The Pauli Principle

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Part I: The Pauli Principle and Atomic Structure

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The Nobel Prize 1945



The Nobel Prize in Physics 1945 was awarded to Wolfgang Pauli *"for the discovery of the Exclusion Principle, also called the Pauli Principle"*.

Pauli's original 1925 formulation: No two electrons (in an atom) can have the same set of 4 quantum numbers: *n*, *l*, *m*, and *s*

Bohr's atomic model of 1913

- The Nobel Prize in Physics 1922 was awarded to Niels Bohr "for his services in the investigation of the structure of atoms and of the radiation emanating from them"
- The electrons orbit the nucleus in shells numbered by the quantum number *n*
- The shells have energy levels

$$E_n = -\frac{e^4 m}{2\hbar^2} \frac{1}{n^2} = -\frac{1}{n^2} Ry$$
 (Rydberg)

- Explained the Rydberg formula in spectroscopy: $\frac{1}{\lambda} = R(\frac{1}{n_f^2} - \frac{1}{n_i^2})$
 - Lyman series $n_i \rightarrow n_f = 1$
 - Balmer Series $n_i \rightarrow n_f = 2$





The Periodic Table



Pauli's quantum numbers:

n=1	l=0	m=0	s=+/-	1 s	1 orbital	2 electrons
n=2	I=0	m=0	s=+/-	2s	1 orbital	2 electrons
	=1	m=-1,0,1	s=+/-	2р	3 orbitals	6 electrons
n=3	I=0	m=0	s=+/-	3s	1 orbital	2 electrons
	=1	m=-1,0,1	s=+/-	3р	3 orbitals	6 electrons
	I=2	m=-2,-1,0,1,2	s=+/-	3d	5 orbitals	10 electrons



Schrödinger's Wave equation

- Schrödinger gives a mathematical explanation of the quantum numbers in 1926.
- Nobel Prize 1933: The Nobel Prize in Physics 1933 was awarded jointly to Erwin Schrödinger and Paul Adrien Maurice Dirac "for the discovery of new productive forms of atomic theory"
- Dirac incorporated Einstein's theory of relativity and predicted the existence of the anti-electron=positron





The Schrödinger Equation

• Schrödinger's equation

$$-\hbar\partial_t \Psi = H\Psi$$

- *H* expresses the energy of the system *E*.
- The quantum states of the system correspond to the standing wave solutions to equation:
- The quantum numbers are related to, e.g., the number of nodes



The General Formulation of the Pauli Principle

- Pauli Principle: Two electrons cannot occupy the same "Quantum State"
- But what is a quantum state?
 - In an atom a state is characterized by (n, l, m, s)
 - In general a quantum state is very complicated to describe, e.g., in a molecule. In fact, even for atoms the Pauli description is only an approximation
- The Pauli principle states that were we able to measure the number of electrons in a *quantum state* we could only get the answers: 0 or 1.
- We shall see how this is necessary to explain the stability of everything we see in our every day macroscopic world!

Particle Statistics: Fermions and Bosons

- All elementary particles fall in two groups:
 - **Fermions**: Those that obey the Pauli principle, e.g., electrons, protons, neutrons, i.e., the particles that make up all normal matter. Fermions are named after **Enrico Fermi** (Nobel prize 1938)
 - Bosons: For which there is no limit to how many can be in the same quantum state, e.g., the photon, i.e., the particle of light, the particles that mediate the weak interaction: W[±], Z or the Higgs particle. Bosons are named after Satyendra Nath Bose





More on Fermions and Bosons

 The prediction that even a macroscopic number of bosons can occupy one state: A Bose-Einstein condensate was shown experimentally in 1995 and won Cornelle, Ketterle and Wieman the 2001 Nobelprize.



- The properties of bosons also explains that certain liquids, e.g., liquid Helium (the isotope Helium 4) become **superfluid**. This was discovered in 1937 by Kapitsa (Nobel 1978), Allen, and Misener and explained shortly after by Landau (Nobel 1962) and Bogoliubov.
- Fermions can also become **superfluid** (Helium 3) or **superconducting** (discovered for mercury in 1911 by Onnes, Nobel 1913). This was explained by Bardeen, Cooper, and Schrieffer in 1957 (Nobel 1972).
- In 2-dimensions mathematics predicts the existence of exotic particles anyons intermediate between *fermions* and *bosons*.

Part II: The Pauli Principle and Stability

- Atomic Stability and the Heisenberg Uncertainty Principle
- Chandrasekhar's Theory of Stability of White Dwarfs
- The Forgotten Question of Stability of Matter
- The Theorem of Stability of Matter by Freeman Dyson and Andrew Lenard
- Matter without the Pauli Principle would be unstable

Atomic Stability the Uncertainty Principle

- In classical physics a hydrogen atom would be **unstable**. The electron would spiral into the nucleus as it radiates light.
- In quantum physics the states are quantized. The **Triumph of Quantum Mechanics:**



The hydrogen atom is stable!

