4.7. S.H.O.

To gain further insight into the quantum mechanics postulates, we consider once again the problem of a one-dimensional simple harmonic oscillator

One-Dimensional SHO:

$$H \equiv \frac{1}{2m} P^2 + \frac{1}{2} m\omega^2 X^2$$

(of course $[X, X] = 0$, $[P, P] = 0$)

with $[X, P] = i\hbar$. The Hamiltonian is conservative, the energy eigenstates $|n\rangle$ obey

$$H|n\rangle = E_n |n\rangle.$$

In the coordinate representation $\{|x\rangle\}$ this yields the energy eigenfunction equation

$$\langle x|H(X,P)|n\rangle = \left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 x^2\right)\psi_n(x)$$
$$= E_n \psi_n(x),$$

with $\psi_n(x) = \langle x|n\rangle$.

Rather than repeat our familiar analysis of this equation, we will work directly with the abstract state vectors and operators in Hilbert space.

In analogy to our wavefunction analysis, we too introduce creation (raising) and annihilation (lowering) operators $a^\dagger$ and a

$$a \equiv \frac{1}{\sqrt{2}}\left[\sqrt{\frac{m\omega}{\hbar}}\,X + i\sqrt{\frac{1}{m\hbar\omega}}\,P\right]$$

and

$$a^\dagger = \frac{1}{\sqrt{2}}\left[\sqrt{\frac{m\omega}{\hbar}}\,X - i\sqrt{\frac{1}{m\hbar\omega}}\,P\right]$$

since $X^\dagger = X$, $P^\dagger = P$. Solving these for X and P we have

$$X = \frac{1}{\sqrt{2}}\sqrt{\frac{\hbar}{m\omega}}\,(a^\dagger + a)\ (= X^\dagger)$$

$$P = \frac{i}{\sqrt{2}}\sqrt{m\hbar\omega}\,(a^\dagger - a)\ (= P^\dagger).$$

Since $[X,P]=i\hbar$, we have

$$[a,a^\dagger]=\frac{1}{2}\left[\sqrt{\frac{m\omega}{\hbar}}X+i\sqrt{\frac{1}{m\hbar\omega}}P,\ \sqrt{\frac{m\omega}{\hbar}}X-i\sqrt{\frac{1}{m\hbar\omega}}P\right]$$

$$=\frac{1}{2}\frac{1}{i\hbar}[X,P]+\frac{1}{2}\frac{i}{\hbar}[P,X]$$

$$=-\frac{i}{\hbar}[X,P]=1$$

Thus $\boxed{[a,a^\dagger]=1}$, and naturally,

$$\boxed{[a,a]=[a^\dagger,a^\dagger]=0}$$

In addition we find that

$$a^\dagger a=\frac{1}{\hbar\omega}\left[\frac{1}{2m}P^2+\frac{1}{2}m\omega^2X^2-\frac{1}{2}\hbar\omega\right]$$

Thus

$$\boxed{H=\hbar\omega\left(a^\dagger a+\frac{1}{2}\right)}.$$

Hence the eigenstates of H are the same as the eigenstates of $a^\dagger a$.

The number operator N is defined as

$$N \equiv a^\dagger a \, .$$

It is hermitian $N = N^\dagger$ and

$$H = \hbar\omega(N + \tfrac{1}{2}) \, .$$

Thus the energy eigenvalue problem is equivalent to the number operator eigenvalue problem,

$$N|n\rangle = n|n\rangle,$$ finding these eigenstates we have that

$$H|n\rangle = \hbar\omega(N+\tfrac{1}{2})|n\rangle$$

$$= \hbar\omega(n+\tfrac{1}{2})|n\rangle = E_n|n\rangle$$

i.e. $E_n = \hbar\omega(n+\tfrac{1}{2})$.

Towards finding n and $|n\rangle$, we exploit the properties of a and

$a^\dagger$. In particular their commutators with N:

$$[N, a] = [a^\dagger a, a],$$

using $[AB, C] = A[B,C] + [A,C]B$,

we have

$$[N,a] = a^\dagger \cancel{[a,a]}^{\,0} + \underbrace{[a^\dagger, a]}_{=-1} a$$

$$= -a.$$

Now $\left([N,a] = -a\right)^\dagger \Rightarrow (Na - aN)^\dagger = -a^\dagger$

or $a^\dagger N^\dagger - N^\dagger a^\dagger = a^\dagger N - N a^\dagger = -a^\dagger$

$\Rightarrow [N, a^\dagger] = +a^\dagger$

(or proceed directly $[N, a^\dagger] = [a^\dagger a, a^\dagger]$).

Hence

$$\boxed{\begin{aligned}[N,a] &= -a \\ [N,a^\dagger] &= +a^\dagger\end{aligned}}$$

We will use these commutators to determine the eigenvalues $\{n\}$ and the eigenstates $\{|n\rangle\}$.

Determination of the Spectrum $\{n\}$

1) Lemma 1: The eigenvalues n of the operator N are positive or zero

$$n \geq 0 .$$

Proof:

$$n = n \frac{\langle n|n\rangle}{\langle n|n\rangle} = \frac{\langle n|N|n\rangle}{\langle n|n\rangle}$$

$$= \frac{\langle n|a^\dagger a|n\rangle}{\langle n|n\rangle} = \frac{\langle\phi|\phi\rangle}{\langle n|n\rangle} \geq 0$$

with $|\phi\rangle \equiv a|n\rangle \Rightarrow \langle\phi| = \langle n|a^\dagger$

and the inner product has

$$\langle\phi|\phi\rangle \geq 0 \;;\; \langle n|n\rangle \geq 0 .$$

2) Lemma 2: Let $|n\rangle$ be a non-zero eigenvector of N with eigenvalue n, then

1) iff $n=0$, $a|n=0\rangle = 0$

2) if $n>0$, the ket $a|n\rangle$ is a non-zero eigenvector of N with eigenvalue $n-1$.

