



Theoretical Nuclear Physics

(SH2011, Second cycle, 6.0cr/ SH3311, Third cycle, 7.5cr)
(March 24, 2014)

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THEORETICAL NUCLEAR PHYSICS
SH2011 | 6.0 CREDITS

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Course overview

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Course plan etc.

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Complex eigenvalue problem

Lanczos approach for the eigenvalue problem

The effect of the spin-orbit coupling in many-body systems

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Theoretical Nuclear Physics

Selection is based on my settings ▾

Main contents

- Nuclear force and second quantization
- Fundamental coupling schemes
- Basic excitations in atomic nuclei and collectivity
- Nuclear deformation
- Magnetic resonances and medical applications
- Normal product and the Wick theorem
- Tamm-Dankoff & Random Phase Approximations
- Nuclear shell model, seniority and computation
- Fission, fusion and nuclear energy
- Nuclear astrophysics and nucleosynthesis

Learning outcome

- The capability to understand the structures and decays of atomic nuclei from a microscopic perspective and to perform basic

New event
Mon 24 mar 13:00-15:00
Föreläsning
Location: FB54
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Latest teacher post
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Comments and corrections are welcome!

Chong Qi, chongq@kth.se

(2*45)

Week 13-22

Mon 24 mar 13:15-15:00

27th March 13:15-15:00

Tue 1 apr 13:15-15:00

April 2, 13:15-15:00

Tue 8 apr 13:15-15:00

Tue 15 apr 13:15-15:00

Tue 22 apr 13:15-15:00 (Guest lecture)

Tue 29 apr 13:15-15:00 (Guest lecture)

Tue 6 may 13:15-15:00

Tue 13 may 13:15-15:00

Mon 19 may 13:15-15:00

Tue May 27, 13:15-15:00

The course contains 12 sections

- ✧ Basic Quantum Mechanics concepts
- ✧ Basic nuclear physics concepts: Pairing, single-particle excitations, square well
- ✧ Magnetic resonances in nuclei
- ✧ Single-particle model and the spin-orbit interaction
- ✧ Nuclear deformation and the Nilsson model, the cranking approximation
- ✧ Two-particle system, LS and jj coupling
- ✧ Modern theory of the nuclear force, isospin symmetry
- ✧ Seniority coupling scheme and neutron-proton coupling scheme
- ✧ One-nucleon operators, gamma and beta decays, ^{14}C -dating β decay
- ✧ Many-body operators and alpha decay
- ✧ Second quantization
- ✧ Hartree-Fock and energy density functional
- ✧ Tamm-Dancoff & Random Phase Approximations

If time allows, we may also cover:

- ✧ Scattering theory and resonances
- ✧ Continuum, nuclear halo and astrophysics

References:

K. Heyde, Basic ideas and concepts in nuclear physics, IOP Publishing 1994

K. Heyde, *The nuclear shell model*, Springer-Verlag 2004

P. J. BRUSSAARD and P. W. M. GLAODEMANS, SHELL -MODEL APPLICATIONS IN NUCLEAR SPECTROSCOPY North-Holland 1977

G.F. Bertsch, Practitioner's Shell Model (North-Holland, New York, 1972)

J. Suhonen, *From Nucleons to Nucleus: Concepts of Microscopic Nuclear Theory*, Springer, Berlin, 2007

D.J Rowe & J.L. Wood, FUNDAMENTALS OF NUCLEAR MODELS, World Scientific, 2010

R. D. Lawson, Theory of the nuclear shell model, Clarendon Press, 1980

I. Talmi, Simple Models of Complex Nuclei (Harwood Academic, Reading, UK, 1993), Chap. 1-13

S.G. Nilsson and I. Ragnarsson: Shapes and Shells in Nuclear Structure, Cambridge Press, 1995

P. Ring and P. Schuck, The Nuclear Many-Body Problem (Springer-Verlag, New York 1980).

Bohr,A.,Mottelson,B. Nuclear.Structure.Vol.I&II.World.Scientific,.1998

Physical Review C <http://prc.aps.org/>

Physical Review Letters <http://prl.aps.org/>

Nuclear Physics A <http://www.sciencedirect.com/science/journal/03759474>

Journal of Physics G, <http://iopscience.iop.org/0954-3899>

European Physical Journal A, <http://www.springerlink.com/content/1434-6001>

<http://arxiv.org/archive/nucl-th>

- Home works (11 in total): Pre-reading + exercises
- projects (note + oral presentation)

Before the lecture

- Finish the exercises and hand in (two copies) in due time.
- Read the lecture notes in advance
 - Pay special attention to the key concepts I mentioned at the beginning of each chapter
 - I will not repeat what is written in the lecture notes.
- Choose one or several projects to work with

During the lecture

- Present your the exercises
- Mark and approve one copy of the others'
- Present your projects
- Group discussion on key concepts



Bases of your assessment. To pass, one should have

>7 Approved homeworks

>1 Approved projects

Higher requirement for PhD and late submission

After the lecture and before you go:

Write on a small piece of paper and leave it to me

- The hard/muddy point
- The interesting point

There will be no Final Exam for this course.

After the course

- Summer projects (2-3 months)
- Master projects
- PhD?

Advanced reading courses

5A5426 Non-Hermitian Quantum Mechanics (7.5 credits)

D.S. Belkic, The principles of Quantum scattering theory, University of Stockholm and own materials

5A5429 Symmetry in Physics (7.5 credits)

J.P. Elliott and P.G. Dawber, Symmetry in Physics (Volume 1 & 2), Oxford

Zhong-Qi Ma, Group Theory For Physicists, World Scientific Publishing Co

5A5427 Quantum Mechanical Many body Problem (7.5 credits)

P. Ring and P. Schuck, Nuclear Many body problem, (Springer, Berlin) 1980 (Chap. 5-8).

D. Rowe, Nuclear collective motion, World Scientific Publishing Co

Own material

Atomic Physics

The physics of the electronic, extra-nuclear structure of atoms

Nuclear Physics

The physics of the atomic nucleus, believed to be *constituted* of neutrons and protons

Elementary Particle Physics

The physics of quarks and gluons, believed to be the constituents of protons and neutrons, and of leptons and gauge bosons and...
who knows what else!

Quarks, gluons, leptons, and gauge bosons are believed to have no substructure.

Who has taken the Nuclear Physics course?
Quantum Physics (Second quantization)?

The dawn of nuclear physics

- *1896: Discovery of radioactivity (Becquerel)
- *1911: Discovery of the nucleus (Rutherford experiment)
- *1932: Discovery of the neutron (Chadwick)
- *1935: Bethe-Weizsaker mass formula
- *1939: Discovery of (neutron-induced) fission
- *1949: Shell model (Goeppert-Mayer, Janssen)
- *1951: Collective model (Bohr, Mottelson, Rainwater)
- *1957: Nuclear superfluidity (Bohr, Mottelson)
- *Since then: Nuclear forces, many-body methods (HF, HFB, RPA, GCM, Green function, etc.)

Nomenclature

Nuclide A specific nuclear species, with a given proton number Z and neutron number N

Isotopes Nuclides of same Z and different N

Isotones Nuclides of same N and different Z

Isobars Nuclides of same mass number A ($A = Z + N$)

Isomer Nuclide in an excited state with a measurable half-life

Nucleon Neutron or proton

Mesons Particles of mass between the electron mass (m_0) and the proton mass (M_H). The best-known mesons are π mesons ($\approx 270 m_0$), which play an important role in nuclear forces, and μ mesons ($207 m_0$) which are important in cosmic-ray phenomena

Natural unit

Natural units are physical units of measurement based only on universal constants. For example the elementary charge e is a natural unit of electric charge, or the speed of light c is a natural unit of speed. In nuclear physics, the most useful units are \hbar , c , fm, MeV.

| | | |
|-----------------|-----------|--|
| Planck constant | h | $6.626\,069\,57(29) \times 10^{-34} \text{ J s}$ $4.135\,667\,516(91) \times 10^{-15} \text{ eV s}$ |
| $h/2\pi$ | \hbar | $1.054\,571\,726(47) \times 10^{-34} \text{ J s}$ $6.582\,119\,28(15) \times 10^{-16} \text{ eV s}$ |
| | $\hbar c$ | $197.326\,9718(44) \text{ MeV fm}$ |

Nuclear masses $\sim 10^{-27} \text{ kg}$

Convenient energy units

$$1 \text{ eV} = 1.602 \times 10^{-19} \text{ J}$$

Atomic Scale ~ eV

Nuclear Scale ~ MeV (10^6 eV)

Particle Scale ~ GeV (10^9 eV)

What is the mass of a nucleon?

