Stability of Matter part 1

1. Introduction
2. Review of QM.

STABILITY OF MATTER

1. INTRODUCTION

Matter: electrons and atomic nuclei.

Forces: electric, magnetic, gravitational

$\downarrow$

most important in the context of atoms and molecules

The electric force between electrons (negative electric charge $-e$) and nuclei (positive charge $+Ze$ with $Z = 1, 2, \dots, 92$ in nature) is attractive and proportional to Ze^2.

In this course we will consider this basic question:

> Why don't the point-like electrons fall into the (nearly) point-like nuclei?

To put it differently: why is the energy of an atom with a point like nucleus not $-\infty$? This would be the case in classical mechanics. Indeed:

recall that in classical mechanics the Hamiltonian is given by

$$H(x,p) = \underbrace{\frac{p^2}{2m}}_{\text{kinetic energy}} + \underbrace{V(x)}_{\text{potential energy}} =: T(p) + V(x)$$

Hydrogen: electron at $x \in \mathbb{R}^3$ surrounding one nucleus at $R=0$

$$\rightsquigarrow V(x) = -\frac{e^2}{|x|}$$

$$\hookrightarrow H(x,p) = \frac{p^2}{2m} - \frac{e^2}{|x|}$$

$$\Longrightarrow \inf_{x\in\mathbb{R}^3, p\in\mathbb{R}^3} H(x,p) = -\infty$$

A succesful answer to the aforementioned question (STABILITY OF FIRST KIND) is given by Quantum Mechanics and Schrödinger's famous equation (1926). This is only 15 years since Rutherford's discovery of the point-like nature of the nucleus.

Second part of the story: STABILITY OF THE SECOND KIND

Question: given the stability of atoms (first kind), is it obvious that bulk matter with a large number N of atoms (say, $N = 10^{23}$) is also stable in the sense that the energy and the volume occupied by $2N$ atoms are twice that of N atoms? Without this property, the world of ordinary matter, as we know it, would not exist.

Question omitted in QM courses → difficult?
First asked by Onsager (1939), solved by Dyson and Lenard in 1967: Pauli principle essential! Bosonic matter would not satisfy the linear (in N) dependence ($\sim N^{7/5}$).

Dyson-Lenard proof complicated
⇝ next Lieb-Thirring who really "understand" what happens ⇝ open a completely new chapter of math-phys and even mathematics.

Course details:

Bibliography: •) "The Stability of Matter in Quantum Mechanics" Lieb - Seiringer

•) Schrödinger operators, e.values, LT ineq - Frank, Laptev, Weidl

•) P.T. Nam - LMU Munich, lecture notes

•) others...

Exam: oral exam

Disclaimer: I will try to make the course as self-contained as possible, sometimes will be impossible...

2. Introduction to QM

Let us briefly recall the main principles of QM. This is well known to you but will set the notation.

•) the state of a quantum mechanical particle is described by a complex valued function

$$\psi : \mathbb{R}^3 \to \mathbb{C}$$

$\uparrow$ physical space (we restrict to 3 dimensions)

•) normalized: $\displaystyle\int_{\mathbb{R}^3} |\psi(x)|^2 = 1$

•) classical energy replaced by energy functional

$$\mathcal{E}(\psi) = T_\psi + V_\psi \quad , \text{ where}$$

kinetic energy expectation value

$$T_\psi = \frac{\hbar^2}{2m} \int_{\mathbb{R}^3} |\nabla\psi(x)|^2 \, dx$$

and potential energy expectation value

$$V_\psi = \int_{\mathbb{R}^3} V(x) \, |\psi(x)|^2 \, dx$$

•) associated Hamiltonian:

$$H = H_0 + V$$

with $H_0 = -\frac{\hbar^2}{2m} \Delta = -\frac{\hbar^2}{2m} \sum_{i=1}^{3} \frac{\partial^2}{\partial (x^i)^2}$