Proof: 1) $\| a|n\rangle \|^2 = \langle n|a^\dagger a|n\rangle$

$= n\langle n|n\rangle$.

So if $n=0$; $\| a|n=0\rangle \|^2 = 0$

$\Rightarrow a|0\rangle = 0$ i.e. the scalar product $\langle\phi|\phi\rangle = 0$ iff $|\phi\rangle = 0$.

Conversely, if $a|0\rangle = 0$,

Then
$$a^{\dagger}a|0\rangle = 0$$
that is $N|0\rangle = 0|0\rangle \Rightarrow n=0$.
Thus any vector for which $a|0\rangle = 0$ has the $n=0$ eigenvalue.

2) if $n>0$ then $a|n\rangle \neq 0$ (this is from above $\| a|n\rangle \|^2 = n\langle n|n\rangle \neq 0$
$$\Rightarrow a|n\rangle \neq 0).$$

Further $a|n\rangle$ is an eigenvector of N
$$N(a|n\rangle) = (Na - aN + aN)|n\rangle$$
$$= \underbrace{[N,a]}_{=-a}|n\rangle + a\underbrace{N|n\rangle}_{=n|n\rangle}$$
$$= -a|n\rangle + an|n\rangle$$
$$= (n-1)(a|n\rangle).$$ Indeed

$a|n\rangle$ is an eigenvector of N with eigenvalue $(n-1)$.

3) Lemma 3: Let $|n\rangle$ be a non-zero eigenvector of N with eigenvalue n, then

1) $a^\dagger|n\rangle$ is always non-zero
2) $a^\dagger|n\rangle$ is an eigenvector of N with eigenvalue $n+1$.

Proof: 1) $\| a^\dagger|n\rangle\|^2 = \langle n|a a^\dagger|n\rangle$

$$= \langle n|aa^\dagger - a^\dagger a + a^\dagger a|n\rangle$$

$$= \langle n|a^\dagger a + [a, a^\dagger]|n\rangle$$

but $a^\dagger a|n\rangle = N|n\rangle = n|n\rangle$ and $[a, a^\dagger] = 1$

$\Rightarrow$ $\| a^\dagger|n\rangle\|^2 = (n+1)\langle n|n\rangle$. Lemma 1 implied $n \geq 0$, therefore $\| a^\dagger|n\rangle\|^2 > 0$

$\Rightarrow$ $\underline{a^\dagger|n\rangle \neq 0}$.

2) As we have just seen

$$N(a^\dagger|n\rangle) = (Na^\dagger - a^\dagger N + a^\dagger N)|n\rangle$$

$$= \underbrace{[N,a^\dagger]}_{=+a^\dagger}|n\rangle + a^\dagger \underbrace{N|n\rangle}_{=n|n\rangle}$$

$$= a^\dagger|n\rangle + a^\dagger n|n\rangle$$

$$= (n+1)(a^\dagger|n\rangle).$$

Thus $a^\dagger|n\rangle$ is an eigenvector of N with eigenvalue $(n+1)$.

Theorem: The spectrum of N is composed of non-negative integers.

Proof: assume n is non-integer valued and non-zero. Then $a|n\rangle$ has eigenvalue $(n-1)$. Since $a|n\rangle$ is non-zero, $aa|n\rangle$ is non-zero with eigenvalue $n-2$. We can continue this indefinitely.

$a^p|n\rangle$ is a non-zero eigenvector of N with eigenvalue $n-p$ by Lemma 2.
At some point $p > n$, then $n-p < 0$, a negative eigenvalue. But by Lemma 1 all eigenvalues of N are non-negative. Hence <u>n must be a non-negative integer.</u>

Suppose n = positive integer or zero. The vectors $a^p|n\rangle$ are non-zero if $p \leq n$. Suppose $p = n$, $a^n|n\rangle$ is a non-zero eigenvector of N with eigenvalue $n-n=0$. Then according to Lemma 2, $a^{n+1}|n\rangle = 0$, the zero vector. The sequence of vectors $a^p|n\rangle$ terminates after $a^n|n\rangle$, which has 0 eigenvalue. Hence only non-negative integer eigenvalues occur, i.e. $n=0,1,2,\ldots$ This series continues indefinitely due to Lemma 3. Since $a^n|n\rangle$ has eigenvalue 0, then

$(a^\dagger)^p(a^n|n\rangle)$ is a non-zero

eigenvector with eigenvalue p and p is any positive integer. Thus $\{n\}$ covers all non-negative integers. Denoting the 0 eigenvalue vector as $|0\rangle$, the eigenvectors are given by

$$|n\rangle = (a^\dagger)^n|0\rangle.$$

(up to a suppressed, complex constant of normalization)

Starting with any $|n\rangle$ we find

$$|n+1\rangle = a^{+}|n\rangle \quad \text{and} \quad |n-1\rangle = a|n\rangle$$

Further the eigenvalues of the Hamiltonian are the eigenvalues of

$$H = \hbar\omega(N + \tfrac{1}{2}). \text{ That is}$$

$$\boxed{E_n = \hbar\omega(n + \tfrac{1}{2}), \quad n = 0, 1, 2, \ldots}$$

Since a^{+} operating on $|n\rangle$ increases the energy by $\hbar\omega$, it is called the raising (or creation) operator; since a operating on $|n\rangle$ gives a state with energy decreased by $\hbar\omega$, it is called the lowering (or annihilation or destruction) operator.

