includes Hamilton's Characteristic action integral SH also known as "reduced" action

$$S_H = \int p \, dx \,, \tag{20.3.35e}$$

The word "Principle" (not "Principal") may be capitalized since it refers to Hamilton's Minimum *Principle*, that is, that S<sub>P</sub> 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)

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

where:

$$p = \frac{\partial S}{\partial x}$$
,  $H = -\frac{\partial S}{\partial t}$  (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 Swavefronts and that a wavefunction such as (20.3.34d) has the form

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

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

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

$$S_{H} = \int_{0}^{t} p_{t} dx_{t} = \int_{0}^{t} \sqrt{2M \left( E_{c} - \frac{M\omega^{2}}{2} x_{t}^{2} \right)} dx_{t} = S_{P} + E_{c}t$$

$$= \frac{x_{t} p_{t}}{2} \Big|_{0}^{t} + \frac{E_{c}}{\omega} \arcsin \left( \frac{M\omega}{\sqrt{2ME_{c}}} x_{t} \right) \Big|_{0}^{t} = \frac{x_{t} p_{t} - x_{0} p_{0}}{2} + E_{c}t$$
(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

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

This yields eigenwave generating functions.

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

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

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

This simplifies the generating expansion.

$$\sum_{n=0}^{\infty} \frac{\left(y_0\right)^n}{n!} H_n(y) = H_0(y) + y_0 H_1(y) + \frac{y_0^2}{2!} H_2(y) + \dots = e^{-\left(y_0^2/4 - yy_0\right)}$$
(20.3.40b)

(20.3.40b) gives successive *Hermite polynomials H<sub>n</sub>(y)* which multiply the Gaussian  $e^{-y^2/2}$ .

$$H_{0}(y) = e^{-\frac{y_{0}^{2}}{4} + yy_{0}} \bigg|_{y_{0} = 0} = 1, \qquad H_{1}(y) = \frac{d}{dy_{0}} e^{-\frac{y_{0}^{2}}{4} + yy_{0}} \bigg|_{y_{0} = 0} = y$$

$$H_{2}(y) = \frac{d^{2}}{dy_{0}^{2}} e^{-\frac{y_{0}^{2}}{4} + yy_{0}} \bigg|_{y_{0} = 0} = y^{2} - \frac{1}{2}, \qquad H_{3}(y) = \frac{d^{3}}{dy_{0}^{3}} e^{-\frac{y_{0}^{2}}{4} + yy_{0}} \bigg|_{y_{0} = 0} = y^{3} - \frac{3}{2}y$$

$$(20.3.40d)$$

In many texts, the Hermite polynomials  $H_n(y)$  are defined as the above multiplied by  $2^n$ . (Let:  $y_0 \rightarrow 2y_0$ .) 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  $e^{-ia\mathbf{p}} = e^{-a\partial/\partial y}$  or boosted by  $e^{ib\mathbf{x}} = e^{iby}$ . We may generalize this to include exponentials of polynomials of generators  $-i\mathbf{p}$  and  $i\mathbf{x}$ . Perhaps, the simplest is the squared or quadratic generator  $(i\mathbf{x})^2 = -y^2$  in an operator  $e^{-s\mathbf{x}^2} = e^{-sy^2}$  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.)

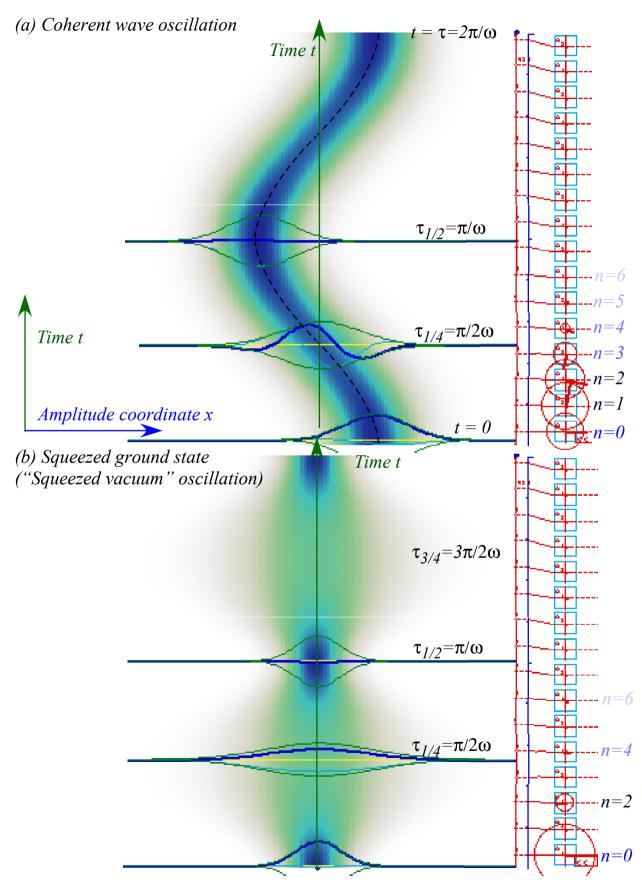


Fig. 20.3.3 (a) Elementary coherent wave. (b) Elementary squeezed ground state wave

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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  $\langle \mathbf{x} \rangle = \overline{x}$  oscillates at the fundamental frequency  $\omega$ , in fact, it follows a classical  $\overline{x} = x_0 \cos \omega t$  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 *uncertain* 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).

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

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.

 $^{\circ}$ High  $\Delta x$  at crest

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

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#### Problems for Chapter 20

#### Uncertain Quantum Viriality

- 1. First: verify equations (20.2.21) to (20.2.22).
- (a) With:  $H=p^2/2M+V(x)$ . show that  $[H, x] = \hbar p/Mi$ .
- (b) With:  $H|j\rangle = \hbar \omega_i |j\rangle$  and  $\Omega_{i1} = \omega_i \omega_1$  show that  $\langle j | p | 1 \rangle = Mi \Omega_{i1} \langle j | x | 1 \rangle$ .
- (d) Show:  $\partial/\partial t \langle k | xp | k \rangle = 0 = i/\hbar \langle k | [H, xp] | k \rangle$ .
- (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:  $\langle k | KE | k \rangle = \langle k | p^2/2M | k \rangle = \langle k | PE | k \rangle P/2$  (A virial theorem)
- (g) Derive energy spectrum and the KE/PE ratio for a hyper-power Hamiltonian  $pQ/2M + Ax^P$ .

#### The Beats Go On

- 2. Consider quantum beats between saturated (50-50) pairs of harmonic oscillator states.
- (a) Derive expected momentum  $\bar{p}$  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  $m\dot{x} = \bar{p}$ ?
- (b) Derive the expected position-squared  $\langle x^2 \rangle$  and momentum-squared  $\langle p^2 \rangle$  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  $m\dot{x} = \overline{p}$ ?

#### Coherent Deviation

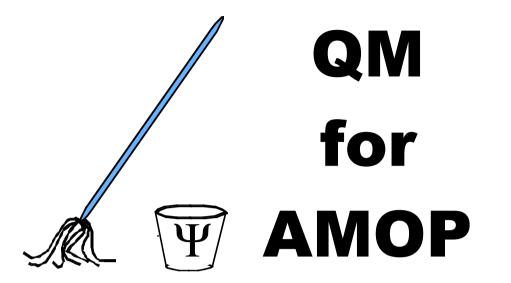
- 3. Here we consider the mean and standard deviation (20.2.20a) or "width" of coherent state distributions for physical quantities.
- (a) Derive a (simple) formula for the coherent state norm  $\langle \alpha | \alpha \rangle$ .
- (b) Derive formulas for the position-squared and momentum-squared expectation 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  $\bar{n}$  of n in the Poisson distribution (20.3.25b).
- (d) Approximate a formula for the width of the Poisson distribution around mean value  $\bar{n}$ .

#### 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.)

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## **Unit 7 Quantum Oscillators**



## **Chapter 21**

# Two-Dimensional Oscillator States and Dynamics

W. G. Harter

Using the 1D-harmonic oscillator algebra from the preceding Chapter 20, the 2D oscillator quantum mechanics is developed. Much of the theory applies to 3D, 4D, and higher dimensional oscillators, as well. Quantum em fields treated in Chapter 22 begin with many-D oscillators, one dimension for each em-mode. However, the main objective of this Chapter 21 is to give the quantum version of the classical ABCD oscillator analogy to quantum spin-1/2, polarization, and other U(2) systems discussed in Chapter 10. This sets the stage for a powerful development, due to Schwinger, of the quantum theory of angular momentum in Chapter 23.

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### Chapter 21. 2D-Harmonic Oscillator States and Dynamics

#### 21.1 Two-Dimensional Harmonic Oscillator Hamiltonians and Bases

So far, most wavefunctions have been one-dimensional. The classical waves in the "Hall of Mirrors" wave-guide and its cavity described in Sec. 6.3 are one exception. Now we extend the oscillator theory of the preceding Chapter 20 to an oscillator system of two (or more) dimensions.

#### (a) 2D-Oscillator basics

As far as symmetry algebra goes it is a big jump to go from a 1D oscillator Hamiltonian with a U (1) phase space (The 1-D phase space has to two real dimensions (x,p) or one complex dimension  $\alpha=x+ip$ ) to a 2D oscillator with a U(2) phase space. The 2-D oscillator phase space has four real *phase space* dimensions  $(x_1, p_1, x_2, p_2)$  or two complex *phasor* dimensions ( $\alpha_1 = x_1 + ip_1$ ,  $\alpha_2 = x_2 + ip_2$ ).

To help understand the physics and mathematics of this formidable system it helps to appeal to the analogy in Sec. 10.1 between a two-dimensional classical oscillator and a two state quantum system. The U(2) catalog in Fig. 10.4.2 showed three archetypes of 2-state Hamiltonians labeled A, B, and C each corresponding to different values of parameters A, B, C, and D that give different symmetry and physics. The goal here is to solve (and more importantly, <u>understand</u>) the eigensolutions of the <u>quantum</u> version of the A, B, and C type oscillators and how their solutions are derived as symmetry varies.

#### (1) Hamiltonians and operators

The first step is easy. We rewrite a classical 2-D Hamiltonian (10.1.3a) with a thick-tip pen!

$$\mathbf{H} = \frac{A}{2} (\mathbf{p}_1^2 + \mathbf{x}_1^2) + B(\mathbf{x}_1 \mathbf{x}_2 + \mathbf{p}_1 \mathbf{p}_2) + C(\mathbf{x}_1 \mathbf{p}_2 - \mathbf{x}_2 \mathbf{p}_1) + \frac{D}{2} (\mathbf{p}_2^2 + \mathbf{x}_2^2)$$
(21.1.1)

The second step is not so hard either. The symmetric form lets us relate each **x** and **p** to creation and destruction operators as in (20.2.1) and (20.2.16). (Here the pesky  $\sqrt{M}$  and  $\hbar$  factors are absorbed in A, B, C, and D.) Each oscillator dimension has a set of operators. First, the number-1 oscillator is set up.

$$\mathbf{a}_1 = (\mathbf{x}_1 + i \, \mathbf{p}_1)/\sqrt{2}$$
  $\mathbf{a}^{\dagger}_1 = (\mathbf{x}_1 - i \, \mathbf{p}_1)/\sqrt{2}$  (21.1.2a)  
 $\mathbf{x}_1 = (\mathbf{a}^{\dagger}_1 + \mathbf{a}_1)/\sqrt{2}$   $\mathbf{p}_1 = i \, (\mathbf{a}^{\dagger}_1 - \mathbf{a}_1)/\sqrt{2}$  (21.1.2b)

Then, the number-2 oscillator gets the same treatment.

$$\mathbf{a}_2 = (\mathbf{x}_2 + i \, \mathbf{p}_2)/\sqrt{2}$$
  $\mathbf{a}^{\dagger}_2 = (\mathbf{x}_2 - i \, \mathbf{p}_2)/\sqrt{2}$  (21.1.2c)  
 $\mathbf{x}_2 = (\mathbf{a}^{\dagger}_2 + \mathbf{a}_2)/\sqrt{2}$   $\mathbf{p}_2 = i \, (\mathbf{a}^{\dagger}_2 - \mathbf{a}_2)/\sqrt{2}$  (21.1.2d)

#### (2) Commutation relations: Bosons and Fermions

The next step involves a little thinking about what sort of commutation relations these operators should obey. It helps to think about what a 2-D oscillator model would model in the real world. Perhaps, the thing that comes to mind is a particle in a 2-D harmonic potential as was shown in Fig. 10.1.2. As

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explained in Appendix 10.A-B, this is also a model for optical polarization described in  $(x, y) = (x_1, x_2)$  space or a charged particle in a very cold magnetic or optical trap.

However, as shown by Fig. 10.1.1 a-b, a 2D oscillator is also a model for two 1D oscillators that may or may not be coupled to each other. In other words, a 2D oscillator could be a <u>two-particle</u> system with particle-1 and particle-2 each having a separate 1D coordinate  $x_1$ , and  $x_2$ , respectively.

Different dimensions for any system are orthogonal and independent. Either can be transformed without affecting the other. For this reason we will demand *inter-dimensional commutivity*.

$$[\mathbf{x}_{1}, \mathbf{p}_{2}] = \mathbf{0} = [\mathbf{x}_{2}, \mathbf{p}_{1}], [\mathbf{a}_{1}, \mathbf{a}^{\dagger}_{2}] = \mathbf{0} = [\mathbf{a}_{2}, \mathbf{a}^{\dagger}_{1}]$$
 (21.1.3)

All number-1 operators commute with all number-2 operators, but the operator commutation relations within the number-1 space or within the number-2 space remain the same as they were for a 1D-oscillator.

$$[\mathbf{a}_{I}, \mathbf{a}^{\dagger}_{I}] = \mathbf{1}, [\mathbf{a}_{2}, \mathbf{a}^{\dagger}_{2}] = \mathbf{1}$$
 (21.1.4)

The commutation relations are summarized for all N-dimensional oscillator problems as follows.

$$[\mathbf{a}_{m}, \mathbf{a}_{n}] = \mathbf{a}_{m} \mathbf{a}_{n} - \mathbf{a}_{n} \mathbf{a}_{m}, \quad [\mathbf{a}_{m}, \mathbf{a}^{\dagger}_{n}] = \mathbf{a}_{m} \mathbf{a}^{\dagger}_{n} - \mathbf{a}^{\dagger}_{n} \mathbf{a}_{m}, \quad [\mathbf{a}^{\dagger}_{m}, \mathbf{a}^{\dagger}_{n}] = \mathbf{a}^{\dagger}_{m} \mathbf{a}^{\dagger}_{n} - \mathbf{a}^{\dagger}_{n} \mathbf{a}^{\dagger}_{m}, \\ = \mathbf{0}.$$

$$(21.1.5b) \qquad (21.1.5c)$$

These are the **a**-operator equivalent of the orthonormality axiom-2 first given in Chapter 2.

