8-5. A transition element which employs the same wave function as both the initial and final states is called an expectation value. Thus the expectation value of $F$ for the ground state $\Phi_0$ of equation (8.83) is

$$\langle \Phi_0 | F | \Phi_0 \rangle = \int \cdots \int \Phi_0^* F \Phi_0 \, dQ_1 \, dQ_2 \cdots dQ_{N-1} \tag{8.84}$$

(The integral over complex variables is defined as equal to the corresponding integral over real normal coordinates $Q_\alpha^c$ and $Q_\alpha^s$.) Show that the following expectation values are correct (for $\alpha \neq 0$).

$$\begin{aligned} \langle \Phi_0^* | Q_\alpha | \Phi_0 \rangle &= \langle \Phi_0^* | Q_\alpha^* | \Phi_0 \rangle = 0 \\ \langle \Phi_0^* | Q_\alpha^2 | \Phi_0 \rangle &= \langle \Phi_0^* | Q_\alpha^{*2} | \Phi_0 \rangle = 0 \\ \langle \Phi_0^* | Q_\alpha^* Q_\alpha | \Phi_0 \rangle &= \frac{\hbar}{2\omega_\alpha} \langle \Phi_0^* | 1 | \Phi_0 \rangle \\ \langle \Phi_0^* | Q_\alpha^* Q_\alpha | \Phi_0 \rangle &= 0, \quad \alpha \neq \beta \end{aligned} \tag{8.85}$$

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From problem 8-4,

$$|\Phi_0|^2 = \Phi_0^* \Phi_0 = \exp\left( -\frac{1}{\hbar} \sum_{\alpha=1}^{N-1} \omega_\alpha \left( (Q_\alpha^c)^2 + (Q_\alpha^s)^2 \right) \right)$$

We will use the following integrals.

$$\int_{-\infty}^{\infty} \exp(-ax^2 + b) \, dx = \sqrt{\frac{\pi}{a}} \exp(b) \tag{1}$$

$$\int_{-\infty}^{\infty} x \exp(-ax^2 + b) \, dx = 0 \tag{2}$$

$$\int_{-\infty}^{\infty} x^2 \exp(-ax^2 + b) \, dx = \frac{1}{2a} \sqrt{\frac{\pi}{a}} \exp(b) \tag{3}$$

Here are some specific examples with $a = \omega_1 / \hbar$.

$$\int_{-\infty}^{\infty} |\Phi_0|^2 \, dQ_1^c = \left( \frac{\pi \hbar}{\omega_1} \right)^{1/2} \exp\left( \frac{\omega_1}{\hbar} (Q_1^c)^2 \right) |\Phi_0|^2 \tag{4}$$

$$\int_{-\infty}^{\infty} Q_1^c |\Phi_0|^2 \, dQ_1^c = 0 \tag{5}$$

$$\int_{-\infty}^{\infty} (Q_1^c)^2 |\Phi_0|^2 \, dQ_1^c = \frac{\hbar}{2\omega_1} \left( \frac{\pi \hbar}{\omega_1} \right)^{1/2} \exp\left( \frac{\omega_1}{\hbar} (Q_1^c)^2 \right) |\Phi_0|^2 \tag{6}$$

Multiplying $|\Phi_0|^2$ by an exponential cancels a factor, i.e., in (1) and (4),

$$\exp(b) = \exp\left(\frac{\omega_1}{\hbar}(Q_1^c)^2\right)|\Phi_0|^2$$

Compute the expectation value for $Q_1$. Let

$$I = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\left(\frac{Q_1^c - iQ_1^s}{\sqrt{2}}\right)|\Phi_0|^2\,dQ_1^c\,dQ_1^s$$

By integral (2), $I = 0$ hence by equation (8.84)

$$\langle\Phi_0^*|Q_1|\Phi_0\rangle = 0$$

Compute the expectation value for $Q_1^*$. Let

$$I = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\left(\frac{Q_1^c + iQ_1^s}{\sqrt{2}}\right)|\Phi_0|^2\,dQ_1^c\,dQ_1^s$$

As above, $I = 0$ hence

$$\langle\Phi_0^*|Q_1^*|\Phi_0\rangle = 0$$

Compute the expectation value for $Q_1^2$. Let

$$I = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\left(\frac{Q_1^c - iQ_1^s}{\sqrt{2}}\right)^2|\Phi_0|^2\,dQ_1^c\,dQ_1^s$$

Rewrite as

$$\begin{aligned}I = &-i\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}Q_1^cQ_1^s|\Phi_0|^2\,dQ_1^c\,dQ_1^s\\&+\frac{1}{2}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}(Q_1^c)^2|\Phi_0|^2\,dQ_1^c\,dQ_1^s - \frac{1}{2}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}(Q_1^s)^2|\Phi_0|^2\,dQ_1^c\,dQ_1^s\end{aligned}$$