Next, we must determine whether there is only one state for each eigenvalue. That is we will show that the <u>energy levels</u> are <u>non-degenerate</u>.

<u>Lemma 4</u>: The ground state (the $n=0$ eigenstate) is non-degenerate.

<u>Proof</u>: The $n=0$ eigenstates obey

$$a|0\rangle = 0 \quad \text{according to Lemma 2.}$$

To show there is only one such state, consider the definition of a

$$a = \frac{1}{\sqrt{2}}\left(\sqrt{\frac{m\omega}{\hbar}}\, X + \frac{i}{\sqrt{m\hbar\omega}}\, P\right).$$

In the coordinate representation with basis vectors $\{|x\rangle\}$, this becomes

$$\langle x|a|0\rangle = 0$$

$$= \frac{1}{\sqrt{2}}\left(\sqrt{\frac{m\omega}{\hbar}}\, \underbrace{\langle x|X|0\rangle}_{= x\langle x|} + \frac{i}{\sqrt{m\hbar\omega}}\, \underbrace{\langle x|P|0\rangle}_{-\frac{\hbar}{i}\frac{d}{dx}\langle x|}\right)$$

Thus we obtain a differential equation,

$$\left(\frac{d}{dx} + \frac{m\omega}{\hbar} x\right)\langle x|0\rangle = 0,$$

for the ground state wavefunction

$$\psi_0(x) = \langle x|0\rangle .$$

This is a first order ordinary differential equation, the general solution is

$$\psi_0(x) = C\, e^{-\frac{1}{2}\frac{m\omega}{\hbar}x^2}$$

with C = constant of integration, the normalization factor for the state. Thus there is only one state corresponding to the ground state, all solutions $\psi_0(x)$ are proportional, C being just the normalization constant.

Hence there exists only one ket vector $|0\rangle$, up to normalization, with N eigenvalue 0. The <u>ground state is non-degenerate</u>.

<u>Lemma 5</u>: All eigenvalues of N are non-degenerate.

<u>Proof</u>: The proof is by induction. Assume, to within normalization, there is only one eigenstate $|n\rangle$ such that $N|n\rangle = n|n\rangle$. Let $|n+1, \alpha\rangle$ be a particular one of the eigenvectors of N with eigenvalue $(n+1)$. It is labelled by α. So $N|n+1, \alpha\rangle = (n+1)|n+1, \alpha\rangle$.

Now by Lemma 2, $a|n+1, \alpha\rangle \neq 0$

and has N-eigenvalue n. Since by hypothesis this ket is non-degenerate, there exists a number c_α such that

$$a|n+1,\alpha\rangle = c_\alpha |n\rangle .$$

We can invert this by applying $a^\dagger$

$$\underbrace{a^\dagger a|n+1,\alpha\rangle} = c_\alpha a^\dagger |n\rangle$$

$$= N|n+1,\alpha\rangle$$

$$= (n+1)|n+1,\alpha\rangle . \quad \text{So}$$

$$\boxed{|n+1,\alpha\rangle = \frac{c_\alpha}{(n+1)} a^\dagger |n\rangle .}$$

Hence, all vectors $|n+1,\alpha\rangle$ with eigenvalue $n+1$ are proportional to eachother and $a^{\dagger}|n\rangle$. Thus the $(n+1)$ eigenvalue is non-degenerate.

<u>Theorem:</u> All eigenvalues of N, and hence H, are non-degenerate.

(Proof: Lemma 4 and Lemma 5.)

So we do not need label α for the eigenstates; $|n\rangle$ is the one eigenvector corresponding to the eigenvalue n, only its normalization is arbitrary.

So the set of all eigenvectors $\{|n\rangle\}$ of N (or H) form a basis for the Hilbert space of onedimensional particle states, $\mathcal{H}$. Let's investigate this basis further. As well we can find the matrix elements of the position, X, and momentum, P, operators in this basis.

Number Operator Eigenvector Basis or Energy Representation

1) The ground state, that is the lowest energy eigenstate $|0\rangle$, as we have seen from lemmas 2 and 4, is defined, up to a complex normalization factor, by

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

We will choose $|0\rangle$ to be normalized to one by convention; $\langle 0|0\rangle \equiv 1$. This fixes the state $|0\rangle$ only up to a constant phase factor i.e.

$$|0'\rangle = e^{i\theta}|0\rangle \quad \text{and still}$$

$$\langle 0'|0'\rangle = \langle 0|0\rangle .$$

2) Excited states have $n \geq 1$. The $n=1$ eigenvector is proportional to $a^\dagger|0\rangle$

$$|n=1\rangle \equiv c_1 a^\dagger |0\rangle \quad , \quad c_1 \in \mathbb{C}.$$

We can conventionally choose c_1 so that

1) $\langle 1|1\rangle \equiv 1$

2) Phase of $|1\rangle$ relative to $|0\rangle$ is such that c_1 is real and positive.

