

Lecture I: Models for Nuclear Interactions

Morten Hjorth-Jensen^{1,2}

¹Department of Physics and Center of Mathematics for Applications
University of Oslo, N-0316 Oslo

²Department of Physics and Astronomy, Michigan State University
East Lansing, Michigan, USA

Lectures at Universidad Complutense Madrid

Outline

Introduction and Motivation to the Lectures

Overview of Nuclear Forces

Nuclear Interactions, from QCD to Effective Theories
Developing Models for the NN force

How to construct an Interaction from chiral perturbation theory

Outline

Introduction and Motivation to the Lectures

Overview of Nuclear Forces

Nuclear Interactions, from QCD to Effective Theories

Developing Models for the NN force

How to construct an Interaction from chiral perturbation theory

Outline

Introduction and Motivation to the Lectures

Overview of Nuclear Forces

Nuclear Interactions, from QCD to Effective Theories

Developing Models for the NN force

How to construct an Interaction from chiral perturbation theory

Outline

Introduction and Motivation to the Lectures

Overview of Nuclear Forces

Nuclear Interactions, from QCD to Effective Theories

Developing Models for the NN force

How to construct an Interaction from chiral perturbation theory

Lecture Plan, see also the link [http:](http://www.fys.uio.no/compphys/cp/software.html)

[//www.fys.uio.no/compphys/cp/software.html](http://www.fys.uio.no/compphys/cp/software.html)

1. First lecture set (Monday 24/1): Nuclear interactions, models and calculational schemes, from one-boson exchange models to effective field theories
2. Second lecture set (Tuesday 25/1): Methods for renormalizing the nucleon-nucleon interaction, Similarity transformation methods and link to many-body methods
3. Third and fourth lecture set (Wednesday 26/1 and Monday 7/2): Many-body methods, we start with Hartree-Fock theory, large scale diagonalization methods (full configuration interaction or shell-model), many-body perturbation theory. Applications of many-body methods and further properties of the different methods, emphasis on shell model and many-body perturbation theory
4. Fifth Lecture set (Tuesday 8/2): Theory for studies of exotic nuclei.

Why CENS and what is it?

Computational Environment for Nuclear Structure (CENS)

- ▶ AIM: To provide you with computational tools for nuclear structure analyses. Useful both for data analysis (finalizing articles, theses etc) as well as for writing proposals.
- ▶ CENS is a graphical user interface (GUI) written in Python which coordinates:
 1. Many programs in Fortran 90/95 for computing effective two-body interactions starting with free nucleon-nucleon interactions (proton-neutron formalism).
 2. A shell-model code and a transition code. Source code in C/C++ (portable to all systems) which allows you to address systems up to 10^9 basic states. Parallel codes for larger systems available upon demand.

Why CENS and what is it?

- ▶ Weblink with codes and lectures:(<http://www.fys.uio.no/compphys/cp/software.html>).
- ▶ Understand how nuclear spectra evolve from the underlying nuclear interactions. Many types of effective interactions.
- ▶ Critical assessment of the methods, pros and cons and their limitations.

Additions to come and further stuff

1. CENS works for Linux/Unix and MAC.
2. For windows, we recommend to install Wubi, Ubuntu on Windows, see <http://www.ubuntu.com/desktop/get-ubuntu/windows-installer>. Can then install Intel's compilers for free academic use.
3. Add possibility to do Coupled-Cluster calculations
4. Include three-body interaction and effective interaction diagrams
5. Code to perform shell-model calculations with and without three-body interactions

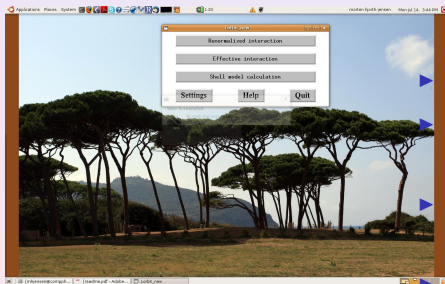
An alternative way to use the GUI

1. For large calculations the GUI is not very practical.
2. Use the GUI to generate the input files to the effective interaction calculation and the shell-model calculations.
3. Then run the shell-model or effective interaction codes on your local computing node(s).
4. **The GUI is then an easy to use tool to generate input files.**
5. This is the most likely usage of the GUI at the end.

Code Developers

Torgeir Engeland, Morten Hjorth-Jensen, Gustav Jansen, Maxim Kartamychev

CENS, with everything installed

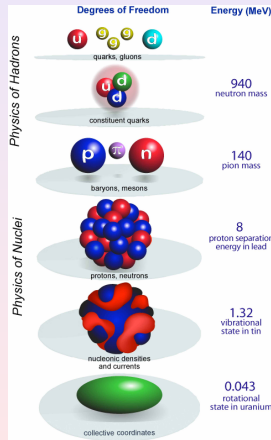


- ▶ Load down the `cens.tar.gz` package and read the README file with installation prescriptions
- ▶ run as **cens**
- ▶ Need python, numpy and Pwm, Tkinter and gnuplot packages
- ▶ Linux: `sudo apt-get install < name - of - package >`
- ▶ C/C++ and Fortran 95 compilers, see <http://software.intel.com/en-us/articles/intel-software-evaluation-cente>

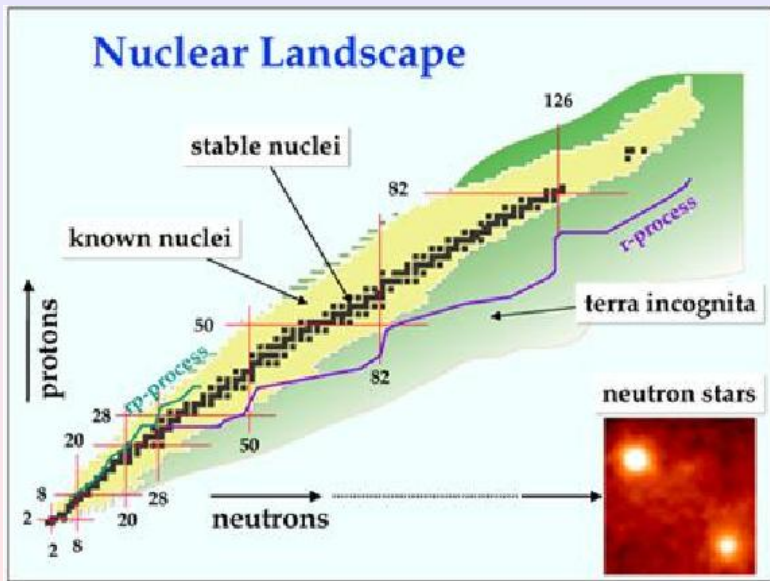
Important questions from QCD to the nuclear many-body problem

- ▶ How to derive the in medium nucleon-nucleon interaction from basic principles?
- ▶ How does the nuclear force depend on the proton-to-neutron ratio?
- ▶ What are the limits for the existence of nuclei?
- ▶ How can collective phenomena be explained from individual motion?
- ▶ Shape transitions in nuclei?

Multiscale Physics: The many scales pose a severe challenge to *ab initio* descriptions of nuclear systems.



The many scales of Nuclear Physics, from baryons to stars



To address these questions one needs a credible theory

Requirements to theory

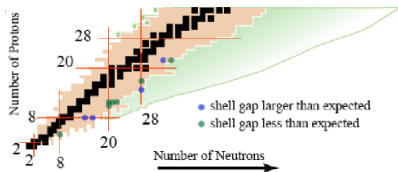
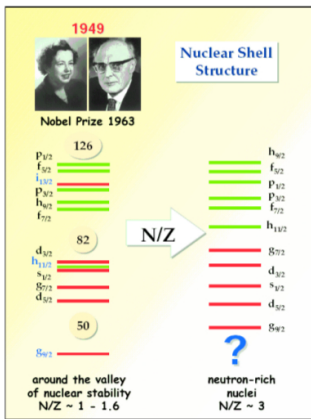
- ▶ It should be fully microscopic and start with present two- and three-body interactions derived from *e.g.*, effective field theory;
- ▶ It can be improved upon systematically, *e.g.*, by inclusion of three-body interactions and more complicated correlations;
- ▶ It allows for description of both closed-shell systems and valence systems;
- ▶ For nuclear systems where shell-model studies are the only feasible ones, viz., a small model space requiring an effective interaction, one should be able to derive effective two and three-body (and more complicated) equations and interactions for the shell model;

Aims, motivations and challenges

Requirements to theory

- ▶ It can be used to generate excited spectra for nuclei like where many shells are involved (It is hard for the traditional shell model to go beyond one major shell. The inclusion of several shells may imply the need of complex effective interactions needed in studies of weakly bound systems); and
- ▶ Finally, nuclear structure results should be used in marrying microscopic many-body results with reaction studies.

Changing shell gaps: one of the challenges

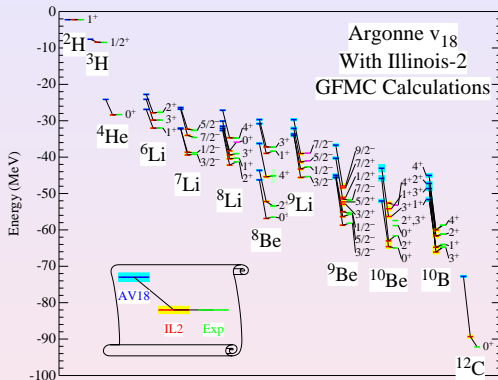


Key intellectual issues

How well do you understand your favourite theory?

1. Can we understand the link between Lattice QCD and Effective field theories?
2. Can we link the cutoff of the interaction with a specific model-space size? That is, can we link many-body theories with effective field theories? All interactions have a cutoff Λ ($\Lambda \sim 500 - 700$ MeV). A cutoff produces always missing many-body physics (intruder states etc).
3. Can we provide proper error estimates (single-particle basis truncation and truncations in number of excitations)?
4. Do we understand how many-body forces evolve as we add more and more particles? What about three-body forces, or more complicated ones?
5. Can we link ab initio methods with density functional theories? Possible road to multiscale physics.

Results, Monte Carlo, Pieper and Wiringa
Ann. Rev. Nucl. Part. Sci. **51**, 53 (2001)



Recently also calculations of several weakly bound and light isotopes. Limit is roughly at $A \leq 12$ for Green's function Monte Carlo approaches (Pieper and Wiringa, ANL). Similar limits apply to large-scale no-core calculations.