- 1MeV
- 1GeV

| | | |
|-----------------------------|----------------|--|
| electron mass | m_e | $9.109\,382\,91(40) \times 10^{-31} \text{ kg}$ $5.485\,799\,0946(22) \times 10^{-4} \text{ u}$ |
| energy equivalent | $m_e c^2$ | $8.187\,105\,06(36) \times 10^{-14} \text{ J}$ $0.510\,998\,928(11) \text{ MeV}$ |
| electron-muon mass ratio | m_e/m_μ | $4.836\,331\,66(12) \times 10^{-3}$ |
| electron-tau mass ratio | m_e/m_τ | $2.875\,92(26) \times 10^{-4}$ |
| electron-proton mass ratio | m_e/m_p | $5.446\,170\,2178(22) \times 10^{-4}$ |
| electron-neutron mass ratio | m_e/m_n | $5.438\,673\,4461(32) \times 10^{-4}$ |
| proton mass | m_p | $1.672\,621\,777(74) \times 10^{-27} \text{ kg}$ |
| energy equivalent | $m_p c^2$ | $1.503\,277\,484(66) \times 10^{-10} \text{ J}$ $938.272\,046(21) \text{ MeV}$ |
| proton-electron mass ratio | m_p/m_e | $1836.152\,672\,45(75)$ |
| proton-neutron mass ratio | m_p/m_n | $0.998\,623\,478\,26(45)$ |
| neutron mass | m_n | $1.674\,927\,351(74) \times 10^{-27} \text{ kg}$ $1.008\,664\,916\,00(43) \text{ u}$ |
| energy equivalent | $m_n c^2$ | $1.505\,349\,631(66) \times 10^{-10} \text{ J}$ $939.565\,379(21) \text{ MeV}$ |
| alpha particle mass | m_α | $6.644\,656\,75(29) \times 10^{-27} \text{ kg}$ $4.001\,506\,179\,125(62) \text{ u}$ |
| energy equivalent | $m_\alpha c^2$ | $5.971\,919\,67(26) \times 10^{-10} \text{ J}$ $3727.379\,240(82) \text{ MeV}$ |

The nuclear constituents

Notation used to represent a given nuclide

Z : atomic number

A : atomic mass number

N : neutron number

X : chemical symbol



$$A = Z + N$$

$$M \approx \text{integer} \times M_H$$

M : the mass of a specific atom

M_H : the mass of a hydrogen atom

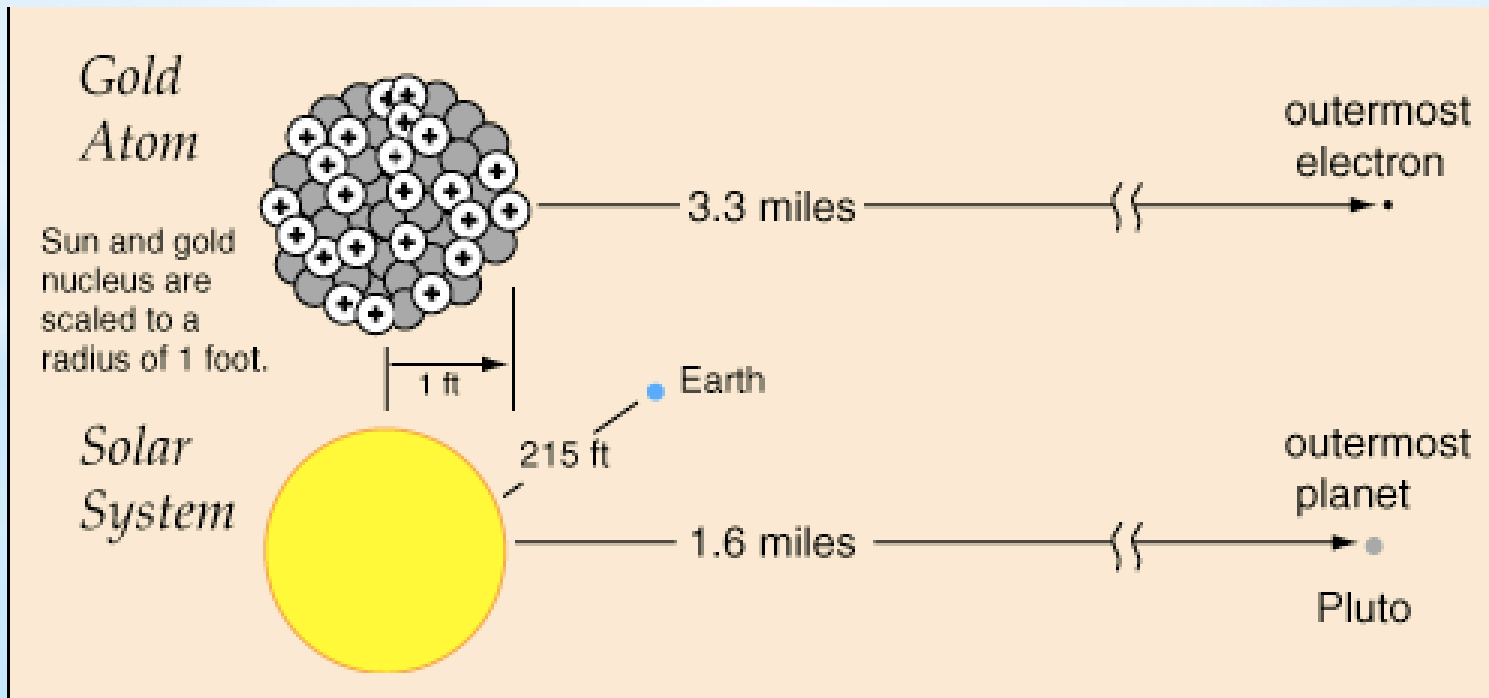
Size of Nuclei

What is the size of the nucleus

- nanometer
- femtometer
- picometer

Atomic radius of aluminum = 1.3×10^{-10} m

Nuclear radius aluminum = 3.6×10^{-15} m



The convenient unit for measuring the nuclear mass

Carbon - 12



u : is called *the atomic mass unit* or for short *amu*.

The mass of a ^{12}C atom (including all six electrons) is defined as **12 amu** (or **12 u**) exact.

$$\begin{aligned} 1\,u &= 1\,amu = 1.6605402(10) \times 10^{-27}\,\text{kg} \\ &= 931.49432(28)\,\text{MeV}/c^2 \end{aligned} \quad (1)$$

The mass of a proton

$$M_p = 1.007276470(12)\,u = 938.27231\,\text{MeV}/c^2$$

The mass of a neutron

$$M_n = 1.008664898(12)\,u = 939.56563\,\text{MeV}/c^2$$

Total binding energy $B(A,Z)$

Definition:

$$B(A, Z) = [ZM_p + NM_n - M(A, Z)]c^2 \quad (2)$$

The total binding energy $B(A,Z)$ is defined as *the total minimum work* that an external agent must do to disintegrate the whole nucleus completely. By doing so the nucleus would no longer be existent but disintegrated into separated nucleons.

This can also be considered as the total amount of energy released when nucleons, with zero kinetic energy initially, come close enough together to form a stable nucleus.

