

Shell model excitations

May 04, 2017

Second quantization

- Fermion basis is given by Slater-determinants

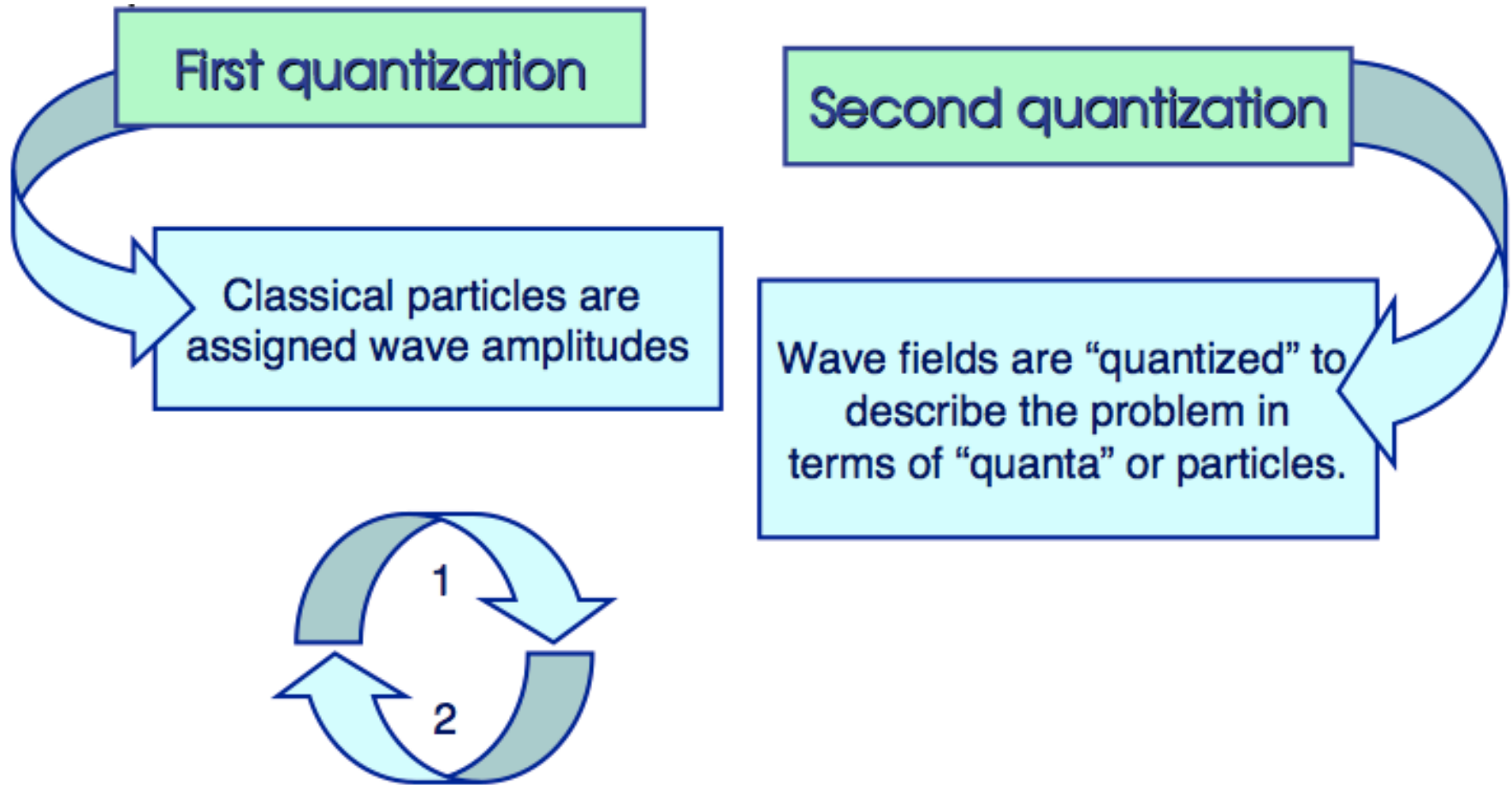
$$\Psi(r_1, r_2, \dots, r_A) = \frac{1}{\sqrt{A}} \sum_{\pi} (-1)^{\pi} \prod_{k=1}^A \psi_k(r_{k_{\pi}})$$

- Meaningful: how many particles populate each state $\psi_k(r)$ = the occupation numbers n_i
 - Fermion?
 - Bosons?
- One can define the many-particle state as an abstract vector in the occupation-number representation

$$|\Psi\rangle = |n_1, n_2, \dots, n_A\rangle$$

Fock space

First & second quantizations



$$|a \otimes b\rangle_B = \frac{1}{\sqrt{2}} (|a_1 \otimes b_2\rangle + |a_2 \otimes b_1\rangle) \quad \text{bosons; symmetric}$$

$$|a \otimes b\rangle_F = \frac{1}{\sqrt{2}} (|a_1 \otimes b_2\rangle - |a_2 \otimes b_1\rangle) \quad \text{fermions; anti - symmetric}$$

- ✧ Convenient to describe processes in which particles are created and annihilated;
- ✧ Convenient to describe interactions.

