Matrix elements for position X and momentum P are the following transition amplitudes.

$$X_{kj} = \int_{-\infty}^{\infty} \psi_k^* \, x \, \psi_j \, dx$$

$$P_{kj} = \int_{-\infty}^{\infty} \psi_k^* \left(-i\hbar \frac{d}{dx} \right) \psi_j \, dx$$

For 4×4 matrices we have

$$X = \left(\frac{\hbar}{2m\omega} \right)^{1/2} \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & \sqrt{2} & 0 \\ 0 & \sqrt{2} & 0 & \sqrt{3} \\ 0 & 0 & \sqrt{3} & 0 \end{pmatrix}$$

$$P = i \left(\frac{\hbar m\omega}{2} \right)^{1/2} \begin{pmatrix} 0 & -1 & 0 & 0 \\ 1 & 0 & -\sqrt{2} & 0 \\ 0 & \sqrt{2} & 0 & -\sqrt{3} \\ 0 & 0 & \sqrt{3} & 0 \end{pmatrix}$$

$$H = \frac{P^2}{2m} + \frac{1}{2} m\omega^2 X^2 = \begin{pmatrix} \frac{1}{2}\hbar\omega & 0 & 0 & 0 \\ 0 & \frac{3}{2}\hbar\omega & 0 & 0 \\ 0 & 0 & \frac{5}{2}\hbar\omega & 0 \\ 0 & 0 & 0 & \frac{7}{2}\hbar\omega \end{pmatrix}$$

H_{33} cannot be computed using 4×4 matrices. The value $\frac{7}{2}\hbar\omega$ is the corrected eigenvalue.

Consider the following eigenfunction.

$$\Psi = \sum_k c_k \psi_k$$

Let us compute the expected value of x for a system in state Ψ.

$$\langle x \rangle = \int_{-\infty}^{\infty} \Psi^* x \Psi \, dx$$

Expand the integrand.

$$\begin{aligned} \langle x \rangle &= \int_{-\infty}^{\infty} \left(\sum_k c_k^* \psi_k^* \right) x \left(\sum_j c_j \psi_j \right) \\ &= \sum_k \sum_j c_k^* c_j \int_{-\infty}^{\infty} \psi_k^* \, x \, \psi_j \, dx \\ &= \sum_k \sum_j c_k^* c_j X_{kj} \end{aligned}$$

Hence

$$\langle x \rangle = \begin{pmatrix} c_0^* & c_1^* & c_2^* & \dots \end{pmatrix} X \begin{pmatrix} c_0 \\ c_1 \\ c_2 \\ \vdots \end{pmatrix}$$