An interesting measured quantity is the averaged binding energy per nucleon

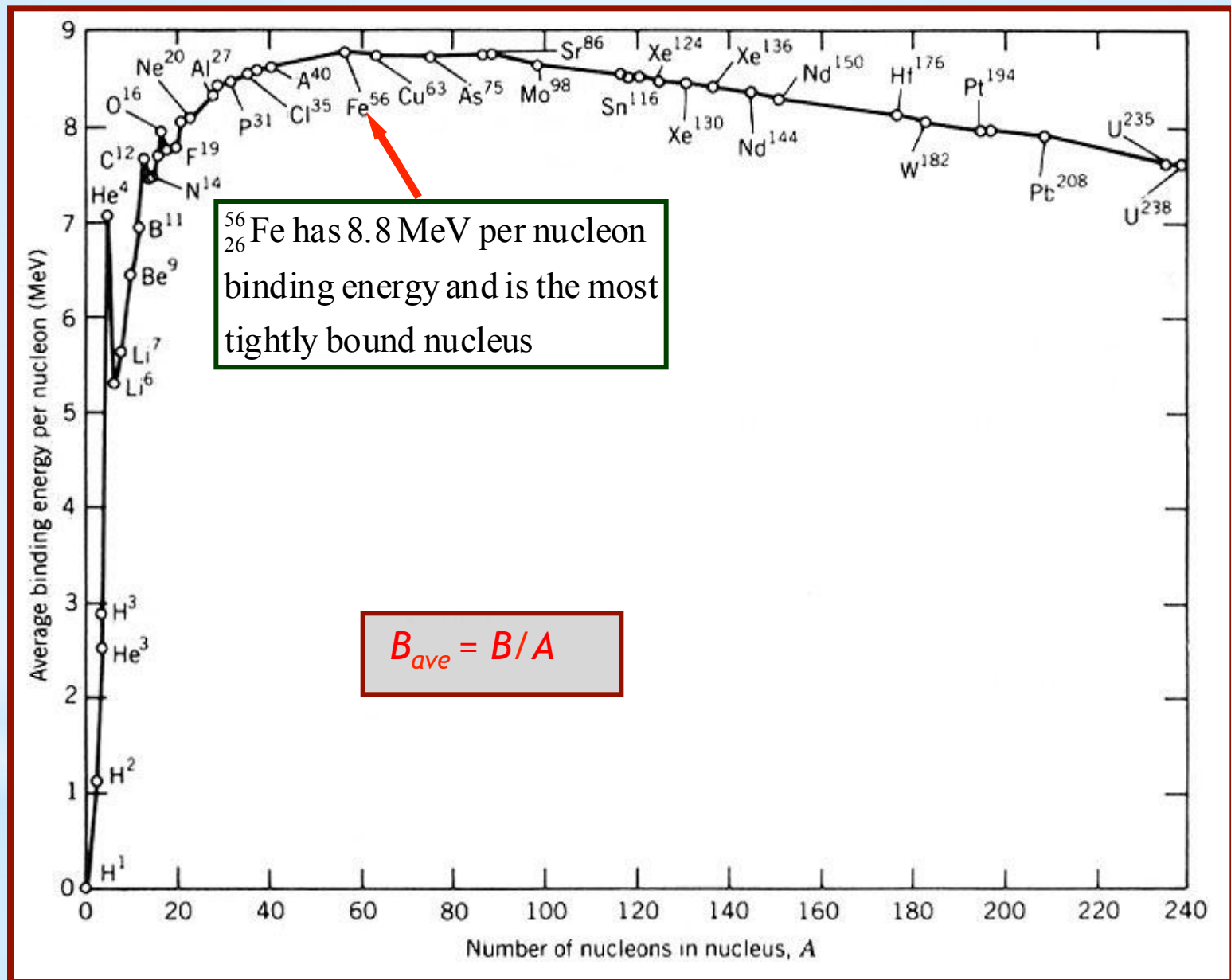
$$B_{ave.}(A, Z) = \frac{B(A, Z)}{A} \quad (3)$$



How large is nuclear binding energy per nucleon?

- 1MeV
- 10MeV

The average binding energy per nucleon versus mass number A



The binding energy of a nucleus

Definition:

$$B(A, Z) = [ZM_p + NM_n - M(A, Z)]c^2 \quad (9)$$

From the liquid drop model – Weizsäcker's formula

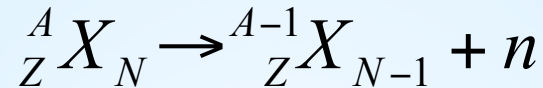
$$B(A, Z) = a_V A - a_S A^{2/3} - a_C \frac{Z^2}{A^{1/3}} - a_A \frac{(N - Z)^2}{A} \pm \delta + \eta \quad (10)$$



Carl Friedrich von Weizsäcker, 1993
A German physicist (1912-2007)

Separation energy (S)

(1). The separation energy of a neutron S_n



$$S_n = [M(A-1, Z) + M_n - M(A, Z)]c^2 \quad (4)$$

$$M(A, Z)c^2 = (ZM_p + NM_n)c^2 - B(A, Z)$$

$$M(A-1, Z)c^2 = [ZM_p + (N-1)M_n]c^2 - B(A-1, Z)$$

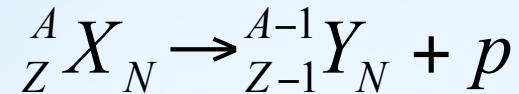
$$\begin{aligned} S_n &= \{[ZM_p + (N-1)M_n]c^2 - B(A-1, Z) + M_nc^2 \\ &\quad - (ZM_p + NM_n)c^2 + B(A, Z)\} \\ &= B(A, Z) - B(A-1, Z) \end{aligned}$$



$$S_n = B(A, Z) - B(A-1, Z) \quad (5)$$

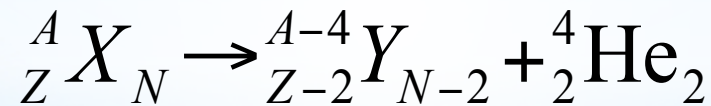
Separation energy (S)

(2). The separation energy of a proton S_p



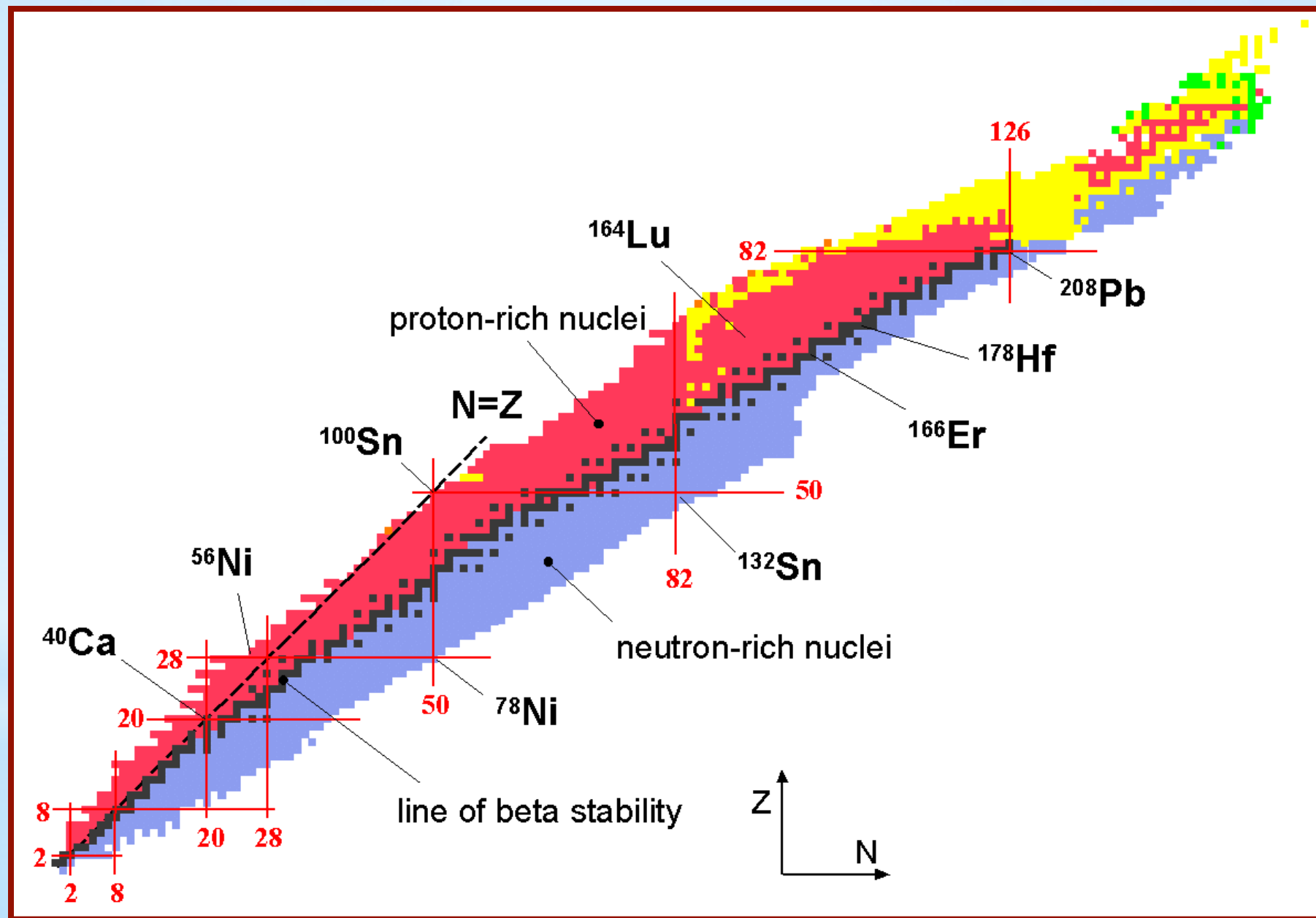
$$S_p = B(A, Z) - B(A-1, Z-1) \quad (6)$$