First quantization:
Slater determinant

Second quantization

$$\Psi_{jk}(q_1, q_2) = \frac{1}{\sqrt{2}} \begin{vmatrix} \psi_j(q_1) & \psi_k(q_2) \\ \psi_j(q_2) & \psi_k(q_2) \end{vmatrix} \quad \Rightarrow \quad |jk\rangle = a_j^\dagger a_k^\dagger |0\rangle$$

$a_i^\dagger |0\rangle$ one-particle state

States $a_i^\dagger a_j^\dagger |0\rangle$ two-particle state

$a_i^\dagger a_j^\dagger \dots a_n^\dagger |0\rangle$ N-particle state

} described by Slater determinants in first quantization

Annihilation and creation operator

- These operators describe the annihilation and creation of excitation in a given single particle state. For boson: $[\hat{a}, \hat{a}] = 0, [\hat{a}^+, \hat{a}^+] = 0, [\hat{a}, \hat{a}^+] = 1, \hat{n} = \hat{a}^+ \hat{a}$
 $\hat{a}|n\rangle = \sqrt{n}|n-1\rangle, \hat{a}^+|n\rangle = \sqrt{n+1}|n+1\rangle$
- \hat{a}^+ and \hat{a} lower and raise, respectively, the eigenvalue of \hat{n} by 1
- For the case of many single-particle (**bosons**) the operators are indexed by i to denote which state they affect $[\hat{a}_i, \hat{a}_j] = 0, [\hat{a}_i^+, \hat{a}_j^+] = 0, [\hat{a}_i, \hat{a}_j^+] = \delta_{ij}, \hat{n}_i = \hat{a}_i^+ \hat{a}_i$

$$\hat{n} = \sum_i \hat{n}_i = \sum_i \hat{a}_i^+ \hat{a}_i$$

$$\hat{a}_i |n_1, n_2, \dots, n_i, \dots\rangle = \sqrt{n_i} |n_1, n_2, \dots, n_i - 1, \dots\rangle$$

$$\hat{a}_i^+ |n_1, n_2, \dots, n_i, \dots\rangle = \sqrt{n_i + 1} |n_1, n_2, \dots, n_i + 1, \dots\rangle$$

Particle-number operator
for each single-particle
state

Second quantization for fermions

- Anti-commutation relations:

$$\{\hat{a}_i, \hat{a}_j\} = 0, \quad \{\hat{a}_i^+, \hat{a}_j^+\} = 0, \quad \{\hat{a}_i, \hat{a}_j^+\} = \delta_{ij}$$

- Vacuum $|-\rangle = |0, 0, \dots\rangle, \quad a_i|-\rangle = 0$

$$|n_1, n_2, \dots, n_i, \dots\rangle = \prod_{\mu} (a_{\mu}^+)^{n_{\mu}} |-\rangle = \hat{a}_1^+ \cdots \hat{a}_i^+ |-\rangle$$

Vacuum

$$\langle 0|0\rangle = 1$$

$$a_k |0\rangle = 0 :$$

$$\langle 0|a_k^\dagger = 0$$

There is no particle to annihilation in “vacuum”

The Fock space

The Hilbert space describing a quantum many-body system with $N = 0, 1, \dots, \infty$ particles is called the Fock space. It is the direct sum of the appropriately symmetrized single-particle Hilbert spaces \mathcal{H} :

$$\bigoplus_{N=0}^{\infty} S_{\pm} \mathcal{H}^{\otimes n} \quad (4.9)$$

where S_+ is the symmetrization operator used for bosons and S_- is the anti-symmetrization operator used for fermions.

In Fock space (a linear vector space), a determinant is represented by an *occupation-number (ON) vector* $|\mathbf{k}\rangle$,

$$|\mathbf{k}\rangle = |k_1, k_2, \dots, k_M\rangle, \quad k_P = \begin{cases} 1 & \phi_P(\mathbf{x}) \text{ occupied} \\ 0 & \phi_P(\mathbf{x}) \text{ unoccupied} \end{cases}$$

For two general vectors in Fock space:

$$|\mathbf{c}\rangle = \sum_{\mathbf{k}} c_{\mathbf{k}} |\mathbf{k}\rangle, \quad |\mathbf{d}\rangle = \sum_{\mathbf{k}} d_{\mathbf{k}} |\mathbf{k}\rangle, \quad \langle \mathbf{c} | \mathbf{d} \rangle = \sum_{\mathbf{k}} c_{\mathbf{k}}^* d_{\mathbf{k}}$$

One-body operators

- Lets translate operators in occupation-number representation
- What is one-body operator?
 - Depends only on the coordinator of one particle.
 - Kinetic energy or external potential
- General form: f_i , which always act on the coordinate of the particle i :

$$\hat{F} = \sum_{i=1}^A \hat{f}_i \quad f_{\nu\nu'} = \langle \nu | \hat{f} | \nu' \rangle$$

$$\hat{F} = \sum_{\nu\nu'} f_{\nu'\nu} a_{\nu}^+ a_{\nu'}$$

Two-body operators

- Two body interaction:
$$\hat{V} = \sum_{k \neq k'} \hat{v}(r_k, r_{k'})$$
$$\hat{V} = \frac{1}{2} \sum_{ijkl} v_{ijkl} \hat{a}_i^+ \hat{a}_j^+ \hat{a}_l \hat{a}_k$$
- Note that the operator can change two single-particle states simultaneously.
- The index order in the operator product has the last two indices interchanged relative to the ordering in the matrix elements.