Orthonormality and unit-scale relations (21.1.2) make it easy to find an **a**-operator expression for the 2D Hamiltonian (21.1.1).

$$\mathbf{H} = H_{11} \left( \mathbf{a}_{1}^{\dagger} \mathbf{a}_{1} + \mathbf{1}/2 \right) + H_{12} \mathbf{a}_{1}^{\dagger} \mathbf{a}_{2} = A \left( \mathbf{a}_{1}^{\dagger} \mathbf{a}_{1} + \mathbf{1}/2 \right) + (B - iC) \mathbf{a}_{1}^{\dagger} \mathbf{a}_{2} + H_{21} \mathbf{a}_{2}^{\dagger} \mathbf{a}_{1} + H_{22} \left( \mathbf{a}_{2}^{\dagger} \mathbf{a}_{2} + \mathbf{1}/2 \right) + (B + iC) \mathbf{a}_{2}^{\dagger} \mathbf{a}_{1} + D \left( \mathbf{a}_{2}^{\dagger} \mathbf{a}_{2} + \mathbf{1}/2 \right)$$
(21.1.6)

This expression was written on two lines in order to emphasize that the 2D quantum oscillator operator  $\mathbf{H}$  has the form of the 2-state *ABCD* Hamiltonian  $\mathbf{H}$  matrix (10.1.1b) used in Chapter 10.

$$\mathbf{H} = \begin{pmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{pmatrix} = \begin{pmatrix} A & B - iC \\ B + iC & D \end{pmatrix}$$
 (21.1.6b)

The ket-bras  $|m\rangle\langle n|$  used in the latter are replaced by symmetrized  $\mathbf{a}^{\dagger}_{m}\mathbf{a}_{n}$  operators. Both serve as elementary "place-holder" operators for the Hamiltonian components  $H_{mn}$  or parameters A,  $B\pm iC$ , and D.

$$|m\rangle\langle n| \rightarrow \left(\mathbf{a}_{m}^{\dagger}\mathbf{a}_{n} + \mathbf{a}_{n}\mathbf{a}_{m}^{\dagger}\right)/2 = \mathbf{a}_{m}^{\dagger}\mathbf{a}_{n} + \delta_{m} \mathbf{1}/2$$
 (21.1.7)

The commutativity embodied in (21.1.5) is commonly known as *Bose symmetry* after Bose who first described the permutational symmetry of photons. The ( $\mathbf{a}_m$ ,  $\mathbf{a}^{\dagger}_n$ ) operators are called *Boson operators* and the quanta or "particles" they create and destroy are known as *Bosons*.

Each time  $\mathbf{a}^{\dagger}_{m}$  is used to raise quantum number of mode-m of an electromagnetic resonator (like the "Hall of Mirrors" cavity) it is equivalent to creating a new *photon*. If  $\mathbf{a}^{\dagger}_{m}$  is used to raise the quantum number of mode-m of a molecule we can say we're creating a new *vibron*. Just put the suffix "-on" onto whatever your favorite oscillator motion is called and you have a cute name for your favorite Boson.

There exists an opposite kind of particle, the *Fermion* named after Enrico Fermi who is credited with describing the permutational anti-symmetry of electrons and nucleons. The creation-destruction operators for Fermions are defined in quite the opposite way using <u>anti-commutators</u>  $\{A,B\} = AB+BA$ .

$$\{\mathbf{c}_{m}, \mathbf{c}_{n}\} = \mathbf{c}_{m}\mathbf{c}_{n} + \mathbf{c}_{n}\mathbf{c}_{m}, \quad \{\mathbf{c}_{m}, \mathbf{c}^{\dagger}_{n}\} = \mathbf{c}_{m}\mathbf{c}^{\dagger}_{n} + \mathbf{c}^{\dagger}_{n}\mathbf{c}_{m}, \quad \{\mathbf{c}^{\dagger}_{m}, \mathbf{c}^{\dagger}_{n}\} = \mathbf{c}^{\dagger}_{m}\mathbf{c}^{\dagger}_{n} + \mathbf{c}^{\dagger}_{n}\mathbf{c}^{\dagger}_{m}, \\ = \mathbf{0}.$$

$$(21.1.8a) \qquad (21.1.8b) \qquad (21.1.8c)$$

The general two-dimensional Fermion Hamiltonian has ket-bras  $|m\rangle\langle n|$  replaced by anti-symmetrized  $\mathbf{c}^{\dagger}_{m}\mathbf{c}_{n}$  operators.

$$|m\rangle\langle n| \rightarrow \left(c_m^{\dagger}c_n - c_nc_m^{\dagger}\right)/2 = c_m^{\dagger}c_n - \delta_{m,n}1/2$$
 (21.1.7)

Fermi operators have a rigid birth-control policy; they are allowed only one Fermion or else, none at all. Creating two Fermions of the same type is punished by death. This is because x=-x implies x=0.

$$\mathbf{c}^{\dagger}{}_{m}\mathbf{c}^{\dagger}{}_{m}\left|0\right\rangle = -\mathbf{c}^{\dagger}{}_{m}\mathbf{c}^{\dagger}{}_{m}\left|0\right\rangle = \mathbf{0} \tag{21.1.8}$$

No two indistinguishable Fermions can occupy the same state. This is called the *Pauli exclusion principle*. Quantum numbers of n=0 and n=1 are the only allowed eigenvalues of the number operator.

$$\mathbf{c}^{\dagger}_{m}\mathbf{c}_{m}|0\rangle = \mathbf{0}$$
,  $\mathbf{c}^{\dagger}_{m}\mathbf{c}_{m}|1\rangle = |1\rangle$ ,  $\mathbf{c}^{\dagger}_{m}\mathbf{c}_{m}|n\rangle = \mathbf{0}$  for:  $n > 1$  (21.1.9)

#### (b) Two-dimensional (or 2-particle) base states

A state for a particle moving in two-dimensions (or two one-dimensional particles) is described using "ket-kets"  $|n_1\rangle|n_2\rangle$  which are outer products of the kets for each single dimension. The dual description is done similarly using "bra-bras"  $\langle n_2|\langle n_1|=(|n_1\rangle|n_2\rangle)^{\dagger}$  which are outer products of the bras. This applies to all types of states  $|\Psi_1\rangle|\Psi_2\rangle$  whether they are eigenstates  $|n_1\rangle|n_2\rangle$ , position states  $|x_1\rangle|x_2\rangle$  and  $\langle x_2|\langle x_1|$ , coherent states  $|\alpha_1\rangle|\alpha_2\rangle$  and  $\langle \alpha_2|\langle \alpha_1|$ , or whatever.

The scalar product is defined so that the two kinds of particles or dimensions will somehow "find" each other and completely ignore the presence of the other kind(s).

$$\langle x_2 | \langle x_1 | \Psi_1 \rangle | \Psi_2 \rangle = \langle x_1 | \Psi_1 \rangle \langle x_2 | \Psi_2 \rangle$$
 (21.1.10a)

This allows the probability axiom-1 to give the correct probability for, say, finding particle-1 at  $x_1$  and particle-2 at  $x_2$ , if state  $|\Psi_1\rangle|\Psi_2\rangle$  is forced to choose between all  $x_1$  and  $x_2$ . Such a probability is a product

$$|\langle x_1, x_2 | \Psi_1, \Psi_2 \rangle|^2 = |\langle x_2 | \langle x_1 | \Psi_1 \rangle | \Psi_2 \rangle|^2 = |\langle x_1 | \Psi_1 \rangle|^2 |\langle x_2 | \Psi_2 \rangle|^2$$
 (21.1.10b)

of the individual probabilities  $|\langle x_I | \Psi_I \rangle|^2$  and  $\langle x_2 | \Psi_2 \rangle|^2$  according to standard probability theory. The shorthand big-bra-big-ket notation  $\langle x_I, x_2 | \Psi_I, \Psi_2 \rangle$  for two-dimensional amplitudes  $\langle x_2 | \langle x_I | \Psi_I \rangle | \Psi_2 \rangle$  is commonly used. Note the 1-2 ordering for both the big-bras and big-kets in the shorthand notation.

To gain a better understanding of the bra-bra and ket-ket structure we will ask the perennial modern question: "How would these structures be stored in a computer program?" The usual answer is in product arrays of some kind. Here we will sketch these objects.

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We begin with an elementary ket basis for each dimension or particle type-1 and type-2.

$$|0_{1}\rangle = \begin{pmatrix} 1\\0\\0\\\vdots \end{pmatrix}, |1_{1}\rangle = \begin{pmatrix} 0\\1\\0\\\vdots \end{pmatrix}, |2_{1}\rangle = \begin{pmatrix} 0\\0\\1\\\vdots \end{pmatrix}, \dots \qquad |0_{2}\rangle = \begin{pmatrix} 1\\0\\0\\\vdots \end{pmatrix}, |1_{2}\rangle = \begin{pmatrix} 0\\1\\0\\\vdots \end{pmatrix}, |2_{2}\rangle = \begin{pmatrix} 0\\0\\1\\\vdots \end{pmatrix}, \dots (21.1.11a)$$

Then Cartesian or outer products are constructed for all states that might have non-zero amplitudes. And, therein lies a conflict between standard analysis and a finite computer. Each ket in (21.1.11) above is a column of  $\infty$ -dimensional and we are about to construct an  $\infty^2$  number of things each of dimension  $\infty^2$ . A computer cannot handle a single  $\infty$ -dimensional ket let alone their outer products.

This is why the finite analysis of Sec. 7.3 is advocated. Constructing sets of adjustable finite sized model systems for each dimension systematizes state counting. Convergence is achieved by orderly upgrades in the number of model "pendulums." Outer products shown below are finite arrays indexed by oscillator quantum labels 0, 1, 2,...(0-based indexing is the default mode in languages such as  $C^{++}$ .)

A 2-wave state product has a lexicographic (00, 01, 02, ...10, 11, 12,..., 20, 21, 22, ...) array indexing.

$$|\Psi_{1}\rangle|\Psi_{2}\rangle = \begin{pmatrix} \langle 0|\Psi_{1}\rangle\\ \langle 1|\Psi_{1}\rangle\\ \langle 2|\Psi_{1}\rangle\\ \vdots \end{pmatrix} \otimes \begin{pmatrix} \langle 0|\Psi_{2}\rangle\\ \langle 1|\Psi_{2}\rangle\\ \langle 2|\Psi_{1}\rangle\\ \vdots \end{pmatrix} = \begin{pmatrix} \langle 0|\Psi_{1}\rangle\langle 0|\Psi_{2}\rangle\\ \langle 0|\Psi_{1}\rangle\langle 1|\Psi_{2}\rangle\\ \langle 1|\Psi_{1}\rangle\langle 0|\Psi_{2}\rangle\\ \langle 1|\Psi_{1}\rangle\langle 1|\Psi_{2}\rangle\\ \langle 2|\Psi_{1}\rangle\langle 0|\Psi_{2}\rangle\\ \langle 1|\Psi_{1}\rangle\langle 0|\Psi_{2}\rangle\\ \langle 1|\Psi_{1}\rangle\langle 1|\Psi_{2}\rangle\\ \langle 2|\Psi_{1}\rangle\langle 1|\Psi_{2}\rangle\\ \vdots \end{pmatrix} = \begin{pmatrix} \langle 0_{1}0_{2}|\Psi_{1}\Psi_{2}\rangle\\ \langle 0_{1}2_{2}|\Psi_{1}\Psi_{2}\rangle\\ \langle 1_{1}0_{2}|\Psi_{1}\Psi_{2}\rangle\\ \langle 1_{1}1_{2}|\Psi_{1}\Psi_{2}\rangle\\ \langle 1_{1}2_{2}|\Psi_{1}\Psi_{2}\rangle\\ \vdots\\ \hline \langle 2_{1}0_{2}|\Psi_{1}\Psi_{2}\rangle\\ \langle 2_{1}1_{2}|\Psi_{1}\Psi_{2}\rangle\\ \langle 2_{1}1_{2}|\Psi_{1}\Psi_{2}\rangle\\ \langle 2_{1}2_{2}|\Psi_{1}\Psi_{2}\rangle\\ \vdots \end{pmatrix}$$

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The same indexing is used for the general 2-particle or 2-dimensional state  $|\Psi\rangle$ .

$$|\Psi\rangle = \begin{pmatrix} \langle 0_{1}0_{2} | \Psi \rangle \\ \langle 0_{1}1_{2} | \Psi \rangle \\ \langle 0_{1}2_{2} | \Psi \rangle \\ \vdots \\ \hline{\langle 1_{1}0_{2} | \Psi \rangle} \\ \langle 1_{1}1_{2} | \Psi \rangle \\ \vdots \\ \hline{\langle 2_{1}0_{2} | \Psi \rangle} \\ \langle 2_{1}1_{2} | \Psi \rangle \\ \langle 2_{1}1_{2} | \Psi \rangle \\ \vdots \\ \hline{\langle 2_{1}0_{2} | \Psi \rangle} \\ \vdots \\ \hline{\Psi_{10}} \\ \Psi_{11} \\ \Psi_{12} \\ \vdots \\ \hline{\Psi_{20}} \\ \Psi_{21} \\ \Psi_{22} \\ \vdots \end{pmatrix}$$

$$(21.1.12c)$$

A word of caution: Do *NOT* assume that a general two-particle state  $|\Psi\rangle$  can be written as a single outer product  $|\Psi_I\rangle|\Psi_2\rangle$  (or even rarer, as  $|\Psi_I\rangle|\Psi_I\rangle$ ) of two single-particle states  $|\Psi_I\rangle$  and  $|\Psi_2\rangle$ . This would be as unusual as having a general matrix operator  $\mathbf{M}$  be a single nilpotent operator  $|1\rangle\langle 2|$  or idempotent  $|1\rangle\langle 1|$ , both of which are singular, that is, have zero determinant. Rather, a general matrix  $\mathbf{M}$  is a full combination

$$\mathbf{M} = \sum_{m} \sum_{n} M_{m,n} |m\rangle\langle n|$$

of <u>all</u> possible ket-bra elementary operator products  $|m\rangle\langle n|$ . So, also, is a general state like (21.1.11) a combination of <u>all</u> possible ket-ket products  $|x_I\rangle\langle x_2\rangle$  made from whichever basis is currently being used.

