Nuclear force theory and its verification using mass spectrometry

1 The Theory of nuclear forces

Ever since it was discovered that the nucleus is made up from protons and neutrons, scientists have been working out how it is held together. The logical answer would be a force, though the only two forces known at the time were the gravitational and the electromagnetic. However, neither of these could be the one as protons and neutrons don't have opposite charges and the gravitational force is far too weak to explain the phenomenon. So it was concluded it must be another force, called the nuclear force. [1]

1.1 Exchange particles and meson theories

The first theory for the nuclear force was developed by Yukawa, introducing his exchange particles. From an intuitive standpoint, the Heisenberg uncertainty principle allows for short term spontaneous creation of particles. These particles can then transfer momentum between two nucleons, by interactions, before vanishing again. This mechanism does impose certain range and strength constraints on the force however, as a stronger force requires more massive exchange particles, giving them less time to exist and travel between nucleons.

Yukawa predicted the properties of suitable exchange particles and when the pion and other suitable mesons were discovered they gave rise to so called meson theories. Many properties of simpler interactions were explained well with One Boson Exchange (OBE) models, where only one exchange of each meson is considered. However, adapting the theory for multiple exchanges wasn't as straight forward and led to the development of many more advanced models (Paris, Bonn, Stony Brook).

1.2 Quantum Chromodynamics

Then Quantum Chromodynamics (QCD) was developed, quarks discovered and the strong force was introduced between them, mediated by gluons. This completely changed the picture of the nuclear force, as the attraction of nucleons was now attributed to residuals of the strong force, delegating the meson theories to models. However, calculating the nuclear force directly from QCD is very difficult for a variety of reasons, QCD is highly nonpertrubative at this range/scale making it is difficult to calculate and even a 2 nucleon interaction would already involve 6 quarks. Still, attempts are made using finite step computer simulations, called Lattice QCD, which are very useful for verifying simple interactions but aren't suitable for regular day-to-day applications.

1.3 Effective Field Theory

Applying Effective Field Theory (EFT) was the next break through, the key is that the significant effects may be studied independently at different scales. To use EFT one must first identify the degrees of freedom (the interacting particles/entities), in our case nucleons and mesons (at the nucleon scale, mesons are the relevant exchange particles). [1] Then one constructs a Lagrangian (which is essentially an expression describing the dynamics of the system) in a certain way. The key is to construct the most general possible Lagrangian that follows the same symmetries as the QCD strong force, as an expansion of Q/Λ. Where Q is the typical momentum of the system and Λ the range at which the EFT interaction model stops being applicable. The EFT application to QCD for modelling the nucleon interactions is called Chiral EFT (CEFT) as chirality (symmetry under reflection) is a key symmetry of the strong force.

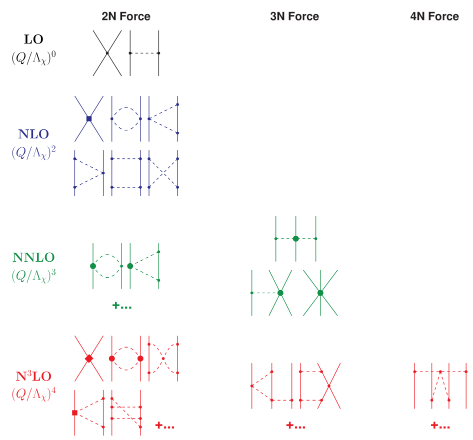

Figure 1: Feynman diagrams showing some of the first interactions that need to be considered when using CEFT. Solid lines represent nucleons and dashed lines pions. Different nodes represent different interactions.

[1]explain later, I'm not sure I get it rn

Using CEFT is a rather involved process but the following tries to provide a short outline of the key features. There are 2 main decisions, the first being how many nucleons do we include, the simplest being 2 nucleons (NN), following with 3 nucleons (3N), 4 nucleons (4N) and many nucleons. The second is how many terms of the mentioned expansion do we take into account, these simplest here is regarded as the Leading Order (LO) followed by Next Leading Order (NLO), Next Next Leading Order (NNLO) and so on. Determining both of these specifies which interactions need to be considered, fig:diagram1 shows Feynman diagrams for some. In these there are different types of nodes each associated with a Low Energy Constant (LEC) which are determined by fitting experimental data and influence how the interaction affects the force.

1.4 Nuclear Shell Theory

The nuclear shell model originates from scientists observing that atoms with certain numbers of protons and neutrons (called magic numbers, covered more later) were more stable than others, which resembled the effects of shell closures in the atomic shell model. Simplest shell models consider the individual nucleons to behave independently, each in a potential formed by the many NN interactions, where this potential results in a central potential with additional spin-orobit, spin-spin and tensor components.