The particle-hole picture

- The lowest state – ground state– of a system of $N=A$ fermions with an energy $E_0 = \sum_{i=1}^A \varepsilon_i$ $|\psi_0\rangle = \prod_{i=1}^A \hat{a}_i^+ |0\rangle$
- Fermi level: the highest occupied state with energy ε_A
- The expectation value of an operator O in the ground state $\langle \Psi_0 | \hat{O} | \Psi_0 \rangle = \langle 0 | \hat{a}_A \cdots \hat{a}_1 \hat{O} \hat{a}_1^+ \cdots \hat{a}_A^+ | 0 \rangle$
- Properties of ground state:

$$\hat{a}_i |\Psi_0\rangle = 0, \quad i > A$$

$$\hat{a}_i^+ |\Psi_0\rangle = 0, \quad i \leq A$$

The simplest excited state

- Lift one particle from an occupied state into an unoccupied one: (one-particle/one-hole state)

$$|\Psi_{mi}\rangle = \hat{a}_m^+ \hat{a}_i |\Psi_0\rangle, \quad m > A, \quad i \leq A$$

$$E_{mi} - E_0 = \varepsilon_m - \varepsilon_i$$

- The next excitation is a two-particle/two-hole

$$|\Psi_{mnij}\rangle = \hat{a}_m^+ \hat{a}_n^+ \hat{a}_i \hat{a}_j |\Psi_0\rangle$$

$$E_{mnij} = \varepsilon_m + \varepsilon_n - \varepsilon_i - \varepsilon_j$$

Hamiltonian with two-body interaction in particle-number representation (2th quantization)

- A microscopic model that describes the structure of the nucleus in terms of the degree of freedom of the nucleons.

$$\hat{H} = \sum_{ij} t_{ij} \hat{a}_i^+ \hat{a}_j + \frac{1}{2} \sum_{ijkl} v_{ijkl} \hat{a}_i^+ \hat{a}_j^+ \hat{a}_l \hat{a}_k$$

- An eigenstate of H:

$$|\Psi\rangle = \sum_{i_1 i_2, \dots, i_A} c_{i_1 i_2, \dots, i_A} \hat{a}_{i_1}^+ \hat{a}_{i_2}^+ \cdots \hat{a}_{i_A}^+ |0\rangle$$

Two-particle outside a closed core (in jj coupled scheme)

$$H = H_0 + V$$

$$H_0|pq; JM\rangle = \varepsilon_p + \varepsilon_q|pq; JM\rangle$$

$\{|\alpha\rangle = |pq; JM\rangle\}$ form the orthonormal bases

$$\sum_{\alpha} |\alpha\rangle\langle\alpha| = \hat{I}$$

$$\sum_{\beta} \langle\alpha|(H_0 + V)|\beta\rangle\langle\beta|n\rangle = E_n\langle\alpha|n\rangle$$

$$\sum_{\beta} \left[(\varepsilon_{\beta} - E_n)\delta_{\alpha\beta} + \langle\alpha|V|\beta\rangle \right] \langle\beta|n\rangle = 0$$

where

$$|\beta\rangle = |rs; JM\rangle, \quad \varepsilon_{\beta} = \varepsilon_r + \varepsilon_s$$

The wave function is

$$|n\rangle = \sum_{\beta} \langle \beta | n \rangle | \beta \rangle, \quad \text{or} \quad |n\rangle = \sum_{p \leq q} X(pq; n) |pq; J\rangle$$

where $X(pq; n) = \langle pq; JM | n \rangle$ and the Hamiltonian equations are

$$\sum_{r \leq s} \left[(\varepsilon_p + \varepsilon_q - E_n) \delta_{pr} \delta_{qs} + \langle pq; J | V | rs; J \rangle \right] X(rs; n) = 0$$