Large-Scale shell-model calculations, Navratil, Quaglioni, Stetcu, Barrett, arXiv:0904.0463

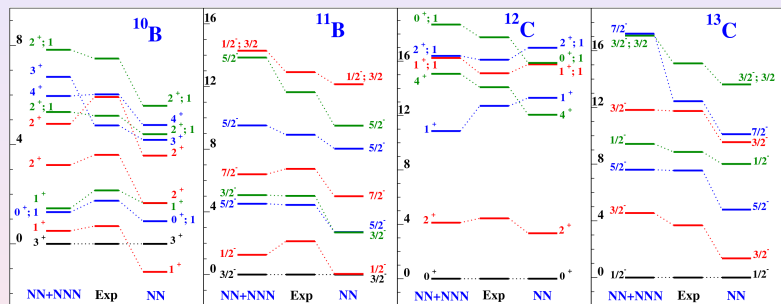
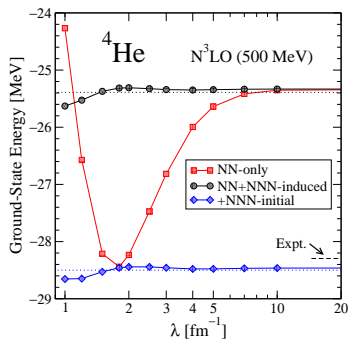
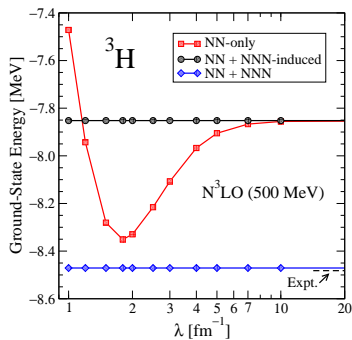
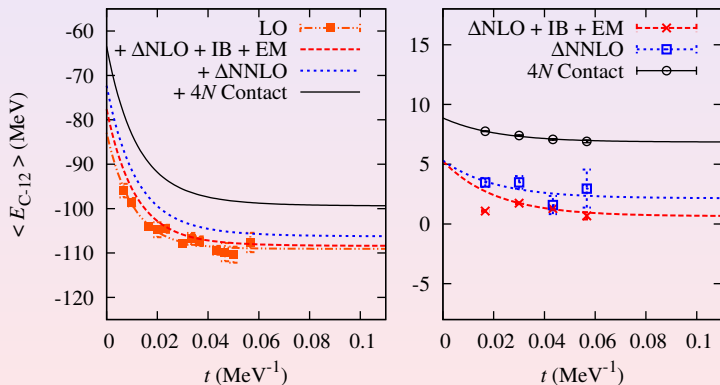


Figure: States dominated by p -shell configurations for ^{10}B , ^{11}B , ^{12}C , and ^{13}C calculated at $N_{\text{max}} = 6$ using $\hbar\Omega = 15$ MeV (14 MeV for ^{10}B). Most of the eigenstates are isospin $T=0$ or $1/2$, the isospin label is explicitly shown only for states with $T=1$ or $3/2$. The excitation energy scales are in MeV.

Similarity Renormalization Group, Jurgenson, Navratil and Furnstahl *et al* PRL 103



N²LO Chiral interactions on the Lattice $A = 3$, ${}^4\text{He}$, ${}^6\text{Li}$
 and ${}^{12}\text{C}$, Epelbaum, Krebs, Dean Lee, Meissner,
 Phys. Rev. Lett. **104**, 142501 (2010), arXiv:0912.4195

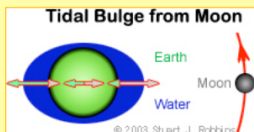


Three-body forces?

- Nucleons are not point particles (i.e. elementary).
- We neglected some internal degrees of freedom (e.g. D-resonance, “polarization effects”, ...), and unconstrained high-momentum modes.

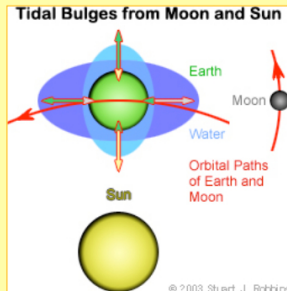
Example from celestial mechanics:

Some tidal effects are included in the two-body interaction



Renormalization group transformation:
Removal of “stiff” degrees of freedom at
expense of additional forces.

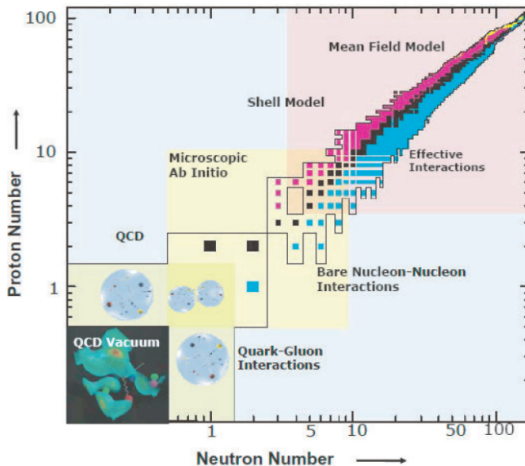
Other tidal effects cannot be included in the two-body interaction! Three-body force unavoidable.



Three-nucleon forces

- ▶ Different NN forces must be associated with different three-nucleon forces
- ▶ Modern understanding that there are no 'TRUE' NN and 3N forces.
- ▶ Question: Is there a consistent and systematic way of relating 3NF's to a given nucleon-nucleon force?
- ▶ Question: Is there a systematic way of linking low- energy nuclear structure with QCD ?
- ▶ Answer: YES! Chiral effective field theory.

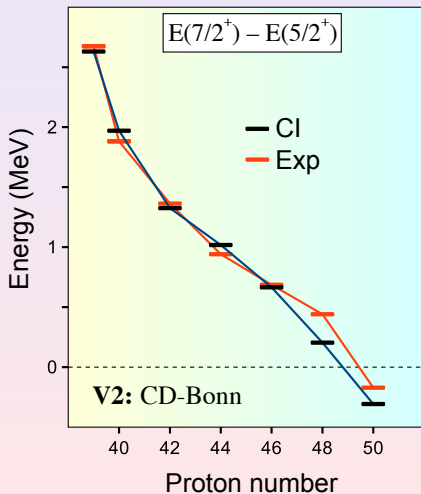
Aim: Bottom up approach to nuclear structure



Nuclear Many-Body Methods

1. Shell-model and No-core shell-model calculations; Large-scale diagonalization
2. Perturbative many-body methods
3. Coupled cluster theory
4. Extension to weakly bound systems, Complex scaling and complex shell model, Gamow shell model
5. DFT and how to link it with ab initio methods
6. Density matrix renormalization group.
7. Variational, Diffusion and Path integral Monte Carlo methods
8. Green's function theory, Unitary operator method....

One possible story: Ground state of ^{101}Sn , Darby *et al*, PRL105, 2010



- ▶ Shell-model calculation with ^{88}Sr as core.
- ▶ Ground state of ^{101}Sn is $7/2^+$!
- ▶ Core-polarization and tensor force crucial
- ▶ One crucial matrix element $\langle (0g_{7/2})^2 J = 0 | V | (0g_{7/2})^2 J = 0 \rangle$

Ground state of ^{101}Sn , Darby *et al*, PRL105, 2010

1. Can we relate the spectrum of the above isotones to specific properties of the nuclear forces?
2. The tools we will present allow you to address questions like: what is the role of the tensor force and other components of the nuclear force?; or what is the structure of the wave function?; can we extract some simple physics messages from complicated many-body calculations?
3. How reliable are our theories? Can we trust the result?

We will try to outline all ingredients needed to study the $N = 50$ isotones and to make a critical analysis of the results.

Before we proceed...some philosophical thoughts...

We wish to interpret data. To do so we need to define what we mean with the concept of an **OBSERVABLE**.

Challenge for this evening:

- ▶ How do you define an observable;
- ▶ Make then a list of observables;
- ▶ and possible links to theoretical descriptions

From Yukawa to Lattice QCD and Effective Field Theory

1930's

Chadwick (1932) discovers the neutron and Heisenberg (1932) proposes the first Phenomenology (Isospin). Yukawa (1935) and his Meson Hypothesis

1940's

Discovery of the pion in cosmic ray (1947) and in the Berkeley Cyclotron Lab (1948). Nobelprize awarded to Yukawa (1949). Rabi (1948) measures quadrupole moment of the deuteron.

1950's

Taketani, Nakamura, Sasaki (1951): 3 ranges. One-Pion-Exchange (OPE): o.k. Multi-pion exchanges: Problems! Taketani, Machida, Onuma (1952); "Pion Theories" Brueckner, Watson (1953).

From Yukawa to Lattice QCD and Effective Field Theory

1960's

Many pions = multi-pion resonances: $\sigma(600)$, $\rho(770)$, $\omega(782)$
etc. One-Boson-Exchange Model. Refined Meson Theories

1970's

Sophisticated models for two-pion exchange: Paris Potential (Lacombe et al., Phys. Rev. C **21**, 861 (1980)) Bonn potential (Machleidt et al., Phys. Rep. **149**, 1 (1987))

1980's

Quark cluster models. Begin of effective field theory studies.

From Yukawa to Lattice QCD and Effective Field Theory

1990's

1993-2001: High-precision NN potentials: Nijmegen I, II, '93, Reid93 (Stoks et al. 1994), Argonne V18 (Wiringa et al, 1995), CD-Bonn (Machleidt et al. 1996 and 2001). Advances in effective field theory: Weinberg (1990); Ordonez, Ray, van Kolck and many more.

3rd Millenium

Another "pion theory"; but now right: constrained by chiral symmetry. Three-body and higher-body forces appear naturally at a given order of the chiral expansion.

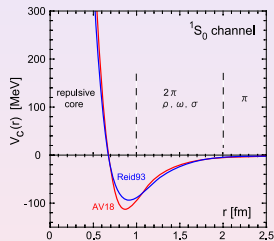
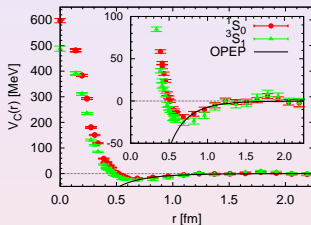
2006

Nucleon-nucleon interaction from Lattice QCD, final confirmation of meson hypothesis of Yukawa?

Progress in our QCD understanding of the NN force

- ▶ Explore the limits of our understanding of the atomic nuclei based on nucleonic and mesonic degrees of freedom. CEBAF, J-Parc, FAIR and LHC offer such perspectives.
- ▶ Experimental plans aim at identifying and exploring the transition from the nucleon/meson description of nuclei to the underlying quark and gluon description.
- ▶ Test the short-range behavior of the NN interaction via deep inelastic scattering
- ▶ Effective field theory has made progress in constructing NN and NNN forces from the underlying symmetries of QCD
- ▶ Three-body and higher-body forces emerge naturally and have explicit expressions at every order in the chiral expansion.
- ▶ Recent progress in Lattice QCD (LQCD) may hold great promise for constraining effective field theories.
- ▶ LQCD will be able to tell us about the interactions of systems that cannot be probed experimentally, but have relevance to astrophysics (nucleon-hyperon interactions), meson-meson and meson-baryon interactions, and other fields of nuclear physics.

Lattice QCD, Ishii *et al*, PRL 2007



The nucleon-nucleon interaction, Phenomenology vs Lattice calculations.

Features of the Nucleon-Nucleon (NN) Force

The aim is to give you an overview over central features of the nucleon-nucleon interaction and how it is constructed, both technical and theoretical approaches.

1. The existence of the deuteron with $J^\pi = 1^+$ indicates that the force between protons and neutrons is attractive at least for the 3S_1 partial wave. Interference between Coulomb and nuclear scattering for the proton-proton partial wave 1S_0 shows that the NN force is attractive at least for the 1S_0 partial wave.
2. It has a short range and strong intermediate attraction.
3. Spin dependent, scattering lengths for triplet and singlet states are different,
4. Spin-orbit force. Observation of large polarizations of scattered nucleons perpendicular to the plane of scattering.