$$\left|\Psi\right\rangle = \sum_{m} \sum_{n} \left|\Psi_{m,n}\right| m \rangle \left|n\right\rangle \tag{21.1.12d}$$

#### (c) Two-dimensional (or 2-particle) matrix operators

When a two-dimensional operator acts on a two-dimensional state, each dimension or particle type-1 or type-2 operator "finds" its corresponding type in the state and goes to work on it while ignoring the other type(s). For creation and destruction operations defined in (20.2.13b) the following happens.

$$\mathbf{a}_{1}^{\dagger} | n_{1} n_{2} \rangle = \mathbf{a}_{1}^{\dagger} | n_{1} \rangle | n_{2} \rangle = \sqrt{n_{1} + 1} | n_{1} + 1 n_{2} \rangle , \qquad \mathbf{a}_{2}^{\dagger} | n_{1} n_{2} \rangle = | n_{1} \rangle \mathbf{a}_{2}^{\dagger} | n_{2} \rangle = \sqrt{n_{2} + 1} | n_{1} n_{2} + 1 \rangle$$

$$\mathbf{a}_{1} | n_{1} n_{2} \rangle = \mathbf{a}_{1} | n_{1} \rangle | n_{2} \rangle = \sqrt{n_{1}} | n_{1} - 1 n_{2} \rangle , \qquad \mathbf{a}_{2} | n_{1} n_{2} \rangle = | n_{1} \rangle \mathbf{a}_{2} | n_{2} \rangle = \sqrt{n_{2}} | n_{1} n_{2} - 1 \rangle$$

$$(21.1.13a) \qquad (21.1.13b)$$

This is consistent with the following general definition of the 2D oscillator base state.

$$|n_1 n_2\rangle = \frac{\left(\mathbf{a}_1^{\dagger}\right)^{n_1} \left(\mathbf{a}_2^{\dagger}\right)^{n_2}}{\sqrt{n_1! n_2!}} |0 0\rangle \tag{21.1.14}$$

The  $\mathbf{a}_m^{\dagger}\mathbf{a}_n$  combinations in the <u>ABCD</u> Hamiltonian **H** in (21.1.6) have fairly simple matrix elements.

$$\mathbf{a}_{1}^{\dagger}\mathbf{a}_{1} | n_{1}n_{2} \rangle = n_{1} | n_{1} n_{2} \rangle , \qquad \mathbf{a}_{1}^{\dagger}\mathbf{a}_{2} | n_{1}n_{2} \rangle = \sqrt{n_{1} + 1} \sqrt{n_{2}} | n_{1} + 1 n_{2} - 1 \rangle$$

$$\mathbf{a}_{2}^{\dagger}\mathbf{a}_{1} | n_{1}n_{2} \rangle = \sqrt{n_{1}} \sqrt{n_{2} + 1} | n_{1} - 1 n_{2} + 1 \rangle , \qquad \mathbf{a}_{2}^{\dagger}\mathbf{a}_{2} | n_{1}n_{2} \rangle = n_{2} | n_{1} n_{2} \rangle$$

$$(21.1.15a)$$

Part of the matrix representation of **H** in creation basis (21.1.14) is shown below.

$\langle \mathbf{H} \rangle =$	: <b>A</b> ( <b>1</b> /2	2) + <b>D</b> ( <b>1</b> /	2)+									
	$ 00\rangle$	$ 01\rangle$	$ 02\rangle$		$ 10\rangle$	$ 11\rangle$	$ 12\rangle$		$ 20\rangle$	$ 21\rangle$	$ 22\rangle$	
(00)	0			•••				•••				•••
$\langle 01  $		D		•••	B+iC	•		•••				•••
(02			2 <i>D</i>			$\sqrt{2}\left(\underline{B}+iC\right)$						•••
<u>:</u>	:	÷	:	٠.	:	:	:	٠.				•••
$\langle 10  $		B-iC			A							•••
(11		•	$\sqrt{2}\left(\underline{B}-iC\right)$			A + D			$\sqrt{2}\left(\mathbf{B}+iC\right)$			•••
(12							A + 2D			$\sqrt{4}\left(\underline{B}+iC\right)$		•••
<u>:</u>	÷	<u>:</u>	<u>:</u>	٠.	÷	:	:	٠.	:	:	:	·
$\langle 20  $					•	$\sqrt{2}(B-iC)$		•••	2 <i>A</i>			•••
(21							$\sqrt{4}\left(B-iC\right)$			2A + D		•••
(22											2A + 2D	
÷					÷	:	:	٠.	:	:	:	٠.
										(	(21.1.15b	))

The eigenstates and eigenvalues for this monster matrix will solve the general quantum 2D harmonic oscillator problem. A little rearrangement of rows and columns brings the matrix to a block-diagonal form in which base states  $|n_1\rangle|n_2\rangle$  with the same *total quantum number*  $v = n_1 + n_2$  are adjacent.

	$ 00\rangle$	01⟩	$ 10\rangle$	$ 02\rangle$	$ 11\rangle$	$ 20\rangle$	$ 03\rangle$	$ 12\rangle$	$ 21\rangle$	$ 30\rangle$	
$\langle 00  $	0										
(01		D	B+iC								
$\langle 10  $		B-iC	$\boldsymbol{A}$								
(02				2 <b>D</b>	$\sqrt{2}(B+iC)$						
(11				$\sqrt{2}(B-iC)$	A + D	$\sqrt{2}\left(B+iC\right)$					
(20					$\sqrt{2}(B-iC)$	2 <i>A</i>					
(03							3 <i>D</i>	$\sqrt{3}(B+iC)$			
(12							$\sqrt{3}(B-iC)$	A + 2D	$\sqrt{4}\left(\underline{B}+iC\right)$		
(21								$\sqrt{4}\left(\underline{B}-iC\right)$	2A + D	$\sqrt{3}(B+iC)$	
(30									$\sqrt{3}(B-iC)$	3 <i>A</i>	
:											T

(21.1.15c)

Note the 2-by-2 sub-space  $|n_1 n_2\rangle = \{|01\rangle, |10\rangle\}$  with total quantum number v=I. It supports a matrix that is identical to the original 2-by-2 Hamiltonian (21.1.6b). (Except, it is up side down and has the zero-point unit matrix added.) A sub-space with unit total quantum number is called the *fundamental* (v=I) vibrational sub-space. Similarity of classical and (v=I) quantum matrices means the fundamental quantum eigenvectors are the same as the classical A, B, AB or C normal mode vectors discussed in Sec. 10.2(a, b, c) and Sec. 10.3(a-b). This leads to analytical solutions to all quantum matrices (21.1.15c).

#### (d) 2D-Oscillator eigensolutions

The analogy between classical 2D-oscillators and a 2-state quantum systems was developed in Sec. 10.5 and solved by special unitary (SU(2)) or rotation (R(3)) group algebra in Appendices 10.A-B. These solutions lead to solutions for the quantum 2D-oscillator Hamiltonian given above in (21.1.15c-d).

#### (1) Fundamental eigenstates

The first step is to diagonalize the fundamental 2-by-2 matrix given in (21.1.15c-d).

$$\langle \mathbf{H} \rangle_{v=1}^{Fundamental} = \begin{vmatrix} n_1, n_2 & |1,0\rangle & |0,1\rangle \\ \langle 1,0| & A & B-iC \\ \langle 0,1| & B+iC & D \end{vmatrix} + \frac{A+D}{2} \mathbf{1}$$
 (21.1.16)

Here we have turned the matrix right-side-up so it matches the Hamiltonian solved in (10.5.10). (A choice of "Little-Endian" indexing (... 10, 01, ...20,11,21...) instead of "Big-Endian" indexing (...01,10, ...02,1...) reorders the states to match.) The eigensolution (10.5.10) uses the Hamilton decomposition coefficients to define a rotation-crank angular rate vector  $\Omega$ 

$$\Omega = (\Omega_X, \Omega_Y, \Omega_Z) = (2B, 2C, A-D) = (\Omega_B, \Omega_C, \Omega_A), \qquad (21.1.17)$$

and the average overall phase rate (including zero-point term (A+D)/2) is

$$\Omega_0 = A + D. \tag{21.1.18}$$

This gives **H** as follows

$$\begin{pmatrix} A & B - iC \\ B + iC & D \end{pmatrix} + \frac{A + D}{2} \mathbf{1} = \begin{pmatrix} A + D \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + 2B \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \frac{1}{2} + 2C \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \frac{1}{2} + \begin{pmatrix} A - D \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \frac{1}{2}$$

in terms of Jordan-Pauli spin operators.

$$\mathbf{H} = \Omega_0 \mathbf{1} + \mathbf{\Omega} \bullet \mathbf{S} = \Omega_0 \mathbf{1} + \Omega_B \mathbf{S}_B + \Omega_C \mathbf{S}_C + \Omega_A \mathbf{S}_A \quad (ABC \ Optical \ vector \ notation)$$

$$= \Omega_0 \mathbf{1} + \Omega_X \mathbf{S}_X + \Omega_Y \mathbf{S}_Y + \Omega_Z \mathbf{S}_Z \quad (XYZ \ Electron \ spin \ notation)$$

The frequency eigenvalues  $\omega_{\pm}$  of **H-** $\Omega_0$ **1/2** and *fundamental transition frequency*  $\Omega = \omega_+$  -  $\omega_-$  are

$$\omega_{\pm} = \frac{\Omega_0 \pm \Omega}{2} = \frac{A + D \pm \sqrt{(2B)^2 + (2C)^2 + (A - D)^2}}{2}$$

$$= \frac{A + D}{2} \pm \sqrt{\left(\frac{A - D}{2}\right)^2 + B^2 + C^2}$$
(21.1.20a)

 $\Omega$  "points out" eigenvectors whose spin vectors **S** align or anti-align with the  $\Omega$ -vector of **H**. The polar angles of the **S**-vector are Euler angles  $(\alpha,\beta)$  in Fig. 10.5.8. Equating  $(\alpha,\beta)$  in an Euler state (10.A.1a) to polar angles  $(\phi,\vartheta)$  of the  $+\Omega$ -vector (or polar angles  $(\phi,\vartheta\pm\pi)$  of the  $-\Omega$ -vector) gives **H** eigenvectors.

$$\left|\omega_{+}\right\rangle = \begin{pmatrix} e^{-i\varphi/2}\cos\frac{\vartheta}{2} \\ e^{i\varphi/2}\sin\frac{\vartheta}{2} \end{pmatrix}, \quad \left|\omega_{-}\right\rangle = \begin{pmatrix} -e^{-i\varphi/2}\sin\frac{\vartheta}{2} \\ e^{i\varphi/2}\cos\frac{\vartheta}{2} \end{pmatrix} \quad \text{where:} \begin{cases} \cos\vartheta = \frac{A-D}{\Omega} \\ \tan\varphi = \frac{C}{B} \end{cases}$$
 (21.1.20b)

The ket eigenvectors are being expressed in terms of  $\{|10\rangle, |01\rangle\}$  bases.

$$\left|\omega_{+}\right\rangle = e^{-i\varphi/2} \left(\cos\frac{\vartheta}{2}\left|10\right\rangle + e^{i\varphi}\sin\frac{\vartheta}{2}\left|01\right\rangle\right), \quad \left|\omega_{-}\right\rangle = e^{-i\varphi/2} \left(-\sin\frac{\vartheta}{2}\left|10\right\rangle + e^{i\varphi}\cos\frac{\vartheta}{2}\left|01\right\rangle\right) \quad (21.1.20c)$$

More important for the general solution, are the eigen-creation operators  $\mathbf{a}^{\dagger}_{+}$  and  $\mathbf{a}^{\dagger}_{-}$  defined by

$$\mathbf{a}_{+}^{\dagger} = e^{-i\varphi/2} \left( \cos \frac{\vartheta}{2} \mathbf{a}_{1}^{\dagger} + e^{i\varphi} \sin \frac{\vartheta}{2} \mathbf{a}_{2}^{\dagger} \right), \quad \mathbf{a}_{-}^{\dagger} = e^{-i\varphi/2} \left( -\sin \frac{\vartheta}{2} \mathbf{a}_{1}^{\dagger} + e^{i\varphi} \cos \frac{\vartheta}{2} \mathbf{a}_{2}^{\dagger} \right) \quad (21.1.20d)$$

The  $\mathbf{a}_{+}^{\dagger}$  create **H** eigenstates (21.1.20c) directly from the ground state.

$$\mathbf{a}_{+}^{\dagger}|0\rangle = |\omega_{+}\rangle$$
,  $\mathbf{a}_{-}^{\dagger}|0\rangle = |\omega_{-}\rangle$  (21.1.20e)

In terms of the eigen- $\mathbf{a}_{\pm}^{\dagger}$  operators, the Hamiltonian has zero off-diagonal components (B=0=C) and is reduced to (at worst) an A-type (Asymmetric Diagonal) or  $C_2^A$ -symmetric operator described in Sec. 10.2(a). But, if the eigenvalues are degenerate ( $\omega_+ = \omega_-$ ) then  $\mathbf{H}$  is a fully SU(2) symmetric unit 2-by-2 Hamiltonian like the case where (B=0=C) and (A=D).

