Mathematical Quantum Mechanics

S. Bachmann

UBC, Fall 2026

1 Introduction

2025 was International Quantum Year, celebrating 100 years of quantum theory, in particular the publication of "On quantum-theoretical reinterpretation of kinematic and mechanical relationships" in *Z. Phys.* by W. Heisenberg.

Quantum mechanics was born around 1900 with works of Planck, Einstein and many others. One of the original problems quantum mechanics solved is that of the "black body radiation", namely the electromagnetic radiation emitted by a physical body as a function of its temperature.

It superseded classical Newtonian mechanics, from which it differs mostly at very small length scales (molecular, $10^{-9}\,\mathrm{m}$, and lower) and very low energy scales (up to $1\,\mathrm{keV} \sim 10^{-20}\,\mathrm{kcal}$).

Among others, quantum mechanics resolves the problem of the *stability of matter*: Why are atoms and molecules stable, namely why does ordinary matter not collapse onto itself?

1.1 Classical mechanics of atoms and molecules

In classical mechanics: The state of the electron in a hydrogen atom is given by

$$(x,p) \in \mathbb{R}^3 \times \mathbb{R}^3,$$

namely its position x and momentum $p = m \cdot v$. Its dynamics is governed by the Hamilton function $H(x,p)$, also known as the energy function, through Hamilton's equations:

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}\, x(t) &= \frac{\partial H\big(x(t),p(t)\big)}{\partial p}, \\ \frac{\mathrm{d}}{\mathrm{d}t}\, p(t) &= -\frac{\partial H\big(x(t),p(t)\big)}{\partial x}. \end{aligned} \tag{1}$$

In the specific case of a single particle,

$$H(x,p) = \frac{1}{2m}\, p^2 + V(x),$$

where $V(x)$ is the potential. Then (1) yields Newton's equations:

$$m\, \frac{\mathrm{d}^2}{\mathrm{d}t^2}\, x(t) = F\big(x(t)\big),$$

where $F(x) = -\nabla V(x)$ is the force.

With N particles, the state is

$$(x_1, \dots, x_N, p_1, \dots, p_N) \in \mathbb{R}^{6N}.$$

A molecular Hamiltonian is given by

$$H_N(x,p) = T(p) + V(x,R),$$

with kinetic energy

$$T(p) = \sum_{i=1}^{N} \frac{1}{2m}\, p_i^2$$

and potential energy

$$V(x,R) = e^2\big(W(x,R) + I(x) + U(R)\big)$$

where

$$W(x,R) = -\sum_{i=1}^{N}\sum_{j=1}^{M} \frac{Z_j}{|x_i - R_j|}$$

is the electrons–nuclei interaction,

$$I(x) = \sum_{1\le i<j\le N} \frac{1}{|x_i - x_j|}$$

is the electron–electron interaction,

$$U(R) = \sum_{1\le i<j\le M} \frac{Z_i Z_j}{|R_i - R_j|}$$

is the nuclei–nuclei interaction. Here: Z_j are the nuclear charges, R_j are the fixed positions of the M nuclei.

The equilibrium state is postulated to be the (x,p) which minimizes $H(x,p)$.

Problem. The function $H(x,p)$ is unbounded below. In classical mechanics, electrons would all collapse onto the nuclei.

1.2 Quantum mechanics of atoms

The state of classical mechanics must be replaced by a function

$$\mathbb{R}^3 \ni x \longmapsto \psi(x) \in \mathbb{C} \qquad \text{"wave function"}$$

whose physical interpretation is: $|\psi(x)|^2$ is the probability density for the presence of the particle at $x \in \mathbb{R}^3$. Hence we must have

$$\int_{\mathbb{R}^3} |\psi(x)|^2\,\mathrm{d}x = 1 = \|\psi\|_2^2$$

(and of course changing the value of $\psi(x)$ on a set of Lebesgue measure zero does not change the probability measure) namely

$$\psi \in L^2(\mathbb{R}^3;\mathbb{C}).$$

Remark. *A constant phase $e^{i\alpha}$, $\alpha \in \mathbb{R}$, does not change the state.*

The classical Hamiltonian function must be replaced by the energy functional $E : L^2(\mathbb{R}^3;\mathbb{C}) \to \mathbb{R}$ defined by

$$E(\psi) = T(\psi) + V(\psi)$$

where

$$T(\psi) = \frac{\hbar^2}{2m}\int_{\mathbb{R}^3} |\nabla\psi(x)|^2\,\mathrm{d}x, \qquad V(\psi) = \int_{\mathbb{R}^3} V(x)\,|\psi(x)|^2\,\mathrm{d}x.$$

where $\hbar$ is the reduced Planck constant.