(3). The separation energy of a α -particle S_α



$$S_\alpha = B(A, Z) - B(A-4, Z-2) - B(4, 2) \quad (7)$$

The naturally occurring nuclei



Total Angular momentum and Nuclear spin

For nuclei:

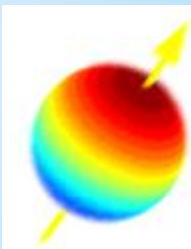
The nucleus is an isolated system and so often acts like a single entity with has a well defined total angular momentum.

It is common practice to represent this total angular momentum of a nucleus by the symbol I and to call it **nuclear spin**.

[Associated with each nuclear spin is a **nuclear magnetic moment** which produces magnetic interactions with its environment.]

For electrons in atoms:

For electrons in atoms we make a clear distinction between **electron spin** and **electron orbital angular momentum** and then combine them to give the **total angular momentum**.



What is spin of the ground state of an even-even nucleus?

- Zero
- Non-zero

The full Hamiltonian

In a non-relativistic approximation, nuclear properties are described by the Schrödinger equation for A nucleons

$$\hat{H}\Psi(1,2,\dots,A) = E\Psi(1,2,\dots,A)$$

$\Psi(1,2,\dots,A)$ denotes an A-body wave function. The Hamiltonian H contains nucleon kinetic energy operators and interactions between nucleons (two-body and three body).

$$\hat{H} = \sum_{i=1}^A \left(-\frac{\hbar^2}{2m} \Delta_i \right) + \sum_{i < j=1}^A W(i,j) + \sum_{i < j < k=1}^A W(i,j,k),$$

\mathbf{r}_i denotes all relevant coordinates of a given particle ($i = 1, 2, \dots, A$).

Practically it is formidable!!



*Prerequisites

- * Basic notions of quantum mechanics

- * Wave function encodes all information about a quantum system
- * Schrödinger equation gives the wave-function

$$\hat{H}\phi_k = E_k\phi_k \quad \equiv \quad \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r}) \right] \phi_k(\mathbf{r}) = E_k\phi_k(\mathbf{r})$$

- * Energy of the system, and its evolution in time is dictated by the Hamiltonian,

$$\hat{H} = \hat{T} + \hat{V}$$

- * Hamiltonian spectrum (eigenvalues of operator) can be

- * Discrete: bound-states, localized
- * Continuous: continuum, resonance, delocalized scattering states

- * To an observable (measurable) quantity corresponds a Hermitian operator

$$\langle \hat{O} \rangle = \langle \Psi | \hat{O} | \Psi \rangle$$

1.2 The Hilbert space

In Quantum Mechanics the states are represented by vectors in an abstract space called Hilbert space. Thus, a state α is a vector which, in Dirac notation, is written as $|\alpha\rangle$. As we will see below, this vector can be associated either to a function $\Psi_\alpha(\vec{r})$, which is regular and square integrable, or to a one-dimensional matrix (spinor). In the first case the metric of the space is defined by the scalar product in the region V of the three-dimensional (physical) space where the functions are square integrable. Usually V includes the whole space. Thus, the scalar product between the vectors $|\alpha\rangle$ and $|\beta\rangle$ is defined by

$$\langle\beta|\alpha\rangle = \int_V d\vec{r} \Psi_\beta^*(\vec{r}) \Psi_\alpha(\vec{r}) \quad (1.6)$$

The vector $\langle\alpha|$ is called "bra" and $|\alpha\rangle$ is called "ket". The scalar product $\langle\alpha|\beta\rangle$ is called "bracket".

Quantum mechanical states are characterized by vectors of a **Hilbert space**

$$|\psi\rangle, |\phi\rangle \in \mathbf{H}.$$

1. The abstract Hilbert space ℓ^2 is given by a set of elements $\mathcal{H} = (|\psi\rangle, |\varphi\rangle, |\chi\rangle, \dots)$, for which addition and multiplication with complex numbers is defined

$$|\psi\rangle + |\varphi\rangle = |\psi + \varphi\rangle \in \mathcal{H} \quad (1.1)$$

$$a |\psi\rangle = |a\psi\rangle \in \mathcal{H} \quad (1.2)$$

together with a scalar product

$$\langle\varphi|\psi\rangle \in \mathcal{C} . \quad (1.3)$$

With respect to (1.1) and (1.2), \mathcal{H} is a linear vector space, i.e.,

$$|\psi\rangle + |\varphi\rangle = |\varphi\rangle + |\psi\rangle$$

$$\begin{aligned}
(|\psi\rangle + |\varphi\rangle) + |x\rangle &= |\psi\rangle + (|\varphi\rangle + |x\rangle) \\
|\psi\rangle + |0\rangle &= |\psi\rangle \\
|\psi\rangle + |-\psi\rangle &= 0
\end{aligned}
\tag{1.4}$$

The last two relations state the existence of a 0-vector and the existence of a negative vector with respect to $|\psi\rangle$.

$$\begin{aligned}
\mathbf{1} |\psi\rangle &= |\psi\rangle \\
a(b |\psi\rangle) &= (ab) |\psi\rangle \\
(a + b) |\psi\rangle &= a |\psi\rangle + b |\psi\rangle \\
a(|\psi\rangle + |\varphi\rangle) &= a |\psi\rangle + a |\varphi\rangle
\end{aligned}
\tag{1.5}$$

One sees from the definition of the scalar product that it is $\langle \alpha | \beta \rangle = \langle \beta | \alpha \rangle^*$. Therefore the norm N_α of a vector $|\alpha\rangle$, i. e. $N_\alpha = \sqrt{\langle \alpha | \alpha \rangle}$ is a real number. In Quantum Mechanics N_α^2 is the probability of measuring the system in the state α . Since the system exists, this probability should be $N_\alpha^2 = 1$. Notice that we assume that the system is stationary, that is all processes are time-independent. Therefore if the system is in the state α , it

II. With respect to the scalar product, \mathcal{H} is a unitary vector space

$$\langle \psi | \psi \rangle \geq 0 \quad (1.6)$$

and

$$\langle \psi | \psi \rangle = 0 \Rightarrow |\psi\rangle = 0 \quad (1.7)$$

$$\begin{aligned} \langle \varphi | \psi \rangle &= \langle \psi | \varphi \rangle^* \\ \langle \varphi | a\psi \rangle &= a\langle \varphi | \psi \rangle \\ \langle \varphi | \psi_1 + \psi_2 \rangle &= \langle \varphi | \psi_1 \rangle + \langle \varphi | \psi_2 \rangle \end{aligned} \quad (1.8)$$

