12. An Operator for Energy & the Schrödinger Equation

12.1 An operator for energy

Let $\hat{H}$ be the operator that 'measures' the value of the energy observable (called the Hamiltonian for historical reasons):

$$\hat{H}\Psi_n = E_n \Psi_n \qquad 12.1$$

Ψ_n energy eigenstate
E_n energy eigenvalue
(in our work on confined particles we already found some examples now we generalize)

Classical physics:

$$E_{TOT} = T + V(\underline{r}) \qquad 12.2$$

we invoke the Correspondence Principle:

$\boxed{\text{The equivalence of classic and quantum physics under appropriate limits}}$

$$\left.\begin{aligned} T = \frac{p^2}{2M} &\longrightarrow \frac{\hat{p}^2}{2M} \\ V(x,y,z) &\longrightarrow \hat{V}(x,y,z) \end{aligned}\right\} \quad * \quad 12.3$$

recall $\hat{p} = -i\hbar\, \partial/\partial x$

In 3d $\quad \frac{\partial}{\partial x} \rightarrow \underline{\nabla} \quad$ Grad operator (del or nabla)

$$\underline{\nabla} = \underline{i}\frac{\partial}{\partial x} + \underline{j}\frac{\partial}{\partial y} + \underline{k}\frac{\partial}{\partial z} \qquad 12.4$$

$$\hat{p} = -i\hbar\,\underline{\nabla}$$

$$\frac{(\hat{p})^2}{2M} = \frac{(-i\hbar \underline{\nabla})^2}{2M} = -\frac{\hbar^2}{2M}\nabla^2 \qquad 12.5$$

where (in Cartesian coord.) (del^2)

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \qquad 12.6$$

12.2 Time-Independent Schrödinger Equation

$$\hat{H} = -\frac{\hbar^2}{2M}\nabla^2 + \hat{V}(\underline{r}) \qquad 12.7$$

- explicitly time independent
  (will come to time dependence in a moment)

For this course we will only consider 1-d

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

$$\left[-\frac{\hbar^2}{2M}\frac{\partial^2}{\partial x^2} + \hat{V}(x)\right]\psi_n(x) = E_n \psi_n(x) \quad (12.8)$$

- Often we can write $\hat{V}(x) = V(x)$
  true if $V(x) = f(x^q)$ (since $\hat{x} = x$)

e.g $V(x) \propto x^2$ or $1/x$

harmonic oscillator   Coulomb potential

then

$$\left[-\frac{\hbar^2}{2M}\frac{\partial^2}{\partial x^2} + V(x)\right]\psi_n(x) = E_n \psi_n(x)$$

12·3 Time-dependent Schrödinger equation

Recall L11 $\quad i\hbar \frac{\partial}{\partial t} \psi(x,t) = E\,\psi(x,t)$

and 12-8 $\quad \hat{H}\psi(x,t) = E_n\,\psi(x,t)$

equating these we obtain

$$\boxed{i\hbar \frac{\partial}{\partial t} \psi_n(x,t) = \left[-\frac{\hbar^2}{2M}\frac{\partial^2}{\partial x^2} + \hat{V}(x,t)\right] \psi_n(x,t)}$$

TDSE [12·9]

- Solutions of this equation $\psi_n(x,t)$ are the wavefunctions of states of definite energy

- An energy eigenvalue equation
- Also the wave-equation for matter waves (Sought by Schrödinger after de Broglie)

- $\psi_n(x,t)$ probability amplitude for position measurements

$\hat{H}$ acts only on spatial part (if $V(x)$ time-independent)

factor $\psi(x,t) = u(x)\, e^{-iE/\hbar\, t}$ [12·10]

$$\hat{H}\psi_n(x,t) = e^{-iE_n/\hbar\, t}\,\hat{H}\,u_n(x)$$

$$= e^{-iE_n/\hbar\, t}\,E_n u_n(x) = E_n\, u_n(x) e^{-iE_n t/\hbar}$$

- An energy eigenstate has a simple temporal dependence

$$\sim e^{-iE_n/\hbar\, t} \qquad [12\cdot11]$$