Maria Goeppert Mayer: a journey through her scientific legacy

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Abstract— One of the most remarkable female scientists of the 20th century was the German physicist and mathematician Maria Goeppert Mayer, who is known for her numerous contributions to the field of physics. This article highlights some of the most important discoveries of Maria Goeppert Mayer, such as the development of the nuclear shell model, which earned her a Nobel Prize in 1963, her studies of double photon emission and the possibility of chemical separation of isotopes as a quantum effect. Acknowledging Goeppert Mayer's contributions is crucial to the understanding of numerous current scientific advances. Moreover, she has been an inspiration for several researchers and a role model for later generations of young female scientists.

Keywords— Nuclear shell model, nucleons, Nobel Prize, double photon emission, isotopes, equilibrium constants.

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1. Introduction

Maria Goeppert Mayer was born on June 28, 1906, in Kattowitz, which was a part of Germany at the time. She grew up in an atmosphere of fascination with science [1]. Her father always encouraged her to grow up to be more than a housewife and to get an education, even though it was difficult for women at the time [2].

She entered the University of Göttingen in 1924, where she intended to study mathematics at first. However, after attending a quantum mechanics seminar taught by Max Born, a prominent figure in physics, she switched her focus to physics [2].

Maria Goeppert Mayer was an accomplished physicist from the start until the very end of her career and she made numerous contributions to the field of physics. She was a pioneer in investigating the phenomenon of double quantum emission and, a few years later, double beta decay [3].

For most of her career, Goeppert Mayer worked without any kind of pay or status, she was 58 before she was able to become a full professor in physics. Nonetheless, she persevered in her research and made major contributions to the growing understanding of nuclear physics, making important discoveries about nuclear structure. She is one of only four women to have won the Nobel Prize in physics (she was the second one, after Marie Curie) for her paper published in 1949, detailing the evidence for the nuclear shell model, which accounts for many properties of atomic nuclei [2], [4].

Additionally, she became a member of the Manhattan Project team during World War II. After the war, she kept on working part-time at Argonne National Laboratory in Chicago. There was the place where she would make her most important scientific discovery [5].

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Goeppert Mayer died due to a heart failure in San Diego, California, in 1972, at age 65.

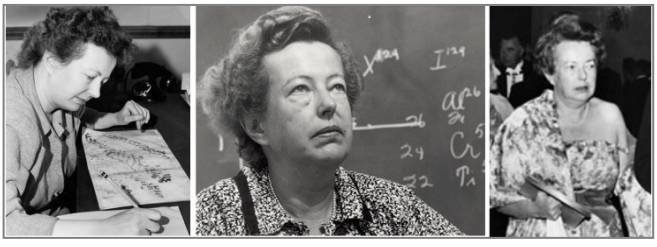

Fig. 1. Maria Goeppert Mayer (1906-1972). Images collected from: [4].

2. Contributions

2.1. Nuclear Shell Model

The nuclear shell model was initially proposed by Dmitri Ivanenko in 1932, however, it was further developed by Maria Goeppert Mayer and simultaneously by physicists Eugene Paul Wigner and J. Hans D. Jensen in 1949. Together they shared the Nobel Prize in Physics in 1963 for their work [6]. Inspired by discussions with Enrico Fermi, Goeppert Mayer proposed that protons and neutrons are arranged in a series of nucleon layers inside the nucleus, like the layers of an onion, with neutrons and protons rotating around their axes and the center of the nucleus at each level (spinning and orbiting, respectively). When these two motions are in opposition, the particle's energy shifts up [4]. The discovery of the magic numbers was crucial for the development of the Nuclear Shell Model. These magic numbers are a series of numbers that provide stability. For instance, 10, 18, 36, 54, and 86 are the magic numbers for the electronic structure of atoms. However, in nuclear physics, the magic numbers are 2, 8, 20, 28, 82 and 126, (see Figure 2).