The first integral vanishes by (2). The remaining integrals cancel hence

$$\langle\Phi_0^*|Q_1^2|\Phi_0\rangle = 0$$

Compute the expectation value for $Q_1^{*2}$. (As above except for a sign change.)

$$\begin{aligned}I = &\,i\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}Q_1^cQ_1^s|\Phi_0|^2\,dQ_1^c\,dQ_1^s\\&+\frac{1}{2}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}(Q_1^c)^2|\Phi_0|^2\,dQ_1^c\,dQ_1^s - \frac{1}{2}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}(Q_1^s)^2|\Phi_0|^2\,dQ_1^c\,dQ_1^s\end{aligned}$$

By the same arguments as $Q_1^2$

$$\langle \Phi_0^* | Q_1^{*2} | \Phi_0 \rangle = 0$$

Compute the expectation value for $Q_1^* Q_1$. Let

$$I = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \left( \frac{(Q_1^c)^2 + (Q_1^s)^2}{2} \right) |\Phi_0|^2 \, dQ_1^c \, dQ_1^s$$

Rewrite as

$$I = \frac{1}{2} \int_{-\infty}^{\infty} \left( \int_{-\infty}^{\infty} (Q_1^c)^2 |\Phi_0|^2 \, dQ_1^c \right) dQ_1^s + \frac{1}{2} \int_{-\infty}^{\infty} \left( \int_{-\infty}^{\infty} (Q_1^s)^2 |\Phi_0|^2 \, dQ_1^s \right) dQ_1^c$$

By integral (3) with $a = \omega_1/\hbar$,

$$\begin{aligned} I = \frac{\hbar}{4\omega_1} \left( \frac{\pi\hbar}{\omega_1} \right)^{1/2} \exp\left( \frac{\omega_1}{\hbar} (Q_1^c)^2 \right) \int_{-\infty}^{\infty} |\Phi_0|^2 \, dQ_1^s \\ + \frac{\hbar}{4\omega_1} \left( \frac{\pi\hbar}{\omega_1} \right)^{1/2} \exp\left( \frac{\omega_1}{\hbar} (Q_1^s)^2 \right) \int_{-\infty}^{\infty} |\Phi_0|^2 \, dQ_1^c \end{aligned}$$

By integral (1),

$$\begin{aligned} I = \frac{\hbar}{4\omega_1} \frac{\pi\hbar}{\omega_1} \exp\left( \frac{\omega_1}{\hbar} (Q_1^c)^2 \right) \exp\left( \frac{\omega_1}{\hbar} (Q_1^s)^2 \right) |\Phi_0|^2 \\ + \frac{\hbar}{4\omega_1} \frac{\pi\hbar}{\omega_1} \exp\left( \frac{\omega_1}{\hbar} (Q_1^s)^2 \right) \exp\left( \frac{\omega_1}{\hbar} (Q_1^c)^2 \right) |\Phi_0|^2 \end{aligned}$$

Integrate over the remaining measure as in (8.84).

$$\begin{aligned} \langle \Phi_0^* | Q_1^* Q_1 | \Phi_0 \rangle &= \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} I \, dQ_2^c \, dQ_2^s \cdots dQ_{N-1}^c \, dQ_{N-1}^s \\ &= \frac{\hbar}{2\omega_1} \frac{\pi\hbar}{\omega_1} \prod_{k=2}^{N-1} \frac{\pi\hbar}{\omega_k} \quad (7) \end{aligned}$$

Note that the exponentials cancel with $u$.

Compute the normalization constant. By integral (1),

$$\langle \Phi_0^* | 1 | \Phi_0 \rangle = \prod_{k=1}^{N-1} \frac{\pi\hbar}{\omega_k} \quad (8)$$

Hence by (7) and (8),

$$\langle\Phi_0^*|Q_1^*Q_1|\Phi_0\rangle = \frac{\hbar}{2\omega_1}\langle\Phi_0^*|1|\Phi_0\rangle$$

Compute the expectation value for $Q_1^*Q_2$. Let

$$I = \int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty}\left(\frac{Q_1^cQ_2^c - Q_1^sQ_2^s - iQ_1^cQ_2^s - iQ_1^sQ_2^c}{2}\right)|\Phi_0|^2\,dQ_1^c\,dQ_1^s\,dQ_2^c\,dQ_2^s$$

By integral (2) we have $I = 0$, hence by equation (8.84)

$$\langle\Phi_0^*|Q_1^*Q_2|\Phi_0\rangle = 0$$