We continue our remarks about $\psi(x_1,\dots,x_N)$:

- 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 $N \gtrsim 10$ or 100) also numerical solutions not feasible

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

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

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

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

  Active research topic: rigorous derivation of such effective equations

- Fact: for $d=3$, wave function is either
  - $\boxed{\text{bosonic}}$, meaning symmetric under exchange of variables, i.e.,

    $$\psi(\dots,x_j,\dots,x_k,\dots) = \psi(\dots,x_k,\dots,x_j,\dots)$$

    $$\Big(\text{i.e., } \psi(x_1,\dots,x_N) = \psi(x_{\sigma(1)},\dots,x_{\sigma(N)}) \ \forall \sigma \in \underset{\text{symmetric group (i.e., permutations of } \{1,\dots,N\})}{S_N}\Big)$$

  - or $\boxed{\text{fermionic}}$, meaning antisymmetric under exchange of variables, i.e.,

    $$\psi(\dots,x_j,\dots,x_k,\dots) = -\psi(\dots,x_k,\dots,x_j,\dots)$$

    $$\Big(\text{i.e., } \psi(x_1,\dots,x_N) = \underbrace{(-1)^\sigma}_{= \operatorname{sgn}(\sigma) = \text{sign of permutation } \sigma = \begin{cases} +1 & \text{for } \sigma \text{ even} \\ -1 & \text{for } \sigma \text{ odd}\end{cases}} \psi(x_{\sigma(1)},\dots,x_{\sigma(N)}) \ \forall \sigma \in S_N\Big)$$

Note: • Only particles of the same kind have these symmetries

(e.g., x_1, x_2 bosons with mass m, y_1, y_2 bosons with mass $\tilde{m} \neq m$, z_1, z_2 fermions, then $\Psi(x_1, x_2, y_1, y_2, z_1, z_2)$ symm. in x_1, x_2, symm. in y_1, y_2, antisymm. in z_1, z_2)

• Bosons: "tend to be in the same state" (see HW 1), which, e.g., leads to Bose-Einstein condensation

• Fermions: "tend to repel each other" (HW 1), which, e.g., leads to the Fermi pressure (neutron stars, ...), superconductivity etc.

• Reason for symm./antisymm. is that really ${}^N\mathbb{R}^d := \underbrace{\{q \subset \mathbb{R}^d : |q| = N\}}_{N \text{ element subsets of } \mathbb{R}^d}$ is the right configuration space, and not $\mathbb{R}^{dN}$ ("all particles are indistinguishable"), for the same particle species; also, we need

$$|\Psi(x_1, \dots, x_N)|^2 = |\Psi(x_{\sigma(1)}, \dots, x_{\sigma(N)})|^2$$

• ${}^N\mathbb{R}^d$ has interesting topology: its connectedness properties lead to the different symmetries

↳ ${}^N\mathbb{R}^3$ is multiply connected, which leads to the boson-fermion alternative

↳ ${}^N\mathbb{R}^2$ is multiply connected "in a worse way", which leads to many more possibilities: anyons, with $\Psi(\dots, x_j, \dots, x_k, \dots) = e^{i\pi\alpha}\Psi(\dots, x_k, \dots, x_j, \dots)$ (relevant for quasi 2 dim. materials)

• Also interesting/relevant is the $\boxed{\text{time-independent Schrödinger equation: } H\phi_E = E\phi_E}$ (an eigenvalue problem).

$E \in \mathbb{R}$

Hamiltonian   wave function

Here, E = eigenvalues/energies ; ϕ_E = eigenfunctions/eigenstates

↳ Give solution $\Psi(t) = e^{-iEt}\phi_E$ to time-dependent Schrödinger equation

(check: $i\partial_t \Psi(t) = i\partial_t e^{-iEt}\phi_E = e^{-iEt}E\phi_E = e^{-iEt}H\phi_E = H\Psi(t)$ ✓)

↳ $E_0 = \inf\{E\} = \inf_{\phi, \|\phi\|=1} \langle \phi, H\phi\rangle$, if it exists, is called ground state energy;

if a minimizer ϕ_{E_0} exists, it is called ground state.

Ground states are very relevant, since matter tends to radiate until it reaches lowest energy state

↳ ϕ_E with $E > E_0$ are called excited states

↳ Active research topics: find/approximate:
- E_0, ϕ_{E_0}
- low lying E, ϕ_E
- (all E, ϕ_E rarely possible)

increasing level of difficulty ↓

- Finally, let us write down the Hamiltonian of non-relativistic matter for N electrons. We treat the nuclei in Born-Oppenheimer approximation (i.e., "classically"), i.e., they are at positions $R_1, \dots, R_M$ ($R_j \in \mathbb{R}^3, j = 1, \dots, M$); they have charges $Z_1, \dots, Z_M$ ($Z_j \in \mathbb{Z}$, i.e., multiples of the elementary charge e). Denoting the electron variables as $x_1, \dots, x_N$ (i.e., the wave function is $\Psi_t(x_1, \dots, x_N)$), the Hamiltonian is:

$$\boxed{H = \sum_{j=1}^{N} \frac{\hbar^2}{2m_e}(-\Delta_{x_j}) + \hbar c\alpha \left(\underbrace{\sum_{1\le j<k\le M} \frac{Z_j Z_k}{|R_j - R_k|}}_{=\text{const}(t) = \text{energy of nuclei}} - \underbrace{\sum_{j=1}^{N}\sum_{k=1}^{M} \frac{Z_k}{|x_j - R_k|}}_{=\text{attractive external field of nuclei}} + \underbrace{\sum_{1\le j<k\le N} \frac{1}{|x_j - x_k|}}_{=\text{repulsive Coulomb interaction of electrons}} \right)}$$

↳ m_e = electron mass

↳ note: for a neutral molecule: $\sum_{j=1}^{M} Z_j = N$

This Hamiltonian describes – sometimes with small modifications – non relativistic matter (e.g., chemistry, conductivity, ...)

Central topic of this class:

For which $\psi(t=0)$ and V does Schrödinger equation have global solutions, and in which sense?

General idea: regard Schrödinger equation as an ODE $i\frac{d}{dt}\psi(t) = H\psi(t)$ for

$$\psi : \mathbb{R} \to \mathcal{H} = \text{some Hilbert space, usually } L^2(\mathbb{R}^{dN})$$

Difficulties: • $\mathcal{H}$ infinite dimensional

• H unbounded