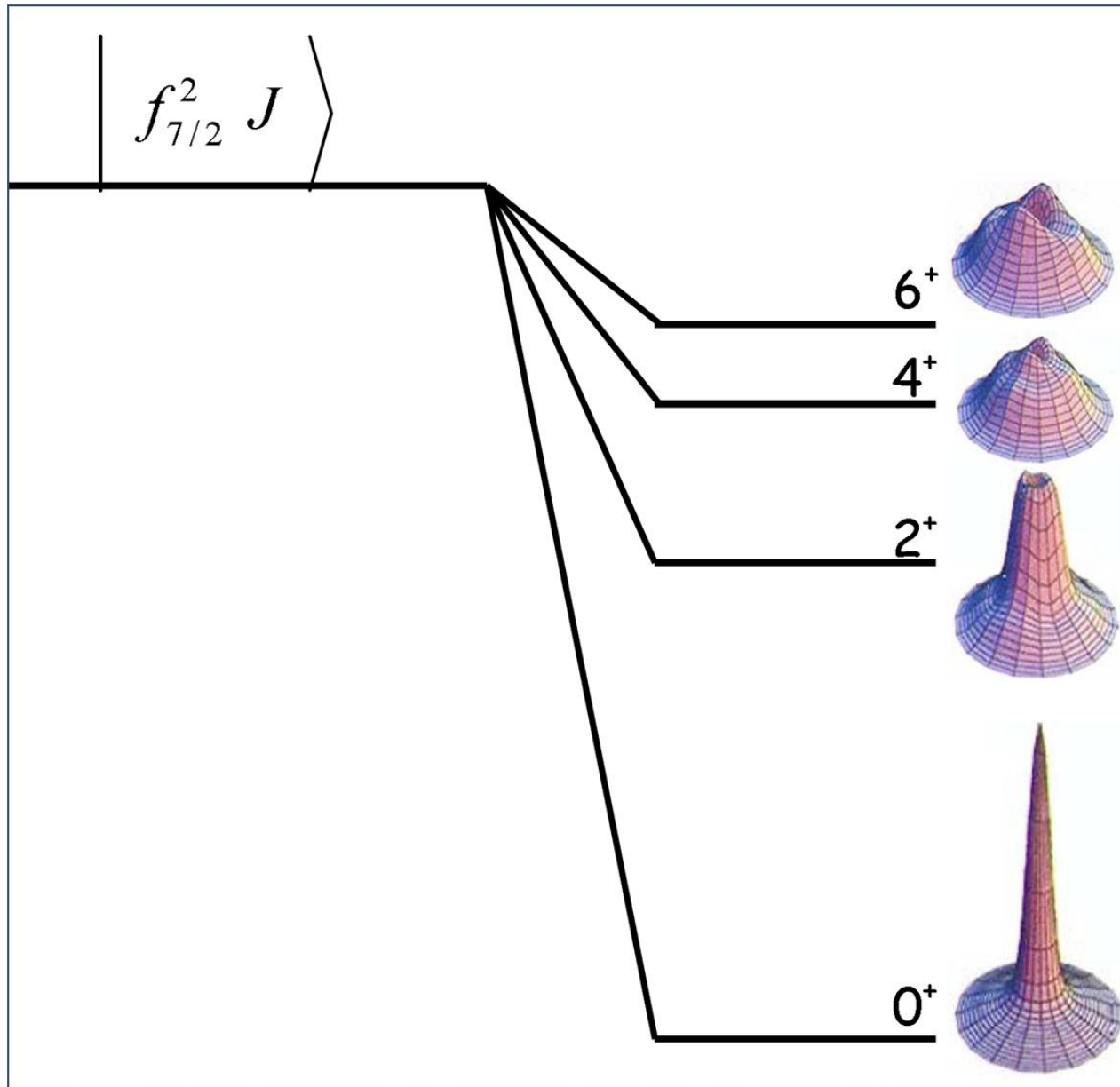
notice that this is M independent.

The two-body interaction

$$\langle pq; J | V | rs; J \rangle$$

Two particles in a single j shell

The $J=0$ pairing interaction is the dominant component of the nuclear interaction.



Configuration mixing

Two nucleons in $p_{1/2}$ and $g_{9/2}$ shells

There are two basis states for 0^+

$$|\alpha\rangle = |(p_{1/2})^2; 0^+\rangle \quad \text{and} \quad |\beta\rangle = |(g_{9/2})^2; 0^+\rangle$$

$$\begin{vmatrix} 2\varepsilon_1 + \langle\alpha|V|\alpha\rangle - E_n & \langle\alpha|V|\beta\rangle \\ \langle\beta|V|\alpha\rangle & 2\varepsilon_2 + \langle\beta|V|\beta\rangle - E_n \end{vmatrix} = 0$$

$$(2\varepsilon_1 + \langle\alpha|V|\alpha\rangle - E_n)(2\varepsilon_2 + \langle\beta|V|\beta\rangle - E_n) - \langle\alpha|V|\beta\rangle^2 = 0$$

calling $V_{\alpha\beta} = \langle\alpha|V|\beta\rangle$ one gets

$$E_n^2 - E_n(2\varepsilon_1 + 2\varepsilon_2 + V_{\alpha\alpha} + V_{\beta\beta}) + (2\varepsilon_1 + V_{\alpha\alpha})(2\varepsilon_2 + V_{\beta\beta}) - V_{\alpha\beta}^2 = 0$$

$$E_n = \varepsilon_1 + \varepsilon_2 + \frac{V_{\alpha\alpha} + V_{\beta\beta}}{2} \pm \left[\left(\varepsilon_1 - \varepsilon_2 + \frac{V_{\alpha\alpha} - V_{\beta\beta}}{2} \right)^2 + V_{\alpha\beta}^2 \right]^{1/2}$$

For the wave functions

$$X(\alpha; n) = \langle \alpha | n \rangle = \langle p_{1/2}^2; 0^+ | n \rangle; \quad X(\beta; n) = \langle \beta | n \rangle = \langle g_{9/2}^2; 0^+ | n \rangle$$

$$\begin{cases} (\varepsilon_\alpha - E_n + V_{\alpha\alpha})X(\alpha; n) + V_{\alpha\beta}X(\beta; n) = 0 \\ V_{\alpha\beta}X(\alpha; n) + (\varepsilon_\beta - E_n + V_{\beta\beta})X(\beta; n) = 0 \end{cases}$$

since we have obtained the energies E_n such that the determinant is 0, it is

$$\begin{cases} (\varepsilon_\alpha - E_n + V_{\alpha\alpha})X(\alpha; n) = -V_{\alpha\beta}X(\beta; n) \\ X^2(\alpha; n) + X^2(\beta; n) = 1 \end{cases}$$