1.5 Outlook

Finally, for a general outlook, most stable nuclei (especially ones in the valley of stability) are modeled well using combinations of the meson theories, CEFT based nuclear shell models (NN is often sufficient for stable isotopes) and other approaches. However for exotic, neutron-rich nuclei the models fall short, at least 3N interactions need to be considered for an accurate model and more measurements are currently being made.

2 Mass Spectrometry

A Mass Spectrometer (MS) is a device used to measure the mass to charge ratio ($\frac{m}{Q}$) of ions. Usually, this charge to mass ratio is calculated from either how much an ion is deflected in a magnetic field or accelerated in an electric field – ions with the same ratio are deflected/accelerated equally. This information can be used for a variety of purposes such as determining an unknown isotope in a mixture or to directly measure nuclear masses.

2.1 Importance to nuclear theory

Mass spectrometers are integral to the study of nuclear theory for identifying or quantifying unknown samples (ions) as well as measuring binding energy of particles to gain information about their nuclear structure. Nuclear mass is a fundamental property which has been responsible for the discovery of many nuclear effects such as shell closures and nucleon-nucleon pairing [2]. MS are used in nuclear physics research to explore exotic nuclei (such as neutron rich calcium isotopes [**wienholtz**]) and isotopes with high neutron to proton ratios are interesting to study as they can develop our understanding of the nuclear force. Examining binding energy is key to understanding the nuclear theory, it is related to the stability of the nuclei so the atoms in the valley of stability have the lowest binding energy as well.

The charge to mass ratio was first measured by J. J. Thomson in the late 19th century [3] and throughout the 20th century MS have evolved with numerous variations and different set ups. This report focuses on 2 types of MS: the Penning trap and the Multiple Reflector Time of-Flight (MR-TOF) mass spectrometer, as both are currently used to measure the mass of exotic nuclei [4].

2.2 How a general MS works

A general MS has three stages components: an ioniser, mass analyser and a detector. A sample must be ionised before entering the mass analyser so it will interact with the magnetic and/or electric fields. In the mass analyser the beam is accelerated/deflected before being incident on a detector. The detector then measured the mass charge ratio based on the time or location of incidence [5]. Ionization methods including thermal ionization ,where the sample is heated and emits electrons on its own, and electron impact, where the sample is bombarded by electrons to excite the sample electrons which are then emitted. At the end of chamber there is a detector usually are electron multiplier like faradays cup, measuring quantity and time of arrival. The more the ions hit a certain part of the detector it means the sample has more of that type of isotope in nature. And from all that, MS can generate the spectrum which is useful for analysing unknown samples.

2.3 Penning traps

Penning traps are the most common development with their currently being 7 active laboratories including CPT, ISOLTRAP, JYFLTRAP, LEBIT, SHIPTRAP, TITAN and TRIGA-TRAP and they also give us the most precise measurement for stable isotopes [6]. Just 15 years ago, the only Penning trap spectrometer publishing the masses of radioactive samples was the pioneering experiment ISOLTRAP, set up at CERN's ISOLDE facility in 1986 [7]. Penning traps are based on a cyclotron design, and they trap the isotopes using a combination of strong longitudinal uniform magnetic and quadrupole electric fields, a high homogeneity also reduces the possibility to field drifts so that they move periodically and then the frequency is related to mass following the equation

$$\nu_c = \frac{1}{2\pi}\frac{qB}{m} \tag{1}$$

the measured quantity is cyclotron frequency which can be essentially measured in high accuracy. Also, the coexistence of trapping and cooling minimizes systematic errors from mass measurement though the time it takes to complete a cycle is the main limitation of mass measurement which tends to limit the range of isotopic species that can be measured [4].

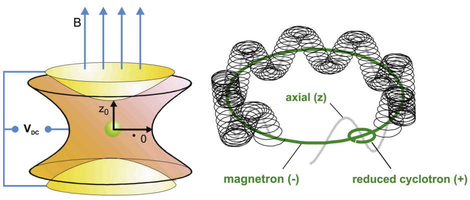

Figure 2: Schematic diagram of a Penning trap.

2.4 MR-TOF mass spectrometers

MR-TOF devices are the newest ion-trap development, first being used in 2013, they are often used accompanied with Penning traps. Their greatest advantage is that they can provide measurements for isotopes with very low production rates and very short half-lives, which is particularly suitable for short lived nuclei as they can resolve in less than 30ms and are suited to rare nuclei as they can resolve small sample sizes. MR-TOF MS works by reflecting the ions back and forth between two electrostatic mirrors in a short tube, effectively increasing the flight path length. The key is that the speed inside depends on the mass-to-charge ratio, so after a while, the isotopes are released, and the mass is calculated from the timing through this equation

$$t = \frac{d}{\sqrt{2U}}\sqrt{\frac{m}{q}} \tag{2}$$

MR-TOF MS are usually faster and more sensitive as a non-scanning device with high ultra-mass resolving power than a Penning trap. It has several advantages compared to a frequency-based mass spectrometer also including the single-ion sensitivity, short cycle time (5ms) and superior resolving power for a measurement time of 1s and mass-to-charge ratio larger than hundreds of amu [8].