Setting (B=0=C) and ( $A=\omega_+$ ) and ( $D=\omega_-$ ) in (21.1.15c) gives diagonal block matrices.  $\langle \mathbf{H} \rangle = \mathbf{A}(\mathbf{1}/2) + \mathbf{D}(\mathbf{1}/2) +$ 

$$\begin{array}{|c|c|c|c|c|c|c|}\hline & |00\rangle & |01\rangle & |10\rangle & |02\rangle & |11\rangle & |20\rangle & |03\rangle & |12\rangle & |21\rangle & |30\rangle & \cdots \\ \hline \hline & |00| & 0 & & & & & & & \\ \hline & |01| & |\omega_{-}| & & & & & & \\ \hline & |01| & |\omega_{+}| & & & & & & \\ \hline & |02| & |\omega_{+}| & & & & & \\ \hline & |03| & |\omega_{+}| & & & & & \\ \hline & |01| & |\omega_{-}| & & & & & \\ \hline & |01| & |\omega_{-}| & & & & & \\ \hline & |01| & |\omega_{-}| & & & & & \\ \hline & |02| & |\omega_{+}| & & & & & \\ \hline & |03| & |\omega_{+}| & & & & \\ \hline & |03| & |\omega_{+}| & & & & \\ \hline & |03| & |\omega_{-}| & & & & \\ \hline & |03| & |\omega_{-}| & & & & \\ \hline & |03| & |\omega_{-}| & & & & \\ \hline & |03| & |\omega_{-}| & & & & \\ \hline & |03| & |\omega_{-}| & & & & \\ \hline & |03| & |\omega_{-}| & & & & \\ \hline & |03| & |\omega_{-}| & & & & \\ \hline & |03| & |\omega_{-}| & & & & \\ \hline & |03| & |\omega_{-}| & & & & \\ \hline & |03| & |\omega_{-}| & & & \\ \hline & |03| & |\omega_{-}| & & & \\ \hline & |03| & |\omega_{-}| & & & \\ \hline & |03| & |\omega_{-}| & & & \\ \hline & |03| & |\omega_{-}| & & & \\ \hline & |03| & |\omega_{-}| & & & \\ \hline & |03| & |\omega_{-}| & & & \\ \hline & |03| & |\omega_{-}| & & & \\ \hline & |03| & |\omega_{-}| & & & \\ \hline & |03| & |\omega_{-}| & & & \\ \hline & |03| & |\omega_{-}| & & & \\ \hline & |03| & |\omega_{-}| & & & \\ \hline & |03| & |\omega_{-}| & & & \\ \hline & |03| & |\omega_{-}| & & & \\ \hline & |03| & |\omega_{-}| & & & \\ \hline & |03| & |\omega_{-}| & & & \\ \hline & |03| & |\omega_{-}| & & & \\ \hline & |03| & |\omega_{-}| & & & \\ \hline & |03| & |\omega_{-}| & & & \\ \hline & |03| & |\omega_{-}| & & & \\ \hline & |03| & |\omega_{-}| & & & \\ \hline & |03| & |\omega_{-}| & & & \\ \hline & |03| & |\omega_{-}| & & & \\ \hline & |03| & |\omega_{-}| & & & \\ \hline & |03| & |\omega_{-}| & & & \\ \hline & |03| & |\omega_{-}| & & & \\ \hline & |03| & |\omega_{-}| & & & \\ \hline & |03| & |\omega_{-}| & & & \\ \hline & |03| & |\omega_{-}| & & & \\ \hline & |03| & |\omega_{-}| & & & \\ \hline & |03| & |\omega_{-}| & & & \\ \hline & |03| & |\omega_{-}| & & & \\ \hline & |03| & |\omega_{-}| & & & \\ \hline & |03| & |\omega_{-}| & & & \\ \hline & |03| & |\omega_{-}| & & & \\ \hline & |03| & |\omega_{-}| & & & \\ \hline & |03| & |\omega_{-}| & & & \\ \hline & |03| & |\omega_{-}| & & & \\ \hline & |03| & |\omega_{-}| & & & \\ \hline & |03| & |\omega_{-}| & & & \\ \hline & |03| & |\omega_{-}| & & & \\ \hline & |03| & |\omega_{-}| & & & \\ \hline & |03| & |\omega_{-}| & & & \\ \hline & |03| & |\omega_{-}| & & & \\ \hline & |03| & |\omega_{-}| & & & \\ \hline & |03| & |\omega_{-}| & & & \\ \hline & |03| & |\omega_{-}| & & & \\ \hline & |03| & |\omega_{-}| & & & \\ \hline & |03| & |\omega_{-}| & & & \\ \hline & |03| & |\omega_{-}| & &$$

The eigenvalue splitting pattern shown in Fig. 21.1.1 is a function of the fundamental splitting frequency.

$$\omega_{+} - \omega_{-} = \Omega = \sqrt{(2B)^{2} + (2C)^{2} + (A - D)^{2}} = A - D$$
 (21.1.22)

For SU(2) symmetry ( $\Omega=0$ ) the spectrum reduces to perfect harmonically spaced levels of eigenfrequency  $\omega=\upsilon+1$  and degeneracy  $\upsilon+I=1,2,3,4,...$  for each total quantum number  $\upsilon=0,1,2,3,...$ , respectively. As will be shown later, this is precisely analogous to the spin angular momentum quantum *multiplet* levels of total angular momentum quantum numbers j=0,1/2,1,3/2,... In fact, each degenerate level corresponds to a different irep of SU(2) and the integral j=0,1,2,... correspond to ireps of the related rotation group R(3) in three dimensions. What we have here is a very powerful way to understand and derive the quantum theory of angular momentum.

As the splitting frequency increases each multiplet splits entirely since the symmetry is reduced to a commutative  $C_2^{A,B,orC}$  subgroup of SU(2) that does not require degeneracy. Every level differs from the nearest neighbor in its multiplet by the same transition frequency  $\Omega$ . So no matter what the value of the

parameters  $\{A, B, C, D\}$ , this model maintains its harmonic spectrum to some extent. However, at rational values of the ratio  $\Omega/\omega$ , there will occur a varying number of degeneracies between levels split off from different multiplets and some interesting effects in the classical and quantum dynamics.

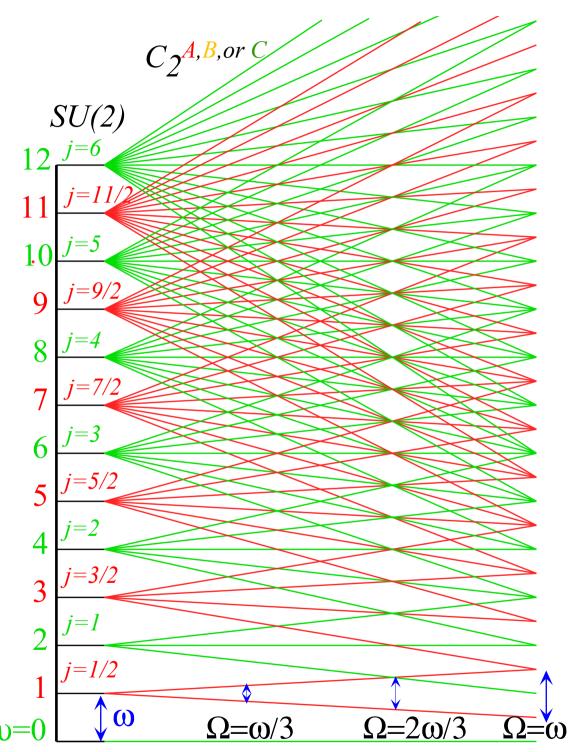


Fig. 21.1.1 Two-Dimensional harmonic oscillator levels with SU(2) degeneracy and C<sub>2</sub> splitting.

#### (2) $U(2) \supset C_2^{\mathbf{A}}$ eigenstates and wavefunctions

The simplest examples of 2D oscillator eigensolutions are found for the type-A or *Asymmetric Diagonal* Hamiltonian **H** in (21.1.1) for which only the parameters A and D are non-zero. (B=0=C)

$$\mathbf{H}^{\mathbf{A}} = \frac{\mathbf{A}}{2} (\mathbf{p}_1^2 + \mathbf{x}_1^2) + \frac{\mathbf{D}}{2} (\mathbf{p}_2^2 + \mathbf{x}_2^2)$$
 (21.1.23)

In terms of **a**-operators, **H** in (21.1.6) reduces to sums of number operators  $\mathbf{a}^{\dagger}_{m}$   $\mathbf{a}_{m}$  or unit operator **1**.

$$\mathbf{H}^{A} = A \left( \mathbf{a}_{1}^{\dagger} \mathbf{a}_{1} + 1/2 \right) + D \left( \mathbf{a}_{2}^{\dagger} \mathbf{a}_{2} + 1/2 \right)$$
 (21.1.24)

Then the **H** matrix (21.1.15) is diagonal, and the eigenvalues are simple combinations of quanta  $n_1$  and  $n_2$ .

$$\varepsilon_{n_{1}n_{2}}^{A} = A \left( n_{1} + \frac{1}{2} \right) + D \left( n_{2} + \frac{1}{2} \right) = \frac{A+D}{2} (n_{1} + n_{2} + 1) + \frac{A-D}{2} (n_{1} - n_{2})$$

$$= \Omega_{0} (n_{1} + n_{2} + 1) + \frac{\Omega}{2} (n_{1} - n_{2}) = \Omega_{0} (\upsilon + 1) + \Omega m$$
(21.1.25a)

Here total quantum number v and half-difference or asymmetry quantum number m

$$v = n_1 + n_2$$
 ,  $m = \frac{n_1 - n_2}{2}$  (21.1.25b)

multiply the fundamental frequency  $\Omega_0 = \omega$  and splitting 1/2-beat frequency  $\Omega$  as seen in Fig. 21.1.2.

$$\omega = \Omega_0 = \frac{A+D}{2}$$
 ,  $\Omega = \frac{A-D}{2}$  (21.1.25c)

The eigenstates for the asymmetric-diagonal  $\mathbf{H}^A$  Hamiltonian are just the base states from (21.1.14).

$$|n_1 n_2\rangle = \frac{\left(\mathbf{a}_1^{\dagger}\right)^{n_1} \left(\mathbf{a}_2^{\dagger}\right)^{n_2}}{\sqrt{n_1! n_2!}} |0 0\rangle$$
 (21.1.26)

The eigenstates belong to the symmetry  $C_2^A$  first discussed in Sec. 10.2(a) and listed near the left hand side of Fig. 10.4.2. The two  $x_1$  and  $x_2$  fundamental normal mode classical vibrations associated with this symmetry are shown in Fig. 10.2.1. If these two motions have the same frequency (A=D) then the symmetry is much higher, indeed. The (A=D)-case has the full U(2) symmetry that a 2D oscillator can have as indicated on the extreme left hand side of Fig. 10.4.2. The U(2)-symmetric Hamiltonian

$$\mathbf{H}^{U(2)} = \mathbf{E} \left( \mathbf{a}_1^{\dagger} \mathbf{a}_1 + \mathbf{a}_2^{\dagger} \mathbf{a}_2 + \mathbf{1} \right) \quad where: \quad \mathbf{A} = \mathbf{E} = \mathbf{D}$$
 (21.1.27a)

has the same eigenvalues as a 1D harmonic oscillator with the zero-point increased from 1/2 to 1.

$$\varepsilon_{n,n_2}^{U(2)} = \Omega_0 \left( n_1 + n_2 + 1 \right) = \omega(\upsilon + 1) \quad (u = 0, 1, 2, 3...)$$
 (21.1.27b)

However, the degeneracy of the  $\upsilon$ -th level is equal to the total quantum number  $\upsilon$  as was shown in Fig. 21.1.2 on the extreme left hand side where the splitting frequency  $\Omega$  is zero.

The redux of the 1D spectrum in a  $C_2^A$ -symmetric two-dimensional system is not surprising if you consider the two-pendulum analogy in Fig. 10.1.1 with equal pendulums or in Fig. 10.2.3 with the coupling spring removed. The result is two independent pendulums. The only effect of having two of them is that the energy level degeneracy and zero-point goes up, but they're just 1D levels.

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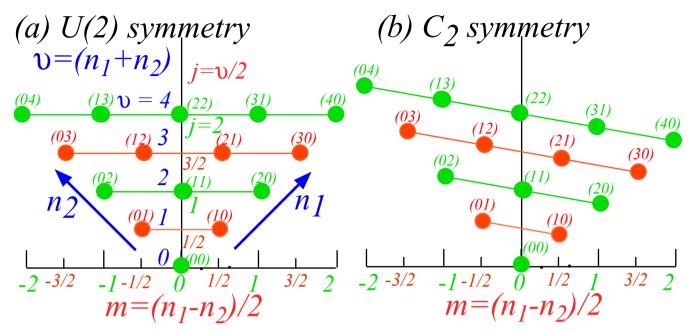


Fig. 21.1.2 Two-Dimensional harmonic oscillator quanta with (a)U(2) degeneracy and (b)  $C_2$  splitting.

A sketch of the energy-quantum-number relation (21.1.27) is shown in Fig. 21.1.2. With U(2) symmetry ( $\Omega$ =0), the degenerate energy values lie along a horizontal line. The states  $|(n_I,n_2)\rangle$  with larger  $n_I$  appear proportionally farther to the right while those with larger  $n_2$  sit to the left. As  $\Omega$  becomes non-zero the lines tip in proportion to  $\Omega$  and the reduction of U(2) to a  $C_2$  symmetry shows up in the splitting of the degenerate levels. The splitting seen in Fig. 21.1.1 is a vertical projection of the tipped points in Fig. 21.1.2 with the  $n_I$  vibrations assumed to be slower (A<D) so they lose frequency in proportion to  $n_I$  while the faster  $n_2$  states gain in proportion to their quantum  $n_2$  -values.

#### (3) $U(2) \supset C_2^A$ oscillator wavefunctions

A two-dimensional oscillator eigenfunction is a simple product of two one-dimensional functions.

$$\langle x_1 x_2 | n_1 n_2 \rangle = \langle x_1 | n_1 \rangle \langle x_2 | n_2 \rangle$$

For example, the ground state eigenfunction  $\langle x_1 x_2 | \theta \theta \rangle$  follows from (20.2.7c) with scale  $M\omega/\hbar = 1$ .

$$\psi_{00}(x_1, x_2) = \langle x_1 | 0 \rangle \langle x_2 | 0 \rangle = \frac{e^{-x_1^2/2}}{(\pi)^{1/4}} \frac{e^{-x_2^2/2}}{(\pi)^{1/4}} = \frac{e^{-(x_1^2 + x_2^2)/2}}{(\pi)^{1/2}}$$
(21.1.28)

This ( $\nu$ =0) Gaussian is plotted in Fig. 21.1.3, and the ( $\nu$ =1) excited state wave doublet in Fig. 21.1.3.

$$\psi_{10}(x_1, x_2) = \frac{\sqrt{2}x_1 e^{-(x_1^2 + x_2^2)/2}}{(\pi)^{1/2}}, \quad \psi_{01}(x_1, x_2) = \frac{\sqrt{2}x_2 e^{-(x_1^2 + x_2^2)/2}}{(\pi)^{1/2}}$$
(21.1.29)

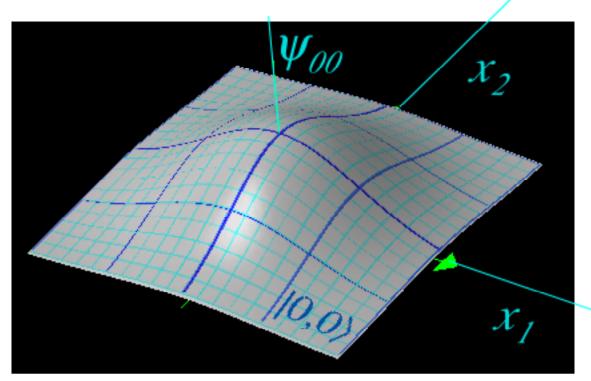


Fig. 21.1.3 2-D harmonic oscillator ground state wave function  $\Psi_{00}(x_1,x_2)$ 

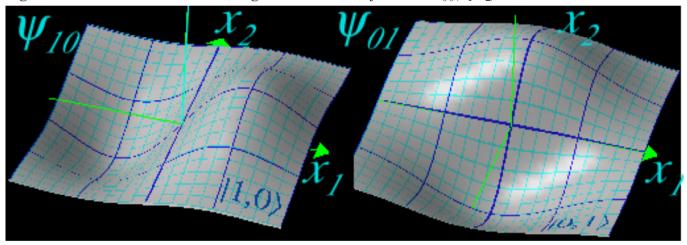
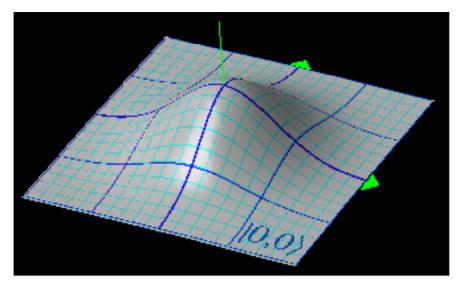


Fig. 21.1.4 2-D harmonic oscillator first excited state wave functions:  $\Psi_{10}(x_1,x_2)$  and  $\Psi_{01}(x_1,x_2)$ .