Explicitly,

$$\langle 1|1\rangle \equiv 1$$

$$= |c_1|^2 \langle 0|a a^\dagger|0\rangle \, , \quad \text{since } (|1\rangle)^\dagger = \langle 1| = c_1^* \langle 0|a \, ,$$

$$= |c_1|^2 \langle 0|a a^\dagger - a^\dagger a + a^\dagger a|0\rangle \, ,$$

but $[a, a^\dagger] = 1$ and the ground state is defined by $a|0\rangle = 0$,

So
$$1 = |c_1|^2 \langle 0|0\rangle = |c_1|^2.$$

Thus
$$c_1 = e^{i\theta_1} \quad \text{by } \langle 1|1\rangle = 1.$$

Next relative to $|0\rangle$, the phase of $|1\rangle$ is such that c_1 is real and positive, to be chosen

but
$$|1\rangle = \underbrace{e^{i\theta_1}} a^\dagger |0\rangle$$

real and positive $\Rightarrow \theta_1 = 0$.

Hence by convention
$$\boxed{|n=1\rangle \equiv a^\dagger |0\rangle}$$

Similarly the second excited state $|n=2\rangle \equiv c_2 a^\dagger |1\rangle$. By convention c_2 is such that 1) $\langle 2|2\rangle \equiv 1$ and 2) the phase of $|2\rangle$ relative to $|1\rangle$ is such that c_2 is real and positive.

So

$$\langle 2|2\rangle \equiv 1$$

$$= |C_2|^2 \langle 1|a a^\dagger|1\rangle$$

$$= |C_2|^2 \langle 1|\underbrace{a a^\dagger - a^\dagger a}_{=1} + a^\dagger a|1\rangle$$

$$= |C_2|^2\langle 1|1\rangle + |C_2|^2 \langle 1|\underbrace{\underbrace{a^\dagger a}_{=N}|1\rangle}_{=1|1\rangle}$$

$$= |C_2|^2 2\langle 1|1\rangle$$

$$= 2|C_2|^2 \Rightarrow \underline{C_2 = \frac{1}{\sqrt{2}} e^{i\theta_2}}$$

but C_2 is to be real and positive $\Rightarrow$

$$\boxed{\theta_2 = 0.}$$

So $C_2 = \frac{1}{\sqrt{2}}$ and

$$\boxed{|2\rangle = \frac{1}{\sqrt{2}} a^\dagger |1\rangle = \frac{1}{\sqrt{2}} (a^\dagger)^2 |0\rangle}$$

Continuing to the n^{th} excited state,

$|n-1\rangle$ normalized to 1

$$|n\rangle \equiv C_n a^\dagger |n-1\rangle$$

with C_n chosen so that 1) $\langle n|n\rangle \equiv 1$

and 2) the phase of $|n\rangle$ relative to $|n-1\rangle$

is such that C_n is real and positive.

$$\Rightarrow \boxed{\langle n|n\rangle \equiv 1}$$

$$= |C_n|^2 \langle n-1| a a^\dagger |n-1\rangle$$

$$= |C_n|^2 \langle n-1| \underbrace{a a^\dagger - a^\dagger a}_{=1} + \underbrace{a^\dagger a}_{=N} |n-1\rangle$$

$$= |C_n|^2 \langle n-1| [1 + (n-1)] |n-1\rangle$$

$$= |C_n|^2 n \langle n-1|n-1\rangle = |C_n|^2 n$$

$$\Rightarrow \quad C_n = e^{i\theta_n} \frac{1}{\sqrt{n}}.$$

C_n is real and positive $\Rightarrow$ $\theta_n = 0$.

So
$$\boxed{|n\rangle = \frac{1}{\sqrt{n}}\, a^\dagger\, |n-1\rangle}$$

But $|n-1\rangle = \frac{1}{\sqrt{n-1}}\, a^\dagger |n-2\rangle$ by a similar construction, and so on

$$|n\rangle = \frac{1}{\sqrt{n}}\frac{1}{\sqrt{n-1}}\frac{1}{\sqrt{n-2}}\cdots\frac{1}{\sqrt{2}}\frac{1}{\sqrt{1}}(a^\dagger)(a^\dagger)\cdots$$

$$\underbrace{\cdots(a^\dagger)(a^\dagger)}_{n\text{-factors of } a^\dagger}|0\rangle$$

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

Since $N = N^\dagger$, for $m \neq n$

$$\langle m|N|n\rangle = n\langle m|n\rangle$$
$$= \langle n|N^\dagger|m\rangle^* = \langle n|N|m\rangle^*$$
$$= m\langle n|m\rangle^* = m\langle m|n\rangle$$
$$\Rightarrow (n-m)\langle m|n\rangle = 0, \text{ for } n \neq m$$
$$\Rightarrow \langle m|n\rangle = 0.$$

Thus the (energy) number operator eigenvectors are orthonormal

$$\boxed{\langle m | n \rangle = \delta_{mn}}$$

(this can also be checked directly from $|n\rangle = \frac{1}{\sqrt{n!}}(a^\dagger)^n|0\rangle$ and $[a,a^\dagger]=1$).

Since N or H is an observable (Postulate 2) we have that $\{|n\rangle\}$ is complete

$$\mathbb{1} = \sum_{n=0}^{\infty} |n\rangle\langle n| \,;$$

That is given any state of our one-dimensional system $|\psi\rangle$ we have

$$|\psi\rangle = \sum_{n=0}^{\infty} \psi_n |n\rangle$$

with

$$\psi_n = \langle n|\psi\rangle .$$

(As we will see, since one can prove that the SHO energy eigenfunctions are complete, one can prove $\{|n\rangle\}$ are a basis.)

