Harmonic Oscillator (2nd quantization only).

This problem is solved at the undergraduate level in term of Hermite polynomials. Here, we will solve the problem without recourse to a specific representation.

The harmonic oscillator problem has the general form, in 1 dimension

$$\hat{H} = \frac{\hat{P}^2}{2M} + \frac{M\omega^2}{2}\hat{Q}^2$$

(rather than the usual $\frac{k}{2}$, we have used $\frac{M\omega^2}{2}$). k is found from $-\frac{\partial W}{\partial Q}$

We begin by replacing $\hat{P}$ and $\hat{Q}$ by dimensionless operators $\hat{p}, \hat{q}$

$$\hat{p} = \left(\frac{1}{M\hbar\omega}\right)^{1/2}\hat{P} \qquad \hat{q} = \left(\frac{M\omega}{\hbar}\right)^{1/2}\hat{Q}$$

So, $$[\hat{q}, \hat{p}] = \left[\left(\frac{M\omega}{\hbar}\right)^{1/2}\hat{Q}, \left(\frac{1}{M\hbar\omega}\right)^{1/2}\hat{P}\right] = \frac{1}{\hbar}[\hat{Q}, \hat{P}] = i$$

In terms of these new variables, the Hamiltonian has the form

$$\hat{H} = \frac{1}{2M}(M\hbar\omega)\hat{p}^2 + \frac{M\omega^2}{2}\left(\frac{\hbar}{M\omega}\right)\hat{q}^2 = \frac{1}{2}\omega\hbar\left(\hat{p}^2 + \hat{q}^2\right).$$

Suppose that we now take linear combinations of $\hat{p}$ & $\hat{q}$ to form

$$\hat{a} = \frac{\hat{q} + i\hat{p}}{\sqrt{2}} \qquad \hat{a}^\dagger = \frac{\hat{q} - i\hat{p}}{\sqrt{2}} \qquad \hat{a} \neq \hat{a}^\dagger \text{ since } \hat{q} = \hat{q}^\dagger; \hat{p} = \hat{p}^\dagger.$$

Further,

$$[\hat{a}, \hat{a}^\dagger] = \frac{1}{2}\left((\hat{q} + i\hat{p})(\hat{q} - i\hat{p}) - (\hat{q} - i\hat{p})(\hat{q} + i\hat{p})\right)$$
$$= \frac{1}{2}\left(\hat{q}^2 + i\hat{p}\hat{q} - i\hat{q}\hat{p} + \hat{p}^2 - \hat{q}^2 - i\hat{q}\hat{p} + i\hat{p}\hat{q} - \hat{p}^2\right)$$
$$= \frac{1}{2}\left(2i\hat{p}\hat{q} - 2i\hat{q}\hat{p}\right) = i[\hat{p}, \hat{q}] = 1.$$

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Substituting back into the Hamiltonians

$$\hat{q} = \frac{1}{\sqrt{2}}(\hat{a}^+ + \hat{a}) \qquad \hat{p} = \frac{1}{\sqrt{2}}(\hat{a}^+ - \hat{a})$$

$$\Rightarrow \hat{H} = \frac{1}{2}\omega\hbar\left(\frac{1}{2}(\hat{a}^+ - \hat{a})^2 + \frac{1}{2}(\hat{a}^+ + \hat{a})^2\right) = \frac{1}{2}\omega\hbar\left(\hat{a}^+\hat{a} + \hat{a}\hat{a}^+\right)$$

But, from the commutation relation $\hat{a}\hat{a}^+ - a^+a = 1 \Rightarrow \hat{a}\hat{a}^+ = 1 + \hat{a}^+\hat{a}$

$$\Rightarrow \hat{H} = \frac{1}{2}\omega\hbar\left(2\hat{a}^+\hat{a} + 1\right) = \omega\hbar\left(\hat{a}^+\hat{a} + 1/2\right)$$

Hence we are solving for $\hat{H}\psi = \omega\hbar(\underline{\underline{\hat{a}^+\hat{a}}} + \frac{1}{2})\psi$

our problem is to find the eigenvalues of this operator, which we define as $\hat{N} = \hat{a}^+\hat{a}$.

Now, need to obtain commutation relations between $\hat{N}$ and $\hat{a}$ or $\hat{a}^+$.