2	8	20	28	50	82	126
			Protons			
He^{4}	O^{16} O^{17} O^{18}	Ca^{40} Ca^{42} Ca^{43} Ca^{44} Ca^{46} Ca^{48}	Ni^{58} Ni^{60} Ni^{61} Ni^{62} Ni^{64}	Sn^{112} Sn^{114} Sn^{115} Sn^{116} Sn^{117} Sn^{118} Sn^{119} Sn^{120} Sn^{122} Sn^{124}	Pb^{204} Pb^{206} Pb^{207} Pb^{208}	
			Neutrons			
He^{4}	N^{15} O^{16}	S^{36} Cl^{37} A^{38} K^{39} Ca^{40}	Ca^{48} Ti^{50} V^{51} Cr^{52} Fe^{54}	Kr^{86} Rb^{87} Sr^{88} Y^{89} Zr^{90} Mo^{92}	Xe^{136} Ba^{138} La^{139} Ce^{140} Pr^{141} Nd^{142} Sm^{144}	Pb^{208} Bi^{209}

Fig. 2. Magic number nuclides. Data collected from: [7].

One remarkable fact is that there are six stable nuclei with 50 neutrons and seven with 82 neutrons, taking into consideration that usually there are only two or three isotopes with the same number of neutrons [7].

Calcium is one of the best examples to explain the effect of magic numbers. Calcium's atomic number is 20, one of the magic numbers mentioned before, and this could be the explanation why it has so many isotopes. ^{40}Ca and ^{48}Ca isotopes have 20 and 28 neutrons respectively, also magic numbers, and they both have more than the expected nuclear binding energy. The nuclear binding energy is the minimum energy needed to divide the nucleus into its parts (protons and neutrons). It can be calculated thanks to the Weizsäcker formula, which is based on the liquid drop model (the previous nuclear model). This formula, as said before, failed to predict ^{40}Ca and ^{48}Ca's binding energy, which means that the nuclear shell model could explain atoms with light nuclei, like these isotopes, better than the liquid drop model [8].

2.1.1. From the atomic model to the nuclear model

The experimental data obtained that led to the discovery of these magic numbers could hardly be explained as a coincidence. At the time, it seemed to be worthwhile to explain them and, from this curiosity, the Nuclear Shell model would arise. At this point, the fact that the electronic model, which is based on a model of shells, also relies on the existence of magic numbers that provide the stability of the atoms, made scientists think that, fundamentally, the nuclear structure could be similar to the current atomic model. This way, it would describe how nucleons are added to shells which increase with energy that orbit around a central potential. Therefore, the nuclear shell model would be based on the Pauli exclusion principle, describing the structure of the nucleus in terms of energy levels [6]. When the highest energy shell in the nucleus is full, then it would be very stable, and when it is not full, the nucleus would be less stable. This explained why certain magic numbers of protons and neutrons created very stable nuclei, while other numbers did not [5].

In analogy with the atomic structure, as explained before, nucleons would move rather independently in distinct orbits. This opened severe doubts. First of all, in the atom, the dominant attraction of the nucleus is key. Second of all, the Coulomb repulsion between the electrons is of long range, which means that the potential acting on one electron does not depend perceptively on the exact position of the others. On the other hand, the forces in the nucleus are of short range, which means that the potential on one nucleon depends strongly on the position of the others. Consequently, it was expected that nucleons would collide with each other. However, these collisions are not critical, thanks to the Pauli principle, which does not allow collisions that would sidetrack nucleons into already filled orbits. Then, most of the expected collisions would not take place and this theory could be pursued [7].

Another difference is that the nucleus contains two kinds of subatomic particles, neutrons and protons. It was assumed that the nuclear potential was the same for protons and neutrons, supported by the fact that the magic numbers were the same for both of them. The Pauli principle requires that each nucleon have a unique set of quantum numbers to describe its motion so a certain level can be occupied by no more than $2(2+\boldsymbol{l})$ nucleons of one kind. For instance, for level 1s ($\boldsymbol{l}$=0), it would have room for two neutrons and two protons (^{4}He). The next level is 1p ($\boldsymbol{l}$=1), which has six states, and then it would have room for eight nucleons of each kind. Since there are two kinds, 16 nucleons can be accommodated, leading to ^{16}O. Thus, the uniquely stable numbers are easily explained for the light nuclei. However, it failed in predicting the properties of heavy nuclei, so they are explained by other nuclear models [7].

According to the nuclear shell model, the motion of each nucleon is governed by the average attractive force of all the other nucleons. The resulting orbits form shells of increasing energy, and as nucleons are added to the nucleus, they drop into the lowest-energy shells allowed by the Pauli Principle, (see Figure 3). This model accurately predicts certain properties of normal nuclei, such as their angular momentum, and describes how much energy is required to move nucleons from one orbit to another and how the quantum numbers change. When a shell is full, the nucleons have used up all of the possible sets of quantum number assignments, and such shell has a total angular momentum equal to zero [9], [10].