Separable Force

An interaction which is often used in nuclear physics is the separable force given by

$$\langle pq; J|V|rs; J\rangle = -G f(pq; J) f(rs; J)$$

$$\sum_{r \leq s} \left[(\varepsilon_p + \varepsilon_q - E_n) \delta_{pr} \delta_{qs} - G f(pq; J) f(rs; J) \right] X(rs; n) = 0$$

$$X(pq; n) = G \frac{f(pq; J)}{\varepsilon_p + \varepsilon_q - E_n} \sum_{r \leq s} f(rs; J) X(rs; n)$$

multiplying by $\sum_{p \leq q} f(pq; J)$ one gets

$$\sum_{p \leq q} f(pq; J) X(pq; n) = G \sum_{p \leq q} \frac{f^2(pq; J)}{\varepsilon_p + \varepsilon_q - E_n} \sum_{r \leq s} f(rs; J) X(rs; n)$$

$$G \sum_{p \leq q} \frac{f^2(pq; J)}{\varepsilon_p + \varepsilon_q - E_n} = 1$$

$$G \left(\frac{f^2(\alpha; 0^+)}{2\varepsilon_1 - E_n} + \frac{f^2(\beta; 0^+)}{2\varepsilon_2 - E_n} \right) = 1$$

$$G = \left(\frac{f^2(\alpha; 0^+)}{2\varepsilon_1 - E_n} + \frac{f^2(\beta; 0^+)}{2\varepsilon_2 - E_n} \right)^{-1}$$

The pairing force in nuclear physics is used for the states 0^+ as

$$f(pq; 0^+) = f(pp; 0^+) = \sqrt{2j_p + 1}$$

For the states in ${}^{90}\text{Zr}$ one has

$$f(\alpha; 0^+) = f(p_{1/2}^2; 0^+) = \sqrt{2}; \quad f(\beta; 0^+) = f(g_{9/2}^2; 0^+) = \sqrt{10}$$

$$G = \left(\frac{2}{2\varepsilon_1 - E_{0_1^+}} + \frac{10}{2\varepsilon_2 - E_{0_1^+}} \right)^{-1}$$

and

$$X(\alpha; n) = G \frac{\sqrt{2}}{2\varepsilon_1 - E_n}, \quad X(\beta; n) = G \frac{\sqrt{10}}{2\varepsilon_2 - E_n}$$

NN interaction and **LST** coupling

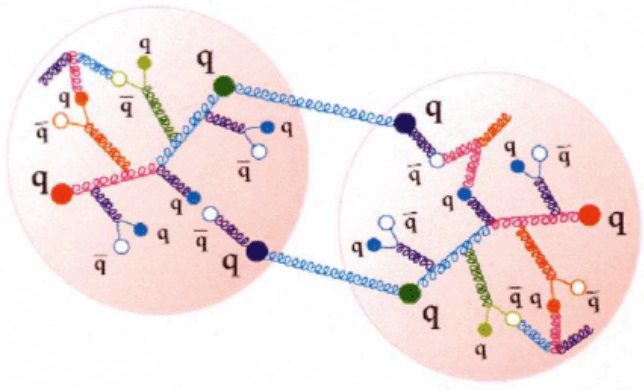
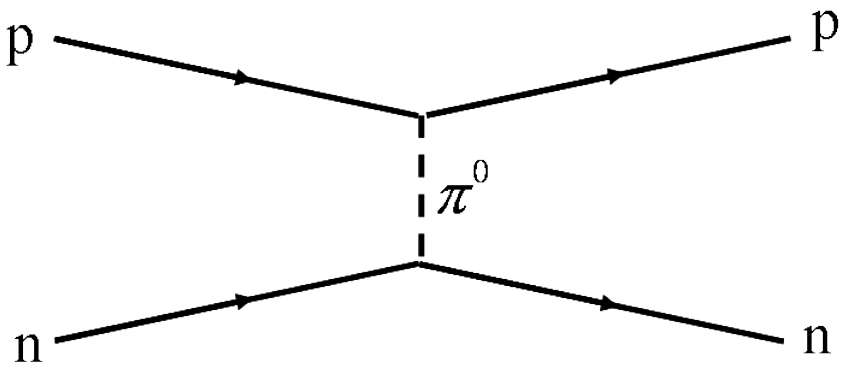
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Philosophical issue: What are the relevant degrees of freedom since it is pretty complicated inside a nucleon?

Answer: It depends on the energy scale!

Nuclear Physics: MeV

The atomic nucleus consists of protons and neutrons (two types of baryons) bound by the nuclear force (also known as the residual strong force). The baryons are further composed of subatomic fundamental particles known as quarks. The residual strong force is a minor residuum of the strong interaction which binds quarks together to form protons and neutrons. **At low energies, the two nucleons “see” each other as structure-less point particles.**



Basic properties of the NN interaction

Properties of nuclear forces :

✧ Nuclear forces are finite range forces. For a distance of the order of 1 fm they are quite strong. *Short-range repulsion (“hard core”)*

✧ **These forces show the property of saturation. It means each nucleon interacts only with its immediate neighbours. Volume and binding energies of nuclei are proportional to the mass number A .**

The distance b is found empirically to be of order $b=1.4\text{fm}$. $V(r)$ is maximally attractive inside 1 fm while for very short distances the nucleon-nucleon interaction becomes repulsive.