The two components of the doublet are related by a 90° rotation in the  $(x_1,x_2)$ -plane. Here, we are looking at the real part of waves that each have their usual complex time factor  $e^{-i\varepsilon_n t/\hbar}$  which in this case is a different frequency  $\omega_{n_1 n_2} = e_{n_1 n_2}/\hbar$  given by (21.1.25a) for each, in general. So these pictures represent snapshots of standing waves that oscillate up and down just like their 1D ancestors in Fig. 20.2.1.

However, their probability distributions shown below in Fig. 21.1.5 are motionless as must be any distribution for a pure-energy eigenstate. The squared wavefunctions are greater than zero everywhere and falls off more rapidly for large x.

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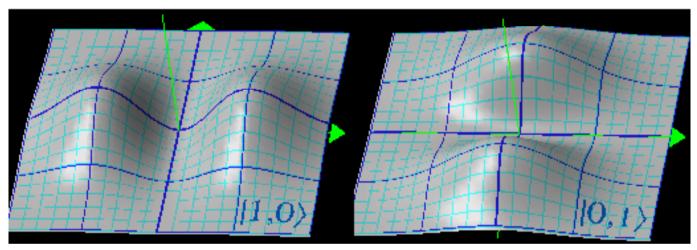


Fig. 21.1.5 2-D oscillator probability distributions:  $|\Psi_{00}(x_1,x_2)|^2$ ,  $|\Psi_{10}(x_1,x_2)|^2$ , and  $|\Psi_{01}(x_1,x_2)|^2$ . Combination wave functions, on the other hand, have moving probability distributions if their component states have different eigenfrequencies. Consider for example, the 50-50 combination of the first two excited states  $|I 0\rangle$  and  $|0 1\rangle$  whose probability distributions are shown for three different times in Fig. 21.1.6. The result is the quantum version of the classical beats shown in Fig. 10.2.2 for uncoupled oscillators and in Fig. 10.2.5 and Fig. 10.2.6 for coupled bilaterally symmetric oscillators.

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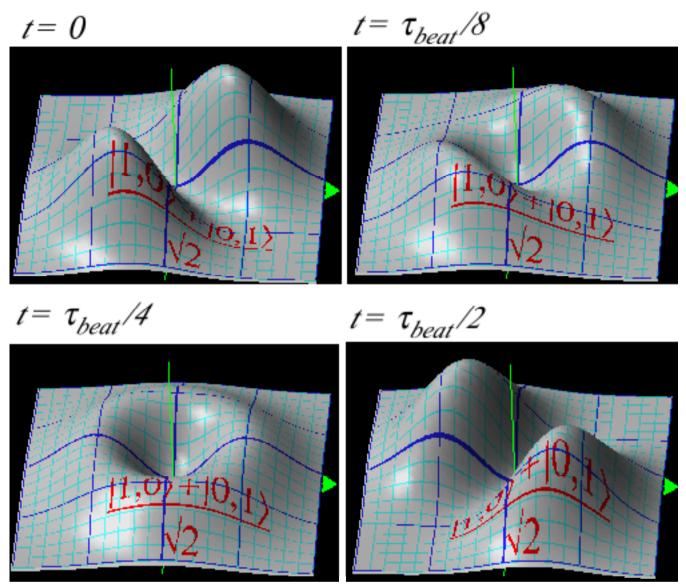


Fig. 21.1.6 2-D oscillator probability distributions:  $|e^{-i\omega_{10}t/\hbar}\Psi_{10}(x_1,x_2) + e^{-i\omega_{01}t/\hbar}\Psi_{01}(x_1,x_2)|^2$ .

The time-dependent wavefunction plotted in Fig. 21.1.6 oscillates with beat period  $\tau_{beat} = 2\pi/(\omega_{10} - \omega_{01})$ .

$$\Psi(x_{1},x_{2},t) = \frac{1}{2} \left| \psi_{10}(x_{1},x_{2}) e^{-i\omega_{10}t} + \psi_{01}(x_{1},x_{2}) e^{-i\omega_{01}t} \right|^{2} e^{-(x_{1}^{2}+x_{2}^{2})} = \frac{e^{-(x_{1}^{2}+x_{2}^{2})}}{2\pi} \left| \sqrt{2}x_{1}e^{-i\omega_{10}t} + \sqrt{2}x_{1}e^{-i\omega_{01}t} \right|^{2} \\
= \frac{e^{-(x_{1}^{2}+x_{2}^{2})}}{\pi} \left( x_{1}^{2} + x_{2}^{2} + 2x_{1}x_{2}\cos(\omega_{10} - \omega_{01})t \right) = \frac{e^{-(x_{1}^{2}+x_{2}^{2})}}{\pi} \begin{cases} \left| x_{1} + x_{2} \right|^{2} & \text{for: } t = 0 \\ x_{1}^{2} + x_{2}^{2} & \text{for: } t = \tau_{\text{beat}} / 4 \\ \left| x_{1} - x_{2} \right|^{2} & \text{for: } t = \tau_{\text{beat}} / 2 \end{cases}$$

At one quarter of beat period ( $\tau_{beat}/4$ ) a circular distribution appears. It is equivalent to the 1/4-wave circular polarization motion shown in the classical model by Fig. 10.2.6(a). The pictures above will apply exactly to a *B*-type oscillator if they are all rotated by  $45^{\circ}$  in the  $(x_1x_2)$ -plane.

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#### 21.2 2D Oscillator Symmetry, Spin, and Wavefunctions

For a given cranking frequency  $\Omega$ , the eigenvalues shown in Fig. 21.1.1 are the same no matter what values we choose for the parameters  $\{A, B, C, D\}$ . However, the eigenvectors or states depend acutely on parameter values as do the underlying symmetries and physics.

The Abelian symmetry analysis in Chapter 8-9 uses  $C_6$  symmetry to dictate a fixed set of eigenvectors, but their eigenvalues depend on the values of six **H**-parameters. However, for non-Abelian  $D_3$  or  $D_6$  symmetry analysis in Chapter 15, both eigenvalues and eigenvectors may vary with the **H**-parameters and the eigenstates may have a range of different local symmetry subgroups and correspondingly different physics. Different choices for local symmetry subgroups or *Maximal Sets of Commuting Observables (MSOCO)* such as in Fig. 15.2.1, gives different types of symmetry states and wave dynamics. So it is with U(2) symmetry that is an infinite non-Abelian group. Its subgroups correspond to a range of different eigensolutions.

For the U(2) model, all parameters  $\{A, B, C, D\}$  have basically the same eigenvalues for a given  $\Omega$  as shown in Fig. 21.1.1, but the eigenvectors or eigenstates will vary according to which U(2) subgroups  $C_2^A(Asymmetric\ diagonal)$ ,  $C_2^B(Bilateral)$ ,  $C_2^{AB}(Mixed\ AB)$ ,  $C_2^C(Circular)$ , or  $C_1^{ABCD}(Elliptical)$  listed in the U(2) catalog of Fig. 10.4.2 are the Abelian sub-group symmetries of the **H**-Hamiltonian. The classical two-dimensional-oscillator and analogous quantum two-state eigenstates for these symmetries are compared in Sections 10.2(a), 10.2(b), 10.3(a-b), 10.2(c), and 10.4(a-b), respectively. Now we compare the corresponding quantum two-dimensional-oscillators having these symmetries. Of these,  $C_2^C$  (Circular) is most useful for understanding quantum angular momentum.

#### (a) Angular momentum eigenstates: $C_2^C$ symmetry

Consider having the *C*-parameter be non-zero.(A=D, B=0,  $C\neq 0$ .) According to Sec. 2.9(c) this corresponds to physics with "*C-ness*", that is, chirality, circular polarization, current states, Coriolis splitting, cyclotron resonance, and anything resembling moving waves with definite right or left-handed momenta. From (21.1.1) with A=D, B=0,  $C\neq 0$ , we have

$$\mathbf{H}^{C} = \frac{\mathbf{A}}{2} (\mathbf{p}_{1}^{2} + \mathbf{x}_{1}^{2} + \mathbf{p}_{2}^{2} + \mathbf{x}_{2}^{2}) + C(\mathbf{x}_{1}\mathbf{p}_{2} - \mathbf{x}_{2}\mathbf{p}_{1})$$
(21.2.1a)

Note that  $\mathbf{H}^C$  contains a term that is C-times the two-dimensional angular momentum operator  $\mathbf{l}_3$ .

$$\mathbf{I}_3 = \mathbf{x}_1 \mathbf{p}_2 - \mathbf{x}_2 \mathbf{p}_1 \tag{21.2.1b}$$

A pure-C Hamiltonian  $\mathbf{H}^C$  with A=D belongs to  $C_2^C$  subgroup of SU(2) and conserves *angular* momentum  $l_3$  which becomes a key observable and quantum label. In terms of **a**-operators,  $\mathbf{H}^C$  is.

$$\mathbf{H}^{C} = \mathbf{A} \left( \mathbf{a}_{1}^{\dagger} \mathbf{a}_{1} + \mathbf{a}_{2}^{\dagger} \mathbf{a}_{2} + \mathbf{1} \right) + iC \left( \mathbf{a}_{2}^{\dagger} \mathbf{a}_{1} - \mathbf{a}_{1}^{\dagger} \mathbf{a}_{2} \right)$$
(21.2.2)

From (21.1.22) it appears that the eigenvalues will be the same as (21.1.25) but with  $\Omega = 2C$ . This will be shown below when the eigenstates are derived. The fundamental representation (21.1.16) of  $\mathbf{H}^C$  is

$$\left\langle \mathbf{H}^{C} \right\rangle_{v=1}^{Fundamental} = \begin{vmatrix} n_{1}, n_{2} & |1,0\rangle & |0,1\rangle \\ \hline \langle 1,0| & A & -iC \\ \langle 0,1| & +iC & A \end{vmatrix} + A\mathbf{1}$$
 (21.2.3)

 $\mathbf{H}^C$  commutes with a complex reflection  $\sigma_C$  and a real continuous rotation  $\mathbf{R}[\phi]$  generated by  $\sigma_C$ .

$$\mathbf{s}_C = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} , \quad \mathbf{R}[\phi] = \begin{pmatrix} \cos \phi & -\sin \phi \\ \sin \phi & \cos \phi \end{pmatrix} = e^{-i\phi \mathbf{s}_C}$$
 (21.2.4)

This means  $\mathbf{H}^C$  is "smooth" or perfectly circular. It does not have any potential valleys or "bumps" which change angular momentum and require standing-or-galloping-wave eigenstates. So its eigenwaves (like those of a Ring Laser) have no nodes or antinodes and are of the form  $e^{\pm im\phi} = (x_1 \pm ix_2)^m$  for which the probability distribution is perfectly circular in the complex phasor plane. Their complex continuous circularity provides some more mnemonic reasons to use the letter "C" to designate such a symmetry.

The complex C-symmetry  $(x_1 \pm ix_2)$ -states differ from the real standing wave  $(x_1 \text{ and } x_2)$  states of  $C_2^A$  symmetry or  $(x_1 \pm x_2)$  states of  $C_2^B$  symmetry described in Sec. 10.2(a) through Sec. 10.3(b). We started by basing our oscillator theory on linear  $(x_1 \text{ and } x_2)$  states of  $C_2^A$ . The A-axis bases will need to be moved to the chiral C-axis of Fig. 10.5.6 using, for example, a  $90^\circ$  rotation around the B-axis. This will be done shortly.

(1) Angular momentum labeling: Fundamental base states  $\{|\uparrow\rangle,|\downarrow\rangle\}$ 

First, let us re-label and "rename" the lowest five U(2) base sets as follows.

$$\begin{vmatrix} j = 0 & \begin{vmatrix} 0 \\ 0 \\ -1 \end{vmatrix} = |00\rangle & \text{"scalar"} \\ \\ j = \frac{1}{2} & \begin{vmatrix} 1/2 \\ 1/2 \\ -1/2 \\ -1/2 \end{vmatrix} = |10\rangle = |1^{\uparrow}\rangle & \text{"spinor"} \\ \\ \begin{vmatrix} \frac{1}{1} \\ -1 \\ -1/2 \\ -1/2 \\ -1/2 \end{vmatrix} = |10\rangle & |11\rangle & \text{"3-vector"} \\ \\ \begin{vmatrix} \frac{1}{1} \\ -1/2 \\$$

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Famous examples of chiral spin objects include electrons, nucleons, neutrinos, and other particles of total spin j=1/2 units of  $\hbar$ . If we choose the fundamental U(2) bases states  $\{|1\rangle,|2\rangle\}$  to be *spin-up*  $|\uparrow\rangle$  and *spin-dn*  $|\downarrow\rangle$  then the quantum theory of angular momentum is mathematically identical to an analysis U(2) oscillator states. Each number-1 boson counts for one-half  $\hbar$ -unit of angular momentum m=+1/2 while each number-2 boson counts for minus one-half  $\hbar$ -unit of angular momentum m=-1/2 along the C-axis or Z-axis.