Features of the Nucleon-Nucleon (NN) Force, continued

1. Hard core. The s -wave phase shift becomes negative at ≈ 250 MeV implying that the singlet S has a hard core with range $0.4 - 0.5$ fm.
2. Charge independence (almost). Two nucleons in a given two-body state always (almost) experience the same force. Modern interactions break charge and isospin symmetry lightly. That means that the pp , neutron-neutron and pn parts of the interaction will be different for the same quantum numbers.
3. Non-central. There is a tensor force. First indications from the quadrupole moment of the deuteron pointing to an admixture in the ground state of both $l = 2$ (3D_1) and $l = 0$ (3S_1) orbital momenta.

Short Range Evidence

Comparison of the binding energies of ${}^2\text{H}$ (deuteron), ${}^3\text{H}$ (triton), ${}^4\text{He}$ (alpha - particle) show that the nuclear force is of finite range (1 – 2 fm) and very strong within that range. For nuclei with $A > 4$, the energy saturates: Volume and binding energies of nuclei are proportional to the mass number A .

Nuclei are also bound. The average distance between nucleons in nuclei is about 2 fm which must roughly correspond to the range of the attractive part.

Charge Dependence

- ▶ After correcting for the electromagnetic interaction, the forces between nucleons (pp, nn, or np) in the same state are almost the same.
- ▶ "Almost the same": Charge-independence is slightly broken.
- ▶ Equality between the pp and nn forces: Charge symmetry.
- ▶ Equality between pp/nn force and np force: Charge independence.
- ▶ Better notation: Isospin symmetry, invariance under rotations in isospin

Charge Dependence, 1S_0 Scattering Lengths

Charge-symmetry breaking (CSB), after electromagnetic effects have been removed:

- ▶ $a_{pp} = -17.3 \pm 0.4\text{fm}$
- ▶ $a_{nn} = -18.8 \pm 0.5\text{fm}$. Note however discrepancy from nd breakup reactions resulting in $a_{nn} = -18.72 \pm 0.13 \pm 0.65\text{fm}$ and $\pi^- + d \rightarrow \gamma + 2n$ reactions giving $a_{nn} = -18.93 \pm 0.27 \pm 0.3\text{fm}$.

Charge-independence breaking (CIB)

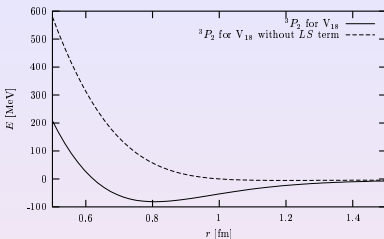
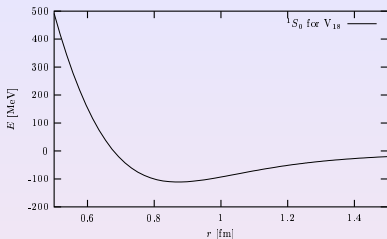
- ▶ $a_{pn} = -23.74 \pm 0.02\text{fm}$

Symmetries of the Nucleon-Nucleon (NN) Force

1. Translation invariance
2. Galilean invariance
3. Rotation invariance
4. Space reflection invariance
5. Time reversal invariance
6. Invariance under the interchange of particle 1 and 2
7. Almost isospin symmetry

CENS options

1. Charge symmetry breaking (CSB): available for N3LO and CD-Bonn interactions. The Argonne V_{18} model includes CSB.
2. Isospin symmetry breaking (ISB): available for N3LO and CD-Bonn interactions. The Argonne V_{18} model includes CSB.
3. Coulomb: Argonne includes Coulomb by default. All other interaction models can or cannot include the Coulomb interaction as an option.







$$V(\mathbf{r}) = \left\{ C_c + C_\sigma \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 + C_T \left(1 + \frac{3}{m_\alpha r} + \frac{3}{(m_\alpha r)^2} \right) S_{12}(\hat{r}) \right. \\ \left. + C_{SL} \left(\frac{1}{m_\alpha r} + \frac{1}{(m_\alpha r)^2} \right) \mathbf{L} \cdot \mathbf{S} \right\} \frac{e^{-m_\alpha r}}{m_\alpha r}$$

How do we derive such terms? (Note: no isospin dependence)

References for Various Phenomenological Interactions

Potentials which are based upon the standard non-relativistic operator structure are called "Phenomenological Potentials" Some historically important examples are

-  Gammel-Thaler potential (Phys. Rev. **107**, 291, 1339 (1957) and the \cdot Hamada-Johnston potential, Nucl. Phys. **34**, 382 (1962)), bot with a hard core. core.
-  Reid potential (Ann. Phys. (N.Y.) **50**, 411 (1968)), soft core.
-  Argonne V_{14} potential (Wiringa et al., Phys. Rev. C **29**, 1207 (1984)) with 14 operators and the Argonne V_{18} potential (Wiringa et al., Phys. Rev. C **51**, 38 (1995)), uses 18 operators
-  A good reference: R. Machleidt, Adv. Nucl. Phys **19**, 189 (1989).

Effective Degrees of Freedom, History

1. From 1950 till approximately 2000: One-Boson-Exchange (OBE) models dominate
2. Now: models based on chiral perturbation theory.

Dramatis Personae

Baryons	Mass (MeV)	Mesons	Mass (MeV)
p, n	938.926	π	138.03
Λ	1116.0	η	548.8
Σ	1197.3	σ	≈ 550.0
Δ	1232.0	ρ	770
		ω	782.6
		δ	983.0
		K	495.8
		K^*	895.0

Lagrangians

To describe the interaction between the various baryons and mesons of the previous table we choose the following phenomenological lagrangians for spin 1/2 baryons

$$\mathcal{L}_{ps} = g^{ps} \bar{\Psi} \gamma^5 \Psi \phi^{(ps)},$$

$$\mathcal{L}_s = g^s \bar{\Psi} \Psi \phi^{(s)},$$

and

$$\mathcal{L}_v = g^v \bar{\Psi} \gamma_\mu \Psi \phi_\mu^{(v)} + g^t \bar{\Psi} \sigma^{\mu\nu} \Psi \left(\partial_\mu \phi_\nu^{(v)} - \partial_\nu \phi_\mu^{(v)} \right),$$

for pseudoscalar (ps), scalar (s) and vector (v) coupling, respectively. The factors g^v and g^t are the vector and tensor coupling constants, respectively.

Spinors for Protons and Neutrons

For spin 1/2 baryons, the fields Ψ are expanded in terms of the Dirac spinors (positive energy solution shown here with $\bar{u}u = 1$)

$$u(k\sigma) = \sqrt{\frac{E(k) + m}{2m}} \begin{pmatrix} \chi \\ \frac{\boldsymbol{\sigma} \mathbf{k}}{E(k) + m} \chi \end{pmatrix},$$

with χ the familiar Pauli spinor and $E(k) = \sqrt{m^2 + |\mathbf{k}|^2}$. The positive energy part of the field Ψ reads

$$\Psi(x) = \frac{1}{(2\pi)^{3/2}} \sum_{\mathbf{k}\sigma} u(k\sigma) e^{-ikx} a_{\mathbf{k}\sigma},$$

with a being a fermion annihilation operator.

The Classical Expression

Expanding the free Dirac spinors in terms of $1/m$ (m is here the mass of the relevant baryon) results, to lowest order, in the familiar non-relativistic expressions for baryon-baryon potentials. The configuration space version of the interaction can be approximated as

$$V(\mathbf{r}) = \left\{ C_C^0 + C_C^1 + C_\sigma \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 + C_T \left(1 + \frac{3}{m_\alpha r} + \frac{3}{(m_\alpha r)^2} \right) S_{12}(\hat{r}) \right. \\ \left. + C_{SL} \left(\frac{1}{m_\alpha r} + \frac{1}{(m_\alpha r)^2} \right) \mathbf{L} \cdot \mathbf{S} \right\} \frac{e^{-m_\alpha r}}{m_\alpha r},$$

where m_α is the mass of the relevant meson and S_{12} is the familiar tensor term.

OBE for Pion Exchange

We derive now the non-relativistic one-pion exchange interaction. Here p_1 , p'_1 , p_2 , p'_2 and $k = p_1 - p'_1$ denote four-momenta. The vertices are given by the pseudovector Lagrangian

$$\mathcal{L}_{p\nu} = \frac{f_\pi}{m_\pi} \bar{\psi} \gamma_5 \gamma_\mu \psi \partial^\mu \phi_\pi.$$

From the Feynman diagram rules we can write the two-body interaction as

$$V^{p\nu} = \frac{f_\pi^2}{m_\pi^2} \frac{\bar{u}(p'_1) \gamma_5 \gamma_\mu (p_1 - p'_1)^\mu u(p_1) \bar{u}(p'_2) \gamma_5 \gamma_\nu (p'_2 - p_2)^\nu u(p_2)}{(p_1 - p'_1)^2 - m_\pi^2}.$$

OBE for Pion Exchange

The factors $p_1 - p'_1 = p'_2 - p_2$ are both the four-momentum of the exchanged meson and come from the derivative of the meson field in the interaction Lagrangian. The Dirac spinors obey

$$\begin{aligned}\gamma_\mu p^\mu u(p) &= m u(p) \\ \bar{u}(p) \gamma_\mu p^\mu &= m \bar{u}(p).\end{aligned}$$

Using these relations, together with $\{\gamma_5, \gamma_\mu\} = 0$, we find

$$\begin{aligned}\bar{u}(p'_1) \gamma_5 \gamma_\mu (p_1 - p'_1)^\mu u(p_1) &= m \bar{u}(p'_1) \gamma_5 u(p_1) + \bar{u}(p'_1) \gamma_\mu p_1'^\mu \gamma_5 u(p_1) \\ &= 2m \bar{u}(p'_1) \gamma_5 u(p_1)\end{aligned}$$

and

$$\bar{u}(p'_2) \gamma_5 \gamma_\mu (p'_2 - p_2)^\mu = -2m \bar{u}(p'_2) \gamma_5 u(p_1).$$

OBE for Pion Exchange

We get

$$V^{p\nu} = -\frac{f_\pi^2}{m_\pi^2} 4m^2 \frac{\bar{u}(p'_1)\gamma_5 u(p_1)\bar{u}(p'_2)\gamma_5 u(p_2)}{(p_1 - p'_1)^2 - m_\pi^2}.$$

By inserting expressions for the Dirac spinors, we find

$$\begin{aligned}\bar{u}(p'_1)\gamma_5 u(p_1) &= \sqrt{\frac{(E'_1 + m)(E_1 + m)}{4m^2}} \begin{pmatrix} \chi^\dagger & -\frac{\boldsymbol{\sigma}_1 \cdot \mathbf{p}_1}{E'_1 + m} \chi^\dagger \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \\ &\quad \times \begin{pmatrix} \chi \\ \frac{\boldsymbol{\sigma}_1 \cdot \mathbf{p}_1}{E_1 + m} \chi \end{pmatrix} \\ &= \sqrt{\frac{(E'_1 + m)(E_1 + m)}{4m^2}} \left(\frac{\boldsymbol{\sigma}_1 \cdot \mathbf{p}_1}{E_1 + m} - \frac{\boldsymbol{\sigma}_1 \cdot \mathbf{p}'_1}{E'_1 + m} \right)\end{aligned}$$