We use

$$[AB, C] = ABC - CAB = ABC - ACB + ACB - CAB = A[B,C] + [A,C]B.$$

$$\Rightarrow [\hat{N}, \hat{a}] = [\hat{a}^+\hat{a}, \hat{a}] = \hat{a}^+[\hat{a}, \hat{a}] + [\hat{a}^+, a]\hat{a} = 0 - \hat{a} = -\hat{a}$$

$$[\hat{N}, \hat{a}^+] = [\hat{a}^+\hat{a}, \hat{a}^+] = \hat{a}^+[\hat{a}, \hat{a}^+] + [\hat{a}^+, \hat{a}^+]\hat{a} = \hat{a}^+(1) + 0 = \hat{a}^+.$$

Suppose now that we have a state $|\nu\rangle$ such that

$\hat{N}|\nu\rangle = \nu|\nu\rangle$ (ν is just some eigenvalue at the moment)

$$\Rightarrow \hat{N}\hat{a}|\nu\rangle = (\hat{a}\hat{N} - \hat{a})|\nu\rangle = (\hat{a}\nu - \hat{a})|\nu\rangle = (\nu - 1)\hat{a}|\nu\rangle$$

So, the operator $\hat{a}$ reduces the eigenvalue by 1 $\rightarrow \hat{a}|\nu\rangle \rightarrow |\nu - 1\rangle$

But what is ν? First, ν is ≥ 0, which can be seen from

$\langle\nu|\hat{N}|\nu\rangle = \langle\nu|\hat{a}^+\rangle\langle\hat{a}|\nu\rangle = |\langle a|\nu\rangle|^2 \geq 0 \longrightarrow \therefore \nu \geq 0$

$\hookrightarrow$ also $= \nu\underbrace{\langle\nu|\nu\rangle}_{\text{positive}}$

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If $\nu \geq 0$, then there must be a minimum value to the sequence

$$\hat{a}\hat{a}\hat{a}\hat{a}|\nu\rangle \to \hat{a}\hat{a}\hat{a}|\nu-1\rangle \to \hat{a}\hat{a}|\nu-2\rangle \dots$$

This implies that we enter negative ν unless we insist that the sequence terminates at $\nu = 0$, and all states $|\nu\rangle$ are characterized by non-negative integers. This hypothesis is consistent with the behavior of $a^+|\nu\rangle$:

$$\hat{N}\hat{a}^+|\nu\rangle = \hat{a}^+ N|\nu\rangle + a^+|\nu\rangle = a^+(\nu+1)|\nu\rangle$$
so $a^+|\nu\rangle \to |\nu+1\rangle$.

In summary so far, the eigenstates are characterized by a non-negative integer n, and
$\hat{N}$ - is the number operator $\hat{N}|n\rangle = n|n\rangle$
$\hat{a}^+$ - is the creation operator
$\hat{a}$ - is the destruction operator.

To find the exact forms of $\hat{a}$, $\hat{a}^+|\nu\rangle$, we write

$$\hat{a}^+|n\rangle = c_n|n+1\rangle.$$

$$\langle n|\hat{a}\;\hat{a}^+|n\rangle = \left(c_n^*\langle n+1|\right)\left(c_n|n+1\rangle\right) = |c_n|^2$$
$$\langle n|a^+a+1|n\rangle = \langle n|\hat{N}+1|n\rangle = n+1 \qquad \therefore c_n = \sqrt{n+1}$$

$$\Rightarrow \hat{a}^+|n\rangle = \sqrt{n+1}\;|n+1\rangle$$
and similarly $\hat{a}|n\rangle = \sqrt{n}\;|n-1\rangle$.

Finally, returning to the Hamiltonian,
$$E_n|n\rangle = (a^+a + 1/2)\hbar\omega|n\rangle$$
$$= (n+1/2)\hbar\omega|n\rangle$$

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In the above, we did not need a specific representation to get the eigenvalues. If we solve in coordinate space, we find

$$\psi_n(x) = \left[\frac{\alpha}{\pi^{1/2} 2^n n!}\right]^{1/2} H_n(\alpha x) e^{-\alpha^2 x^2/2}$$

where $\alpha = (M\omega/\hbar)^{1/2}$

and $H_n(z)$ are the Hermite polynomials

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