3 Nuclei mass measurements with regard to nuclear force theory

3.1 Nucleon pairing energy

Besides the standard investigations, we can also investigate the neutron pairing energy of finite nuclei. We can study a range of odd and even pairs of N/Z numbers; to investigate the strong nuclear force [9]. So far, the idea is that the (N)even-(Z)even nucleus (although energy depends on factors such as the kind of particles and state it is occupied) we known for a fact that odd(N)- odd(A) nucleus is 1/2 to 2/3 times smaller, this is when they are given in the same shell and the mass numbers A are very close to one another. This strange character is due to the nucleon-nucleon potential resulting from the strong force. [10]

There is a model known as the liquid drop model, which underpredicts the binding energy of magic nuclei, magic nuclei referrer to nuclei where N or Z are a magic number, for the stable atoms these are 2, 8, 20, 28, 50, 82 and 126. The neutron/ proton separation energy peaks if N(Z) equals a magic number; on the zigzag graph, we see this as the last point before the significant drop. There is a more stable isotope if Z is a magic number and a more stable isotone if N is a magic number. If either N or Z or both are magic numbers, then the energies of the excited state will be much higher than the ground state. Another discovery is that elements with Z equal to a magic number have a more prominent natural abundance than nearby elements. [11]

3.2 Liquid drop model and the investigation of magic numbers

The magic number can further be explained by the shell closure model of the nucleus. This is done by considering each nucleon to be moving in some potential and classifying the energy level in terms of quantum numbers n l j, like how the wavefunction of individual electrons are classified in atomic physics. The energy eigenvalues depend on the principal quantum number, n, orbital angular momentum. The energy level comes in shells, with a large gap just above each shell. [12]

3.3 Nucleon driplines

In particle physics, we often use the idea of drip lines to categorize our particles. We have a one or two-particle drip line, which is a result of the idea that odd and even nucleon numbers, as we know, it has a significant effect on binding energy. We will be looking at one particle drip line for an odd(Z) or odd(N) nuclei. Two particle drip line occurs when the energy of the separation of two-particle becomes negative. Experimentally, we determined the one and two neutron drip lines up to neon. [??tobedone??]

4 Applications of MS outside nuclear force theory

Mass spectrometry has a long history and wide adoption out with nuclear physics both in research and commercially. MS are essential for chemical analysis – often used to determine the isotopes present in a mixture. In chemical and biomedical research, they are used frequently for structural elucidation where MS can give information about molecular structure. [13]

One exciting area of study where MS are fundamental is neutrino physics. Penning traps are especially well suited to this study due to their high sensitivity while neutrinos are not short lived so do not require the quickest resolving time (that a MR-TOF could provide). The neutrino is the most abundant particle with mass - roughly a thousand trillion pass through your body every second. [14] Yet the incredibly light particles are elusive and difficult to detect as they only interact with the weak force and gravity so surprisingly little is known about them. [15] Research in neutrino science could further the understanding of the standard model and they could be important in explaining why there is matter in the universe and not antimatter [16] – it is thought that neutrinos could be their own antimatter, unlike any other fermion in the standard model [8]. Another interesting behaviour they have is neutrino oscillometry where the particle can change flavour (electron, muon, tau) as it travels. It was this behaviour which proved that not only do neutrinos have mass but that they are a quantum superposition of 3 masses [16]. Since neutrinos are chargeless themselves, an upper limit to their rest mass can be measured by the mass difference between mother and daughter nucleotides from a nuclear decay. [17] For example the -decay: ?? with Rhenium as the mother nucleotide and Osmium the daughter. [18] The current upper limit of this mass is 1. 1eV measured at the Karlsruhe Tritium Neutrino (KATRIN) spectrometer. [19] Although KATRIN is an electron spectrometer and not a MS, PENTATRAP is a new five Penning trap facility being built in Heidelberg, Germany and is expected to reduce this upper mass limit even further [18].

MR-TOF MS also have many applications outside nuclear physics. Due to their compact size and relative affordability compared to Penning traps, MR-TOF's are suited to in situ applications[7 check source]. One potential application is waste water management where the MS could identify pollutants [8] – during COVID-19 pandemic waste water analysis was used to model the spread of the disease [20]. One current application of the technology is in biomedical analysis where a variation of the device (MALDI-TOF MS) is used routinely as an accurate and fast method to identify of microorganisms which reduces costs as it requires minimum consumables. [11]

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