$$(H\psi)(x) = -\frac{\hbar^2}{2m} (\Delta\psi)(x) + V(x)\,\psi(x) .$$

•) Then

$$\mathcal{E}(\psi) = (\psi, H\psi) \quad , \quad (f,g) = \int_{\mathbb{R}^3} \bar{f}(x) g(x) \, dx$$

for sufficiently nice functions

•) $$(\varphi, H\varphi) = \int_{\mathbb{R}^3} \left(\frac{\hbar^2}{2m} (\overline{\nabla\varphi})(x) \cdot (\nabla\varphi)(x) + V(x) \, \overline{\varphi(x)} \, \varphi(x) \right) dx \qquad (*)$$

Problem: LHS does not always make sense for arbitrary φ's.

In this course: interpret $(\varphi, H\varphi)$ as RHS of $(*)$

Well defined if ψ and $\varphi \in H^1(\mathbb{R}^3)$!

The Sobolev space $H^1(\mathbb{R}^3)$

Df A function $f \in L^2(\mathbb{R}^3)$ is weakly differentiable if there exists a function $g \in L^2(\mathbb{R}^3, \mathbb{C}^3)$ such that for all $\phi \in C_0^\infty(\mathbb{R}^3; \mathbb{C}^3)$

$$\int_{\mathbb{R}^3} \overline{\nabla \phi(x)}\, f(x)\, dx = \int_{\mathbb{R}^3} \overline{\phi(x)}\, g(x)\, dx.$$

We then define

$$\nabla f := g.$$

Df The Sobolev space $H^1(\mathbb{R}^3)$ is the space of all functions $f \in L^2(\mathbb{R}^3)$ that are weakly differentiable. It is a Hilbert space with the inner product given by

$$(f, g)_{H^1} = \int_{\mathbb{R}^3} \bar{f}(x)\, g(x)\, dx + \int_{\mathbb{R}^3} \overline{(\nabla f)(x)}\, (\nabla g)(x)\, dx$$

and the corresponding norm:

$$\|f\|_{H^1} = \left(\int_{\mathbb{R}^3} |f(x)|^2\, dx + \int_{\mathbb{R}^3} |\nabla f(x)|^2\, dx \right)^{1/2}.$$

Remark $H^1(\mathbb{R}^3)$ is the space of $L^2(\mathbb{R}^3)$ functions that have distributional first order derivatives that are also in $L^2(\mathbb{R}^3)$.

Remark Clearly $H^1(\mathbb{R}^3) \subset L^2(\mathbb{R}^3)$.

Fourier Transform

Convenient way of rewriting the kinetic energy is via Fourier Transform and the momentum representation.

$$\hat{\varphi}(k) = \int_{\mathbb{R}^d} \varphi(x)\, e^{-2\pi i k\cdot x}\, dx$$

well defined for all $\varphi \in L^2(\mathbb{R}^d)$.

•) Inverse:

$$\varphi(x) = \int_{\mathbb{R}^d} \hat{\varphi}(k)\, e^{2\pi i k x}\, dk$$

•) Plancherel's identity

$$\int_{\mathbb{R}^d} |\varphi(x)|^2 dx = \int_{\mathbb{R}^d} |\hat{\varphi}(k)|^2 dk.$$

•) Non-relativistic kinetic energy:

$$\int_{\mathbb{R}^d} |\nabla \varphi(x)|^2 dx = \int_{\mathbb{R}^d} (2\pi k)^2\, |\hat{\varphi}(k)|^2 dk.$$

Remark:

$\varphi \in L^2(\mathbb{R}^d)$ is in $H^1(\mathbb{R}^d) \Longleftrightarrow |k|\,\hat{\varphi}(k) \in L^2(\mathbb{R}^d)$

Stability of the first kind:

$\boxed{E_0 > -\infty}$ where $E_0 = \inf\{\mathcal{E}(\varphi) : \|\varphi\|_2 = 1\}$