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Time Evolving States

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References

Quantum Chemistry, D. A. McQuarrie, Chapter 2 (Chem QD462 M25).

Molecular Quantum Mechanics, P. W. Atkins, §2.3 (Chem QD462 A84).

Time evolution for an energy eigenstate

If the Hamiltonian (operator) is

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + V(r),$$

the time evolution of a wave function is determined by How fast ψ changes in time

$$i\hbar\frac{\partial\psi(r,t)}{\partial t} = \hat{H}\psi(r,t). \qquad (1)$$

A state with well-defined energy has the form

$$\psi(r,t) = e^{-iE_nt/\hbar}\psi_n(r) \qquad (2)$$

with

$$\hat{H}\psi_n(r) = E_n\psi_n(r)$$

determining both $\psi_n(r)$ and E_n.

A superposition of energy eigenstates

Because of the linearity of (1), any linear combination of terms of the form (2) is also a solution to (1). Thus,

$$\psi(r,t) = \sum_n c_n e^{-iE_nt/\hbar}\psi_n(r)$$

(with $\{c_n\}$ *any* set of constants) describes a time evolving state function that started ($t = 0$) in state

$$\psi(r,0) = \sum_n c_n\psi_n(r).$$