OBE for Pion Exchange

Similarly

$$\bar{u}(p'_2)\gamma_5 u(p_2) = \sqrt{\frac{(E'_2 + m)(E_2 + m)}{4m^2}} \left(\frac{\sigma_2 \cdot \mathbf{p}_2}{E_2 + m} - \frac{\sigma_2 \cdot \mathbf{p}'_2}{E'_2 + m} \right).$$

In the CM system we have $\mathbf{p}_2 = -\mathbf{p}_1$, $\mathbf{p}'_2 = -\mathbf{p}'_1$ and so $E_2 = E_1$, $E'_2 = E'_1$. We can then write down the relativistic contribution to the NN potential in the CM system:

$$\begin{aligned} V^{pv} &= -\frac{f_\pi^2}{m_\pi^2} 4m^2 \frac{1}{(p_1 - p'_1)^2 - m_\pi^2} \frac{(E_1 + m)(E'_1 + m)}{4m^2} \\ &\times \left(\frac{\sigma_1 \cdot \mathbf{p}_1}{E_1 + m} - \frac{\sigma_1 \cdot \mathbf{p}'_1}{E'_1 + m} \right) \left(\frac{\sigma_2 \cdot \mathbf{p}_1}{E_1 + m} - \frac{\sigma_2 \cdot \mathbf{p}'_1}{E'_1 + m} \right). \end{aligned}$$

OBE for Pion Exchange

In the non-relativistic limit we have to lowest order

$$E_1 = \sqrt{\mathbf{p}_1^2 + m^2} \approx m \approx E'_1$$

and then $(p_1 - p'_1)^2 = -\mathbf{k}^2$, so we get for the contribution to the NN potential

$$\begin{aligned} V^{p\nu} &= -\frac{f_\pi^2}{m_\pi^2} 4m^2 \frac{1}{\mathbf{k}^2 + m^2} \frac{2m \cdot 2m}{4m^2} \frac{\sigma_1}{2m} \cdot (\mathbf{p}_1 - \mathbf{p}'_1) \frac{\sigma_2}{2m} \cdot (\mathbf{p}_1 - \mathbf{p}'_1) \\ &= -\frac{f_\pi^2}{m_\pi^2} \frac{(\sigma_1 \cdot \mathbf{k})(\sigma_2 \cdot \mathbf{k})}{\mathbf{k}^2 + m_\pi^2}. \end{aligned}$$

We have omitted exchange terms and the isospin term $\boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2$.

OBE for Pion Exchange, from k -space to r -space

We have

$$V^{pv}(k) = -\frac{f_\pi^2}{m_\pi^2} \frac{(\sigma_1 \cdot \mathbf{k})(\sigma_2 \cdot \mathbf{k})}{\mathbf{k}^2 + m_\pi^2}.$$

In coordinate space we have

$$V^{pv}(r) = \int \frac{d^3k}{(2\pi)^3} e^{i\mathbf{k}\mathbf{r}} V^{pv}(k)$$

resulting in

$$V^{pv}(r) = -\frac{f_\pi^2}{m_\pi^2} \sigma_1 \cdot \nabla \sigma_2 \cdot \nabla \int \frac{d^3k}{(2\pi)^3} e^{i\mathbf{k}\mathbf{r}} \frac{1}{\mathbf{k}^2 + m_\pi^2}.$$

We obtain

$$V^{pv}(r) = -\frac{f_\pi^2}{m_\pi^2} \sigma_1 \cdot \nabla \sigma_2 \cdot \nabla \frac{e^{-m_\pi r}}{r}.$$

OBE for Pion Exchange, really the last Step (I promise)

Carrying out the differentiation of

$$V^{pv}(r) = -\frac{f_\pi^2}{m_\pi^2} \sigma_1 \cdot \nabla \sigma_2 \cdot \nabla \frac{e^{-m_\pi r}}{r}.$$

we arrive at the famous one-pion exchange potential with central and tensor parts

$$V(\mathbf{r}) = -\frac{f_\pi^2}{m_\pi^2} \left\{ \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 + C_T \left(1 + \frac{3}{m_\alpha r} + \frac{3}{(m_\alpha r)^2} \right) S_{12}(\hat{r}) \right\} \frac{e^{-m_\pi r}}{m_\pi r}.$$

For the full potential add the exchange part and the $\boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2$ term as well. (Subtle point: there is a divergence which gets cancelled by using cutoffs).

Other Mesons: Collecting Terms, σ

When we perform similar non-relativistic expansions for scalar and vector mesons we obtain for the σ meson

$$V^\sigma = g_{\sigma NN}^2 \frac{1}{\mathbf{k}^2 + m_\sigma^2} \left(-1 + \frac{\mathbf{q}^2}{2M_N^2} - \frac{\mathbf{k}^2}{8M_N^2} - \frac{\mathbf{L}\mathbf{S}}{2M_N^2} \right).$$

We note an attractive central force and spin-orbit force. This term has an intermediate range. We have defined $1/2(p_1 + p_1') = \mathbf{q}$. For the full potential add the exchange part and the isospin dependence as well.

Other Mesons: Collecting Terms, ω

We obtain for the ω meson

$$V^\omega = g_{\omega NN}^2 \frac{1}{\mathbf{k}^2 + m_\omega^2} \left(1 - 3 \frac{\mathbf{L} \cdot \mathbf{S}}{2M_N^2} \right).$$

We note a repulsive central force and an attractive spin-orbit force. This term has short range. For the full potential add the exchange part and the isospin dependence as well.

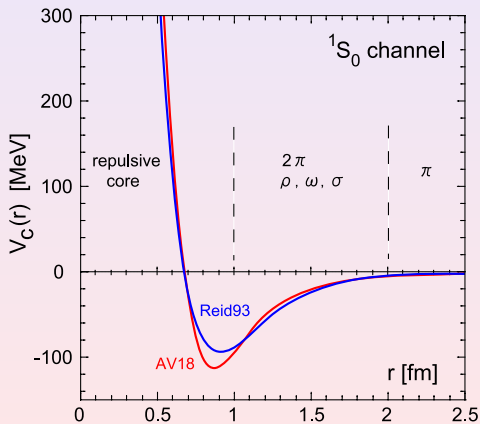
Other Mesons: Collecting Terms, ρ

Finally for the ρ meson

$$V^\rho = g_{\rho NN}^2 \frac{\mathbf{k}^2}{\mathbf{k}^2 + m_\rho^2} \left(-2\sigma_1\sigma_2 + S_{12}(\hat{k}) \right) \tau_1\tau_2.$$

We note a tensor force with sign opposite to that of the pion. This term has short range. For the full potential add the exchange part and the isospin dependence as well.

Summarizing, in terms of a boson exchange picture



CENS options

1. You can compute a pure one-pion exchange interaction, option OPEP
2. Or you can just study the role of the LS interaction
3. Or just the tensor force.

All these options are derived using the parameterizations of the Argonne V8 interaction model.

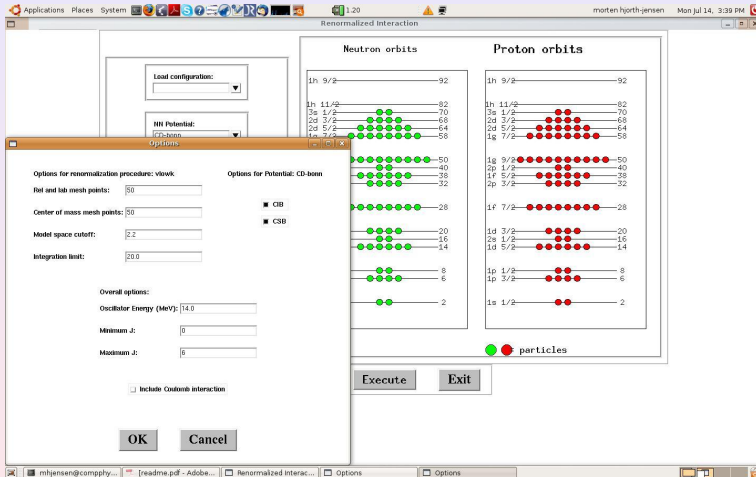
Brief summary of properties of the NN interaction

1. Can use a one-boson exchange picture to construct a nucleon-nucleon interaction a la QED
2. Non-relativistic approximation yields amongst other things a spin-orbit force which is much stronger than in atoms.
3. At large intermediate distances pion exchange dominates while pion resonances (other mesons) dominate at intermediate and short range
4. Potentials are parameterized to fit selected two-nucleon data, binding energies and scattering phase shifts.
5. Nowadays, chiral perturbation theory gives an effective theory that allows a systematic expansion in terms of controllable parameters. Good basis for many-body physics

CENS options

1. You can choose to omit or include particular partial waves under the **options** knob of the renormalization part. The variables refer to the minimum and maximum J in the relative coordinates.
2. Note that the Argonne model is parameterized with $J \leq 4$.
3. Data are scanty above $J > 5$ and the other interaction models give therefore only theoretical predictions.
4. For the no-core, vlowk, v-krg and v-nrg options, beyond $J > 6$ the Hamiltonian is given by kinetic energy only.

CENS image



How do I construct the interaction: Lippman-Schwinger Equation

To parameterize the nucleon-nucleon interaction we solve the Lippman-Schwinger equation

$$T_{ll'}^\alpha(kk'K) = V_{ll'}^\alpha(kk') + \frac{2}{\pi} \sum_{l''} \int_0^\infty dq q^2 V_{ll''}^\alpha(kq) \frac{1}{k^2 - q^2 + i\epsilon} T_{l''l'}^\alpha(qk'K).$$

The shorthand notation

$$T(\hat{V})_{ll'}^\alpha(kk'K\omega) = \langle kKlL\mathcal{J}ST | T(\omega) | k'Kl'L\mathcal{J}ST \rangle,$$

denotes the $T(V)$ -matrix with momenta k and k' and orbital momenta l and l' of the relative motion, and K is the corresponding momentum of the center-of-mass motion. Further, L , \mathcal{J} , S and T are the orbital momentum of the center-of-mass motion, the total angular momentum, spin and isospin, respectively.

Numerical Solution

For scattering states, the energy is positive, $E > 0$. The Lippman-Schwinger equation, which is the non-relativistic version of the Bethe-Salpeter equation discussed above, is an integral equation where we have to deal with the amplitude $R(k, k')$ (reaction matrix, which is the real part of the full complex T -matrix) defined through the integral equation for one partial wave (no coupled-channels)

$$R_l(k, k') = V_l(k, k') + \frac{2}{\pi} \mathcal{P} \int_0^\infty dq q^2 V_l(k, q) \frac{1}{E - q^2/m} R_l(q, k').$$

For negative energies (bound states) and intermediate states scattering states blocked by occupied states below the Fermi level.