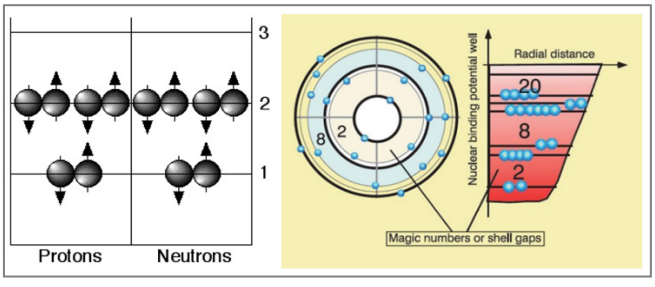

Fig. 3. Nucleons occupying different shells (left) and magic numbers (right). Data collected and modified from: [9], [11].

The fact that nuclei with a magic number of nucleons were especially stable had been noticed before, but physicists were convinced that a shell model could not be correct, because of the success of the liquid drop model (an alternative model that treats the nucleus as a homogene-

ous drop of a liquid) in explaining fission and other properties of nuclei. Furthermore, physicists assumed that the interactions between nucleons would be too strong, so they could not be treated as independent particles. Yet, Goeppert Mayer was less biased by the liquid drop model, so she considered other nuclear properties and collected evidence that pointed to supporting that the nuclear shell model was correct [2].

2.2. Calculation of Equilibrium constants

Goeppert Mayer published with Jacob Bigeleisen a paper in 1947 on equilibrium constants providing important information that demonstrated that the chemical separation of isotopes was a quantum effect [12].

The calculations of equilibrium constants for isotopic exchange reactions from spectroscopic data can be greatly simplified: they can be calculated without any knowledge of the moments of inertia of the molecules.

For gaseous substances, the Helmholtz free energy is connected to the partition function by a relation where Q is the partition function of the molecule.

$$F = -RTlnQ/N \quad (1)$$

The partition function is defined as:

$$Q = \sum_n e^{-\epsilon_n/kT} \quad (2)$$

The Helmholtz free energy change would be:

$$\Delta F = -RTlnK \quad (3)$$

By combining (1), (2) and (3), the equilibrium constant is obtained:

$$K = \frac{\prod Q_{products}}{\prod Q_{reactants}} \quad (4)$$

A calculation of Q allows for the calculation of equilibrium constants for chemical reactions.

It is likely that the calculation of $\boldsymbol{RTlnK}$ as the difference of the total free energies of the reactants and products leads to significant errors. A much simpler and more accurate method is obtained by calculating the differences in the free energies or the ratios of the partition functions directly.

The chemical separation of isotopes is a quantum-mechanical effect. The potential energies for molecules differing only in isotopic constituents are alike. The ratio of the partition functions of two isotopic molecules is, therefore, considered to reduce to the inverse ratio of the symmetry numbers multiplied by the mass ratio of the different isotopes raised to the 3/2 power:

$$\frac{Q}{Q'} = \frac{s'}{s}\left(\frac{m}{m'}\right)^{\frac{3}{2}} \quad (5)$$

We have to consider the ratio of the quantum mechanical to classical correction to the partition function for each of the molecules. The fundamental approximation that was made was the failure of the interaction between rotation and vibration, as well as the anharmonicity of the vibrations. These corrections can be very small if the frequency in the ground state and the zero-point energy is correctly chosen [13].

The Bigeleisen–Mayer equation is based on the Born–Oppenheimer approximation. In this equation, isotope-independent potential energy is used, and simple harmonic vibrations are assumed in its derivation [14].

Those errors have become one of the biggest mistakes in the prediction of equilibrium isotopic fractionation. In addition, a lot of researchers still use this equation to handle Hydrogen–deuterium exchange reactions [15].

For a lot of years, this method (called the Urey model too) has been one of the most stable equations of isotope geochemistry. The advantage of using the Bigeleisen-Mayer equation is that it simplified so much the calculation. That is possible because it cancels out as many identical energy terms as possible [16].

"In all isotopic exchange reactions partial cancellation of the separative effect must occur", said Maria in her article [13].