U(2) levels from Fig. 21.1.1 are separated and labeled according to angular momentum notation in Fig. 21.2.1. *Odd-v* and half-integral j = 1/2, 3/2,... *levels* are sketched on the left-hand side while the *even-v* and integral j = 0, 1, 2,... *levels* are sketched on the right-hand side. Common names "*spinor*", "*vector*" and "*tensor*" are applied to multiplets j = 1/2, 1, and 2, respectively. The half-integral-j side is generally associated with the group U(2) that works on complex 2-dimensional "spinor" space, while the integral-j side (which belongs to U(2), too) is generally associated with real 3-dimensional R(3) rotations in optical ABC-space or in a real XYZ-space, not entirely different from the one in which we live.

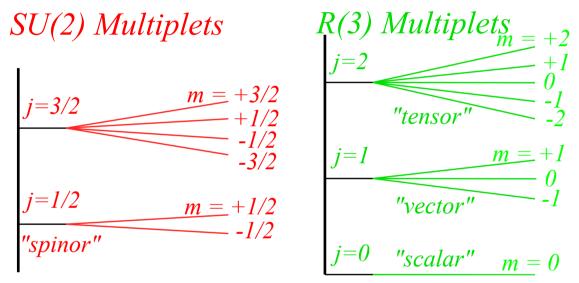


Fig. 21.2.1 SU(2) and R(3) angular momentum levels labeled by j and m.

A *C*-Hamiltonian is diagonalized by a  $\Theta = 90^{\circ}$  rotation around the *X* or *B*-axis which takes a spin vector **S** on the *Z* or *A*-axis down to the *Y* or *C*-axis. *X*-rotations have polar angles  $[\phi = 0^{\circ}, \vartheta = 90^{\circ}]$ . Putting these angles into a Darboux rotation matrix (2.10.15d) gives

$$\left\langle \mathbf{R}_{B}(90^{\circ})\right\rangle = \left\langle \mathbf{R}\left[\varphi = 0^{\circ}, \vartheta = 90^{\circ}, \Theta = 90^{\circ}\right]\right\rangle = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{-i}{\sqrt{2}} \\ \frac{-i}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} = \begin{pmatrix} \left\langle R \middle| x_{1} \right\rangle & \left\langle R \middle| x_{2} \right\rangle \\ \left\langle L \middle| x_{1} \right\rangle & \left\langle L \middle| x_{2} \right\rangle \end{pmatrix} \tag{21.2.6a}$$

This is a transformation between linear optical polarization states  $\{|x_1\rangle, |x_2\rangle\}$  and states of circular right-or-left-polarization  $\{|R\rangle, |L\rangle\}$  or electronic states of spin-up-or-dn  $\{|\uparrow\rangle = |+^{1}/_{2}\rangle, |\downarrow\rangle = |-^{1}/_{2}\rangle\}$ 

$$|R\rangle = |\uparrow\rangle = \left|\frac{1/2}{+1/2}\right\rangle = \frac{|x_1\rangle + i|x_2\rangle}{\sqrt{2}}, \qquad |L\rangle = |\downarrow\rangle = \left|\frac{1/2}{-1/2}\right\rangle = \frac{i|x_1\rangle + |x_2\rangle}{\sqrt{2}},$$

$$\langle R| = \langle\uparrow\rangle = \left\langle\frac{1/2}{+1/2}\right| = \frac{\langle x_1| - i\langle x_2|}{\sqrt{2}}, \qquad \langle L| = \langle\downarrow\rangle = \left\langle\frac{1/2}{-1/2}\right| = \frac{-i\langle x_1| + \langle x_2|}{\sqrt{2}}.$$
(21.2.6b)

This must also be the transformation between the corresponding sets of  $\{\mathbf{a}^{\dagger}_{1}, \mathbf{a}^{\dagger}_{2}\}$  and  $\{\mathbf{a}^{\dagger}\uparrow, \mathbf{a}^{\dagger}\downarrow\}$  operators which create the base states  $\{|x_{I}\rangle=\mathbf{a}^{\dagger}_{1}|0\rangle, |x_{2}\rangle=\mathbf{a}^{\dagger}_{2}|0\rangle\}$  and  $\{|\uparrow\rangle=\mathbf{a}^{\dagger}\uparrow|0\rangle, |\downarrow\rangle=\mathbf{a}^{\dagger}\downarrow|0\rangle\}$ .

$$\mathbf{a}_{R}^{\dagger} = \mathbf{a}_{\uparrow}^{\dagger} = \mathbf{a}_{+1/2}^{\dagger} = \frac{\mathbf{a}_{1}^{\dagger} + i\mathbf{a}_{2}^{\dagger}}{\sqrt{2}}, \qquad \mathbf{a}_{L}^{\dagger} = \mathbf{a}_{-1/2}^{\dagger} = \frac{i\mathbf{a}_{1}^{\dagger} + \mathbf{a}_{2}^{\dagger}}{\sqrt{2}},$$

$$\mathbf{a}_{R} = \mathbf{a}_{\uparrow} = \mathbf{a}_{+1/2} = \frac{\mathbf{a}_{1} - i\mathbf{a}_{2}}{\sqrt{2}}, \qquad \mathbf{a}_{L} = \mathbf{a}_{\downarrow} = \mathbf{a}_{-1/2} = \frac{-i\mathbf{a}_{1}^{\dagger} + \mathbf{a}_{2}^{\dagger}}{\sqrt{2}}.$$

$$(21.2.6c)$$

It does indeed diagonalize the fundamental (v=I) or (j=I/2) **H**-submatrix (21.1.16) for  $C_2^C$  symmetry.

$$\begin{pmatrix} \left\langle \uparrow \middle| x_{1} \right\rangle & \left\langle \uparrow \middle| x_{2} \right\rangle \\ \left\langle \downarrow \middle| x_{1} \right\rangle & \left\langle \downarrow \middle| x_{2} \right\rangle \end{pmatrix} \cdot \begin{pmatrix} \left\langle x_{1} \middle| \mathbf{H} \middle| x_{1} \right\rangle & \left\langle x_{1} \middle| \mathbf{H} \middle| x_{2} \right\rangle \\ \left\langle x_{2} \middle| \mathbf{H} \middle| x_{1} \right\rangle & \left\langle x_{2} \middle| \mathbf{H} \middle| x_{2} \right\rangle \end{pmatrix} \cdot \begin{pmatrix} \left\langle x_{1} \middle| \uparrow \right\rangle & \left\langle x_{1} \middle| \downarrow \right\rangle \\ \left\langle x_{2} \middle| \uparrow \right\rangle & \left\langle x_{2} \middle| \downarrow \right\rangle \end{pmatrix} = \begin{pmatrix} \left\langle \uparrow \middle| \mathbf{H} \middle| \uparrow \right\rangle & \left\langle \uparrow \middle| \mathbf{H} \middle| x_{2} \right\rangle \\ \left\langle \downarrow \middle| \mathbf{H} \middle| \uparrow \right\rangle & \left\langle \downarrow \middle| \mathbf{H} \middle| \downarrow \right\rangle \end{pmatrix} \\ \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{-i}{\sqrt{2}} \\ \frac{-i}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} \cdot \begin{pmatrix} 0 & -iC \\ iC & 0 \end{pmatrix} \cdot \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{-i}{\sqrt{2}} \\ \frac{-i}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} = \begin{pmatrix} C & 0 \\ 0 & -C \end{pmatrix} \tag{21.2.6d}$$

The resulting wave functions are a complex-conjugate pair of two-dimensional Gaussians.

$$\psi_{1\uparrow 0\downarrow}(x_1, x_2) = \frac{\sqrt{2}(x_1 + ix_2)e^{-(x_1^2 + x_2^2)/2}}{(\pi)^{1/2}}, \psi_{0\uparrow 1\downarrow}(x_1, x_2) = \frac{\sqrt{2}(x_1 - ix_2)e^{-(x_1^2 + x_2^2)/2}}{(\pi)^{1/2}}$$
(21.2.7)

The two have identical probability distribution which is plotted in Fig. 21.2.2. (Also, recall Fig. 21.1.6.)

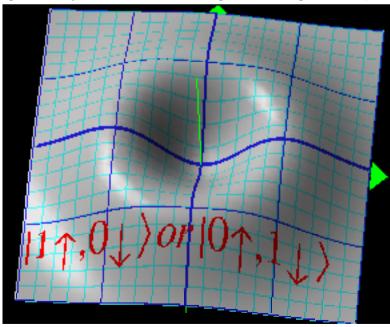


Fig. 21.2.2 2-D Oscillator probability distributions:  $|\Psi_{1\uparrow0\downarrow}(x_1,x_2)|^2$  or  $|\Psi_{0\uparrow1\downarrow}(x_1,x_2)|^2$ .

Notice how the probability drops to zero quickly near the origin. This is a general property of an eigentate with non-zero momentum  $\ell$  in  $\ell$ -conserving systems. As a particle approaches the origin with non-zero angular momentum, it gains speed and kinetic energy without limit, like a dust particle in a perfect vortex. However, if energy is also conserved then particles simply must avoid the origin.

#### (2) 3-Vector base states (v=2) or (i=1)

The preceding procedures may be used to find the eigenvectors of the excited (v=2, 3, 4...) **H**-submatrices. For example, the (v=2) or (j=1) eigenvectors of a  $C_2^C$  symmetric **H** must be the following.

$$\begin{aligned} \left| 2_{\uparrow} 0_{\downarrow} \right\rangle &= \frac{\mathbf{a}_{\uparrow}^{\dagger 2}}{\sqrt{2!}} |0\rangle &= \frac{\left( \mathbf{a}_{1}^{\dagger} + i \mathbf{a}_{2}^{\dagger} \right)^{2}}{2\sqrt{2!}} |0\rangle &= \frac{\mathbf{a}_{1}^{\dagger 2} + 2i \mathbf{a}_{1}^{\dagger} \mathbf{a}_{2}^{\dagger} - \mathbf{a}_{2}^{\dagger 2}}{2\sqrt{2}} |0\rangle &= \frac{1}{2} |2_{1} 0_{2}\rangle + \frac{i}{\sqrt{2}} |1_{1} 1_{2}\rangle - \frac{1}{2} |0_{1} 2_{2}\rangle \\ \left| 1_{\uparrow} 1_{\downarrow} \right\rangle &= \frac{\mathbf{a}_{\uparrow}^{\dagger} \mathbf{a}_{\downarrow}^{\dagger}}{\sqrt{1!} \sqrt{1!}} |0\rangle &= \frac{\left( \mathbf{a}_{1}^{\dagger} + i \mathbf{a}_{2}^{\dagger} \right) \left( \mathbf{a}_{1}^{\dagger} - i \mathbf{a}_{2}^{\dagger} \right)}{2} |0\rangle &= \frac{\mathbf{a}_{1}^{\dagger 2} + \mathbf{a}_{2}^{\dagger 2}}{2} |0\rangle &= \frac{1}{\sqrt{2}} |2_{1} 0_{2}\rangle &+ \frac{1}{\sqrt{2}} |0_{1} 2_{2}\rangle \\ \left| 0_{\uparrow} 2_{\downarrow} \right\rangle &= \frac{\mathbf{a}_{\downarrow}^{\dagger 2}}{\sqrt{2!}} |0\rangle &= \frac{\mathbf{a}_{1}^{\dagger 2} - 2i \mathbf{a}_{1}^{\dagger} \mathbf{a}_{2}^{\dagger} - \mathbf{a}_{2}^{\dagger 2}}{2\sqrt{2}} |0\rangle &= \frac{1}{2} |2_{1} 0_{2}\rangle - \frac{i}{\sqrt{2}} |1_{1} 1_{2}\rangle - \frac{1}{2} |0_{1} 2_{2}\rangle \end{aligned}$$

$$(21.2.8)$$

We verify that the resulting vectors are eigenvectors of the 3-by-3 submatrix of (21.1.15c).

The splitting between neighboring levels is  $\Omega = 2C$  as required by (21.1.22)

The (v=2) eigenfunctions  $\langle x_1 x_2 | n_1 n_2 \rangle$  in the *A*-basis are products of 1-D waves (20.3.40).

$$\psi_{2_{1}0_{1}}(x_{1},x_{2}) = \langle x_{1}|2\rangle\langle x_{2}|0\rangle , \quad \psi_{1_{1}1_{1}}(x_{1},x_{2}) = \langle x_{1}|1\rangle\langle x_{2}|1\rangle , \quad \psi_{1_{1}1_{1}}(x_{1},x_{2}) = \langle x_{1}|0\rangle\langle x_{2}|2\rangle$$

$$= Ne^{-(x_{1}^{2}+x_{2}^{2})/2}\sqrt{2}\left(x_{1}^{2}-\frac{1}{2}\right) , \quad = Ne^{-(x_{1}^{2}+x_{2}^{2})/2}2\left(x_{1}x_{2}\right) , \quad = Ne^{-(x_{1}^{2}+x_{2}^{2})/2}\sqrt{2}\left(x_{2}^{2}-\frac{1}{2}\right)$$

$$(21.2.10a) \qquad (21.2.10b) \qquad (21.2.10c)$$

Combining them according to (21.2.8) gives the ( $\nu$ =2) eigenwaves for a *C*-type Hamiltonian.

$$\psi_{2\uparrow 0\downarrow} = \frac{1}{2} \psi_{2\downarrow 0\downarrow} + \frac{i\sqrt{2}}{2} \psi_{1\downarrow 1\downarrow} - \frac{1}{2} \psi_{0\downarrow 1\downarrow} = Ne^{-\frac{r^2}{2}} \frac{x_1^2 + 2ix_1x_2 - x_2^2}{\sqrt{2}} = Ne^{-\frac{r^2}{2}} \frac{\left(x_1 + ix_2\right)^2}{\sqrt{2}}$$
(21.2.10d)  
$$\psi_{1\uparrow 1\downarrow} = \frac{1}{\sqrt{2}} \psi_{2\downarrow 0\downarrow} + \frac{1}{\sqrt{2}} \psi_{0\downarrow 1\downarrow} = Ne^{-\frac{r^2}{2}} \frac{\sqrt{2} \left(x_1^2 + x_2^2 - 1\right)}{\sqrt{2}} = Ne^{-\frac{r^2}{2}} \left(x_1^2 + x_2^2 - 1\right)$$
(21.2.10e)  
$$\psi_{0\uparrow 2\downarrow} = \frac{1}{2} \psi_{2\downarrow 0\downarrow} - \frac{i\sqrt{2}}{2} \psi_{1\downarrow 1\downarrow} - \frac{1}{2} \psi_{0\downarrow 1\downarrow} = Ne^{-\frac{r^2}{2}} \frac{x_1^2 + 2ix_1x_2 - x_2^2}{\sqrt{2}} = Ne^{-\frac{r^2}{2}} \frac{\left(x_1 - ix_2\right)^2}{\sqrt{2}}$$
(21.2.10f)

The *A*-type waves  $\psi_{2102}$  and  $\psi_{1112}$  plotted in Fig. 21.2.3 have lumps and bumps that are aligned to Cartesian  $(x_1 \ x_2)$  coordinates.