The phaseshift codes are at <http://www.fys.uio.no/compphys/cp/software.html>

See applet at <http://people.ccmr.cornell.edu/~emuellet/well.html>

Relation to data

The symbol \mathcal{P} in the previous slide indicates that Cauchy's principal-value prescription is used in order to avoid the singularity arising from the zero of the denominator.

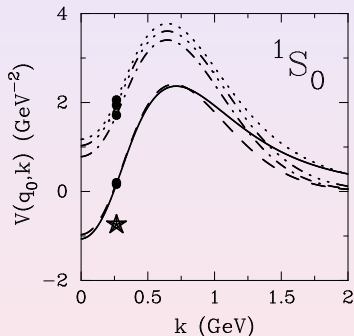
The total kinetic energy of the two incoming particles in the center-of-mass system is

$$E = \frac{k_0^2}{m}.$$

The matrix $R_I(k, k')$ relates to the the phase shifts through its diagonal elements as

$$R_I(k_0, k_0) = -\frac{\tan \delta_I}{mk_0}.$$

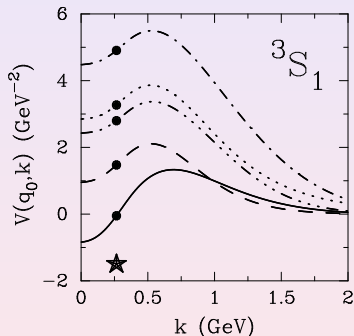
T-matrix and V



1S_0

Matrix elements $V(q_0, k)$ for the 1S_0 partial wave for the CD-Bonn (solid line), Nijm-I (dashed), Nijm-II (dash-dot), Argonne V_{18} (dash-triple-dot) and Reid93 (dotted) potentials. The diagonal matrix elements with $k = q_0 = 265 \text{ MeV}/c$ (equivalent to $T_{lab} = 150 \text{ MeV}$) are marked by a solid dot. The corresponding matrix element of the full scattering R -matrix is marked by the star.

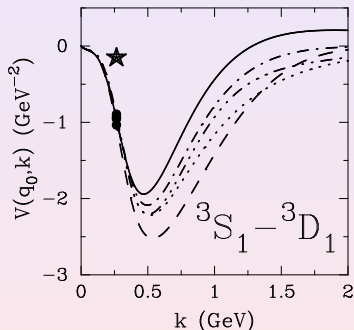
T-matrix and V



3S_1

Matrix elements for the 3S_1 for the CD-Bonn (solid line), Nijm-I (dashed), Nijm-II (dash-dot), Argonne V_{18} (dash-triple-dot) and Reid93 (dotted) potentials. The diagonal matrix elements with $k = q_0 = 265$ MeV/c (equivalent to $T_{lab} = 150$ MeV) are marked by a solid dot. The corresponding matrix element of the full scattering R -matrix is marked by the star.

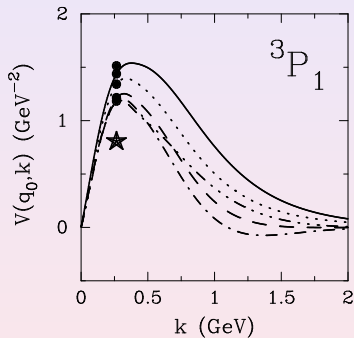
T-matrix and V



3S_1 - 3D_1

Matrix elements for 3S_1 - 3D_1 for the CD-Bonn (solid line), Nijm-I (dashed), Nijm-II (dash-dot), Argonne V_{18} (dash-triple-dot) and Reid93 (dotted) potentials. The diagonal matrix elements with $k = q_0 = 265 \text{ MeV}/c$ (equivalent to $T_{lab} = 150 \text{ MeV}$) are marked by a solid dot. The corresponding matrix element of the full scattering R -matrix is marked by the star.

T -matrix and V



3P_1

Matrix elements for 3P_1 for the CD-Bonn (solid line), Nijm-I (dashed), Nijm-II (dash-dot), Argonne V_{18} (dash-triple-dot) and Reid93 (dotted) potentials. The diagonal matrix elements with $k = q_0 = 265$ MeV/c (equivalent to $T_{lab} = 150$ MeV) are marked by a solid dot. The corresponding matrix element of the full scattering R -matrix is marked by the star.

Something to ponder about

The behavior seen here has important consequences for renormalizations in a nuclear medium.

All interactions yield the same on-shell T -matrix, although V and its off-shell character can be very different from interaction model to interaction model and may lead to for example different nuclear binding energies for different interaction models.

Question: Is this off-shell character something which can be constrained by data? Can you see some potential problems in a many-body context?

Exercises Day 1)

1. Install the software and make sure everything runs smoothly.
2. List all partial waves with isospin projection T_z , spin S , orbital angular momentum l and total spin J for $J \leq 2$.
3. Show that the spin-orbit force **LS** gives a zero contribution for S -waves (orbital angular momentum $l = 0$).

Effective Field Theories

We want to describe the low-energy scenario of QCD by an Effective Field Theory (EFT). The steps to take:

- ▶ Write down the most general Lagrangian including all terms consistent with the assumed symmetries, particularly, spontaneously broken chiral symmetry.
- ▶ Calculate Feynman diagrams. Note: There will be infinitely many diagrams.
- ▶ Find a scheme for assessing the importance of the various diagrams, because we cannot calculate infinitely many diagrams.

Chiral Perturbation Theory

The starting point for the derivation of the NN interaction is an effective chiral Lagrangian

$$\mathcal{L} = \mathcal{L}_{\pi N} + \mathcal{L}_{\pi\pi} + \mathcal{L}_{NN},$$

which is given by a series of terms of increasing chiral dimension,

$$\mathcal{L}_{\pi N} = \mathcal{L}_{\pi N}^{(1)} + \mathcal{L}_{\pi N}^{(2)} + \mathcal{L}_{\pi N}^{(3)} + \dots,$$

$$\mathcal{L}_{\pi\pi} = \mathcal{L}_{\pi\pi}^{(2)} + \dots,$$

$$\mathcal{L}_{NN} = \mathcal{L}_{NN}^{(0)} + \mathcal{L}_{NN}^{(2)} + \mathcal{L}_{NN}^{(4)} + \dots,$$

where the superscript refers to the number of derivatives or pion mass insertions (chiral dimension). Good review: Epelbaum, Prog. Part. Nucl. Phys. **57**, 654 (2006).

NN and 3NF Interaction

Chiral order	2N force	3N force	4N force
$\nu = 0$	$V_{1\pi} + V_{\text{cont}}$	—	—
$\nu = 1$	—	—	—
$\nu = 2$	$V_{1\pi} + V_{2\pi} + V_{\text{cont}}$	—	—
$\nu = 3$	$V_{1\pi} + V_{2\pi}$	$V_{2\pi} + V_{1\pi, \text{cont}} + V_{\text{cont}}$	—
$\nu = 4$	$V_{1\pi} + V_{2\pi} + V_{3\pi} + V_{\text{cont}}$	work in progress	work in progress

Chiral Perturbation Theory

Common to apply the heavy baryon (HB) formulation of chiral perturbation theory in which the relativistic Lagrangian is subjected to an expansion in terms of powers of $1/M_N$ (kind of a nonrelativistic expansion), the lowest order of which is

$$\begin{aligned}\hat{\mathcal{L}}_{\pi N}^{(1)} &= \bar{N} \left(iD_0 - \frac{g_A}{2} \vec{\sigma} \cdot \vec{u} \right) N \\ &\approx \bar{N} \left[i\partial_0 - \frac{1}{4f_\pi^2} \vec{\tau} \cdot (\vec{\pi} \times \partial_0 \vec{\pi}) - \frac{g_A}{2f_\pi} \vec{\tau} \cdot (\vec{\sigma} \cdot \vec{\nabla}) \vec{\pi} \right] N + \dots\end{aligned}$$

For the parameters that occur in the leading order Lagrangian, we apply $M_N = 938.919$ MeV, $m_\pi = 138.04$ MeV, $f_\pi = 92.4$ MeV, and $g_A = g_{\pi NN} f_\pi / M_N = 1.29$, which is equivalent to $g_{\pi NN}^2 / 4\pi = 13.67$.

NN Interaction

The chiral NN force has the general form

$$V_{2N} = V_{\pi} + V_{\text{cont}} ,$$

where V_{cont} denotes the short-range terms represented by NN contact interactions and V_{π} corresponds to the long-range part associated with the pion-exchange contributions. Both V_{π} and V_{cont} are determined within the low-momentum expansion.

Notice that the nucleon kinetic energy contributes to $\mathcal{L}^{(2)}$. The above terms determine the nuclear potential up to $N^2\text{LO}$ (with the exception of the NN contact terms at NLO) in the limit of exact isospin symmetry.

NN Interaction

Consider now pion-exchange contributions to the potential

$$V_{\pi} = V_{1\pi} + V_{2\pi} + V_{3\pi} + \dots ,$$

where one-, two- and three-pion exchange (3PE) contributions $V_{1\pi}$, $V_{2\pi}$ and $V_{3\pi}$ can be written in the low-momentum expansion as

$$\begin{aligned} V_{1\pi} &= V_{1\pi}^{(0)} + V_{1\pi}^{(2)} + V_{1\pi}^{(3)} + V_{1\pi}^{(4)} + \dots , \\ V_{2\pi} &= V_{2\pi}^{(2)} + V_{2\pi}^{(3)} + V_{2\pi}^{(4)} + \dots , \\ V_{3\pi} &= V_{3\pi}^{(4)} + \dots . \end{aligned}$$

Here, the superscripts denote the corresponding chiral order and the ellipses refer to $(Q/\Lambda)^5$ - and higher order terms. Contributions due to the exchange of four- and more pions are further suppressed: n -pion exchange diagrams start to contribute at the order $(Q/\Lambda)^{2n-2}$.

NN Interaction

The static 1PE potential at N³LO has the form

$$V_{1\pi}^{(0)} + V_{1\pi}^{(2)} + V_{1\pi}^{(3)} + V_{1\pi}^{(4)} = - \left(\frac{g_A}{2F_\pi} \right)^2 (1 + \delta)^2 \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 \frac{\vec{\sigma}_1 \cdot \vec{q} \vec{\sigma}_2 \cdot \vec{q}}{\vec{q}^2 + M_\pi^2} .$$

Chiral Perturbation Theory

Q^0

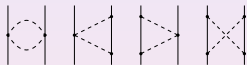


1 π Exchange

χ^{PT}

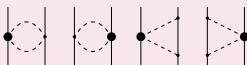
- ▶ The most important irreducible one- and two-pion exchange contributions to the NN interaction up to order Q^3 .
- ▶ Vertices denoted by small dots are from $\hat{\mathcal{L}}_{\pi N}^{(1)}$.
- ▶ Large dots refer to $\hat{\mathcal{L}}_{\pi N, \text{ct}}^{(2)}$

Q^2

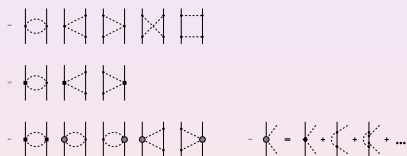


2 π Exchange

Q^3

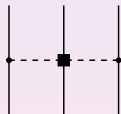


2 π -Exchange

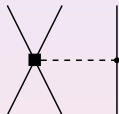


Leading $((\frac{Q}{\Lambda})^2)$, subleading $((\frac{Q}{\Lambda})^3)$ and sub-subleading $((\frac{Q}{\Lambda})^4)$ contributions to the chiral 2 π -exchange potential. Solid (dashed) lines correspond to nucleons (pions). Solid dots, filled rectangles and filled diamonds represent vertices with $\Delta_i = 0, 1$ and 2 , respectively. Shaded blob denotes the next-to-next-to-leading order contribution to the pion-nucleon scattering amplitude.

