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Time Evolving States

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Time Evolving States

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

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

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

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

A state with well-defined energy has the form

$$\psi(\mathbf{r}, t) = e^{-iE_n t/\hbar}\psi_n(\mathbf{r}) \quad (2)$$

with

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

determining both $\psi_n(\mathbf{r})$ 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,

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

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

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