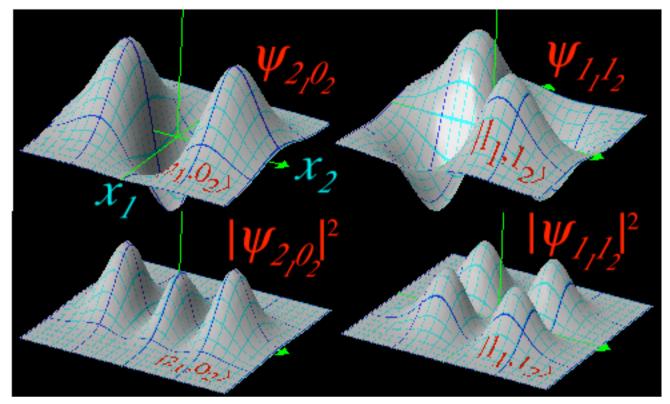


Fig. 21.2.3 (v=2) Type-A standing waves and distributions:  $|\Psi_{2_10_2}(x_1,x_2)|^2$  and  $|\Psi_{I_1I_2}(x_1,x_2)|^2$ .

In contrast, the *C*-type waves  $\psi_{2\uparrow0\downarrow}$  and  $\psi_{I\uparrow1\downarrow}$  plotted in Fig. 21.2.4 are waves moving around in circular orbits with vibrational angular momentum of  $\pm 2$  and 0.

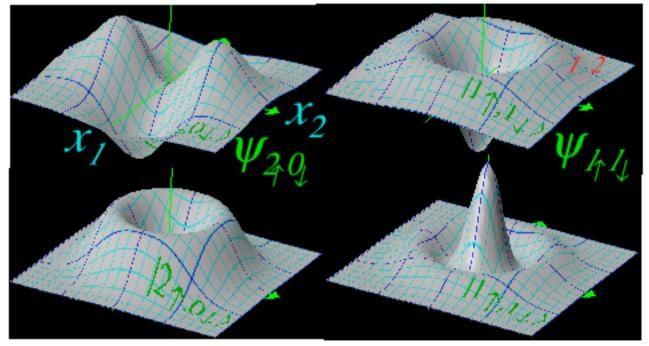


Fig. 21.2.4 (v=2) Type-C moving waves and distributions:  $|\Psi_{2\uparrow0\downarrow}(x_1,x_2)|^2$  and  $|\Psi_{1\uparrow1\downarrow}(x_1,x_2)|^2$ . The angular momentum structure can be seen by rewriting the wavefunctions in polar coordinates.

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$$\psi_{2\uparrow 0\downarrow} = Ne^{-\frac{r^2}{2}} \frac{\left(x_1 + ix_2\right)^2}{\sqrt{2}} = \psi_{2m=2}^{2j=2} = Ne^{-\frac{r^2}{2}} \frac{r^2 e^{i2\theta}}{\sqrt{2}}$$
(21.2.10d)

$$\psi_{1_{\uparrow}1_{\downarrow}} = Ne^{-\frac{r^2}{2}} \left( x_1^2 + x_2^2 - 1 \right) = \psi_{2m=0}^{2j=2} = Ne^{-\frac{r^2}{2}} \left( r^2 - 1 \right) e^{i0\theta}$$
 (21.2.10d)

$$\psi_{0\uparrow 2\downarrow} = Ne^{-\frac{r^2}{2}} \frac{\left(x_1 - ix_2\right)^2}{\sqrt{2}} = \psi_{2m=-2}^{2j=2} = Ne^{-\frac{r^2}{2}} \frac{r^2 e^{-i2\theta}}{\sqrt{2}}$$
(21.2.10d)

Quantum numbers for *C*-type vibrational states are the *radial quantum number* (v=2j) and the *vibrational angular momentum quantum number*  $\mu$ .

$$v = 2j = n \uparrow + n \downarrow$$
 ,  $\mu = 2m = n \uparrow - n \downarrow$  (21.2.11)

A *C*-type vibrational eigenstate has  $\mu$  angular waves and  $2\mu$  angular moving wave zeros (two for each wave). For larger angular momentum the wave tends to avoid the origin more and more as shown in Fig. 21.2.5 below in a comparison between a  $\mu$ =I and a  $\mu$ =I probability distribution.

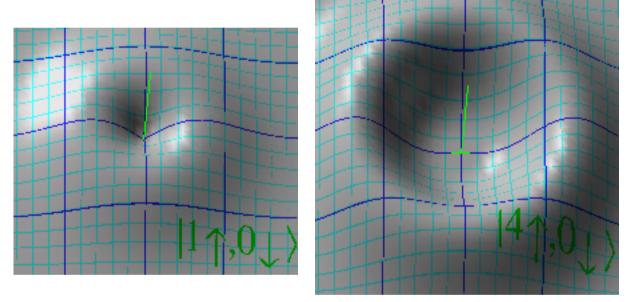


Fig. 21.2.5 (v=2) Type-C moving wave distributions:  $|\Psi_{1\uparrow0\downarrow}(x_1,x_2)|^2$  and  $|\Psi_{4\uparrow0\downarrow}(x_1,x_2)|^2$ .

As the azimuthal angualr momentum quantum number  $\mu=2m$  increases, the location of the circular orbital radius becomes more and more clearly defined.

#### (b) Polar coordinates: $C_2^C$ symmetry variable separation

An alternative (and historically much older) way to obtain C-symmetry eigenfunctions is to use coordinates based on circular symmetry, namely, polar coordinates  $(r,\phi)$  instead of Cartesian (x,y) or

$$x = x_1 = r \cos \phi$$
,  $y = x_2 = r \sin \phi$ . (21.2.12)

The Jacobian transformation between the Cartesian and polar coordinates relates their derivatives.

$$\begin{pmatrix} \frac{\partial}{\partial r} \\ \frac{\partial}{\partial \phi} \end{pmatrix} = \begin{pmatrix} \frac{\partial x}{\partial r} & \frac{\partial y}{\partial r} \\ \frac{\partial x}{\partial \phi} & \frac{\partial y}{\partial \phi} \end{pmatrix} \begin{pmatrix} \frac{\partial}{\partial x} \\ \frac{\partial}{\partial y} \end{pmatrix} = \begin{pmatrix} \cos \phi & \sin \phi \\ -r \sin \phi & r \cos \phi \end{pmatrix} \begin{pmatrix} \frac{\partial}{\partial x} \\ \frac{\partial}{\partial y} \end{pmatrix} \tag{21.2.13a}$$

The inverse (Kajobian) transformation lets us rewrite the Cartesian Schrodinger equation.

$$\begin{pmatrix} \frac{\partial}{\partial x} \\ \frac{\partial}{\partial y} \end{pmatrix} = \begin{pmatrix} \frac{\partial r}{\partial x} & \frac{\partial \phi}{\partial x} \\ \frac{\partial r}{\partial y} & \frac{\partial \phi}{\partial y} \end{pmatrix} \begin{pmatrix} \frac{\partial}{\partial r} \\ \frac{\partial}{\partial \phi} \end{pmatrix} = \begin{pmatrix} \cos \phi & -\frac{1}{r} \sin \phi \\ \sin \phi & \frac{1}{r} \cos \phi \end{pmatrix} \begin{pmatrix} \frac{\partial}{\partial r} \\ \frac{\partial}{\partial \phi} \end{pmatrix} \tag{21.2.13b}$$

The oscillator Schrodinger equation in Cartesian coordinates

$$\frac{\partial^2 \Psi}{\partial x^2} + \frac{\partial^2 \Psi}{\partial y^2} \qquad -\frac{2M}{\hbar^2} \left( \frac{M\omega^2}{2} (x^2 + y^2) - E \right) \Psi = 0 , \qquad (21.2.14a)$$

is rewritten as follows in polar coordinates.

$$\frac{\partial^2 \Psi}{\partial r^2} + \frac{1}{r} \frac{\partial \Psi}{\partial r} + \frac{1}{r^2} \frac{\partial^2 \Psi}{\partial \phi^2} - \frac{2M}{\hbar^2} \left( \frac{M\omega^2}{2} r^2 - E \right) \Psi = 0$$

(21.2.14a)

Separation of coordinate variables r and  $\phi$  into a wavefunction  $\Psi(r,\phi)=R(r)\phi(\phi)$  is similar to the separation  $\Psi(x,y)=\psi_x(x)\psi_y(y)$  for Cartesian coordinates and results in the following equation separation.

$$\frac{r^2}{R} \left[ \frac{d^2 R}{dr^2} + \frac{1}{r} \frac{dR}{dr} \right] - \frac{2Mr^2}{\hbar^2} \left( \frac{M\omega^2}{2} r^2 - E \right) = -\frac{1}{\varphi} \frac{\partial^2 \varphi}{\partial \phi^2} = const. = m^2$$
 (21.2.15a)

Equality of the two ordinary equations of independent r and  $\phi$  implies both equal a constant. Azimuthal symmetry and boundary conditions  $\varphi(\phi) = \varphi(\phi \pm 2\pi)$  force m-quantization, so the constant is the square of azimuthal angular momentum quantum number  $m = 0, \pm 1, \pm 2...$ 

$$\frac{\partial^2 \varphi}{\partial \phi^2} = -m^2 \varphi \qquad \text{or:} \qquad \varphi(\phi) = Ae^{im\phi} + Be^{-im\phi}$$
 (21.2.15b)

The radial equation involves the constant  $m^2$  in a more complicated way.

$$\frac{d^2R}{dr^2} + \frac{1}{r}\frac{dR}{dr} - \left[\frac{M^2\omega^2}{\hbar^2}r^2 + \frac{2M}{\hbar^2}E - \frac{m^2}{r^2}\right]R = 0$$
(21.2.15c)

C-symmetry makes the angular moving waves in the  $\phi$ -direction independent of the radial wave except through the constant  $m^2$ . Such a constant is called a *separation constant*.

As in the 1-D case of (20.1.12) it helps to factor out a Gaussian scaling function  $s(r) = e^{-\alpha r^2}$  such that the factor  $\rho(r)$  in the radial wave  $R(r) = s(r)\rho(r)$  is a simpler function and preferably an r polynomial.

$$R = \rho e^{-\alpha r^2}$$

$$R' = (\rho' - 2\alpha r \rho) e^{-\alpha r^2}$$

$$R'' = (\rho'' - 4\alpha r \rho' + \left[ 4\alpha^2 r^2 - 2\alpha \right] \rho) e^{-\alpha r^2}$$
(21.2.16)

Dropping the Gaussian converts (21.2.15c) to an equation of similar form.

$$R'' + \frac{R'}{r} - \left[ \frac{M^2 \omega^2}{\hbar^2} r^2 - \frac{2M}{\hbar^2} E + \frac{m^2}{r^2} \right] R = 0$$

$$\rho'' + \left[ \frac{1}{r} - 4\alpha r \right] \rho' + \left[ \left( 4\alpha^2 - \frac{M^2 \omega^2}{\hbar^2} \right) r^2 + \frac{2M}{\hbar^2} E - 4\alpha - \frac{m^2}{r^2} \right] \rho = 0$$
(21.2.17a)

This simplifies if we use the same Gaussian parameter  $\alpha = M\omega/2\hbar$  from (20.1.10b) and set  $E = \hbar\omega\epsilon$ .

$$\rho'' + \left[\frac{1}{r} - 4\alpha r\right]\rho' + \left[4\alpha(\varepsilon - 1) - \frac{m^2}{r^2}\right]\rho = 0 = r^2\rho'' + \left[r - 4\alpha r^3\right]\rho' + \left[4\alpha(\varepsilon - 1)r^2 - m^2\right]\rho \quad (21.2.17b)$$

Now a polynomial analysis will work by expanding the radial wave and its derivatives. Let  $\varepsilon = \varepsilon - 1$ .

$$\rho = a_0 + a_1 r + a_2 r^2 + a_3 r^3 + a_4 r^4 + \dots = \sum_{k=0}^{\infty} a_k r^k 
\rho' = a_1 + 2a_2 r + 3a_3 r^2 + 4a_4 r^4 + 5a_5 r^5 + \dots = \sum_{k=1}^{\infty} k a_k r^{k-1} 
\rho'' = 2a_2 + 6a_3 r + 12a_3 r^2 + 20a_4 r^4 + 30a_5 r^5 + \dots = \sum_{k=2}^{\infty} k (k-1)a_k r^{k-2}$$
(21.2.18)

Putting this into each term of the radial equation gives series whose grand sum must be zero.

$$-m^{2}\rho = -m^{2}a_{0} - m^{2}a_{1}r - m^{2}a_{2}r^{2} - m^{2}a_{3}r^{3} - m^{2}a_{4}r^{4} + \dots = \sum_{k=0}^{\infty} -m^{2}a_{k} r^{k}$$

$$4\alpha\varepsilon_{-}r^{2}\rho = 4\alpha\varepsilon_{-}a_{0}r^{2} + 4\alpha\varepsilon_{-}a_{1}r^{3} + 4\alpha\varepsilon_{-}a_{2}r^{4} + \dots = \sum_{k=2}^{\infty} 4\alpha\varepsilon_{-}a_{k-2} r^{k}$$

$$r\rho' = a_{1}r + 2a_{2}r^{2} + 3a_{3}r^{3} + 4a_{4}r^{4} + \dots = \sum_{k=1}^{\infty} ka_{k} r^{k}$$

$$r^{2}\rho'' = 2a_{2}r^{2} + 6a_{3}r^{3} + 12a_{4}r^{4} + \dots = \sum_{k=2}^{\infty} k(k-1)a_{k} r^{k}$$

$$-4\alpha\varepsilon_{-}r^{3}\rho' = -4\alpha\alpha_{1}r^{3} - 8\alpha\alpha_{2}r^{4} + \dots = \sum_{k=3}^{\infty} -4\alpha(k-2)a_{k-2} r^{k}$$

$$(21.2.19)$$

The sum of coefficients of each power lying in each column above must vanish. The  $\theta$ -column gives

$$m^2a_0=0$$

This says that wave amplitude  $a_0$  must vanish for all non-zero momentum m. We noted after Fig. 21.2.5 that orbiting particles avoid the origin. Consider the general column or power-k as listed on the right hand side above. Setting the sum of the k- coefficients to zero leads to a *recursion relation*.

$$\left[4\alpha\varepsilon_{-} - 4\alpha(k-2)\right]a_{k-2} = -\left[k(k-1) + k - m^{2}\right]a_{k}$$
(21.2.20a)

This may be used as a *bottom-up* relation or else as a *top-down* relation.