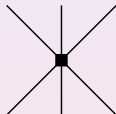
Three-Nucleon Force at order $\nu = 3$.



(a)



(b)



(c)

3NF Interaction

The first non-vanishing 3NF contribution appears at order $\nu = 3$, i.e. at N²LO. The contribution from graph (a)

$$V_{2\pi}^{(3)} = \sum_{i \neq j \neq k} \frac{1}{2} \left(\frac{g_A}{2F_\pi} \right)^2 \frac{(\vec{\sigma}_i \cdot \vec{q}_i)(\vec{\sigma}_j \cdot \vec{q}_j)}{(\vec{q}_i^2 + M_\pi^2)(\vec{q}_j^2 + M_\pi^2)} F_{ijk}^{\alpha\beta} \tau_i^\alpha \tau_j^\beta,$$

where $\vec{q}_i \equiv \vec{p}_i' - \vec{p}_i$; \vec{p}_i (\vec{p}_i') is the initial (final) momentum of the nucleon i and

$$F_{ijk}^{\alpha\beta} = \delta^{\alpha\beta} \left[-\frac{4c_1 M_\pi^2}{F_\pi^2} + \frac{2c_3}{F_\pi^2} \vec{q}_i \cdot \vec{q}_j \right] + \sum_\gamma \frac{c_4}{F_\pi^2} \epsilon^{\alpha\beta\gamma} \tau_k^\gamma \vec{\sigma}_k \cdot [\vec{q}_i \times \vec{q}_j].$$

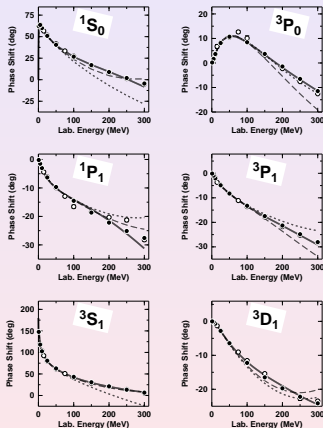
3NF Interaction

The contributions from the remaining graphs (b) and (c) take the form

$$V_{1\pi, \text{cont}}^{(3)} = - \sum_{i \neq j \neq k} \frac{g_A}{8F_\pi^2} D \frac{\vec{\sigma}_j \cdot \vec{q}_j}{\vec{q}_j^2 + M_\pi^2} (\boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j) (\vec{\sigma}_i \cdot \vec{q}_j), \quad V_{\text{cont}}^{(3)} = \frac{1}{2} \sum_{j \neq k} E (\boldsymbol{\tau}_j \cdot \boldsymbol{\tau}_k),$$

where D and E are the corresponding low-energy constants from the Lagrangian of order $\nu = 1$.

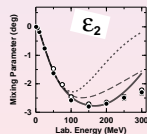
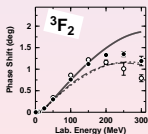
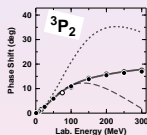
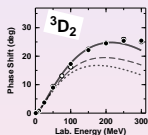
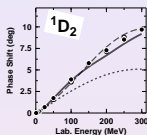
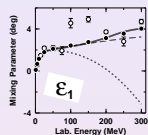
Results with NN interaction to $\nu = 4$



Phase Shifts

- ▶ np phase parameters below 300 MeV lab. energy for partial waves with $J \leq 2$. The solid line is the result at N³LO.
- ▶ The dotted and dashed lines are the phase shifts at NLO and NNLO, respectively.
- ▶ The solid dots show the Nijmegen multi-energy np phase shift analysis

Results with NN interaction to $\nu = 4$



Phase Shifts

- ▶ np phase parameters below 300 MeV lab. energy for partial waves with $J \leq 2$. The solid line is the result at N³LO.
- ▶ The dotted and dashed lines are the phase shifts at NLO and NNLO, respectively.
- ▶ The solid dots show the Nijmegen multi-energy np phase shift analysis

Mathematical Intermezzo, two-body Schrödinger in k -space

The Schrödinger equation in abstract vector representation is

$$(T + V) |\psi_n\rangle = E_n |\psi_n\rangle \quad (1)$$

Here T is the kinetic energy operator and V is the potential operator. The eigenstates form a complete orthonormal set according to

$$\mathbf{1} = \sum_n |\psi_n\rangle \langle \psi_n|, \quad \langle \psi_n | \psi_{n'} \rangle = \delta_{n,n'}$$

Mathematical Intermezzo, two-body Schrödinger in k -space

The most commonly used representations of equation 1 are the coordinate and the momentum space representations. They define the completeness relations

$$\mathbf{1} = \int d\mathbf{r} |\mathbf{r}\rangle\langle\mathbf{r}|, \quad \langle\mathbf{r}|\mathbf{r}'\rangle = \delta(\mathbf{r} - \mathbf{r}') \quad (2)$$

$$\mathbf{1} = \int d\mathbf{k} |\mathbf{k}\rangle\langle\mathbf{k}|, \quad \langle\mathbf{k}|\mathbf{k}'\rangle = \delta(\mathbf{k} - \mathbf{k}') \quad (3)$$

Here the basis states in both \mathbf{r} - and \mathbf{k} -space are dirac-delta function normalized. From this it follows that the plane-wave states are given by,

$$\langle\mathbf{r}|\mathbf{k}\rangle = \left(\frac{1}{2\pi}\right)^{3/2} \exp(i\mathbf{k} \cdot \mathbf{r}) \quad (4)$$

which is a transformation function defining the mapping from the abstract $|\mathbf{k}\rangle$ to the abstract $|\mathbf{r}\rangle$ space.

Mathematical Intermezzo, two-body Schrödinger in k -space

That the \mathbf{r} -space basis states are delta-function normalized follows from

$$\delta(\mathbf{r} - \mathbf{r}') = \langle \mathbf{r} | \mathbf{r}' \rangle = \langle \mathbf{r} | \mathbf{1} | \mathbf{r}' \rangle = \int d\mathbf{k} \langle \mathbf{r} | \mathbf{k} \rangle \langle \mathbf{k} | \mathbf{r}' \rangle = \left(\frac{1}{2\pi} \right)^3 \int d\mathbf{k} e^{i\mathbf{k}(\mathbf{r} - \mathbf{r}')} \quad (5)$$

and the same for the momentum space basis states,

$$\delta(\mathbf{k} - \mathbf{k}') = \langle \mathbf{k} | \mathbf{k}' \rangle = \langle \mathbf{k} | \mathbf{1} | \mathbf{k}' \rangle = \int d\mathbf{r} \langle \mathbf{k} | \mathbf{r} \rangle \langle \mathbf{r} | \mathbf{k}' \rangle = \left(\frac{1}{2\pi} \right)^3 \int d\mathbf{r} e^{i\mathbf{r}(\mathbf{k} - \mathbf{k}')} \quad (6)$$

Mathematical Intermezzo, two-body Schrödinger in k -space

Projecting equation 1 on momentum states the momentum space Schrödinger equation is obtained,

$$\frac{\hbar^2}{2\mu} k^2 \psi_n(\mathbf{k}) + \int d\mathbf{k}' V(\mathbf{k}, \mathbf{k}') \psi_n(\mathbf{k}') = E_n \psi_n(\mathbf{k}) \quad (7)$$

Here the notation $\psi_n(\mathbf{k}) = \langle \mathbf{k} | \psi_n \rangle$ and $\langle \mathbf{k} | V | \mathbf{k}' \rangle = V(\mathbf{k}, \mathbf{k}')$ has been introduced. The potential in momentum space is given by a double Fourier-transform of the potential in coordinate space, i.e.

$$V(\mathbf{k}, \mathbf{k}') = \left(\frac{1}{2\pi} \right)^3 \int d\mathbf{r} \int d\mathbf{r}' e^{-i\mathbf{k}\mathbf{r}} V(\mathbf{r}, \mathbf{r}') e^{i\mathbf{k}'\mathbf{r}'} \quad (8)$$

Mathematical Intermezzo, two-body Schrödinger in k -space

Here it is assumed that the potential interaction does not contain any spin dependence. Instead of a differential equation in coordinate space, the Schrödinger equation becomes an integral equation in momentum space. This has many tractable features. Firstly, most realistic nucleon-nucleon interactions derived from field-theory are given explicitly in momentum space. Secondly, the boundary conditions imposed on the differential equation in coordinate space are automatically built into the integral equation. And last, but not least, integral equations are easy to numerically implement, and convergence is obtained by just increasing the number of integration points. Instead of solving the three-dimensional integral equation given in equation (7), an infinite set of 1-dimensional equations can be obtained via a partial wave expansion.

Mathematical Intermezzo, two-body Schrödinger in k -space

The wave function $\psi_n(\mathbf{k})$ can be expanded in a complete set of spherical harmonics, i.e.

$$\psi_n(\mathbf{k}) = \sum_{lm} \psi_{nlm}(k) Y_{lm}(\hat{k}), \quad \psi_{nlm}(k) = \int d\hat{k} Y_{lm}^*(\hat{k}) \psi_n(\mathbf{k}). \quad (9)$$

By inserting equation 9 in equation 7, and projecting from the left $Y_{lm}(\hat{k})$, the three-dimensional Schrödinger equation (7) is reduced to an infinite set of 1-dimensional angular momentum coupled integral equations,

$$\left(\frac{\hbar^2}{2\mu} k^2 - E_{nlm} \right) \psi_{nlm}(k) = - \sum_{l'm'} \int_0^\infty dk' k'^2 V_{lm,l'm'}(k, k') \psi_{nl'm'}(k') \quad (10)$$

where the angular momentum projected potential takes the form,

$$V_{lm,l'm'}(k, k') = \int d\hat{k} \int d\hat{k}' Y_{lm}^*(\hat{k}) V(\mathbf{k}, \mathbf{k}') Y_{l'm'}(\hat{k}') \quad (11)$$

here $d\hat{k} = d\theta \sin \theta d\varphi$.

