Session 2
Feb. 5, 2020

single particle QM: wave function $\Psi(t,x)$

Law of motion: Schrödinger equation (SE) (Schrödinger, 1926)

$$i\hbar \frac{\partial}{\partial t} \Psi(t,x) = -\frac{\hbar^2}{2m} \Delta_x \Psi(t,x) + V(x)\Psi(t,x) := H\Psi(t,x)$$

- m = mass, $\hbar$ = Planck's constant
- $V: \mathbb{R}^d \to \mathbb{R}$ called potential, e.g., Coulomb potential $V^{\text{Coul}}(x) = -\hbar c \alpha \frac{1}{|x|}$

  describes hydrogen atom

  α = fine structure constant
- $\Delta_x := \sum_{j=1}^{d} \frac{\partial^2}{\partial x_j^2}$ Laplacian (Laplace operator)
- H = Hamiltonian (Hamilton operator)

important notes:
- SE linear ($\Rightarrow$ superpositions)
- SE first-order in t ($\Psi(t=0)$ determines $\Psi(t)$)

solution theory of SE central topic of this class

Very brief comparison to classical mechanics:

↳ particles with position $q(t) \in \mathbb{R}^d$

↳ potential $V(x)$, i.e., force $F(x) = -\nabla_x V(x)$

$\Rightarrow$ Newton's law: $m \frac{d^2}{dt^2} q(t) = F(q(t)) = -\nabla V(q(t))$

$\Rightarrow$ second order ODE, $q(0)$ and $\dot{q}(0)$ determine $q(t)$ (for "nice" V)

other formulation: introduce momentum $p(t) = m \frac{dq(t)}{dt}$

• define classical Hamilton function $H(q,p) = \frac{p^2}{2m} + V(q)$

$\Rightarrow$ Newton's law becomes $\frac{d}{dt}\begin{pmatrix} q(t) \\ p(t) \end{pmatrix} = \begin{pmatrix} \frac{1}{m} p(t) \\ -\nabla q(t) \end{pmatrix} = \underbrace{\begin{pmatrix} \nabla_p \\ -\nabla_q \end{pmatrix}}_{} H(q,p)$

$$= \underbrace{\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}}_{\text{symplectic matrix}} \begin{pmatrix} \nabla_q \\ \nabla_p \end{pmatrix}$$

Note: • $(q,p) \in \mathbb{R}^{2d}$ is called phase space (it has a natural symplectic structure)

• formal correspondence between QM H and $H(q,p)$ by setting $p = -i\hbar\nabla_x$

↳ active research topic: derive classical mechanics from QM in appropriate limits

↳ mathematical recipes to "make a classical theory quantum" (like replacing p by $-i\hbar\nabla_x$ in $H(q,p)$) are called quantization

1.3 QM for Many Particles

• for N particles, we need $(x_1, \dots, x_N) \in (\mathbb{R}^d)^N = \mathbb{R}^{dN}$ (configuration space)

• wave function $\psi: \mathbb{R} \times \mathbb{R}^{dN} \to \mathbb{C}$

• $|\psi(t, x_1, \dots, x_N)|^2$ = probability density for particles to be at $x_1, \dots, x_N$

Schrödinger equation: $i\hbar \frac{\partial}{\partial t} \psi(t, x_1, \dots, x_N) = H \psi(t, x_1, \dots, x_N)$

with $H = \left(-\frac{\hbar^2}{2} \sum_{j=1}^{N} \frac{\Delta_{x_j}}{m_j} + V(x_1, \dots, x_N) \right)$

Remarks:

- usually $V(x_1,\dots,x_N) = \lambda \underbrace{\sum_{i<j} v(x_i - x_j)}_{\text{pair interaction}} + \tilde{\lambda} \underbrace{\sum_{i=1}^{N} V^{ext}(x_i)}_{\text{external field}}$ $\quad$ ($\lambda, \tilde{\lambda} \in \mathbb{R}$ coupling constants)

- the fact that $\psi_t = \psi_t(x_1,\dots,x_N)$ is the source of entanglement

  ↳ roughly: if $\psi_t(x_1,\dots,x_N) \neq \prod_{j=1}^{N} \varphi^{(j)}(x_j)$ then ψ_t is called entangled

  ⟹ statistics of particle j can "depend on" particle $k \neq j$

  ⟹ "all particles in the universe are connected"

  active research topic: • measures for "how much" entanglement
  • non-locality, Bell's inequality

- for $N \geq 2$ (and $V \neq 0$) explicit solutions not feasible (Helium atom?)

- for "large N" (in practice $N \geq 10$ or 100) also numerical solutions not feasible

  ↳ divide $\mathbb{R}$ into M lattice points

  ⟹ need M^{dN} lattice points to approximate $\psi_t(x_1,\dots,x_N)$

  e.g., $M = 100$ (very little!), $N = 10$ ⟹ $M^N = 100^{10} = 10^{20} \approx 100\,000\,000$ Terabyte

  ↳ need simplified / approximate / coarse-grained = effective descriptions

  active research topic: rigorous derivation of such effective equations