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$$a_{k+2} = \frac{-4\alpha(\varepsilon_{-} - k)}{(k+2)^{2} - m^{2}} a_{k}$$
,  $a_{k-2} = \frac{m^{2} - k^{2}}{4\alpha(\varepsilon_{-} - k + 2)} a_{k}$  (21.2.20b)

The first starts with bottom coefficient  $a_0$  or  $a_1$  and computes the higher ones. The other works down. The bottom-up relation leads to the *quantization condition* 

$$\varepsilon_{-} = N = k_{>} , \qquad (21.2.20c)$$

for some integer *principal quantum number N* in order that the polynomial order is finite and the wave is bounded by the Gaussian. The top-down relation leads to a *centrifugal exclusion condition* 

$$k < = |m|,$$
 (21.2.20d)

which limits the lowest degree k < m allowed by a given angular momentum m. High powers  $r^k$  are "center-fleeing" with low radial wave near r = 0. Momentum magnitude is restricted between zero and N.

$$0 \le |m| \le N$$

The quantization condition agrees with the energy spectrum previously derived in (21.1.25).

$$\hbar\omega\varepsilon = \hbar\omega(\varepsilon-1) = \hbar\omega N$$
,

where we use  $E = \hbar \omega \varepsilon$  and  $\varepsilon = \varepsilon - I$  from (21.2.17).

$$E = \hbar \omega \varepsilon = \hbar \omega (N+1) \tag{21.2.20e}$$

Note the principal quantum number N is the total quantum number  $\nu$  defined previously in (21.1.25).

$$N = v = n_1 + n_2$$

The  $N=2=\varepsilon$  wave for m=0 in (21.2.10b) follows from (21.2.20b)

$$a_2 = \frac{-4\alpha\varepsilon_-}{(2)^2 - 0^2} a_0 = -2\alpha a_0 = -\frac{M\omega}{\hbar} a_0$$
 (21.2.21)

In units such that  $M\omega/\hbar = 1$  or  $\alpha = 1/2$  this agrees with (21.2.10b).

$$R(r) = a_0 (1-r^2)$$

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#### 21.3 N-Dimensional Oscillator Levels

The quantum levels  $(1,2,3,4,...,\upsilon,...)$  of a 1D oscillator are singlet levels (no degeneracy). However, an isotropic (U(2) symmetric) 2D oscillator has levels whose degeneracy  $\ell = \upsilon$  equals the principal quantum number.  $\upsilon = n_1 + n_2 = (1,2,3,4,...,\upsilon,...)$ , as seen in Fig. 21.1.1.

The degeneracies of isotropic (U(N) symmetric) N-D oscillators increase more rapidly. For a U(3) symmetric 3D oscillator the degeneracy numbers are  $\ell = (1,3,6,10,...,\upsilon(\upsilon+1)/2,...)$ . These are known as *triangular numbers*. Here we consider ways to describe oscillator levels.

#### (a) Pascal triangle and U(N) degeneracy

There are some geometric ways to organize and label oscillator degeneracy. The first uses Pascal's triangle of binomial coefficients as shown in Fig. 21.3.1. Each Pascal number is the sum of the two numbers directly above it as shown in Fig. 21.3.1(a). Numbers along a given *N*-diagonal are the degeneracy  $\ell$  for each quantum number  $\nu$  listed along the opposing  $(\nu)$ -diagonal. It's a binomial coefficient  $C_n^n = \binom{n}{n}$  that means the number of combinations of *n* things taken  $\nu$  at a time.

$$\ell = C_{v}^{N-1+v} = {N-1+v \choose v} = \frac{(N-1+v)!}{v!(N-1)!} = {N-1+v \choose N-1}$$
(23.1.1)

(a) N-D Oscillator Degeneracy  $\ell$  of quamtum level  $\upsilon$ 

(b) Stacking numbers

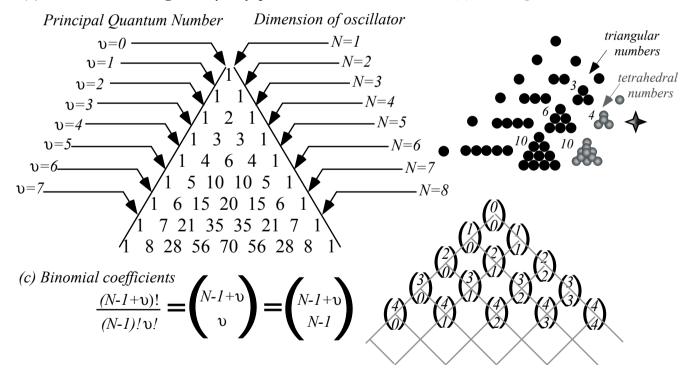


Fig. 21.3.1 Pascal binomial numbers related to oscillator level degeneracy.

The plot in Fig. 21.1.2 of the principal quantum number  $v = n_1 + n_2$  versus individual U(2) oscillator quantum numbers  $n_1$  and  $n_2$  shows why Pascal's triangular numbers are relevant to oscillator degeneracy. An analogous plot of  $v = n_1 + n_2 + n_3$  for a U(3) oscillator produces equilateral triangles stacked a diagonal distance  $v = n_1 + n_2 + n_3$  from the corner of three Cartesian planes defining  $n_1$ ,  $n_2$ , and  $n_3$  axes.

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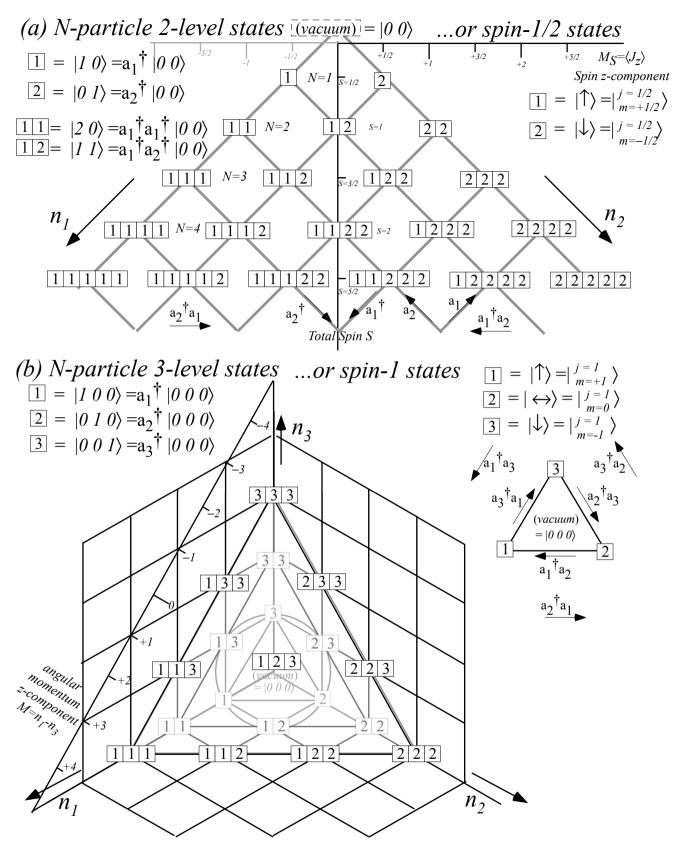


Fig. 21.3.2 N-quanta ("particle") multiplets (a) 2-Levels ("states"): Spin-1/2. (b) 3-Levels: Spin-1

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Fig. 21.1.3(a) displays the 2D oscillator states in a way that is similar but upside down to Fig. 23.1.2(a). Each level has the same total number  $N=v=n_1+n_2$  of quanta. We may think of each level as an N-particle state where by "particle" we mean a photon, vibron, libron, or any of a number of excitons that occupy our attention in modern physics. It is only important that each "X-on" or "Enr-on" may be created in arbitrary order, that is, has Bose symmetry as stated in (21.1.5) or again below.

$$[\mathbf{a}_m, \mathbf{a}_n] = \mathbf{a}_m \mathbf{a}_n - \mathbf{a}_n \mathbf{a}_m , \quad [\mathbf{a}_m, \mathbf{a}^{\dagger}_n] = \mathbf{a}_m \mathbf{a}^{\dagger}_n - \mathbf{a}^{\dagger}_n \mathbf{a}_m , \quad [\mathbf{a}^{\dagger}_m, \mathbf{a}^{\dagger}_n] = \mathbf{a}^{\dagger}_m \mathbf{a}^{\dagger}_n - \mathbf{a}^{\dagger}_n \mathbf{a}^{\dagger}_m ,$$

$$= \mathbf{0} .$$

This is indicated by a *Young Tableaux* notation of boxes holding numbers that indicated the state or X-on numbers. Numbers may be permuted with in the rows without changing their meaning. Only the sum

$$N = S/2 = v = n_1 + n_2 \tag{21.3.2}$$

or difference

$$C = S_z/2 = n_1 - n_2 \tag{21.3.3}$$

Has physical significance. In the following Chapter 22, these numbers will define the photon "spin" that characterizes the intensity N and *one* of the polarization A, B, or C components in a quantum light beam. In Chapter 23, these quantum numbers will define total spin angular momentum S and its z-component  $S_z$  in the Schwinger development of rotational quanta.

Fig. 21.1.3(b) displays the 3D oscillator states in an analogous but 3-dimensional way with the 2D oscillator  $n_1$ -axis and  $n_2$ -axis lying on the floor of a Cartesian octant or "room" whose vertical  $n_3$ -axis is the number of quanta or "particles" in the 3<sup>rd</sup> oscillator state. Again any kind of "X-on" may use this geometry and the total number  $N=v=n_1+n_2+n_3$  of these "particles" would be marked off on a (1,1,1)-axis coming straight out of this Fig. 21.3.2(b). With three dimensions or quanta  $n_1$ ,  $n_2$ , and  $n_3$  there are lots more ways that they can sum to a given N. That number is one of the triangular numbers 1,3,6,10,... listed in Pascal's triangle on the N=3 diagonal of Fig. 21.3.1(a) and indicated in Fig. 21.3.1(b). The triangles for N=v=0, 1, 2, and 3 are "stacked" in Fig. 21.3.2(b) with their Young tableaux state labeling.

These stacks make larger and larger tetrahedrons. Such tetrahedrons are just what are needed to make the next higher 4D-oscillator states whose degeneracy (for an isotropic oscillator) will be the tetrahedral numbers 1,4,10,15.. listed in Fig. 21.3.1(b). These are the number of cannonballs in an *N*-sided stack seen sitting dissolutely in Civil War monuments throughout the educationally miasmic Southern states of a United States so tortured by its apparent need for that and other wars.

In contrast, there is much to learn about the quantum states by considering the geometry and algebra of these curious stacks and considering how it is that the idea of quantum *particles*, on one hand and quantum *states*, on the other, can be clearly defined in some cases and quite mixed up in others.

#### **Problems for Chapter 21**

From A to B

21.1.1. Consider a *B*-type 2D oscillator Hamiltonian:

$$\mathsf{H}^{B} = \frac{A}{2} \Big( \mathsf{p}_{1}^{2} + \mathsf{x}_{1}^{2} + \mathsf{p}_{2}^{2} + \mathsf{x}_{2}^{2} \Big) + B \Big( \mathsf{p}_{1} \mathsf{p}_{2} + \mathsf{x}_{1} \mathsf{x}_{2} \Big)$$

- (a) Express it in terms of A-basis creation-destruction operators  $\mathbf{a}_i = (\mathbf{x}_i + i \mathbf{p}_i)/\sqrt{2}$  (j=1,2).
- (b) Compute its A-basis representation for the first five levels: N=0, 1, 2, 3, 4,...
- (c) Plot the  $H^B$  eigenvalues for fixed A=1 and varying between B=-1 and B=+1.
- (d) Diagonalize the representation for the three N=2 levels and display the 3-by-3 trans-formation matrix  $T_{B\leftarrow A}$  which effectively transforms from the A-basis to the B-basis. Does T depend on A or B?

Lines of degeneracy

21.1.2. The eigenvalues in Fig. 21.1.1 exhibit quite a number of degeneracy points as the splitting or beat frequency  $\Omega$  varies relative to static oscillator frequency  $\omega$ . Give a sketch of the algebra, geometry, or arithmetic that might shed some light on this. The revival crossings described in Ch. 9 might be relevant.

From B to C

21.1.3. Consider a *C*-type 2D oscillator Hamiltonian:

$$\mathsf{H}^{C} = \frac{A}{2} \Big( \mathsf{p}_{1}^{2} + \mathsf{x}_{1}^{2} + \mathsf{p}_{2}^{2} + \mathsf{x}_{2}^{2} \Big) + C \Big( \mathsf{x}_{1} \mathsf{p}_{2} - \mathsf{x}_{2} \mathsf{p}_{1} \Big)$$

- (a) The (N=2)-transformation  $T_{B\leftarrow A}$  from an A-basis to a B-basis derived in Exercise 21.1.1(d) might also be capable of continuing on from a B-basis to a C-basis. Does  $T_{B\leftarrow A}=T_{C\leftarrow B}$ ? Check this. How is  $T_{C\leftarrow A}$  related to these two?
- (b) (For Ch. 23) How are these matrices related to the irreducible representations  $D^{(I)}(\varphi, \vartheta, \Theta)$ ?

From 2 to 3

- 21.3.1. Using a ruler and a compass plot out the N-exciton states of a 3D isotropic harmonic oscillator for N=3 and for N=4 (as in Fig. 21.3.2(b). Label each plot with tableaux state labels.
- (a) Show how the energy levels would split for N=1, 2, 3, and 4 if oscillator-3 shifted up by 0.1  $\omega$ .
- (b) Plot the 2D oscillator states (as in Fig. 21.3.2(a) that belong to each level that splits out.

*To 4* 

- 21.3.2. How would you plot the states and their tableaux for a four dimensional (4D) oscillator?
- (a) Do it for principal quantum number or "X-on" number N=1, 2, and 3.
- (b) Show how the energy levels would split if oscillator-4  $\,$  shifted up by 0.1  $\omega.$

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