Mathematical Intermezzo, two-body Schrödinger in k -space

Often the potential is given in position space, so it is convenient to establish the connection between $V_{lm,l'm'}(k, k')$ and $V_{lm,l'm'}(r, r')$. Inserting position space completeness in equation (11) gives

$$\begin{aligned} V_{lm,l'm'}(k, k') &= \int d\mathbf{r} \int d\mathbf{r}' \int d\hat{k} \int d\hat{k}' Y_{lm}^*(\hat{k}) \langle \mathbf{k} | \mathbf{r} \rangle \langle \mathbf{r} | V | \mathbf{r}' \rangle \langle \mathbf{r}' | \mathbf{k}' \rangle Y_{lm}(\hat{k}') \\ &= \int d\mathbf{r} \int d\mathbf{r}' \left\{ \int d\hat{k} Y_{lm}^*(\hat{k}) \langle \mathbf{k} | \mathbf{r} \rangle \right\} \\ &\quad \times \langle \mathbf{r} | V | \mathbf{r}' \rangle \left\{ \int d\hat{k}' Y_{lm}(\hat{k}') \langle \mathbf{r}' | \mathbf{k}' \rangle \right\} \end{aligned} \quad (12)$$

Mathematical Intermezzo, two-body Schrödinger in k -space

Since the plane waves depend only on the absolute values of position and momentum, $|\mathbf{k}|$, $|\mathbf{r}|$, and the angle between them, θ_{kr} , they may be expanded in terms of bipolar harmonics of zero rank, i.e.

$$e^{i\mathbf{k}\cdot\mathbf{r}} = 4\pi \sum_{l=0}^{\infty} i^l j_l(kr) \left(Y_l(\hat{k}) \cdot Y_l(\hat{r}) \right) = \sum_{l=0}^{\infty} (2l+1) i^l j_l(kr) P_l(\cos \theta_{kr}) \quad (13)$$

where the addition theorem for spherical harmonics has been used in order to write the expansion in terms of Legendre polynomials. The spherical Bessel functions, $j_l(z)$, are given in terms of Bessel functions of the first kind with half integer orders,

$$j_l(z) = \sqrt{\frac{\pi}{2z}} J_{l+1/2}(z).$$

Mathematical Intermezzo, two-body Schrödinger in k -space

Inserting the plane-wave expansion into the brackets of equation (12) yields,

$$\begin{aligned}\int d\hat{k} Y_{lm}^*(\hat{k}) \langle \mathbf{k} | \mathbf{r} \rangle &= \left(\frac{1}{2\pi} \right)^{3/2} 4\pi i^{-l} j_l(kr) Y_{lm}^*(\hat{r}), \\ \int d\hat{k}' Y_{lm}(\hat{k}') \langle \mathbf{r}' | \mathbf{k}' \rangle &= \left(\frac{1}{2\pi} \right)^{3/2} 4\pi i^{l'} j_{l'}(k' r') Y_{l' m'}(\hat{r}).\end{aligned}$$

Mathematical Intermezzo, two-body Schrödinger in k -space

The connection between the momentum- and position space angular momentum projected potentials are then given,

$$V_{lm,l'm'}(k, k') = \frac{2}{\pi} i^{l'-l} \int_0^\infty dr r^2 \int_0^\infty dr' r'^2 j_l(kr) V_{lm,l'm'}(r, r') j_{l'}(k'r') \quad (14)$$

which is known as a double Fourier-Bessel transform. The position space angular momentum projected potential is given by

$$V_{lm,l'm'}(r, r') = \int d\hat{r} \int d\hat{r}' Y_{lm}^*(\hat{r}) V(\mathbf{r}, \mathbf{r}') Y_{l'm'}(\hat{r}'). \quad (15)$$

Mathematical Intermezzo, two-body Schrödinger in k -space

No assumptions of locality/non-locality and deformation of the interaction has so far been made, and the result in equation (14) is general. In position space the Schrödinger equation takes form of an integro-differential equation in case of a non-local interaction, in momentum space the Schrödinger equation is an ordinary integral equation of the Fredholm type, see equation (10). This is a further advantage of the momentum space approach as compared to the standard position space approach. If we assume that the interaction is of local character, i.e.

$$\langle \mathbf{r} | V | \mathbf{r}' \rangle = V(\mathbf{r}) \delta(\mathbf{r} - \mathbf{r}') = V(\mathbf{r}) \frac{\delta(r - r')}{r^2} \delta(\cos \theta - \cos \theta') \delta(\varphi - \varphi'),$$

then equation (15) reduces to

$$V_{lm,l'm'}(r, r') = \frac{\delta(r - r')}{r^2} \int d\hat{r} Y_{lm}^*(\hat{r}) V(\mathbf{r}) Y_{l'm'}(\hat{r}), \quad (16)$$

Mathematical Intermezzo, two-body Schrödinger in k -space

and equation (14) reduces to

$$V_{lm,l'm'}(k, k') = \frac{2}{\pi} i^{l'-l} \int_0^\infty dr r^2 j_l(kr) V_{lm,l'm'}(r) j_{l'}(k'r) \quad (17)$$

where

$$V_{lm,l'm'}(r) = \int d\hat{r} Y_{lm}^*(\hat{r}) V(\mathbf{r}) Y_{l'm'}(\hat{r}), \quad (18)$$

Mathematical Intermezzo, two-body Schrödinger in k -space

In the case that the interaction is central, $V(\mathbf{r}) = V(r)$, then

$$V_{lm,l'm'}(r) = V(r) \int d\hat{r} Y_{lm}^*(\hat{r}) Y_{l'm'}(\hat{r}) = V(r) \delta_{l,l'} \delta_{m,m'}, \quad (19)$$

and

$$V_{lm,l'm'}(k, k') = \frac{2}{\pi} \int_0^\infty dr r^2 j_l(kr) V(r) j_{l'}(k'r) \delta_{l,l'} \delta_{m,m'} = V_l(k, k') \delta_{l,l'} \delta_{m,m'} \quad (20)$$

where the momentum space representation of the interaction finally reads,

$$V_l(k, k') = \frac{2}{\pi} \int_0^\infty dr r^2 j_l(kr) V(r) j_l(k'r). \quad (21)$$

Mathematical Intermezzo, two-body Schrödinger in k -space

For a local and spherical symmetric potential, the coupled momentum space Schrödinger equations given in equation (10) decouples in angular momentum, giving

$$\frac{\hbar^2}{2\mu} k^2 \psi_{nl}(k) + \int_0^\infty dk' k'^2 V_l(k, k') \psi_{nl}(k') = E_{nl} \psi_{nl}(k) \quad (22)$$

Where we have written $\psi_{nl}(k) = \psi_{nlm}(k)$, since the equation becomes independent of the projection m for spherical symmetric interactions. The momentum space wave functions $\psi_{nl}(k)$ defines a complete orthogonal set of functions, which spans the space of functions with a positive finite Euclidean norm (also called l^2 -norm), $\sqrt{\langle \psi_n | \psi_n \rangle}$, which is a Hilbert space. The corresponding normalized wave function in coordinate space is given by the Fourier-Bessel transform

$$\phi_{nl}(r) = \sqrt{\frac{2}{\pi}} \int dk k^2 j_l(kr) \psi_{nl}(k) \quad (23)$$

Bethe-Salpeter Equation

In order to obtain the parameters which define an NN potential derived from OBE or chiral perturbation theory models, the Bethe-Salpeter equation is used as the starting point for most calculations. This equation serves to define a two-particle interaction \mathcal{T} , meant to reproduce properties like low-energy scattering data. The fully covariant Bethe-Salpeter equation reads (suppressing spin and isospin) in an arbitrary frame

$$\begin{aligned}\langle p'_1 p'_2 | \mathcal{T} | p_1 p_2 \rangle &= \langle p'_1 p'_2 | \mathcal{V} | p_1 p_2 \rangle \\ &+ \frac{i}{(2\pi)^4} \int d^4 k \langle p'_1 p'_2 | \mathcal{V} | P + k, P - k \rangle \\ &\times S_{(1)}(P + k) S_{(2)}(P - k) \langle P + k, P - k | \mathcal{T} | p_1 p_2 \rangle .\end{aligned}$$

Bethe-Salpeter Equation, contn.

Here we have defined P to be *half* the total four-momentum, i.e. $P = \frac{1}{2}(p_1 + p_2)$, and k to be the relative four-momentum. The term $S_{(i)}$ is the fermion propagator, which for e.g. positive energy spin 1/2 baryons reads

$$S_{(i)}(p) = (\not{p}_i - m_i + i\epsilon)^{-1},$$

with the subscript i referring to baryon i .

Bethe-Salpeter Equation, contn.

In principle \mathcal{V} is supposed to represent all kinds of irreducible two-particle interactions, though it is commonly approximated by the lowest order two-particle diagram. With this prescription we obtain the familiar ladder approach to the Bethe-Salpeter equation, similar to the approach discussed in connection with the G -matrix. The schematic structure of the ladder equation is representative for both the scattering matrix and the reaction matrix G . It is a four-dimensional integral equation, which is rather tedious to solve numerically.

Bethe-Salpeter Equation, contn.

It is therefore commonly replaced by a three-dimensional quasi-potential equation, where the time components of the four-momenta of the incoming and outgoing particles have been fixed by some adequate choice. Still in an arbitrary frame we get

$$\begin{aligned}\langle \mathbf{p}'_1 \mathbf{p}'_2 | T | \mathbf{p}_1 \mathbf{p}_2 \rangle &= \langle \mathbf{p}'_1 \mathbf{p}'_2 | V | \mathbf{p}_1 \mathbf{p}_2 \rangle \\ &+ \frac{1}{(2\pi)^3} \int d^3 k \langle \mathbf{p}'_1 \mathbf{p}'_2 | V | \mathbf{P} + \mathbf{k}, \mathbf{P} - \mathbf{k} \rangle \\ &g(\mathbf{k}, s) \langle \mathbf{P} + \mathbf{k}, \mathbf{P} - \mathbf{k} | T | \mathbf{p}_1 \mathbf{p}_2 \rangle .\end{aligned}$$

V is now the so-called “quasi-potential”, with fixed time components of the in- and outgoing particle momenta. As such, it is no longer an independent quantity. A much favored choice is to fix $p_1^0 = p_2^0 = \frac{1}{2}\sqrt{s}$, $s = (p_1 + p_2)^2$.

Bethe-Salpeter Equation, contn.

This prescription puts the two particles symmetrically off-shell, and is used in connection with the Blankenbecler-Sugar equation. The latter is one possibility of several three-dimensional reductions of the Bethe-Salpeter equation. The quantity g is related to the baryon propagators $S_{(1)}S_{(2)}$ through

$$g(\mathbf{k}, s) = -i \int dk_0 S_{(1)}(k) S_{(2)}(-k).$$

The Blankenbecler-Sugar choice for g is (assuming $m_1 = m_2$ and spin 1/2 fermions)

$$g(\mathbf{k}, s) = \frac{m^2}{E_k} \frac{\Lambda_{(1)}^+(\mathbf{k}) \Lambda_{(2)}^+(-\mathbf{k})}{\frac{1}{4}s - E_k^2 + i\epsilon}.$$

All NN potentials reproduce essentially the same set of low-energy NN scattering data ($E_{lab} \leq 350$ MeV) and properties of the deuteron. These are referred to as the “on-shell” properties of an NN potential, since all potential models result in a roughly similar on-shell scattering matrix T . The crucial point is then the differing off-shell behavior of the NN potentials in nuclear structure studies. The Bethe-Salpeter equation reads in the center-of-mass system (omitting angular momentum, isospin, spin etc. assignments)

$$T(\mathbf{k}, \mathbf{k}') = V(\mathbf{k}, \mathbf{k}') + \int_0^\infty \frac{d^3q}{(2\pi)^3} V(\mathbf{k}, \mathbf{q}) \frac{M_N^2}{E_q} \frac{\Lambda_{(1)}^+(\mathbf{q}) \Lambda_{(2)}^+(-\mathbf{q})}{\mathbf{k}^2 - \mathbf{q}^2 + i\epsilon} T(\mathbf{q}, \mathbf{k}'),$$

where $E_q = \sqrt{M_N^2 + \mathbf{q}^2}$.