Because of (1.6) a Norm can be defined

$$\| \psi \| = \sqrt{\langle \psi | \psi \rangle} , \quad (1.9)$$

1.2 Eigenvalues and eigenvectors of matrices

The word "eigenvector" almost always means a "right column" vector that must be placed to the "right" of the matrix A . The eigenvalue equation for a matrix A is

$$Av - \lambda v = 0 \tag{1.4}$$

In matrix form we can write,

$$\begin{pmatrix} A_{1,1} & A_{1,2} & \dots & A_{1,n} \\ A_{2,1} & A_{2,2} & \dots & A_{2,n} \\ \vdots & \vdots & \ddots & \vdots \\ A_{n,1} & A_{n,2} & \dots & A_{n,n} \end{pmatrix} \begin{pmatrix} v_1 \\ v_2 \\ \vdots \\ v_n \end{pmatrix} = \lambda \begin{pmatrix} v_1 \\ v_2 \\ \vdots \\ v_n \end{pmatrix}$$

where for each element we have,

$$w_i = A_{i1}v_1 + A_{i2}v_2 + \dots + A_{in}v_n = \sum_{j=1}^n A_{ij}v_j = \lambda v_i.$$

For a 2×2 matrix the eigenvalues are found to be

$$\lambda = \frac{\text{tr}(A) \pm \sqrt{\text{tr}^2(A) - 4\det(A)}}{2}. \quad (1.14)$$

For the eigen vectors we have

$$\frac{v_1}{v_2} = \frac{A_{12}}{\lambda - A_{11}} = \frac{\lambda - A_{22}}{A_{21}}. \quad (1.15)$$

1.3 Hermitian operators

The relation between $|\alpha\rangle$ and $|\beta\rangle$ is $A|\alpha\rangle = |\beta\rangle$. The corresponding adjoint operator \hat{A}^\dagger is defined by $\langle\beta| = \langle\alpha|\hat{A}^\dagger$. Taking the scalar product with another vector γ one gets, $\langle\gamma|\hat{A}|\alpha\rangle = \langle\gamma|\beta\rangle = \langle\beta|\gamma\rangle^* = \langle\alpha|\hat{A}^\dagger|\gamma\rangle^*$. The operator \hat{A} is called Hermitian if

$$\hat{A}^\dagger = \hat{A} \quad \text{Hermitian} \quad (1.9)$$

The eigenvalues a and eigenvectors $|\alpha\rangle$ of the operator \hat{A} satisfy the equation

$$\hat{A}|\alpha\rangle = a|\alpha\rangle \quad (1.10)$$

and for the adjoint operator \hat{A}^\dagger it is,

$$\langle\alpha|\hat{A}^\dagger = a^*\langle\alpha| \quad (1.11)$$

If the operator \hat{A} is Hermitian one has

$$\langle\beta|\hat{A}|\alpha\rangle = \langle\beta|\hat{A}^\dagger|\alpha\rangle \quad (1.12)$$

If, in addition, $|\alpha\rangle$ and $|\beta\rangle$ are eigenvectors of \hat{A} , then one gets

$$a\langle\beta|\alpha\rangle = b^*\langle\beta|\alpha\rangle \quad (1.13)$$

Which implies that

$$\begin{cases} |\alpha\rangle \neq |\beta\rangle; & \langle\beta|\alpha\rangle = 0 \\ |\alpha\rangle = |\beta\rangle; & a \text{ real} \end{cases} \quad (1.14)$$

A hermitian operator has then and only then a complete system of Eigenfunctions, if it is self-adjoint.

The eigenvectors of Hermitian operators are the corresponding wave functions that allow one to evaluate all probabilities, in particular transition probabilities. Besides, they

play a fundamental role in Quantum Mechanics. Thus, normalizing the eigenvectors in Eq. (1.13) as $\langle\alpha|\alpha\rangle = 1$ and from Eq. (1.14) one finds that they satisfy

$$\langle\alpha|\beta\rangle = \delta_{\alpha\beta} \quad (1.15)$$

which means that they form an orthonormal set of vectors in the Hilbert space. They can be used as a basis to describe any vector belonging to the space. In a more rigorous statement one can say that the eigenvectors of an Hermitian operator span the Hilbert space on which the operator acts. To see the great importance of this property, assume a Hilbert space of dimension N and a Hermitian operator \hat{A} acting on this space such that,

$$\hat{A}|\alpha_i\rangle = a_i|\alpha_i\rangle, \quad i = 1, 2, \dots, N \quad (1.16)$$

Any vector $|v\rangle$ in the space spanned by the basis $\{|\alpha\rangle\}$ can be written as

$$|v\rangle = \sum_{i=1}^N c_i |\alpha_i\rangle \quad (1.17)$$

Representations and their use

From Eq. (1.15) one obtains

$$c_i = \langle \alpha_i | v \rangle \quad (1.18)$$

The numbers $\langle \alpha_i | v \rangle$ are called "amplitudes". If the vector $|v\rangle$ represents a physical (quantum) state, then the amplitudes have to obey the normality relation given by,

$$\langle v | v \rangle = \sum_{i=1}^N c_i \langle v | \alpha_i \rangle = \sum_{i=1}^N \langle v | \alpha_i \rangle^* \langle v | \alpha_i \rangle = \sum_{i=1}^N |\langle v | \alpha_i \rangle|^2 = 1 \quad (1.19)$$

From Eq. (1.18) the vector $|v\rangle$ can be written as,

$$|v\rangle = \sum_{i=1}^N \langle \alpha_i | v \rangle |\alpha_i\rangle = \sum_{i=1}^N |\alpha_i\rangle \langle \alpha_i | v \rangle \quad (1.20)$$

which shows that

$$\sum_{i=1}^N |\alpha_i\rangle \langle \alpha_i| = \hat{I} \quad (1.21)$$

This is the projector into the space spanned by the set $\{|\alpha\rangle\}$. We will use the projector often in these lectures.

For the case of an N-dimensional spinor the vector α is associated to the one-dimensional matrix given by

$$\begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \cdot \\ \cdot \\ \cdot \\ \alpha_N \end{pmatrix} \quad (1.7)$$

and the scalar product between the vectors α and β is given by

$$\langle \beta | \alpha \rangle = (\beta_1^*, \beta_2^*, \cdot, \cdot, \cdot, \beta_N^*) \begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \cdot \\ \cdot \\ \cdot \\ \alpha_N \end{pmatrix} = \sum_{i=1}^N \beta_i^* \alpha_i \quad (1.8)$$

Translation symmetry

The translation operator \hat{T} is defined by,

$$\hat{T}(\Delta\mathbf{r})|\mathbf{r}\rangle = |\mathbf{r} + \Delta\mathbf{r}\rangle \quad (1.36)$$

which applied to the vector $|\Psi\rangle$ gives,

$$\hat{T}(\Delta\mathbf{r})|\Psi\rangle = \int d\mathbf{r}' \hat{T}(\Delta\mathbf{r})|\mathbf{r}'\rangle \langle\mathbf{r}'|\Psi\rangle = \int d\mathbf{r}' |\mathbf{r}' + \Delta\mathbf{r}\rangle \langle\mathbf{r}'|\Psi\rangle \quad (1.37)$$

and, in r-representation, the translated function is

$$\Psi_t(\mathbf{r}) = \langle\mathbf{r}|\hat{T}(\Delta\mathbf{r})|\Psi\rangle = \int d\mathbf{r}' \delta(\mathbf{r} - \mathbf{r}' - \Delta\mathbf{r}) \langle\mathbf{r}'|\Psi\rangle = \Psi(\mathbf{r} - \Delta\mathbf{r}) \quad (1.38)$$

Since

$$\langle\mathbf{r}|\hat{T}^\dagger(\Delta\mathbf{r})\hat{T}(\Delta\mathbf{r})|\mathbf{r}\rangle = \langle\mathbf{r} + \Delta\mathbf{r}|\mathbf{r} + \Delta\mathbf{r}\rangle = 1 \quad (1.39)$$

one obtains

$$\hat{T}^\dagger\hat{T} = 1 \quad (1.40)$$

which defines the operator \hat{T} as unitary.