Matrix Elements of Operators in the $\{|n\rangle\}$ Basis

For the SHO, all observables can be expressed in terms of X and P, like the energy operator $H = \frac{1}{2m}P^2 + \frac{1}{2}m\omega^2 X^2$

Since X and P are linear combinations of $a, a^\dagger$, we can express all operators as functions of a and $a^\dagger$.

Hence it is useful to express the raising and lowering operators in the number operator eigenvector basis (energy basis).

With the above phase conventions

$$a^\dagger|n\rangle = \sqrt{n+1}\ |n+1\rangle$$, $a^\dagger$ raises the N-eigenvalue by 1; and

$$\begin{aligned} a|n\rangle &= a\left(\frac{1}{\sqrt{n}}\, a^\dagger|n-1\rangle\right) \\ &= \frac{1}{\sqrt{n}}\left(aa^\dagger - a^\dagger a + a^\dagger a\right)|n-1\rangle \\ &= \frac{1}{\sqrt{n}}(N+1)|n-1\rangle = \sqrt{n}\,|n-1\rangle \\ &= \sqrt{n}\ |n-1\rangle \end{aligned}$$

, a lowers the N-eigenvalue by 1. Since the $\{|n\rangle\}$ are orthonormal we find the matrix elements of $a, a^\dagger$ to be

$$\boxed{\begin{aligned} \langle m|a^\dagger|n\rangle &= \sqrt{n+1}\ \delta_{m,n+1} \\ \langle m|a|n\rangle &= \sqrt{n}\ \delta_{m,n-1} \end{aligned}}$$

.

So in the $\{|n\rangle\}$ basis we can represent the eigenstates $|n\rangle$ by ∞-dimensional column vectors, the conjugate states $\langle n|$ by ∞-dimensional row vectors, and the raising and lowering operators by ∞-dimensional matrices.

$$|n\rangle \longrightarrow \begin{array}{cl} \left(\begin{array}{c} 0 \\ \vdots \\ 0 \\ 1 \\ 0 \\ \vdots \\ 0 \end{array}\right) & \begin{array}{l} \\ \\ \\ \leftarrow \text{1 in the } n^{\text{th}} \text{ row} \\ \\ \\ \\ \end{array} \end{array}$$

$$\langle n| \longrightarrow \begin{array}{c} \left(0 \cdots 0 \;\; 1 \;\; 0 \cdots 0\right) \\ \uparrow \\ \text{1 in the } n^{\text{th}} \text{ column} \end{array}$$

Since $\langle m|a|n\rangle = \sqrt{n}\,\delta_{m,n-1}$

we have

$$
(a) = \begin{array}{c|cccccccc}
m\backslash n & 0 & 1 & 2 & 3 & \cdots & n & \cdots \\
\hline
0 & 0 & \sqrt{1} & 0 & 0 & \cdots & & \\
1 & 0 & 0 & \sqrt{2} & 0 & \cdots & & \\
2 & 0 & 0 & 0 & \sqrt{3} & 0 & \cdots & \\
3 & 0 & 0 & 0 & 0 & \ddots & & \\
\vdots & \vdots & \vdots & 0 & 0 & \ddots & & \\
n-1 & \vdots & \vdots & \vdots & \vdots & \ddots & \sqrt{n} & 0 \; \cdots \\
\vdots & & & & & & 0 & \ddots \\
 & & & & & & 0 & \ddots
\end{array}
$$

i.e.

$$
= \begin{bmatrix}
0 & \sqrt{1} & & & \\
 & 0 & \sqrt{2} & & \Large 0 \\
 & & 0 & \sqrt{3} & \\
 & \Large 0 & & 0 & \ddots \\
 & & & & \ddots
\end{bmatrix}
$$

And since $\langle m|a^\dagger|n\rangle = \sqrt{n+1}\,\delta_{m,n+1}$

we have

$$
(a^{\dagger}) = \begin{array}{c|cccccccc}
m \backslash n & 0 & 1 & 2 & 3 & \cdots & n & \cdots & \\
\hline
0 & 0 & & & & & & & \\
1 & \sqrt{1} & 0 & & & & O & & \\
2 & & \sqrt{2} & 0 & & & & & \\
3 & & & \sqrt{3} & 0 & & & & \\
\vdots & & O & & & \ddots & & & \\
& & & & & & 0 & & \\
n+1 & & & & & & \sqrt{n+1} & 0 & \\
\vdots & & & & & & & \ddots & \ddots
\end{array}
$$

i.e.

$$
= \begin{bmatrix}
0 & & & & \\
\sqrt{1} & 0 & & O & \\
 & \sqrt{2} & 0 & & \\
 & & \sqrt{3} & 0 & \\
 & O & & \ddots & \ddots
\end{bmatrix}.
$$

Note that

$$
(a^{\dagger})(a) = \begin{bmatrix}
0 & & & & \\
 & 1 & & O & \\
 & & 2 & & \\
 & O & & 3 & \\
 & & & & \ddots
\end{bmatrix}
$$

while

$$
(a)(a^{\dagger}) = \begin{bmatrix}
1 & & & \\
 & 2 & O & \\
 O & & 3 & \\
 & & & \ddots
\end{bmatrix}
$$

