

1.2 Single Particle QM

d = dimension of space ($d=1,2,3$ usually)

Wave function for one particle is $\psi: \mathbb{R}_t \times \mathbb{R}_x^d \rightarrow \mathbb{C}, (t,x) \mapsto \psi(t,x)$

Normalization: $\int_{\mathbb{R}^d} |\psi(t,x)|^2 dx = 1 \quad \forall t \in \mathbb{R}$

$|\psi(t,x)|^2 =: \rho(t,x)$ = probability density for particle to be at position x at time t

In other words: for $\Lambda \subset \mathbb{R}^d$: $P(Q(t) \in \Lambda) \equiv \mathbb{P}^{\psi_t}(\Lambda) = \int_{\Lambda} |\psi(t,x)|^2 dx$ is the probability that particle is in region Λ (at time t)

Note: ρ is only a probability density, not a charge or mass density!

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

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

with:

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

• $\Delta_x := \sum_{j=1}^d \frac{\partial^2}{\partial x_j^2}$ 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 is one of the central topics of this class.

Very brief comparison to classical mechanics:

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

\hookrightarrow 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 $\frac{d}{dt} \begin{pmatrix} q(t) \\ p(t) \end{pmatrix} = \begin{pmatrix} \frac{1}{m} p(t) \\ -\nabla V(q(t)) \end{pmatrix} = \begin{pmatrix} \nabla_p \\ -\nabla_q \end{pmatrix} H(q, p) \Big|_{\substack{q=q(t) \\ p=p(t)}}$

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

Note: • $\{(q,p)\} = \mathbb{R}^{2d}$ 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 $\Psi: \mathbb{R} \times (\mathbb{R}^d)^N \rightarrow \mathbb{C}$ (or \mathbb{C}^n if there is spin)

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

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

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

Remarks:

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

(If $\Psi(x_1, \dots, x_N) = \varphi^1(x_1) \dots \varphi^N(x_N)$, then each particle has its own probability distribution; in terms of random variables: the particle positions would be independent)

⇒ "all particles in the universe are connected"

Active research topics: • measures for "how much" entanglement

• non-locality, Bell's inequality

• For $N \geq 2$ (and $V \neq 0$) explicit solutions not feasible

↳ already for the Helium atom ($N=2$) no explicit solution is known

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

↳ divide \mathbb{R}^3 into M (lattice points)

⇒ need M^N (lattice points) to approximate $\Psi_t(x_1, \dots, x_N)$

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

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

Active research topic: rigorous derivation of such effective equations