Parity symmetry

The parity operator $\hat{\pi}$ is defined as,

$$\hat{\pi}|x\rangle = |-x\rangle \quad (1.72)$$

it is $\hat{\pi}^\dagger = \hat{\pi}$ (exercise) The eigenvalues of the parity operator are obtained as,

$$\hat{\pi}|\Psi_\lambda\rangle = \lambda|\Psi_\lambda\rangle \implies \hat{\pi}^2|\Psi_\lambda\rangle = \lambda^2|\Psi_\lambda\rangle \quad (1.73)$$

since

$$\hat{\pi}^2|x\rangle = |x\rangle \quad (1.74)$$

one gets

$$\lambda^2|\Psi_\lambda\rangle = |\Psi_\lambda\rangle \implies \lambda = \pm 1 \quad (1.75)$$

in x -space it is

$$\langle x|\hat{\pi}|\Psi_\lambda\rangle = \langle -x|\Psi_\lambda\rangle = \Psi_\lambda(-x) = \lambda\Psi_\lambda(x) \quad (1.76)$$

$$\Psi_\lambda(x) = \begin{cases} \text{even,} & \lambda = 1 \\ \text{odd,} & \lambda = -1 \end{cases} \quad (1.77)$$

If $[H, \hat{\pi}] = 0$, as it happens with potentials with reflection symmetry, parity is conserved and λ is a good quantum number.

1.5 Sum of angular momenta

We will here analyze the possible angular momenta values of a two-particle system. The angular momenta of the particles are \mathbf{L}_1 and \mathbf{L}_2 and the total angular momentum is $\mathbf{L} = \mathbf{L}_1 + \mathbf{L}_2$. The components $\hat{L}_x, \hat{L}_y, \hat{L}_z$ of \mathbf{L} satisfy the commutation relations

$$[\hat{\mathbf{L}}^2, \hat{L}_i] = 0 \quad (i = x, y, z) \quad (1.78)$$

$$[\hat{L}_x, \hat{L}_y] = i\hbar\hat{L}_z, \quad [\hat{L}_y, \hat{L}_z] = i\hbar\hat{L}_x, \quad [\hat{L}_z, \hat{L}_x] = i\hbar\hat{L}_y \quad (1.79)$$

and the same for \mathbf{L}_1 and \mathbf{L}_2 .

Besides, since the degrees of freedom of the particles are independent of each other one also has,

$$[\hat{\mathbf{L}}_1, \hat{\mathbf{L}}_2] = 0, \quad [\hat{\mathbf{L}}^2, \hat{\mathbf{L}}_1] = [\hat{\mathbf{L}}^2, \hat{\mathbf{L}}_2] = 0 \quad (1.80)$$

The eigenvectors corresponding to these operators are given by

$$\begin{aligned} \hat{\mathbf{L}}_1^2 |l_1 m_1\rangle &= \hbar^2 l_1(l_1 + 1) |l_1 m_1\rangle & ; & \quad \hat{L}_{1z} |l_1 m_1\rangle = \hbar m_1 |l_1 m_1\rangle \\ \hat{\mathbf{L}}_2^2 |l_2 m_2\rangle &= \hbar^2 l_2(l_2 + 1) |l_2 m_2\rangle & ; & \quad \hat{L}_{2z} |l_2 m_2\rangle = \hbar m_2 |l_2 m_2\rangle \\ \hat{\mathbf{L}}^2 |lm\rangle &= \hbar^2 l(l + 1) |lm\rangle & ; & \quad \hat{L}_z |lm\rangle = \hbar m |lm\rangle \end{aligned} \quad (1.81)$$

$$|l_1 - l_2| \leq l \leq l_1 + l_2, \quad m = m_1 + m_2 \quad (1.82)$$

$$-l_i \leq m_i \leq l_i, \quad -l \leq m \leq l \quad (1.83)$$

Not all the quantum numbers related to these operators can be used to label the states. In other words, not all of them can be taken as good quantum numbers. To see the reason for this we will analyze the behavior of commuting operators.

Symmetry properties of the Clebsch-Gordan coefficient

The Clebsch-Gordan coefficient can best be written in terms of the 3-j symbol defined as

$$\begin{pmatrix} l_1 & l_2 & l \\ m_1 & m_2 & -m \end{pmatrix} = \frac{(-1)^{l_1-l_2+m}}{\sqrt{2l+1}} \langle l_1 m_1 l_2 m_2 | l m \rangle \quad (1.91)$$

with the properties that

1. $\begin{pmatrix} l_1 & l_2 & l \\ m_1 & m_2 & m \end{pmatrix} = \begin{pmatrix} l_2 & l & l_1 \\ m_2 & m & m_1 \end{pmatrix} = \begin{pmatrix} l & l_1 & l_2 \\ m & m_1 & m_2 \end{pmatrix}$
2. $\begin{pmatrix} l_1 & l_2 & l \\ m_1 & m_2 & m \end{pmatrix} = (-1)^{l_1+l_2+l} \begin{pmatrix} l_2 & l_1 & l \\ m_2 & m_1 & m \end{pmatrix}$
3. $\begin{pmatrix} l_1 & l_2 & l \\ -m_1 & -m_2 & -m \end{pmatrix} = (-1)^{l_1+l_2+l} \begin{pmatrix} l_1 & l_2 & l \\ m_1 & m_2 & m \end{pmatrix}$
4. $m_1 + m_2 - m = 0$

6-j symbols

In the sum of three angular momenta one can choose the partition

$$\mathbf{J} = \mathbf{j}_1 + \mathbf{j}_2 + \mathbf{j}_3 = \mathbf{J}_{12} + \mathbf{j}_3 = \mathbf{j}_1 + \mathbf{J}_{23} \quad (1.101)$$

where

$$\mathbf{J}_{12} = \mathbf{j}_1 + \mathbf{j}_2, \quad \mathbf{J}_{23} = \mathbf{j}_2 + \mathbf{j}_3 \quad (1.102)$$

One can write the basis vector in one representation in terms of the other representation as

$$|(j_1 j_2) J_{12} j_3; JM\rangle = \sum_{J_{23}} \langle j_1 (j_2 j_3) J_{23}; J | (j_1 j_2) J_{12} j_3; J \rangle |j_1 (j_2 j_3) J_{23}; JM\rangle \quad (1.103)$$

The symmetry properties of the expansion coefficient can best be seen by introducing the 6-j symbol as

$$\begin{aligned} \langle j_1 (j_2 j_3) J_{23}; J | (j_1 j_2) J_{12} j_3; J \rangle \\ = (-1)^{j_1 + j_2 + j_3 + J} \sqrt{(2J_{12} + 1)(2J_{23} + 1)} \left\{ \begin{matrix} j_1 & j_2 & J_{12} \\ j_3 & J & J_{23} \end{matrix} \right\} \end{aligned} \quad (1.104)$$

which is a real number (therefore it is the same for $\langle (j_1 j_2) J_{12} j_3; J | j_1 (j_2 j_3) J_{23}; J \rangle$). The 6-j symbol does not change if two columns are inter changed, for instance

$$\left\{ \begin{matrix} j_1 & j_2 & J_{12} \\ j_3 & J & J_{23} \end{matrix} \right\} = \left\{ \begin{matrix} j_1 & J_{12} & j_2 \\ j_3 & J_{23} & J \end{matrix} \right\}. \quad (1.105)$$

The angular momentum triangular relation must be satisfied for (j_1, j_2, J_{12}) , (j_1, J, J_{23}) , (j_3, j_2, J_{23}) and (j_3, J, J_{12}) . Thus, e.g.,

$$\left\{ \begin{array}{ccc} 1/2 & 1/2 & 0 \\ 1/2 & 1/2 & 2 \end{array} \right\} = 0 \quad (1.107)$$

In general, When $j_6 = 0$ the expression for the 6-j symbol can be written as

$$\left\{ \begin{array}{ccc} j_1 & j_2 & j_3 \\ j_4 & j_5 & 0 \end{array} \right\} = \frac{\delta_{j_2, j_4} \delta_{j_1, j_5}}{\sqrt{(2j_1 + 1)(2j_2 + 1)}} (-1)^{j_1 + j_2 + j_3} \{j_1, j_2, j_3\}. \quad (1.108)$$

The function $\{ \}$ is equal to 1 when the triad satisfies the triangle conditions, and zero otherwise.

