Harmonic Oscillators Are Ubiquitous

Suppose $V(x)$ is a 1-dimensional potential with a minimum at x_0. Then if $V(x)$ is smooth, near x_0 it will look like its Taylor series

$$V(x) = V(x_0) + \frac{(x-x_0)^2}{2} V''(x_0)$$

with the $(x-x_0)V'(x_0)$ term missing since $V'(x_0)=0$.

So for this $V(x)$, the ground state will be the ground state of the harmonic oscillator with

$$m\omega^2 = V''(x_0).$$

Now go to 3 dimensions. Suppose $V(x,y,z) = V(x_1,x_2,x_3) = V(\vec{r}) = V(\vec{x})$ is a smooth potential with a minimum at $\vec{x}_0$. Then all its first derivatives will vanish at $\vec{x}_0$, and the first 3 terms of its Taylor series will be

$$V(\vec{r}) = V(\vec{r}_0) + \frac{(x-x_0)^2}{2} V_{xx}(\vec{r}_0) + \frac{(y-y_0)^2}{2} V_{yy}(\vec{r}_0)$$
$$+ \frac{(z-z_0)^2}{2} V_{zz}(\vec{r}_0) + (x-x_0)(y-y_0) V_{xy}(\vec{r}_0)$$
$$+ (y-y_0)(z-z_0) V_{yz}(\vec{x}_0) + (x-x_0)(z-z_0) V_{xz}(\vec{r}_0)$$

in which I used the notation

$$V_{yz}(\vec{r}_0) = \left.\frac{\partial^2 V(\vec{r})}{\partial y \partial z}\right|_{r=r_0} .$$

The matrix of derivatives V_2 is

$$V_2 = \begin{pmatrix} V_{xx} & V_{xy} & V_{xz} \\ V_{yx} & V_{yy} & V_{yz} \\ V_{zx} & V_{zy} & V_{zz} \end{pmatrix}$$

and in term of it $V(\vec{r})$ near $\vec{r}_0$ is

$$V(\vec{r}) = V(\vec{r}_0) + \tfrac{1}{2}(\overrightarrow{r-r_0})^T V_{22} (\overrightarrow{r-r_0})$$

in which $(\overrightarrow{r-r_0})$ is a column 3-vector. The function $V(\vec{r})$ is real, so the matrix V_2 is real and symmetric. It can therefore be diagonalized by a real unitary matrix, i.e., by an orthogonal matrix O

$$1 = O^\dagger O = O^T O$$

$$O^T V_2 O = m \begin{pmatrix} \omega_1^2 & 0 & 0 \\ 0 & \omega_2^2 & 0 \\ 0 & 0 & \omega_3^2 \end{pmatrix} = m\Omega^2.$$

The e-vals $m\omega_i^2$ are all positive because $V(\vec{r}_0)$ is a minimum.

Every 3×3 orthogonal matrix represents a rotation or a reflection or both. These matrices form a group called $O(3)$.

Note that since the determinant of a product of matrices is the product of the determinants,

$$1 = O^T O \qquad \text{implies that}$$

$$1 = |O^T||O| = |O|^2$$

since $|O^T| = |O|$. So

$$|O| = \pm 1.$$

The subgroup with $|O| = 1$ is called $SO(3)$. This group $SO(3)$ is the group of rotations in 3 dimensions.

Change to the new coordinates

$$\frac{1}{2}(\vec{r-r_0})^T V_{22} (\vec{r-r_0}) = \frac{1}{2}(r-r_0)^T O^T m\Omega^2 O(r-r_0)$$

The new coordinates are $\vec{R-R_0} = O(\vec{r-r_0})$. In terms of them, the potential is

$$V(\vec{R}) = V(R_0) + \frac{1}{2}m(\vec{R-R_0})^T \Omega^2 (\vec{R-R_0}).$$

So the hamiltonian (near $\vec{r}_0$) is

$$H = \frac{\vec{P}^2}{2m} + \frac{1}{2} m \sum_{i=1}^{3} \omega_i^2 (R_i - R_{0i})^2 .$$

That's just 3 harmonic oscillators.

The energy e-vals are

$$E_{n_1 n_2 n_3} = \sum_{i=1}^{3} \hbar \omega_i (n_i + \tfrac{1}{2}) .$$

The e-vecs are

$$|n_1 n_2 n_3\rangle = \frac{(a_3^+)^{n_3} (a_2^+)^{n_2} (a_1^+)^{n_1}}{\sqrt{n_3!}\,\sqrt{n_2!}\,\sqrt{n_1!}} |0\rangle .$$