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 Φ_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_α^c and Q_α^s.) Show that the following expectation values are correct (for $\alpha \neq 0$).

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

Recall that

$$Q_\alpha = \frac{1}{\sqrt{2}} (Q_\alpha^c - i Q_\alpha^s)$$

Hence

$$Q_\alpha^* Q_\alpha = \frac{1}{2} (Q_\alpha^c)^2 + \frac{1}{2} (Q_\alpha^s)^2 \tag{1}$$

Here is equation (8.83).

$$\Phi_0 = A \exp\left(-\frac{1}{2\hbar} \sum_{\alpha=1}^{N-1} \omega_\alpha Q_\alpha^* Q_\alpha \right) \tag{8.83}$$

Compute $\Phi_0^* \Phi_0$.

$$\begin{aligned}
\Phi_0^* \Phi_0 &= A^2 \exp\left(-\frac{1}{2\hbar} \sum_{\alpha=1}^{N-1} \omega_\alpha Q_\alpha Q_\alpha^* \right) \exp\left(-\frac{1}{2\hbar} \sum_{\alpha=1}^{N-1} \omega_\alpha Q_\alpha^* Q_\alpha \right) \\
&= A^2 \exp\left(-\frac{1}{\hbar} \sum_{\alpha=1}^{N-1} \omega_\alpha Q_\alpha^* Q_\alpha \right) \qquad (2)
\end{aligned}$$

Substitute (1) into (2).

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

For brevity in the following formulas, let

$$u = \Psi_0^* \Psi_0$$

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 $a = \omega_1 / 2\hbar$.

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

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

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

Note that multiplying u by an exponential cancels that factor in u, i.e.,

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

Compute the expectation value for Q_1. Let

$$I = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} u \frac{Q_1^c - iQ_1^s}{\sqrt{2}}\, dQ_1^c\, dQ_1^s$$

By equation (2) we have

$$I = 0$$

Since $I = 0$ there is no need to continue integrating as in (8.84). Hence

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

Compute the expectation value for Q_1^*. Let

$$I = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} u \frac{Q_1^c + iQ_1^s}{\sqrt{2}}\, dQ_1^c\, dQ_1^s$$

As above, $I = 0$ hence

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

Compute the expectation value for Q_1^2. Let

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

Rewrite as

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

The first integral vanishes by (1). The remaining integrals cancel by symmetry, hence

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

Compute the expectation value for Q_1^{*2}. (As above except the first integral is positive.)

$$\begin{aligned} \langle \Phi_0^* | Q_1^{*2} | \Phi_0 \rangle = i \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} u Q_1^c Q_1^s \, dQ_1^c \, dQ_1^s \\ + \frac{1}{2} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} u (Q_1^c)^2 \, dQ_1^c \, dQ_1^s - \frac{1}{2} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} u (Q_1^s)^2 \, dQ_1^c \, dQ_1^s \end{aligned}$$

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

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

Rewrite as

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

By equations (3) and (6)

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

By equations (1) and (4)

$$I = \frac{\hbar}{2\omega_1}\frac{2\pi\hbar}{\omega_1}\exp\left(\frac{\omega_1}{2\hbar}(Q_1^c)^2\right)\exp\left(\frac{\omega_1}{2\hbar}(Q_1^s)^2\right)u + \frac{\hbar}{2\omega_1}\frac{2\pi\hbar}{\omega_1}\exp\left(\frac{\omega_1}{2\hbar}(Q_1^c)^2\right)\exp\left(\frac{\omega_1}{2\hbar}(Q_1^s)^2\right)u$$

Now integrate over the remaining measure as in (8.84).

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

By equation (1)

$$\langle\Phi_0^*|1|\Phi_0\rangle = \prod_{k=1}^{N-1}\frac{2\pi\hbar}{\omega_k}$$