The 6-j symbols satisfy the orthogonality relation,

$$\sum_{j_3} (2j_3 + 1) \left\{ \begin{array}{ccc} j_1 & j_2 & j_3 \\ j_4 & j_5 & j_6 \end{array} \right\} \left\{ \begin{array}{ccc} j_1 & j_2 & j_3 \\ j_4 & j_5 & j'_6 \end{array} \right\} = \frac{\delta_{j_6, j'_6}}{2j_6 + 1} \{j_1, j_5, j_6\} \{j_4, j_2, j_6\}. \quad (1.109)$$

9-j symbols

In the case of 4 angular momenta

$$\mathbf{J} = \mathbf{j}_1 + \mathbf{j}_2 + \mathbf{j}_3 + \mathbf{j}_4 \quad (1.110)$$

one can write, e.g.,

$$\mathbf{J} = \mathbf{J}_{12} + \mathbf{J}_{34} = \mathbf{J}_{13} + \mathbf{J}_{24} \quad (1.111)$$

where $\mathbf{J}_{12} = \mathbf{j}_1 + \mathbf{j}_2$, $\mathbf{J}_{34} = \mathbf{j}_3 + \mathbf{j}_4$, $\mathbf{J}_{13} = \mathbf{j}_1 + \mathbf{j}_3$ and $\mathbf{J}_{24} = \mathbf{j}_2 + \mathbf{j}_4$.

One can thus write

$$\begin{aligned} |(j_1 j_3) J_{13} (j_2 j_4) J_{24}; JM\rangle &= \sum_{J_{12} J_{34}} \langle (j_1 j_2) J_{12} (j_3 j_4) J_{34}; J | (j_1 j_3) J_{13} (j_2 j_4) J_{24}; JM \rangle \\ &\times |(j_1 j_2) J_{12} (j_3 j_4) J_{34}; J \rangle \end{aligned} \quad (1.112)$$

and the 9-j symbol is defined by,

$$\begin{aligned} &\langle (j_1 j_2) J_{12} (j_3 j_4) J_{34}; J | (j_1 j_3) J_{13} (j_2 j_4) J_{24}; J \rangle \\ &= \sqrt{(2J_{12} + 1)(2J_{34} + 1)(2J_{13} + 1)(2J_{24} + 1)} \left\{ \begin{array}{ccc} j_1 & j_2 & J_{12} \\ j_3 & j_4 & J_{34} \\ J_{13} & J_{24} & J \end{array} \right\} \end{aligned} \quad (1.113)$$

which is also a real number.

The symmetry properties of the 9-j symbols are

1. Any permutation of rows and columns does not change the 9-j symbol except the sign, which is plus if the permutation is even and $(-1)^S$, where S is the sum of all angular momenta, if the permutation is odd.

For example, we have,

$$\left\{ \begin{matrix} j_1 & j_2 & j_3 \\ j_4 & j_5 & j_6 \\ j_7 & j_8 & j_9 \end{matrix} \right\} = (-1)^S \left\{ \begin{matrix} j_4 & j_5 & j_6 \\ j_1 & j_2 & j_3 \\ j_7 & j_8 & j_9 \end{matrix} \right\} = (-1)^S \left\{ \begin{matrix} j_2 & j_1 & j_3 \\ j_5 & j_4 & j_6 \\ j_8 & j_7 & j_9 \end{matrix} \right\}, \quad (1.114)$$

where

$$S = \sum_{i=1}^9 j_i. \quad (1.115)$$

2. The 9-j symbol does not change under a reflection about either diagonal.

$$\left\{ \begin{matrix} j_1 & j_2 & j_3 \\ j_4 & j_5 & j_6 \\ j_7 & j_8 & j_9 \end{matrix} \right\} = \left\{ \begin{matrix} j_1 & j_4 & j_7 \\ j_2 & j_5 & j_8 \\ j_3 & j_6 & j_9 \end{matrix} \right\} = \left\{ \begin{matrix} j_9 & j_6 & j_3 \\ j_8 & j_5 & j_2 \\ j_7 & j_4 & j_1 \end{matrix} \right\} \quad (1.116)$$

The 9-j symbols can be calculated as sums over triple-products of 6-j symbols where the summation extends over all "x" admitted by the triangle condition,

$$\left\{ \begin{matrix} j_1 & j_2 & j_3 \\ j_4 & j_5 & j_6 \\ j_7 & j_8 & j_9 \end{matrix} \right\} = \sum_x (-1)^{2x} (2x+1) \left\{ \begin{matrix} j_1 & j_4 & j_7 \\ j_8 & j_9 & x \end{matrix} \right\} \left\{ \begin{matrix} j_2 & j_5 & j_8 \\ j_4 & x & j_6 \end{matrix} \right\} \left\{ \begin{matrix} j_3 & j_6 & j_9 \\ x & j_1 & j_2 \end{matrix} \right\}. \quad (1.117)$$

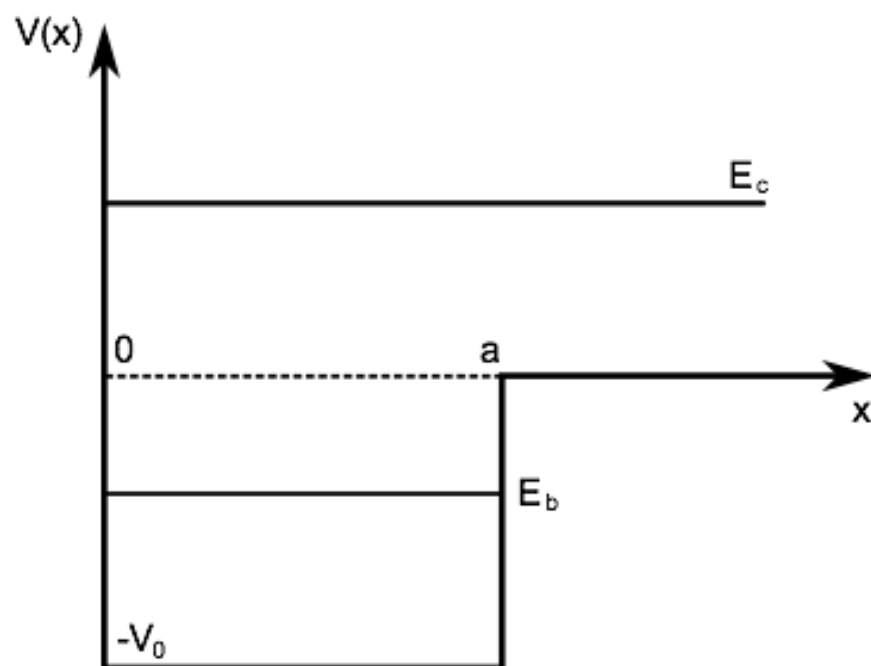


Figure 2.1: Square well potential in one-dimension. The range of the potential is a and the depth is $-V_0$. For $x < 0$ the potential is infinite and, therefore, the wave function vanishes at $x = 0$. E_b (E_c) is the energy of a bound (continuum) state.