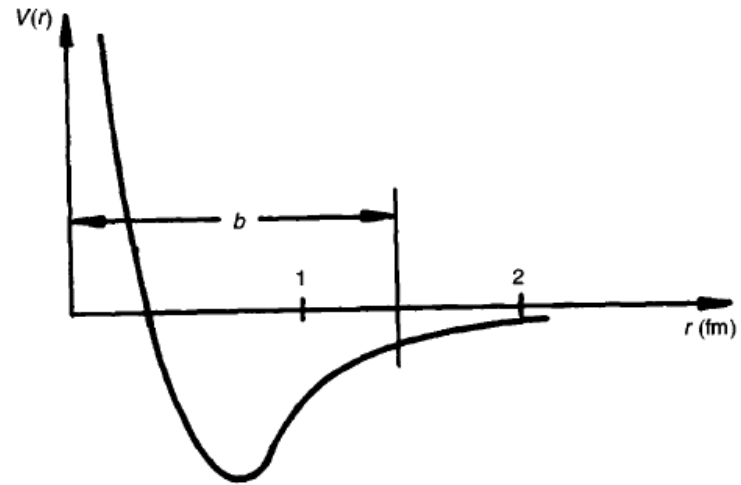


Fig. 13.1. Schematic illustration of the radial dependence of the nucleon–nucleon interaction.

A brief history of NN interactions

1935 – Yukawa (meson theory or Meson Hypothesis)

1950's – Full One-Pion-Exchange potential (OPEP)

--Hamada-Jonston

1960's – non-relativistic One-Boson-Exchange potential (OBEP) (pions, Many pions, scalar mesons, 782(ω), 770(ρ), 600(σ))

1970's – fully relativistic OBEPs

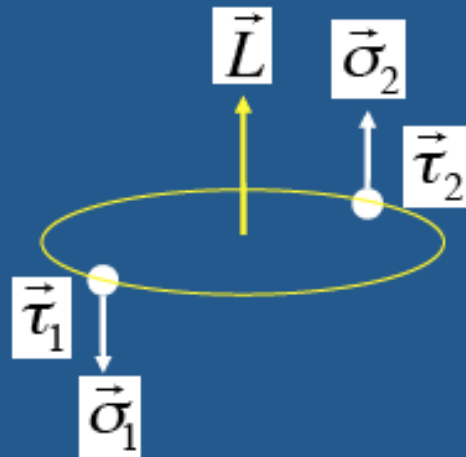
-- 2-pion exchange

-- Paris, Bonn potential

1990's – High-precision Nijmegen, Argonne V18, Reid93, Bonn potentials

1990-2000's – Chiral or Effective Field Theory potentials (2 and 3 body), Lattice QCD

N-N quantum states



$$\vec{L} = \vec{r} \times \vec{p}$$

orbital ang. momentum

$$\vec{S} = \frac{\hbar}{2}(\vec{\sigma}_1 + \vec{\sigma}_2)$$

spin of N-N pair

$$\vec{J} = \vec{L} + \vec{S}$$

total ang. momentum

$$\vec{T} = \frac{1}{2}(\vec{\tau}_1 + \vec{\tau}_2)$$

isospin of N-N pair

Spectroscopic notation:

$$(2S+1)L_J$$

use S,P,D,... for L=0,1,2,...

N-N state vector:

$$|\Psi(1,2)\rangle = |LS; JM_J\rangle \otimes |T, T_z\rangle$$

The total spin is either $S = 1$ (triplet) or $S = 0$ (singlet), whose wave functions take the form (problem 13.2)

$$\chi_m^{S=1} = \begin{cases} \alpha(1)\alpha(2) & , m = 1 \\ \beta(1)\beta(2) & , m = -1 \\ (1/\sqrt{2}) [\alpha(1)\beta(2) + \beta(1)\alpha(2)] & , m = 0 \end{cases}$$

$$\chi_0^{S=0} = \frac{1}{\sqrt{2}} [\alpha(1)\beta(2) - \beta(1)\alpha(2)]$$

It is evident that the triplet wave function is symmetric in the spin variables while the singlet wave function is antisymmetric. Thus, for identical particles, even L must be combined with $S = 0$ and odd L with $S = 1$. These wave

Antisymmetric two-particle wave functions

For identical nucleons, i.e. either protons or neutrons, the Pauli exclusion principle requires that a many-nucleon wave function be antisymmetric in all particle coordinates. Thus if the space and spin variables of any two protons or any two neutrons are interchanged, the wave function must reverse its sign.

Isospin symmetry requires that the wave function reverse its sign upon an odd permutation of all coordinates (i.e. space, spin and isospin) of any two nucleons.

This property is strongly connected with the symmetry of the two-particle wave function $|12\rangle$. Since nucleons are fermions, they have to be totally antisymmetric. For example, if we take a product wave function built out of ordinary space, a spin and an isospin part

$$\langle \mathbf{r}_1 s_1 t_1, \mathbf{r}_2 s_2 t_2 | 12 \rangle = \varphi(\mathbf{r}_1, \mathbf{r}_2) \chi(s_1, s_2) \zeta(t_1, t_2)$$

we have four combinations compatible with the Pauli principle.

φ	χ	abbreviation	ζ
even	singlet	es	+
even	triplet	et	-
odd	singlet	os	-
odd	triplet	ot	+

Table 13.1. Possible states defined by internal spin S , orbital angular momentum L , total angular momentum J and parity π applicable to the NP (neutron-proton) and NN and PP systems, respectively. In the last column, the corresponding isospin is given. Only those states having $L \leq 3$ are indicated.