The stability of matter problem in quantum mechanics is thus rephrased as: Is

$$E_0 := \inf\big\{\, E(\psi) \;:\; \psi\in L^2(\mathbb{R}^3,\mathbb{C}) \text{ and } \nabla\psi\in L^2(\mathbb{R}^3,\mathbb{C}),\;\|\psi\|_2 = 1 \,\big\}$$

finite? Note that the constraint $\nabla\psi\in L^2(\mathbb{R}^3,\mathbb{C})$ is needed for $T(\psi)$ to be defined. This is a problem in the calculus of variations.

More specific question: if $E_0 > -\infty$, is the infimum a minimum, namely is there a ground state ψ_0 such that

$$E_0 = E(\psi_0)$$

and is that state unique?

Classically, the positive T could not compensate the negative V. Quantum mechanically T and V are not independent: This fact is generically referred to as the *uncertainty principle*.

1. *Heisenberg*: for any $\|\psi\|_2 = 1$,

$$\int |\nabla\psi(x)|^2\,\mathrm{d}x \;\geq\; C\left(\int |\psi(x)|^2 x^2\,\mathrm{d}x\right)^{-1}.$$

   Equivalently $T(\psi) \geq \frac{\hbar^2}{2m} C\big(\int |\psi|^2 x^2\,\mathrm{d}x\big)^{-1}$. In other words, if the particle is well localized close to $x = 0$ where its potential energy is large and negative, then its kinetic energy must be very large and positive.

2. A more useful one: *Gagliardo–Nirenberg–Sobolev*. If ψ vanishes at infinity, i.e.

$$\big|\{x : |\psi(x)| > a\}\big| < \infty \quad \text{for all } a > 0,$$

   and $\nabla\psi\in L^2(\mathbb{R}^3;\mathbb{C})$, then $\psi\in L^6(\mathbb{R}^3;\mathbb{C})$ and

$$S\|\psi\|_6^2 \leq \|\nabla\psi\|_2^2, \qquad S = \tfrac{3}{4}\,(2\pi^2)^{2/3} = 3\left(\tfrac{\pi}{2}\right)^{4/3} \tag{2}$$

   Here, 6 is the Sobolev conjugate of 2, namely $\dfrac{1}{p^*} = \dfrac{1}{p} - \dfrac{1}{d} = \dfrac{1}{2} - \dfrac{1}{3}$. Written explicitly,

$$\underbrace{\int_{\mathbb{R}^3} |\nabla\psi(x)|^2\,\mathrm{d}x}_{=\frac{2m}{\hbar^2}T(\psi)} \;\geq\; \tfrac{3}{4}\,(2\pi^2)^{2/3}\underbrace{\left(\int |\psi(x)|^6\,\mathrm{d}x\right)^{1/3}}_{\text{relate to } V(\psi)}.$$

These elementary inequalities, together with *Hölder's inequality*: for any $1 \leq p, q \leq \infty$ s.t. $p^{-1} + q^{-1} = 1$,

$$\left|\int \overline{f(x)}\,g(x)\,\mathrm{d}x\right| \leq \int |f(x)||g(x)|\,\mathrm{d}x \leq \|f\|_p\|g\|_q$$

provided $f\in L^p(\mathbb{R}^3;\mathbb{C})$, $g\in L^q(\mathbb{R}^3;\mathbb{C})$, yield a proof of stability of matter (of the first kind), which we sketch now.

