

4) The Hamiltonian of a system, and therefore the eigenvalues  $E_n$  of the energy, are functions of some parameter  $\lambda$ . Show that  $(\partial H / \partial \lambda)_{nn} = \partial E_n / \partial \lambda$ .

In other words, show  $\langle n | \frac{\partial H}{\partial \lambda} | n \rangle = \frac{\partial E_n}{\partial \lambda}$ . Starting

from the eigenvalue equation  $\hat{H} \psi_n = E_n \psi_n$  we have

$(\hat{H} - E_n) \psi_n = 0$ , indicating  $\psi_n$  is an eigenstate.

Differentiating:  $\frac{\partial}{\partial \lambda} [(\hat{H} - E_n) \psi_n] = 0$

$$\Leftrightarrow (\partial_\lambda \hat{H}) \psi_n - (\partial_\lambda E_n) \psi_n + (\hat{H} - E_n) \frac{\partial \psi_n}{\partial \lambda} = 0$$

Multiplying with  $\psi_n^*$ :  $\psi_n^* (\hat{H} - E_n) \frac{\partial \psi_n}{\partial \lambda} = \psi_n^* \left( \frac{\partial E_n}{\partial \lambda} - \frac{\partial \hat{H}}{\partial \lambda} \right) \psi_n$

and integrating both sides over all space  $q$

$$\int \psi_n^* (\hat{H} - E_n) \frac{\partial \psi_n}{\partial \lambda} dq = \int \psi_n^* \left( \frac{\partial E_n}{\partial \lambda} - \frac{\partial \hat{H}}{\partial \lambda} \right) \psi_n dq \quad (i)$$

Using the Hermiticity of  $\hat{H}$  on LHS we see that

$$\int \psi_n^* (\hat{H} - E_n) \frac{\partial \psi_n}{\partial \lambda} dq = \int \frac{\partial \psi_n}{\partial \lambda} (\hat{H} - E_n) \psi_n^* dq = 0$$

since  $(\hat{H} - E_n) \psi = 0 \Rightarrow (\hat{H} - E_n) \psi^* = 0$ . The RHS of (i)

$$\int \psi_n^* \left( \frac{\partial E_n}{\partial \lambda} - \frac{\partial \hat{H}}{\partial \lambda} \right) \psi_n dq = 0 \quad \text{and splitting terms:}$$

$$\frac{\partial E_n}{\partial \lambda} \int |\psi_n|^2 dq - \int \psi_n^* \frac{\partial \hat{H}}{\partial \lambda} \psi_n dq = 0$$

Leaves us with  $\frac{\partial E}{\partial \lambda} = \int \psi_n^* \frac{\partial \hat{H}}{\partial \lambda} \psi_n dq$

or in other words:

$$\frac{\partial E_n}{\partial \lambda} = \langle \psi_n | \frac{\partial \hat{H}}{\partial \lambda} | \psi_n \rangle \quad \square$$

The important thing to take away is the fact that if we tweak a parameter in the Hamiltonian then the change in energy will be the average of how ~~the~~ the Hamiltonian changes in that state.