	S	L	J^P	Symmetry	Notation	Isospin T
NP only	1	0	1^+	symmetric in	3S_1	0
	1	2	$1^+, 2^+, 3^+$		${}^3D_{1,2,3}$	
	0	1	1^-	spin + position	1P_1	
	0	3	3^-		1F_3	
NN PP	1	1	$0^-, 1^-, 2^-$	antisymmetric in	${}^3P_{0,1,2}$	1
	1	3	$2^-, 3^-, 4^-$		${}^3F_{2,3,4}$	
and NP	0	0	0^+	spin + position	1S_0	
	0	2	2^+		1D_2	

The deuteron and low-energy nucleon-nucleon scattering data

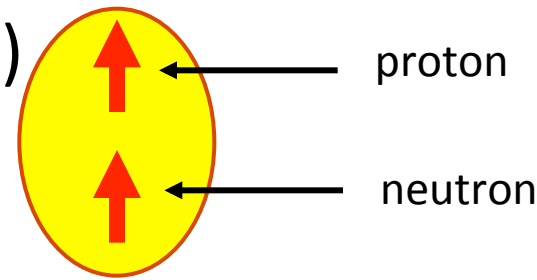
In the 1940s and early 1950s information about the nucleon–nucleon interaction came largely from studying the simplest non-trivial nucleus, the deuteron, denoted d or ${}^2\text{H}$, consisting of a neutron and a proton. For the deuteron the most important properties, known since the 1930s are the following

binding energy	$E_B = 2.25 \text{ MeV}$
spin, parity	$J^\pi = 1^+$
isospin	$T = 0$
magnetic moment	$\mu = 0.8574 \text{ n.m.} = \mu_p + \mu_n - 0.0222 \text{ n.m.}$
quadrupole moment	$Q = 2.82 \times 10^{-3} \text{ barn}$

Much more information about the nucleon-nucleon interaction has been obtained from the scattering of proton and neutron projectiles against protons and neutrons.

Deuteron : ground state $J = 1$ (Total spin $S=1$)

The deuteron is the only bound state of 2 nucleons, with isospin $T = 0$, spin-parity $J^\pi = 1^+$, and binding energy $E_B=2.225$ MeV. For two spin $\frac{1}{2}$ nucleons, only total spins $S = 0, 1$ are allowed. Then the orbital angular momentum is restricted to $J - 1 < l < J + 1$, i.e., $l = 0, 1$ or 2 . Since the parity is $\pi = (-)^l = +$, only $l = 0$ and $l = 2$ are allowed; this also implies that we have $S = 1$.



$$\psi_d = a \left| {}^3S_1 \right\rangle + b \left| {}^3D_1 \right\rangle$$

Relative motion : S wave ($L=0$) + D wave ($L=2$)

Tensor force does mix

$$V_T = (\tau_1 \tau_2) ([\sigma_1 \sigma_2]^{(2)} Y^{(2)}(\Omega)) Z(r)$$

contributes
only to $S=1$ states

relative motion

The tensor force is crucial to bind the deuteron. Without tensor force, deuteron is unbound.

No S wave to S wave coupling by tensor force because of Y_2 spherical harmonics

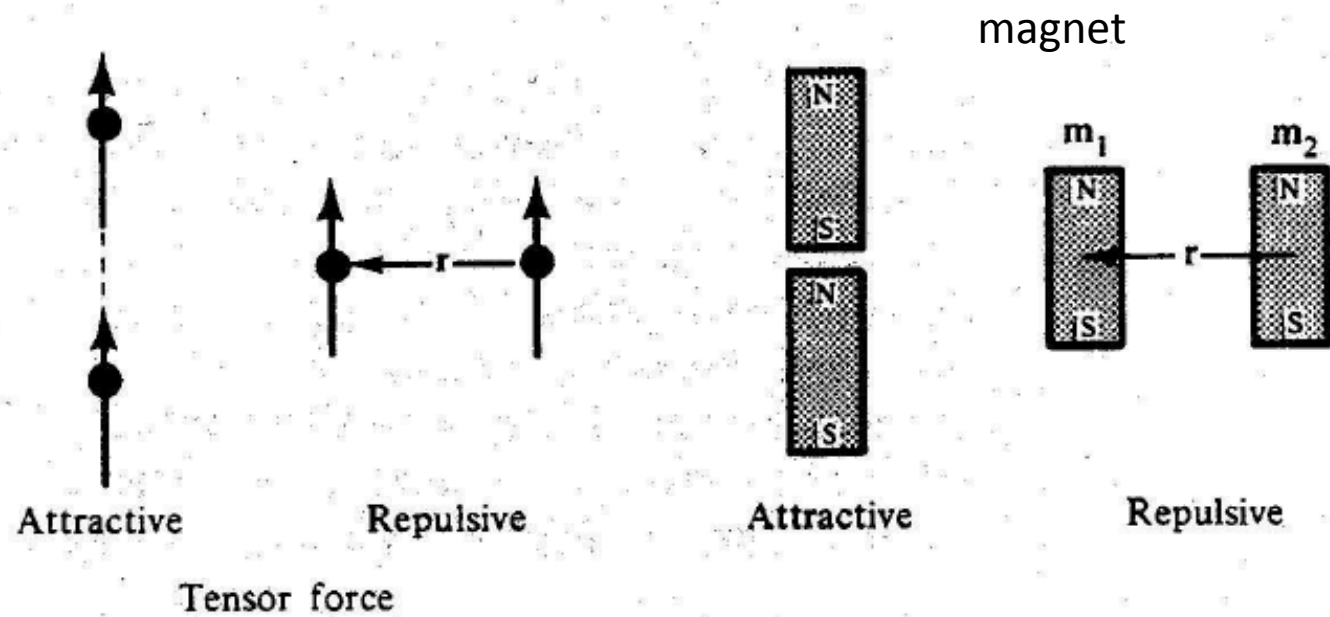


Fig. 14.11. The tensor force in the deuteron is attractive in the cigar-shaped configuration and repulsive in the disk-shaped one. Two bar magnets provide a classical example of a tensor force.

