

Feynman-Hellmann Theorem - for stationary states

Let $|\psi\rangle$ be a bound state of \hat{H} with energy E satisfying:

$$\hat{H}|\psi\rangle = E|\psi\rangle.$$

If $\hat{H} \equiv \hat{H}(\lambda)$ ANALYTIC dependence on parameter, (not near singular points)
then $E \equiv E(\lambda)$ and $|\psi\rangle \equiv |\psi(\lambda)\rangle$.

Start with matrix element of Schrödinger equation:

$$\langle\psi|\hat{H}|\psi\rangle = E\langle\psi|\psi\rangle$$

Differentiate:

$$\begin{aligned} \frac{dE}{d\lambda} \langle\psi|\psi\rangle &= \frac{d}{d\lambda} (\langle\psi|\hat{H}|\psi\rangle) \\ &= \left(\frac{d}{d\lambda}\langle\psi|\right) \hat{H}|\psi\rangle + \langle\psi|\frac{d\hat{H}}{d\lambda}|\psi\rangle + \langle\psi|\hat{H}\left(\frac{d}{d\lambda}|\psi\rangle\right) \\ &= E \left[\left(\frac{d}{d\lambda}\langle\psi|\right)|\psi\rangle + \langle\psi|\left(\frac{d}{d\lambda}|\psi\rangle\right) \right] + \langle\psi|\frac{d\hat{H}}{d\lambda}|\psi\rangle \\ &= E \underbrace{\frac{d}{d\lambda}(\langle\psi|\psi\rangle)}_0 + \langle\psi|\frac{d\hat{H}}{d\lambda}|\psi\rangle \end{aligned}$$

$$\boxed{\frac{dE}{d\lambda} = \langle\psi|\frac{d\hat{H}}{d\lambda}|\psi\rangle}$$

Feynman-Hellmann theorem.

Power of theorem: expectation value in RHS is evaluated at $|\psi\rangle$ for fixed λ .

Exact parametric dependence of λ on $|\psi\rangle$ need not be known.

(Numerically obtained $|\psi\rangle$ would suffice!)

Caveat = Must be at an analytic point in complex λ -plane!

Can't study interacting spectrum starting from free theory.