So
$$[(a),(a^\dagger)] = \begin{pmatrix} 1 & 0 & \\ 0 & 1 & \\ & & 1\ldots \end{pmatrix} = (\mathbb{1}) \text{, as it should}$$

Further, X and P operators are just related to a and $a^\dagger$ by

$$X = \sqrt{\frac{\hbar}{2m\omega}}\,(a^\dagger + a)$$
$$P = i\sqrt{\frac{m\hbar\omega}{2}}\,(a^\dagger - a)\ .$$ Hence the

matrix representation of X and P in the $\{|n\rangle\}$ basis is just given by the sum and difference of the above (a) and $(a^\dagger)$ matrices.

$$\langle m|X|n\rangle = \sqrt{\frac{\hbar}{2m\omega}}\left[\sqrt{n+1}\,\delta_{m,n+1} + \sqrt{n}\,\delta_{m,n-1}\right]$$

$$\langle m|P|n\rangle = i\sqrt{\frac{m\hbar\omega}{2}}\left[\sqrt{n+1}\,\delta_{m,n+1} - \sqrt{n}\,\delta_{m,n-1}\right].$$

Explicitly,

$$(X) = \sqrt{\frac{\hbar}{2m\omega}} \begin{bmatrix} 0 & \sqrt{1} & & & \\ \sqrt{1} & 0 & \sqrt{2} & & 0 \\ & \sqrt{2} & 0 & \sqrt{3} & \\ & & \sqrt{3} & 0 & \ddots \\ & 0 & & \ddots & \ddots \end{bmatrix}$$

$$(P) = i\sqrt{\frac{m\hbar\omega}{2}} \begin{bmatrix} 0 & -\sqrt{1} & & & \\ \sqrt{1} & 0 & -\sqrt{2} & & 0 \\ & \sqrt{2} & 0 & -\sqrt{3} & \\ & & \sqrt{3} & 0 & \ddots \\ & 0 & & \ddots & \ddots \end{bmatrix}.$$

Since $\{|n\rangle\}$ are the number operator eigenstates, N and hence H are diagonal in this basis

$$\langle m|N|n\rangle = n\delta_{m,n}$$

$$\langle m|H|n\rangle = \hbar\omega(n+\tfrac{1}{2})\delta_{m,n} .$$

Explicitly

$$(N) = \begin{pmatrix} 0 & & 0 \\ & 1 & \\ 0 & & 2 \\ & & & \ddots \end{pmatrix}$$

$$(H) = \hbar\omega \begin{bmatrix} 1/2 & & & \\ & 3/2 & & 0 \\ & & 5/2 & \\ 0 & & & \ddots \end{bmatrix}.$$

An arbitrary state at time t, $|\psi(t)\rangle$, obeys the Schrödinger equation

$$i\hbar \frac{d}{dt} |\psi(t)\rangle = H |\psi(t)\rangle$$

or

$$|\psi(t)\rangle = U(t,t_0) |\psi(t_0)\rangle$$

with the time-evolution operator

$$U(t,t_0) = e^{-\frac{i}{\hbar} H(t-t_0)}.$$

The state at time t_0 can be expanded in terms of the eigenstates of H, $\{|n\rangle\}$,

$$|\psi(t_0)\rangle = \sum_{n=0}^{\infty} \psi_n(t_0) |n\rangle,$$

with $\psi_n(t_0) = \langle n|\psi(t_0)\rangle$.

Then

$$|\psi(t)\rangle = \sum_{n=0}^{\infty} e^{-iE_n(t-t_0)/\hbar} \psi_n(t_0)\,|n\rangle$$

where $E_n = \hbar\omega(n+\frac{1}{2})$; $n = 0, 1, 2, \ldots$

The probability that the system is in an energy eigenstate (i.e. that we measure the energy E_n) $|n\rangle$ at time t is

$$P(n;t) = |\langle n|\psi(t)\rangle|^2$$

$$= \left| e^{-iE_n(t-t_0)/\hbar} \psi_n(t_0) \right|^2$$

$$= |\psi_n(t_0)|^2 = |\langle n|\psi(t_0)\rangle|^2$$

$$= P(n;t_0) \, ,$$

the same as at time t_0; it is independent of time.

Finally, let's consider the connection of the energy eigenstates to the SHO energy eigenfunctions of wave mechanics. That is, let's expand the energy eigenvectors in terms of the position coordinate eigenvector basis $\{|x\rangle\}$ where

$$X|x\rangle = x|x\rangle$$

and $$\langle x'|x\rangle = \delta(x-x')$$

while $$\int_{-\infty}^{+\infty} dx\, |x\rangle\langle x| = \mathbb{1}.$$

Thus $$|n\rangle = \int_{-\infty}^{+\infty} dx\, \psi_n(x)\,|x\rangle$$

with $$\psi_n(x) = \langle x|n\rangle.$$

We already found that $a|0\rangle = 0 \Rightarrow$

(p. -385-) $$\psi_0(x) = \langle x|0\rangle = C\, e^{-\frac{1}{2}\frac{m\omega}{\hbar}x^2}.$$

By our normalization conventions

$$\langle 0|0\rangle \equiv 1 = \int_{-\infty}^{+\infty} dx\, \psi_0^*(x)\,\psi_0(x)$$

$\Rightarrow$

$$1 = |C|^2 \int_{-\infty}^{+\infty} dx\, e^{-\frac{m\omega}{\hbar} x^2} = |C|^2 \sqrt{\frac{\hbar\pi}{m\omega}}$$

Thus

$$C = \left(\frac{m\omega}{\hbar\pi}\right)^{1/4} e^{i\theta_0} .$$

Without loss of generality we can choose $\theta_0 = 0$.

