

We continue our remarks about $\Psi(x_1, \dots, x_n)$:

- fact: for $d=3$, wave function is either

- **bosonic**, meaning symmetric under exchange of variables, i.e.,

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

$$(i.e., \Psi(x_1, \dots, x_n) = \Psi(x_{\sigma(1)}, \dots, x_{\sigma(n)}) \quad \forall \sigma \in S_n)$$

symmetric group (i.e., permutations of $\{1, \dots, n\}$)

- or **fermionic**, meaning antisymmetric under exchange of variables, i.e.,

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

$$(i.e., \underbrace{\Psi(x_1, \dots, x_n)}_{=} = (-1)^6 \Psi(x_{\sigma(1)}, \dots, x_{\sigma(n)}) \quad \forall \sigma \in S_n)$$

$= \text{sgn}(\sigma) = \text{sign of permutation } \sigma = \begin{cases} +1 & \text{for } \sigma \text{ even} \\ -1 & \text{for } \sigma \text{ odd} \end{cases}$

Note:

- only particles of the same kind have these symmetries

(e.g., x_1, x_2 bosons with mass m , γ_1, γ_2 bosons with mass $\tilde{m} \neq m$, z_1, z_2 fermions, then

$\Psi(x_1, x_2, \gamma_1, \gamma_2, z_1, z_2)$ symm. in x_1, x_2 , symm. in γ_1, γ_2 , antisym. 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.

N element subsets of \mathbb{R}^d

- reason for symm./antisymm. is that really " $\mathbb{R}^d := \{q \in \mathbb{R}^d : |q|=N\}$ " is the right configuration space, and not \mathbb{R}^{dN} ("all particles are indistinguishable"), for the same particle species; also, we need

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

- " \mathbb{R}^d " has interesting topology: its connectedness properties lead to the different symmetries

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

↳ \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 time-independent Schrödinger equation: (an eigenvalue problem).

$$H \phi_E = E \phi_E$$

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: $i\partial_t \Psi(t) = i\partial_t e^{-iEt} \phi_E = e^{-iEt} (-iE) \phi_E = e^{-iEt} H \phi_E = H \Psi(t) \quad \checkmark$)

↳ $E_0 = \inf \{E\} = \inf_{\|\phi\|=1} \langle \phi, H \phi \rangle$; 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

↳ 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 $Y_1(t), \dots, Y_M(t)$ ($Y_j(t) \in \mathbb{R}^3$); 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:

$$H = \sum_{j=1}^N \frac{\hbar^2}{2m_e} (-\Delta x_j) + \hbar c \alpha \left(\underbrace{\sum_{1 \leq j < k \leq M} \frac{z_j z_k}{|Y_j(t) - Y_k(t)|}}_{= \text{const}(t) = \text{energy of nuclei}} - \underbrace{\sum_{j=1}^N \sum_{k=1}^M \frac{z_k}{|x_j - Y_k(t)|}}_{= \text{attractive external field of nuclei}} + \underbrace{\sum_{1 \leq j < k \leq N} \frac{1}{|x_j - x_k|}}_{= \text{repulsive Coulomb interaction of electrons}} \right)$$

↳ 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

$\Psi: \mathbb{R} \rightarrow \mathcal{H}$ = some Hilbert space, usually $L^2(\mathbb{R}^{dn})$

difficulty:

- \mathcal{H} infinite dimensional
- H unbounded