urm.math.uni-tuebingen.de

Sec. 1.2 The Schrödinger eq.

$$i\hbar \frac{\partial \psi}{\partial t} = -\sum_{i=1}^{N} \frac{\hbar^2}{2m_i} \nabla_i^2 \psi + V\psi$$

$\psi = \psi_t = \psi_t(\underline{x}_1, \dots, \underline{x}_N)$, $\psi : \mathbb{R}_t \times \mathbb{R}_q^{3N} \to \mathbb{C}$

$q = (\underline{x}_1, \dots, \underline{x}_N)$ $\quad \underline{x}_i \in \mathbb{R}^3$ $\quad \hbar = \frac{h}{2\pi}$

$$\nabla_i = \left(\frac{\partial}{\partial x_{i1}}, \frac{\partial}{\partial x_{i2}}, \frac{\partial}{\partial x_{i3}} \right)$$

$$\nabla_i^2 = \frac{\partial^2}{\partial x_{i1}^2} + \frac{\partial^2}{\partial x_{i2}^2} + \frac{\partial^2}{\partial x_{i3}^2}$$ Laplacian

V = potential $= V(\underline{x}_1, \dots, \underline{x}_N)$, fundamentally

$$V = \sum_{1 \le i < j \le N} \frac{e_i e_j / 4\pi\varepsilon_0}{|\underline{x}_j - \underline{x}_i|} - \sum_{1 \le i < j \le N} \frac{G m_i m_j}{|\underline{x}_j - \underline{x}_i|}$$

Coulomb, $|\underline{x}| = \sqrt{x_1^2 + x_2^2 + x_3^2}$ Euclidean norm

$$H = -\sum_{i=1}^{N} \frac{\hbar^2}{2m_i} \nabla_i^2 + V$$ Hamiltonian operator

Schr. eq. $i\hbar \frac{\partial \psi}{\partial t} = H\psi$. PDE

Born's Rule. If we measure the system's configuration at time t, then the outcome ~~...~~ is random with prob. density

$$\rho_t(q) = |\psi_t(q)|^2 . \quad \forall q \in \mathbb{R}^{3N}$$

outcome X, $\mathbb{P}(X = x) = 0$.

$$\mathbb{P}(X \in B) = \int_B \rho(q) \underbrace{d^{3N}q}_{dq} .$$

$B \subseteq \mathbb{R}^{3N}$

$\rho(q) \geq 0$, $\quad \int_{\mathbb{R}^{3N}} \rho(q)\, dq = 1$

gaussian density in $\mathbb{R}^1$

$$\rho(x) = \frac{1}{\sqrt{2\pi}\,\sigma} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$$

mean μ

= expectation

$$\mathbb{E}(X) = \int x\,\rho(x)\,dx$$

σ = standard deviation

$$SD(X) = \sqrt{\underbrace{\mathbb{E}\left[(X-\mathbb{E}X)^2\right]}_{Var(X)}}$$

We need that

$$\int_{\mathbb{R}^{3N}} |\psi_t(q)|^2 \, dq = 1$$

If true at $t=0$ $\xrightarrow{\text{Schr. eq.}}$ true at any t.

Schr. eq $\Rightarrow$ $\underbrace{\int_{\mathbb{R}^{3N}} |\psi_t(q)|^2 dq}_{\|\psi_t\|^2} = \underbrace{\int_{\mathbb{R}^{3N}} |\psi_0(q)|^2 dq}_{\|\psi_0\|^2}$

L^2 norm

conservation law

local conservation

continuity eq. $$\frac{\partial \rho}{\partial t} = -\sum_{\alpha=1}^{d} \frac{\partial j_\alpha}{\partial x_\alpha}$$

$(d=3N)$

$\rho=\rho(t, x_1 \dots x_d)$

$j=j_\alpha(t, x_1, \dots, x_d)$ current

t-dep. vector field on $\mathbb{R}^d$

Why cont. eq. expresses local conservation:

Ostrogradski-Gauss integral theorem

vector field $\underline{F}$ in $\mathbb{R}^n$

$$\int_A \operatorname{div} \underline{F}(\underline{x})\, d^n\underline{x} = \int_{\partial A} \underline{F}(\underline{x}) \cdot \underline{n}(\underline{x})\, d^{n-1}\underline{x}$$

flux integral

where $\operatorname{div} \underline{F} = \dfrac{\partial F_1}{\partial x_1} + \dots + \dfrac{\partial F_n}{\partial x_n}$

A is n-dim with piecewise smooth boundary ∂A

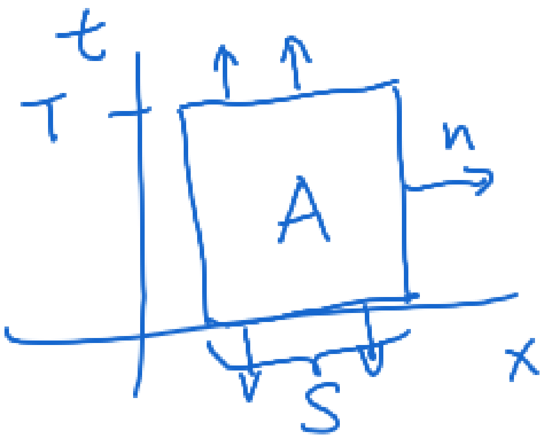
$A \subseteq \mathbb{R}^n$

$\underline{n}(\underline{x})$ = outward unit normal vector to ∂A

Now $n = d+1$

$\underline{F} = (\rho, j_1, \dots, j_d)$ has $\operatorname{div} \underline{F} = 0$

$A = [0,T] \times S$, $\quad S \subseteq \mathbb{R}^d$ has piecewise smooth $\partial S \subseteq \mathbb{R}^d$



$$\cancel{0} \cancel{=} \int_S \rho_T - \int_S \rho_0 + \int_0^T dt \int_{\partial S} dx^{d-1}$$

$j(x,t) \cdot n_{\partial S}$

If no flux to ∞, i.e. $\int_{\partial S} d^{d-1}x \, j \cdot n_{\partial S} \to 0$ as $S \to \mathbb{R}^d$.

then $\int_{\mathbb{R}^d} \rho_T = \int_{\mathbb{R}^d} \rho_0$.

Schr eq $\Rightarrow$ cont. eq.