Three-dimensional Reduction

For positive-energy spinors

$$T(\mathbf{k}, \mathbf{k}') = V(\mathbf{k}, \mathbf{k}') + \int_0^\infty \frac{d^3 q}{(2\pi)^3} V(\mathbf{k}, \mathbf{q}) \frac{M_N^2}{E_q} \frac{1}{\mathbf{k}^2 - \mathbf{q}^2 + i\epsilon} T(\mathbf{q}, \mathbf{k}').$$

Using

$$\hat{T}(\mathbf{k}, \mathbf{k}') = \sqrt{\frac{M_N}{E_{k'}}} T(\mathbf{k}, \mathbf{k}') \sqrt{\frac{M_N}{E_k}},$$

and

$$\hat{V}(\mathbf{k}, \mathbf{k}') = \sqrt{\frac{M_N}{E_{k'}}} V(\mathbf{k}, \mathbf{k}') \sqrt{\frac{M_N}{E_k}},$$

gives

$$\hat{T}(\mathbf{k}, \mathbf{k}') = \hat{V}(\mathbf{k}, \mathbf{k}') + \int_0^\infty \frac{d^3 q}{(2\pi)^3} \hat{V}(\mathbf{k}, \mathbf{q}) \frac{1}{\mathbf{k}^2 - \mathbf{q}^2 + i\epsilon} \hat{T}(\mathbf{q}, \mathbf{k}').$$

First Solution Step

In terms of the relative and center-of-mass momenta \mathbf{k} and \mathbf{K} , the potential in momentum space is related to the nonlocal operator $V(\mathbf{r}, \mathbf{r}')$ by

$$\langle \mathbf{k}' \mathbf{K}' | V | \mathbf{k} \mathbf{K} \rangle = \int d\mathbf{r} d\mathbf{r}' e^{-i\mathbf{k}' \mathbf{r}'} V(\mathbf{r}', \mathbf{r}) e^{i\mathbf{k} \mathbf{r}} \delta(\mathbf{K}, \mathbf{K}').$$

We will assume that the interaction is spherically symmetric. Can separate the radial part of the wave function from its angular dependence. The wave function of the relative motion is described in terms of plane waves as

$$e^{i\mathbf{k} \mathbf{r}} = \langle \mathbf{r} | \mathbf{k} \rangle = 4\pi \sum_{lm} i^l j_l(kr) Y_{lm}^*(\hat{\mathbf{k}}) Y_{lm}(\hat{\mathbf{r}}),$$

where j_l is a spherical Bessel function and Y_{lm} the spherical harmonic.

Decomposing the NN Force

This partial wave basis is useful for defining the operator for the nucleon-nucleon interaction, which is symmetric with respect to rotations, parity and isospin transformations. These symmetries imply that the interaction is diagonal with respect to the quantum numbers of total angular momentum J , spin S and isospin T . Using the above plane wave expansion, and coupling to final J , S and T we get

$$\begin{aligned} \langle \mathbf{k}' | V | \mathbf{k} \rangle &= (4\pi)^2 \sum_{STl'l'mJ} i^{l+l'} Y_{lm}^*(\hat{\mathbf{k}}) Y_{l'm'}(\hat{\mathbf{k}}') \\ &\times C_{m'M_S M}^{l'SJ} C_{mM_S M}^{lSJ} \langle k'l'STJM | V | kISTJM \rangle, \end{aligned}$$

where we have defined

$$\langle k'l'STJM | V | kISTJM \rangle = \int j_{l'}(k'r') \langle l'STJM | V(r', r) | ISTJM \rangle j_l(kr) r'^2$$

The general structure of the T -matrix is

$$T_{ll'}^\alpha(kk'K\omega) = V_{ll'}^\alpha(kk') + \frac{2}{\pi} \sum_{l''mM_S} \int_0^\infty d\mathbf{q} (C_{mM_S}^{l''S\mathcal{J}})^2 \frac{Y_{l''m}^*(\hat{\mathbf{q}}) Y_{l''m}(\hat{\mathbf{q}}) V_{ll''}^\alpha(kq) T_{l''l'}^\alpha(qk'K\omega)}{\omega - H_0},$$

The shorthand notation

$$T_{ll'}^\alpha(kk'K\omega) = \langle kKlL\mathcal{J}ST | T(\omega) | k'Kl'L\mathcal{J}ST \rangle,$$

denotes the T -matrix with momenta k and k' and orbital momenta l and l' of the relative motion, and K is the corresponding momentum of the center-of-mass motion. Further, L , \mathcal{J} , S and T are the orbital momentum of the center-of-mass motion, the total angular momentum, spin and isospin, respectively.

Using the orthogonality properties of the Clebsch-Gordan coefficients and the spherical harmonics, we obtain the well-known one-dimensional angle independent integral equation

$$T_{ll'}^{\alpha}(kk'K\omega) = V_{ll'}^{\alpha}(kk') + \frac{2}{\pi} \sum_{l''} \int_0^{\infty} dq q^2 \frac{V_{ll''}^{\alpha}(kq) T_{l''l'}^{\alpha}(qk'K\omega)}{\omega - H_0}.$$

Inserting the denominators for the Blankenbecler-Sugar of the full Bethe-Salpeter equation we arrive at

$$\hat{T}_{ll'}^{\alpha}(kk'K) = \hat{V}_{ll'}^{\alpha}(kk') + \frac{2}{\pi} \sum_{l''} \int_0^{\infty} dq q^2 \hat{V}_{ll''}^{\alpha}(kq) \frac{1}{k^2 - q^2 + i\epsilon} \hat{T}_{l''l'}^{\alpha}(qk'K).$$

Recipe I

From now on we will drop the subscript l in all equations. In order to solve the Lippman-Schwinger equation in momentum space, we need first to write a function which sets up the mesh points. We need to do that since we are going to approximate an integral through

$$\int_a^b f(x) dx \approx \sum_{i=1}^N w_i f(x_i),$$

where we have fixed N lattice points through the corresponding weights w_i and points x_i . Typically obtained via methods like Gaussian quadrature, see my course on computational physics (all material in english) [http:](http://www.uio.no/studier/emner/matnat/fys/FYS3150/h08/)

[//www.uio.no/studier/emner/matnat/fys/FYS3150/h08/](http://www.uio.no/studier/emner/matnat/fys/FYS3150/h08/)

Recipe II

If you use Gauss-Legendre the points are determined for the interval $x_i \in [-1, 1]$ You map these points over to the limits in your integral. You can then use the following mapping

$$k_i = \text{const} \times \tan \left\{ \frac{\pi}{4} (1 + x_i) \right\},$$

and

$$\omega_i = \text{const} \frac{\pi}{4} \frac{w_i}{\cos^2 \left(\frac{\pi}{4} (1 + x_i) \right)}.$$

If you choose units fm^{-1} for k , set $\text{const} = 1$. If you choose to work with MeV, set $\text{const} \sim 200$ ($\hbar c = 197 \text{ MeVfm}$).

Recipe III

The principal value integral is rather tricky to evaluate numerically, mainly since computers have limited precision. We will here use a subtraction trick often used when dealing with singular integrals in numerical calculations. We introduce first the calculus relation

$$\int_{-\infty}^{\infty} \frac{dk}{k - k_0} = 0.$$

It means that the curve $1/(k - k_0)$ has equal and opposite areas on both sides of the singular point k_0 . If we break the integral into one over positive k and one over negative k , a change of variable $k \rightarrow -k$ allows us to rewrite the last equation as

$$\int_0^{\infty} \frac{dk}{k^2 - k_0^2} = 0.$$

Recipe IV

We can then express a principal values integral as

$$\mathcal{P} \int_0^\infty \frac{f(k)dk}{k^2 - k_0^2} = \int_0^\infty \frac{(f(k) - f(k_0))dk}{k^2 - k_0^2},$$

where the right-hand side is no longer singular at $k = k_0$, it is proportional to the derivative df/dk , and can be evaluated numerically as any other integral.

Recipe V

We can then use this trick to obtain

$$R(k, k') = V(k, k') + \frac{2}{\pi} \int_0^\infty dq \frac{q^2 V(k, q) R(q, k') - k_0^2 V(k, k_0) R(k_0, k')}{(k_0^2 - q^2)/m}.$$

This is the equation to solve numerically in order to calculate the phase shifts. We are interested in obtaining $R(k_0, k_0)$.

Recipe VI

How do we proceed?

Using the mesh points k_j and the weights ω_j , we reach

$$R(k, k') = V(k, k') + \frac{2}{\pi} \sum_{j=1}^N \frac{\omega_j k_j^2 V(k, k_j) R(k_j, k')}{(k_0^2 - k_j^2)/m} - \frac{2}{\pi} k_0^2 V(k, k_0) R(k_0, k')$$

Recipe VII

This equation contains now the unknowns $R(k_i, k_j)$ (with dimension $N \times N$) and $R(k_0, k_0)$.

We can turn it into an equation with dimension $(N + 1) \times (N + 1)$ with a mesh which contains the original mesh points k_j for $j = 1, N$ and the point which corresponds to the energy k_0 .

Consider the latter as the 'observable' point. The mesh points become then k_j for $j = 1, n$ and $k_{N+1} = k_0$.

With these new mesh points we define the matrix

$$A_{i,j} = \delta_{i,j} - V(k_i, k_j)u_j,$$

Recipe VIII

where δ is the Kronecker δ and

$$u_j = \frac{2}{\pi} \frac{\omega_j k_j^2}{(k_0^2 - k_j^2)/m} \quad j = 1, N$$

and

$$u_{N+1} = -\frac{2}{\pi} \sum_{j=1}^N \frac{k_0^2 \omega_j}{(k_0^2 - k_j^2)/m}.$$

Recipe IX

The first task is then to set up the matrix A for a given k_0 . This is an $(N+1) \times (N+1)$ matrix. It can be convenient to have an outer loop which runs over the chosen observable values for the energy k_0^2/m . *Note that all mesh points k_j for $j = 1, N$ must be different from k_0 . Note also that $V(k_i, k_j)$ is an $(N+1) \times (N+1)$ matrix.* With the matrix A we can rewrite the problem as a matrix problem of dimension $(N+1) \times (N+1)$. All matrices R , A and V have this dimension and we get

$$A_{i,l} R_{l,j} = V_{i,j},$$

or just

$$AR = V.$$

Recipe X

Since you already have defined A and V (these are stored as $(N + 1) \times (N + 1)$ matrices) The final equation involves only the unknown R . We obtain it by matrix inversion, i.e.,

$$R = A^{-1}V.$$

Thus, to obtain R , you will need to set up the matrices A and V and invert the matrix A . With the inverse A^{-1} , perform a matrix multiplication with V results in R .

With R you can then evaluate the phase shifts by noting that

$$R(k_{N+1}, k_{N+1}) = R(k_0, k_0) = -\frac{\tan \delta}{mk_0},$$

where δ are the phase shifts.