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.

$$\Psi = \sum_{k=0}^{3} c_k \psi_k$$

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.

$$\begin{aligned} \langle x \rangle &= \int_{-\infty}^{\infty} \left(\sum_{k=0}^{3} c_k^* \psi_k^*\right) x \left(\sum_{j=0}^{3} c_j \psi_j\right) \\ &= \sum_{k=0}^{3} \sum_{j=0}^{3} c_k^* c_j \int_{-\infty}^{\infty} \psi_k^* \, x \, \psi_j \, dx \\ &= \sum_{k=0}^{3} \sum_{j=0}^{3} c_k^* c_j X_{kj} \end{aligned} \tag{1}$$

Noting that $X_{kj} = 0$ for $|k - j| \neq 1$ we have

$$\langle x \rangle = \sum_{k=0}^{2} \left(c_k^* c_{k+1} X_{k,k+1} + c_{k+1}^* c_k X_{k+1,k}\right)$$

Noting that $X_{k,k+1} = X_{k+1,k}$ we have

$$\begin{aligned}\langle x \rangle &= \sum_{k=0}^{2} \left(c_k^* c_{k+1} + c_{k+1}^* c_k \right) X_{k,k+1} \\ &= (c_0^* c_1 + c_1^* c_0) X_{01} + (c_1^* c_2 + c_2^* c_1) X_{12} + (c_2^* c_3 + c_3^* c_2) X_{23}\end{aligned}$$

From equation (1) above, the expected value of x can also be computed this way.

$$\langle x \rangle = \begin{pmatrix} c_0^* & c_1^* & c_2^* & c_3^* \end{pmatrix} X \begin{pmatrix} c_0 \\ c_1 \\ c_2 \\ c_3 \end{pmatrix}$$