• The **energy** of hydrogen cannot become arbitrarily negative:

 $E = \frac{p^2}{2m} - \frac{e^2}{|x|} \ge -\frac{e^4m}{2\hbar^2}$ (Recall Bohr's formula)

• This does not reply on the Pauli principle, but is another expression of the **Heisenberg Uncertainty Principle:**

$$\Delta x \Delta p \geq \frac{\hbar}{2}$$

• The Nobel Prize in Physics 1932 was awarded to Werner Heisenberg "for the creation of quantum mechanics, the application of which has, inter alia, led to the discovery of the allotropic forms of hydrogen".

Stability of White Dwarfs

- The Nobel Prize in Physics 1983 was divided equally between Subramanyan Chandrasekhar "for his theoretical studies of the physical processes of importance to the structure and evolution of the stars" and William Alfred Fowler "for his theoretical and experimental studies of the nuclear reactions of importance in the formation of the chemical elements in the universe".
- Chandrasekhar explained how certain not too heavy stars at the end of their lifetimes when they no longer burn nuclear energy would not collapse to black holes, but form *white dwarfs* stabilized by the *Pauli degeneracy pressure* against gravitational collapse
- The *Pauli degeneracy pressure* is the pressure created by electrons in the star due to the *Pauli Principle*
- Chandrasekhar gives a formula for the limit to how heavy a star can be to resist gravitational collapse. (1.4 solar masses)
- The sun can become a white dwarf!
- Chandrasekhar's theory relies on special relativity. Without relativistic effects all stars would be stable. There would be no limit!



Chandrasekhar's Theory: simple minded derivation

• The **degeneracy pressure** for a gas of *N* electrons confined to ball of radius *R* would give an **energy**

$$\sim \frac{N^{\frac{5}{3}}}{R^2}$$

• The **gravitational energy** will be (the mass is not with the electrons but with the nucleons close to the electrons)

$$\sim -\frac{N^2}{R}$$

- These balance when $R \sim N^{-1/3}$
- For **relativistic particles** (moving almost with the speed of light). The degeneracy energy is

$$\sum \frac{N^{4/3}}{R}$$

 Now an upper bound (The Chandrasekhar limit) on N is needed to avoid collapse!!

The Question of Stability of Matter

- The forgotten question: Stability of macroscopic Matter.
- Stability of matter is also an issue of energy:
- Why does the energy contents grow proportionally with the amount of matter? Why does it make sense to say Joule/gram?
- The first to raise the question was **Lars Onsager** (Nobel prize chemistry 1968) in 1937:
- "In the electrostatic theory of crystals and liquids the existence of an additive lower bound for the electrostatic energy is generally taken for granted ... and it does appear that a rigorous proof... has ever been attempted"

Specific Energy and Energy Density						
	Specific Energy	Density	Chemical			
Fuel	kj/g	KWH/gal	Formula			
Propane	50.36	26.8	C3H8			
Ethanol	32.72	24.7	CH3CH2OH			
Gasoline	47.36	36.6	C7H16			
Diesel	44.75	40.6	C12H26			
Methane	55.82	26.8	CH4			
Oil	49.11	40.5	C14H30			
Wood	14.89	11.3	approx weight			
Coal	30.24	22.9	approx weight			
H2	141.89	2.5	H2			

Source: College of the Desert, Green Econometrics research

Serving size 100 g	acts
Amount	% Daily Value
Calories 80	



The Theorem on Stability of Matter

• In 1967 Freeman Dyson and Andrew Lenard finally showed that Stability of Matter consisting of electrons and nuclei is a consequence of Quantum Mechanics and in particular they need the Pauli Principle:

 $E \ge -const N Ry$

• In 1973 **Elliott Lieb** and **Joel Lebowitz** show the Onsager additivity of energy

$$E \sim -N Ry$$

• Both derivations are mathematically extremely sophisticated and are usually not presented in textbooks on quantum physics.





Instability of Matter without the Pauli principle?

• Freeman Dyson proved in 1967 that Stability of Matter fails if the electrons do not obey the Pauli principle. In fact, he showed that in this case:

$$E < -A_1 N^{\frac{7}{5}} R y$$

• Notice

$$\frac{7}{5} = 1.4 > 1$$

- The Onsager additivity fails!
- Dyson derives this by showing that a **superfluid state** can form.
- Dyson predicted that weakly interacting charged bosons could not exist. He was wrong: $W^{\pm}, Z!!$

Dyson's conjecture

- It is interesting that Dyson needed to imagine a **superfluid** state to show the instability.
- **Bose-Einstein condensation** of the "electrons" would not in itself cause instability.
- Dyson asks whether a superfluid state would really form: *"More interesting than making piecemeal improvements is the determination of the best possible coefficient* A₁*in*

$$E < -A_1 N^{\frac{\prime}{5}} R y$$

- Dyson states what he believes it should be and I confirmed it in 2006! Establishing that a superfluid state would indeed form.
- If somebody turned of the Pauli Principle of the electron. The earth would collapse to the size of an atomic nucleus!



Conclusion

- The Pauli Principle explains the structure of the periodic table of the elements and their basic chemical properties.
- The Pauli Principle is not needed to understand the stability of atoms only their structure.
- The Pauli Principle explains the stability of white dwarf stars
- The Pauli Principle is needed to explain the stability of everything around us: The Macroscopic Stability of Matter
- Without the Pauli Principle matter would collapse to a superfluid state