$$\psi_d = a \left| {}^3S_1 \right\rangle + b \left| {}^3D_1 \right\rangle$$

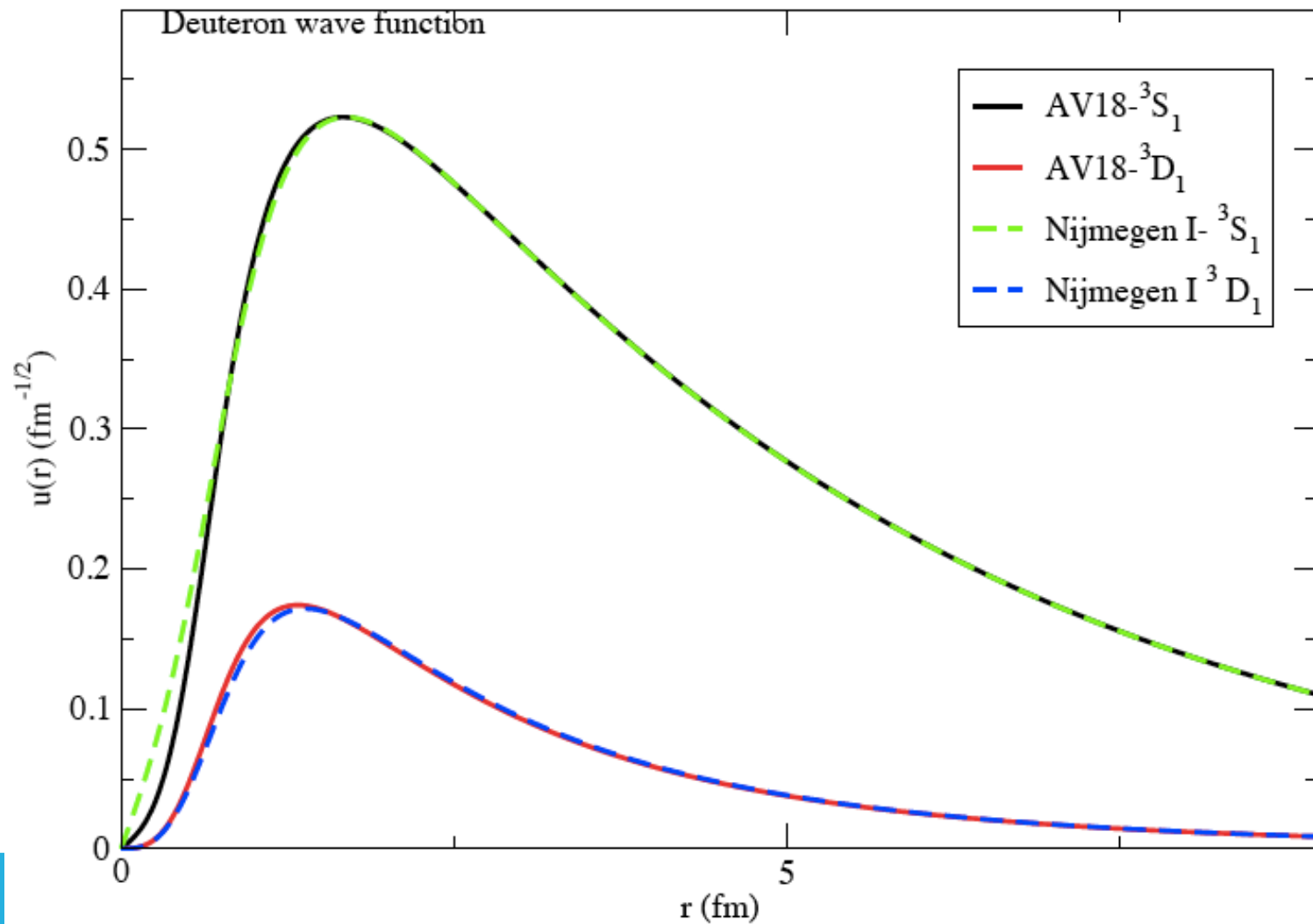
$$H = -\frac{\hbar^2}{M} \frac{1}{r} \frac{d^2}{dr^2} r + \frac{\hbar^2}{M} \frac{L^2}{r^2} + V_C(r) + V_T(r) S_{12}$$

we find the radial equations

$$\left[\frac{\hbar^2}{M} \frac{d^2}{dr^2} + E - V_c(r) \right] u_S = \sqrt{8} V_T(r) u_D$$

$$\left[\frac{\hbar^2}{M} \left(\frac{d^2}{dr^2} - \frac{6}{r^2} \right) + E + 2V_T(r) - V_c(r) \right] u_D = \sqrt{8} V_T(r) u_S$$

These equations can be solved numerically.



<http://www.phy.anl.gov/theory/movie-run.html>

Anybody has a better solution?