Chapter 2

Gamow states and the Berggren representation

One-particle Hamiltonian in one dimension

The one-dimension Hamiltonian is.

$$\left[-\frac{\hbar^2}{2\mu} \frac{d^2}{dx^2} + V(x) \right] \Phi_n(x) = E_n \Phi_n(x) \quad (2.3)$$

and we will consider the square well potential shown in Fig. 2.1. To solve the eigenvalue problem given by Eq. (2.3) we notice that there are two regions:

Region (1): $0 < x < a$; $V(x) = -V_0$

Region (2): $x \geq a$; $V(x) = 0$

There are also two possibilities for the energy: Continue ($E = E_c > 0$) and Bound ($E = -E_b < 0$)

$$\text{Region (1):} \quad \left[-\frac{\hbar^2}{2\mu} \frac{d^2}{dx^2} - V_0 \right] \Phi_n^{(1)}(x) = E_n \Phi_n^{(1)}(x)$$

$$\text{Region (2):} \quad \left[-\frac{\hbar^2}{2\mu} \frac{d^2}{dx^2} \right] \Phi_n^{(2)}(x) = E_n \Phi_n^{(2)}(x)$$

with

$$q^2 = \frac{2\mu}{\hbar^2}(E_n + V_0); \quad k^2 = \frac{2\mu}{\hbar^2}E_n$$

the eigenvectors solution of the eigenvalue problem are

$$\begin{cases} \Phi_n^{(1)}(x) = A_n e^{iqx} + B_n e^{-iqx} \\ \Phi_n^{(2)}(x) = C_n e^{ikx} + D_n e^{-ikx} \end{cases}$$

To determine the constant A_n , B_n , C_n and D_n , the boundary conditions of continuity of density and current have to be applied. In addition, since $V(x) = \infty$ for $x \leq 0$, one has

$$\Phi_n^{(1)}(x=0) = 0 \implies A_n + B_n = 0$$

I) Bound states

$$q^2 = \frac{2\mu}{\hbar^2}(V_0 - E_b) > 0; \quad k^2 = -\frac{2\mu}{\hbar^2}E_b < 0$$

Notice that we assume $E_b > 0$ and, therefore, the energy of the bound state is $-E_b$.

$$k = \pm i\chi; \quad \chi = \sqrt{\frac{2\mu E_b}{\hbar^2}}$$

$$\begin{cases} \Phi_n^{(1)}(a) = \Phi_n^{(2)}(a) \\ \left. \frac{d}{dx}\Phi_n^{(1)}(x) \right|_{x=a} = \left. \frac{d}{dx}\Phi_n^{(2)}(x) \right|_{x=a} \end{cases}$$

An additional condition in $\Phi_n^{(2)}(x) = C_n e^{-\chi x} + D_n e^{\chi x}$ is that since $e^{\chi x}$ diverges as $x \rightarrow \infty$ one has to impose $D_n = 0$. Besides there is the normalization condition. With the constants thus evaluated one obtains the possible energies as those for which the continuity relations are satisfied.

II) Continuum

$$q^2 = \frac{2\mu}{\hbar^2}(V_0 + E_c) > 0; \quad k^2 = \frac{2\mu}{\hbar^2}E_c > 0$$

assuming that the system is confined in the region

$$0 < x < L \implies \int_0^L |\Phi_n(x)|^2 dx = 1$$

Notice that all energies $E_c > 0$ are allowed in the continuum, but only a discrete number of energies $-E_b < 0$ are allowed as bound states.

2.1 Gamow states

The wave function of a resonance with a peak at energy E_0 and a width Γ can be factorized as

$$\Phi(E, \mathbf{r}) = \sqrt{\frac{\Gamma/2}{\pi [(E - E_0)^2 + (\Gamma/2)^2]}} \Psi(\mathbf{r}), \quad (2.4)$$

where $\Psi(\mathbf{r}) = \sqrt{\pi\Gamma/2} \Phi(E_0, \mathbf{r})$. Through the Fourier transform, we obtain the time evolution of the resonance

$$\Phi(t, \mathbf{r}) = \int_{-\infty}^{\infty} \Phi(E, \mathbf{r}) e^{-iEt/\hbar} dE = \Psi(\mathbf{r}) e^{-i\tilde{E}t/\hbar}, \quad (2.5)$$

which gives us the resonance in the form of a stationary state, but with a complex energy

$$\tilde{E} = E_0 - i\frac{\Gamma}{2}. \quad (2.6)$$

The probability of measuring the system at t is given by

$$|\Phi(t, \mathbf{r})|^2 = |\Psi(\mathbf{r})|^2 e^{-\Gamma t/\hbar}. \quad (2.7)$$

The half-life of the resonance can be obtained from

$$T_{1/2} = \frac{\hbar \ln 2}{\Gamma}. \quad (2.8)$$

$$\tilde{E}_n = \frac{\hbar^2}{2\mu} k_n^2. \quad (2.9)$$

They can be written as

$$k_n = \kappa_n + i\gamma_n. \quad (2.10)$$

The states can be classified into four classes, namely:

1. bound states, for which $\kappa_n = 0$ and $\gamma_n > 0$;
2. antibound states with $\kappa_n = 0$ and $\gamma_n < 0$;
3. decay resonant states with $\kappa_n > 0$ and $\gamma_n < 0$;
4. capture resonant states with $\kappa_n < 0$ and $\gamma_n < 0$.

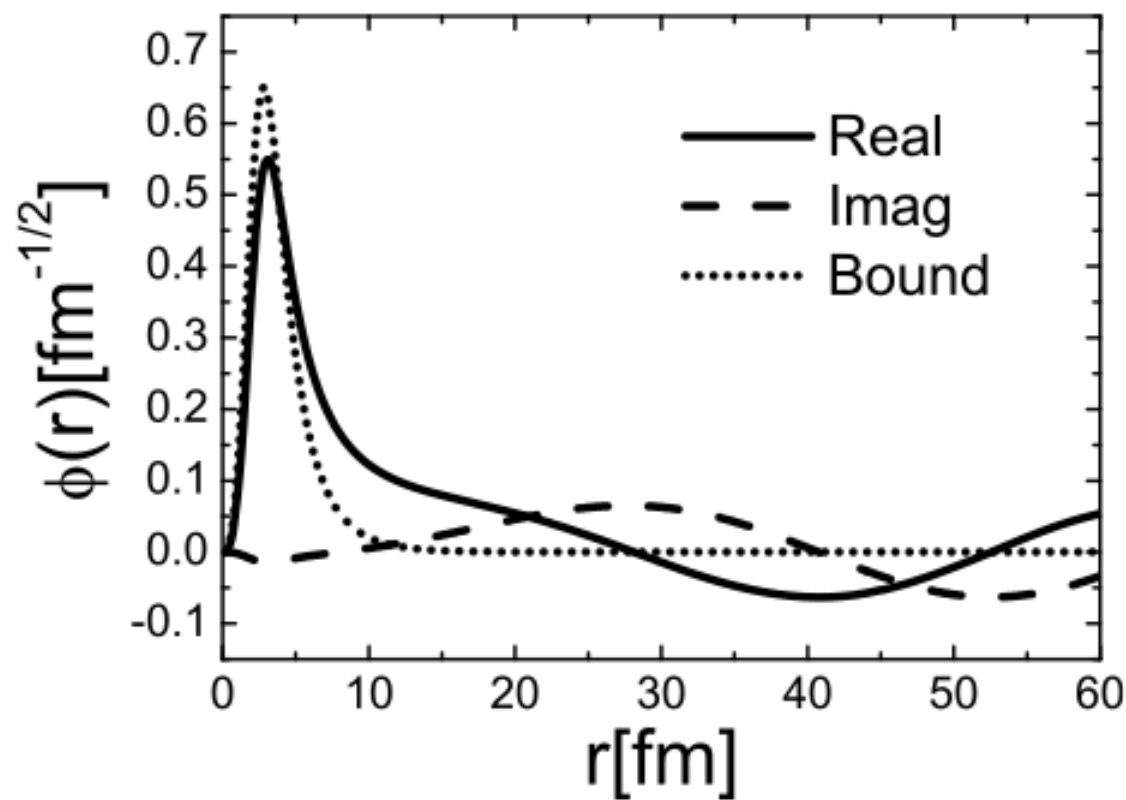


Figure 2.2: Radial function of a narrow resonance and a bound state. The solid and the dashed line denote the real and imaginary part of the wave function of a narrow resonance respectively, while the dotted line denotes the wave function of a bound state.

Since the radial wave function has the form of $w(E_n, r) \sim e^{ik_n r}$, one can see that the wave function of the resonant states will diverge at infinity. However a narrow resonance can still be treated stationary since the wave function does not diverge at small distance.

2.2 Berggren completeness relation

The eigenvectors of a Hamiltonian provide a representation projector which allows one to write

$$\delta(r - r') = \sum_n w_n(r)w_n(r') + \int_0^\infty dE u(r, E)u(r', E), \quad (2.11)$$

where $w_n(r)$ are the wave functions of the bound states and $u(r, E)$ are the scattering states. The integration contour is along the real energy axis, and all the energies and radial wave functions are real, or more precisely, can be chosen to be real. Notice that only bound states and scattering states enter in Eq. (2.11).

Projects:

- Diagonalization of the matrix and the Lanczos method
- Solution of a square well