Thus the normalized ground state wavefunction is just the Gaussian

$$\boxed{\psi_0(x) = \left(\frac{m\omega}{\hbar\pi}\right)^{1/4} e^{-\frac{1}{2}\frac{m\omega}{\hbar} x^2} .}$$

The n^{th} excited state is given by

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

with $\langle n|n\rangle = 1$. Thus its wavefunction is

$$\psi_n(x) = \langle x|n\rangle = \frac{1}{\sqrt{n!}} \langle x|(a^\dagger)^n|0\rangle .$$

But with any state $|\phi\rangle$, we have

$$\langle x|a^\dagger|\phi\rangle = \frac{1}{\sqrt{2}}\langle x|\sqrt{\frac{m\omega}{\hbar}}\,X - i\sqrt{\frac{1}{m\hbar\omega}}\,P|\phi\rangle$$

$$= \frac{1}{\sqrt{2}}\left(\sqrt{\frac{m\omega}{\hbar}}\,x - i\sqrt{\frac{1}{m\hbar\omega}}\,\frac{\hbar}{i}\frac{d}{dx}\right)\langle x|\phi\rangle.$$

This implies

$$\psi_n(x) = \frac{1}{\sqrt{n!}}\,\frac{1}{2^{n/2}}\left(\sqrt{\frac{m\omega}{\hbar}}\,x - \sqrt{\frac{\hbar}{m\omega}}\,\frac{d}{dx}\right)^n \langle x|0\rangle$$

Recall p. -133- to -148-, with $\xi = \sqrt{\frac{m\omega}{\hbar}}\,x$

This becomes

$$\boxed{\begin{aligned}\psi_n(x) &= \frac{1}{\sqrt{2^n n!}}\left(\xi - \frac{d}{d\xi}\right)^n \psi_0(x)\\ &= \left(\frac{m\omega}{\hbar\pi}\right)^{1/4}\frac{1}{\sqrt{2^n n!}}\left(\xi - \frac{d}{d\xi}\right)^n e^{-\frac{1}{2}\xi^2}\end{aligned}}$$

the SHO wavefunction, since

$$H_n(\xi) = (-1)^n e^{+\frac{1}{2}\xi^2}\left(\frac{d}{d\xi} - \xi\right)^n e^{-\frac{1}{2}\xi^2}.$$

(p. -142-)

In fact the creation and annihilation operators in the coordinate representation are

$$\langle x|a = \frac{1}{\sqrt{2}}\left(\xi + \frac{d}{d\xi}\right)\langle x|$$

$$\langle x|a^\dagger = \frac{1}{\sqrt{2}}\left(\xi - \frac{d}{d\xi}\right)\langle x|,$$

nothing but the differential operators introduced to analyze the SHO wave equation earlier.

Thus we find that

$$\boxed{\begin{aligned}\psi_n(x) &= \langle x|n\rangle \\ &= \left(\frac{m\omega}{\hbar\pi}\right)^{1/4}\frac{1}{\sqrt{2^n n!}}\,H_n\!\left(\sqrt{\frac{m\omega}{\hbar}}\,x\right)e^{-\frac{1}{2}\frac{m\omega}{\hbar}x^2}\end{aligned}}$$

Since $\langle m|n\rangle = \delta_{mn} = \int_{-\infty}^{+\infty} dx\, \psi_m^*(x)\,\psi_n(x)$,

as we checked explicitly earlier using the properties of the Hermite polynomials.

Also the Hermite polynomials are complete, as can be shown mathematically, in $L^2(R^1)$; hence we have that

$$\mathbb{1} = \sum_{n=0}^{\infty} |n\rangle\langle n| \quad \text{yields}$$

$$\langle x'|x\rangle = \sum_{n=0}^{\infty} \langle x'|n\rangle\langle n|x\rangle$$

$$= \sum_{n=0}^{\infty} \psi_n^*(x)\psi_n(x')$$

but

$$\langle x'|x\rangle = \delta(x-x')$$

$$= \sum_{n=0}^{\infty} \psi_n^*(x)\psi_n(x'),$$

the expression of completeness in wavefunction space.

Rather than working in the Schrödinger picture, as above, it is instructive to work in the Heisenberg picture in which X and P now depend on time. Letting the pictures coincide at $t=0$, we have, of course, that the Hamiltonian is still time independent

$$H = \frac{1}{2m} P^2(t) + \frac{1}{2} m\omega^2 X^2(t)$$

but that $X(t)$ and $P(t)$ now depend on time (i.e.

$$A_H(t) = U^{-1}(t,0)\, A_S\, U(t,0))$$

and obey the Heisenberg equations of motion

$$\frac{d}{dt} X(t) = \frac{i}{\hbar}[H, X(t)]$$

$$\frac{d}{dt} P(t) = \frac{i}{\hbar}[H, P(t)].$$

Since $[P(t), X(t)] = \frac{\hbar}{i}\mathbb{1}$ still, the Heisenberg equations become coupled linear differential equations ("Hamilton's" equations for X and P). That is

$$[H, X(t)] = \frac{-i\hbar}{m} P(t)$$

$$[H, P(t)] = i\hbar m\omega^2 X(t) \quad \text{so}$$

$$\boxed{\begin{aligned} \frac{d}{dt} X(t) &= \frac{1}{m} P(t) \\ \frac{d}{dt} P(t) &= -m\omega^2 X(t) \end{aligned}}$$