After these mistakes, a lot of corrections about the harmonic level to the Bigeleisen–Mayer equation have been discussed and compared. Nowadays, this first equation is not the most accurate [15].

2.3. Double photon emission

The absorption of light by atoms and molecules is a known phenomenon in Quantum Physics. The transition between a ground state and an excited state can be carried out by absorbing one, two or more photons, (see Figure 4). The theoretical expression for the absorption of two photons was published by Maria Goeppert-Mayer in 1930 and experimentally confirmed 30 years later after the invention of the laser (light amplification by stimulated emission radiation) [17].

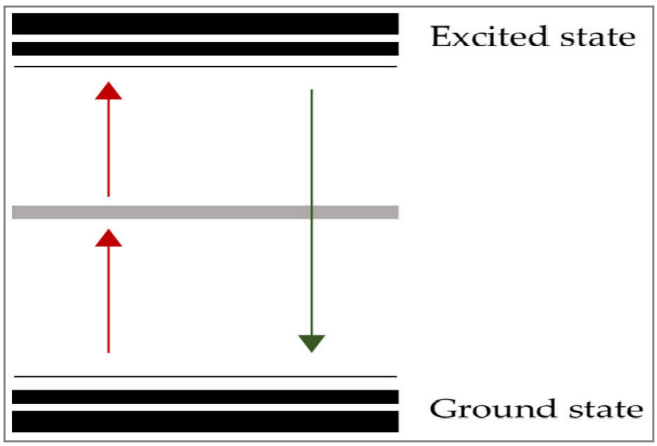

Fig. 4. Schematic of a two-photon emission process. Both photons are absorbed simultaneously. Upward arrows mean absorbed; downward arrows mean emitted photons.

Two non-resonant photons are used for excitation simultaneously that results in the occupation of an energy state at the sum of the frequencies of the absorbed photons. "When light falls upon the atom with a frequency smaller than the corresponding atomic eigenfrequency, another stimulated double emission occurs during which the atom divides its energy into one incident and one frequency-difference photon" [18]. Kramers and Heisenberg did calculate the probability of this last process according to the corresponding principle. Moreover, the reversal of this process is considered, that is, where two photons, whose sum of frequencies equals the excitation frequency of the atom, co-act to excite the atom.

Maria Goeppert's research went deeper to attempt an explanation of this phenomenon through a process whereby, simultaneously, in one elementary action, the molecule or atom takes the energy from the emitted electron up and sends out light. Then, it remains in a state of "discrete" [18] energy able to emit a spectral line of the discrete spectrum in a second, independent process. This consideration shares some similarities to the Raman effect, which can also be regarded as the coincidence of two processes in one elementary process. Because such a single process occurs the moment the collision affects the atom, it would explain all phenomena which cannot be interpreted through a recombination radiation, because it refers to the absorption of a free electron by an ion and the subsequent radiation of the excess energy as photons, causing the recombination line spectra [19]. The calculation of the double-photon emission yields a non-zero probability for such a process, the character of which was discussed in Goeppert's paper.

The two-photon emission phenomenon is currently used in skin surface microscopy, in the diagnosis of tissue lesions, or the testing of drug distribution in the skin. More techniques like photodynamic therapy and multiphoton tomography come from the application of Maria Goeppert's research [1].

3. Conclusions

The influence of Maria Goeppert Mayer on science continues to be significant. The importance of her achievements was a turning point in the field of physics and an inspiration for later generations of female scientists. The development of the nuclear shell model was a fundamental change in how physicists thought of what was going on inside the nucleus of an atom, and the idea quickly spread throughout the world. Although Maria Goeppert Mayer had to face multiple obstacles during her career due to gender inequality, she became a successful researcher in her field. The Maria Goeppert Mayer Award was created posthumously in her honor, to recognize and enhance outstanding achievements by female physicists in the early years of their careers.

Based on the legacy that Goeppert Mayer left behind, scientific progress is still going on. Although the nuclear shell model is more than 70 years old, physicists continue studying it. Goeppert Mayer's discovery could answer some of the deepest questions scientists asked about, such as what we are made of and where we came from. She was a pioneering thinker whose ideas are still at the core of research in current science [20].

YouTube video

The authors have summarized this paper in a video with the same title, that you can find clicking the following link:

https://youtu.be/c313y7RqB0k

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