If $V \in L^{3/2}(\mathbb{R}^3;\mathbb{R})$,

$$\begin{aligned} |V(\psi)| &\le \int |\psi(x)|^2 |V(x)| \,\mathrm{d}x \\ &\le \big\| |\psi|^2 \big\|_3 \big\| |V| \big\|_{3/2} \qquad \left(\tfrac{1}{3} + \tfrac{2}{3} = 1\right) \end{aligned}$$

Noting that $\||\psi|^2\|_3 = \left(\int |\psi(x)|^6\right)^{1/3}$ and with (2),

$$\frac{2m}{\hbar^2}\, T(\psi) \;\ge\; \tfrac{3}{4}\,(2\pi^2)^{2/3}\, \frac{1}{\|V\|_{3/2}}\, |V(\psi)|,$$

and so, since $V(\psi) \ge -|V(\psi)|$,

$$T(\psi) + V(\psi) \;\ge\; \left(\frac{3\hbar^2}{8m}\, \frac{(2\pi^2)^{2/3}}{\|V\|_{3/2}} - 1 \right) |V(\psi)|.$$

We conclude that

$$E(\psi) \ge 0 \quad \text{for all } \psi \in L^2(\mathbb{R}^3;\mathbb{C}),\ \nabla\psi \in L^2(\mathbb{R}^3;\mathbb{C}), \qquad \text{provided } \ \|V\|_{3/2} \le \frac{3\hbar^2}{8m}\,(2\pi^2)^{2/3}.$$

Note that the Coulomb potential $V(x) = -|x|^{-1}$ is not in the right space: $|x|^{-3/2}$ is integrable at 0 in three dimensions, but it is not at ∞, so we need a bit more gymnastics. If

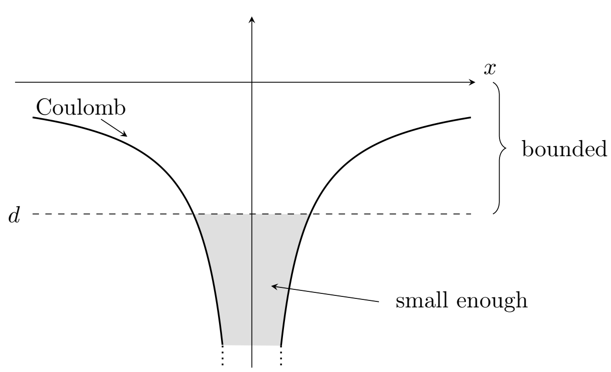
$$V(x) = V_1(x) + V_2(x), \qquad V_1 \in L^{3/2}(\mathbb{R}^3;\mathbb{C}), \quad V_2 \in L^\infty(\mathbb{R}^3;\mathbb{C}) \text{ (i.e. bounded)},$$

we pick $d \in \mathbb{R}$ (with $d < 0$) s.t.

$$v(x) = \min\big(V_1(x) - d,\, 0\big)$$

is such that

$$\|v\|_{3/2} \le \frac{1}{2} \cdot \frac{3\hbar^2}{8m}\,(2\pi^2)^{2/3}.$$



Then $v(\psi) \ge -\frac{1}{2} T(\psi)$, and since $V_1 - d \ge v$ we get

$$T(\psi) + V(\psi) = T(\psi) + \big(V_1(\psi) - d\big) + d + V_2(\psi) \ge \tfrac{1}{2} T(\psi) + d - \|V_2\|_\infty$$

since

$$\int |V_2(x)| |\psi(x)|^2 \,\mathrm{d}x \le \|V_2\|_\infty \int |\psi(x)|^2 \,\mathrm{d}x.$$

All in all, and since $T(\psi) \ge 0$, we conclude that

$$E_0 \ge d - \|V_2\|_\infty > -\infty.$$

Remark. *The power of the method lies in its generality. Stability is not specific to the hydrogen atom* $V(x) \propto -|x|^{-1}$.

In the specific case of the hydrogen atom

$$E(\psi) = \int \left(\frac{\hbar^2}{2m} |\nabla \psi(x)|^2 - \frac{\alpha}{|x|} |\psi(x)|^2 \right) \mathrm{d}x,$$

the minimizer is unique and explicit,

$$\psi_0 = Ce^{-|x|/a}, \qquad a = \frac{\hbar^2}{m\alpha},$$

and

$$E_0 = E(\psi_0) = -\frac{m\alpha^2}{2\hbar^2}.$$

Quantum mechanics further yields the *stability of matter of the second kind*: For a system of N electrons and M nuclei, the ground state energy per particle is bounded below,

$$\frac{1}{N} \inf_{\substack{\|\psi\|=1 \\ \psi \text{ antisymmetric}}} \langle \psi, H_N \psi \rangle > -C(M)$$

uniformly in N and in the positions R of the nuclei, for a positive constant $C(M)$.