We can solve these by diagonalizing the "Hamilton's" equations i.e. group these into a matrix equation

$$\frac{d}{dt}\begin{pmatrix} X(t) \\ P(t) \end{pmatrix} = \begin{pmatrix} 0 & \frac{1}{m} \\ -m\omega^2 & 0 \end{pmatrix}\begin{pmatrix} X(t) \\ P(t) \end{pmatrix} \quad \text{and}$$

multiply by the constant diagonalization matrix $\mathcal{U}$

$$\frac{d}{dt}\,\mathcal{U}\begin{pmatrix} X(t) \\ P(t) \end{pmatrix} = \mathcal{U}\begin{pmatrix} 0 & \frac{1}{m} \\ -m\omega^2 & 0 \end{pmatrix}\mathcal{U}^{-1}\,\mathcal{U}\begin{pmatrix} X(t) \\ P(t) \end{pmatrix}.$$

From our previous analysis we found the form of $\mathcal{U}$; that is

$$\begin{pmatrix} a(t) \\ a^\dagger(t) \end{pmatrix} \equiv \mathcal{U}\begin{pmatrix} X(t) \\ P(t) \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} \sqrt{\frac{m\omega}{\hbar}}\,X(t) + i\sqrt{\frac{1}{m\hbar\omega}}\,P(t) \\ \sqrt{\frac{m\omega}{\hbar}}\,X(t) - i\sqrt{\frac{1}{m\hbar\omega}}\,P(t) \end{pmatrix}$$

$$\Rightarrow \quad \mathcal{U} = \frac{1}{\sqrt{2\hbar}}\begin{pmatrix} \sqrt{m\omega} & \frac{i}{\sqrt{m\omega}} \\ \sqrt{m\omega} & \frac{-i}{\sqrt{m\omega}} \end{pmatrix}.$$

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i.e. $$\mathcal{U}\begin{pmatrix} 0 & \frac{1}{m} \\ -m\omega^2 & 0 \end{pmatrix}\mathcal{U}^{-1} = \begin{pmatrix} -i\omega & 0 \\ 0 & +i\omega \end{pmatrix}$$

So $$\frac{d}{dt}\begin{pmatrix} a(t) \\ a^\dagger(t) \end{pmatrix} = \begin{pmatrix} -i\omega & 0 \\ 0 & +i\omega \end{pmatrix}\begin{pmatrix} a(t) \\ a^\dagger(t) \end{pmatrix}.$$

This yields

$$a(t) = e^{-i\omega t}\, a(0) \equiv e^{-i\omega t}\, a$$
$$a^{\dagger}(t) = e^{+i\omega t}\, a^{\dagger}(0) \equiv e^{+i\omega t}\, a^{\dagger} .$$

As before, we obtain the creation and annihilation operator commutation relation.

$$[a(t), a^{\dagger}(t)] = 1 = [a, a^{\dagger}] .$$

The Hamiltonian takes the simple form

$$H = \left(X(t)\ P(t)\right) \begin{pmatrix} \frac{1}{2}m\omega^2 & 0 \\ 0 & \frac{1}{2m} \end{pmatrix} \begin{pmatrix} X(t) \\ P(t) \end{pmatrix}$$

$$= \left(a^{\dagger}(t)\ a(t)\right) U^{-1\dagger} \begin{pmatrix} \frac{1}{2}m\omega^2 & 0 \\ 0 & \frac{1}{2m} \end{pmatrix} U^{-1} \begin{pmatrix} a(t) \\ a^{\dagger}(t) \end{pmatrix}$$

but

$$U^{-1} = i\sqrt{\frac{\hbar}{2}} \begin{pmatrix} \frac{-i}{\sqrt{m\omega}} & \frac{-i}{\sqrt{m\omega}} \\ -\sqrt{m\omega} & \sqrt{m\omega} \end{pmatrix}$$

So $$H = \frac{\hbar\omega}{2} \left(a^{\dagger}\ a\right) \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} a \\ a^{\dagger} \end{pmatrix}$$

$$H = \frac{1}{2}\hbar\omega\left(a^{\dagger}(t)a(t) + \underbrace{a(t)\,a^{\dagger}(t)}_{= a^{\dagger}(t)a(t)+1}\right)$$

$$H = \hbar\omega\left[a^{\dagger}(t)a(t) + \tfrac{1}{2}\right]$$

but $a(t)\,a^{\dagger}(t) = aa^{\dagger}$

$a^{\dagger}(t)\,a(t) = a^{\dagger}a$ independent of time

So

$$\boxed{\begin{aligned} H &= \tfrac{1}{2}\hbar\omega\left[a^{\dagger}a + aa^{\dagger}\right] \\ &= \hbar\omega\left[a^{\dagger}a + \tfrac{1}{2}\right] \end{aligned}}$$

As earlier, we can represent the creation and annihilation operator algebra, $[a,a^{\dagger}]=1$; $[a,a]=0$, $[a^{\dagger},a^{\dagger}]=0$, on the number operator, $N \equiv a^{\dagger}a$, eigenvectors $N|n\rangle = n|n\rangle$.