

# No-Core Shell Model and Related Areas (NCSM\*)

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## Lecture 1: Hamiltonian

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# Overview

## ■ **Lecture 1: Hamiltonian**

Prelude • Nuclear Hamiltonian • Matrix Elements • Two-Body Problem • Correlations & Unitary Transformations

## ■ **Lecture 2: Light Nuclei**

Similarity Renormalization Group • Many-Body Problem • Configuration Interaction • No-Core Shell Model • Hypernuclei

## ■ **Lecture 3: Beyond Light Nuclei**

Normal Ordering • Coupled-Cluster Theory • In-Medium Similarity Renormalization Group

## ■ **Hands-On: Do-It-Yourself NCSM**

Three-Body Problem • Numerical SRG Evolution • NCSM Eigenvalue Problem • Lanczos Algorithm

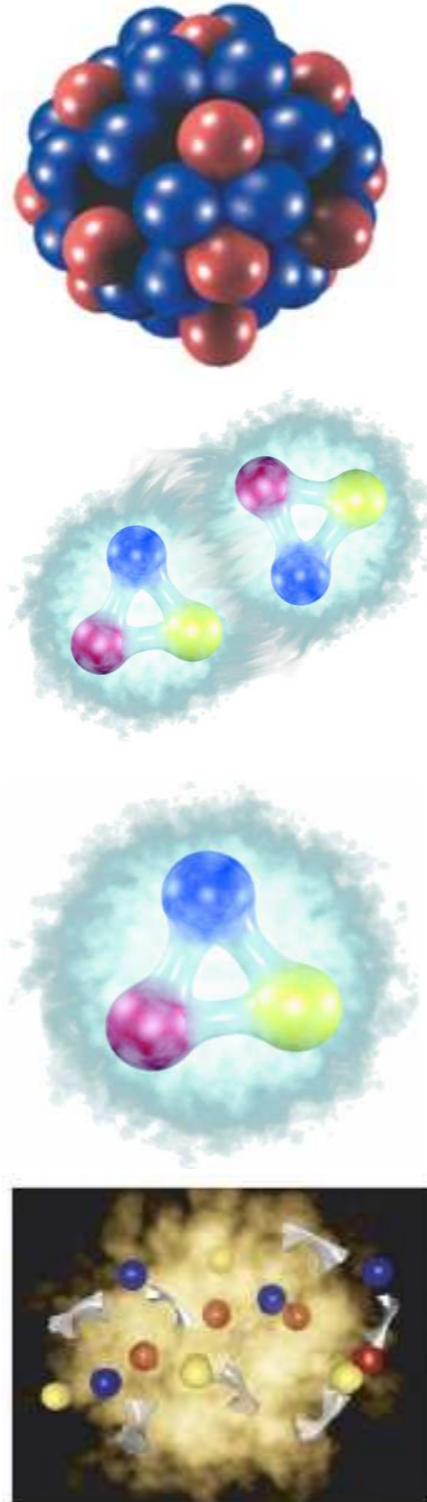
# Prelude

# Theoretical Context

better resolution / more fundamental

Quantum Chromodynamics

Nuclear Structure



- finite nuclei
- few-nucleon systems
- nuclear interaction
- hadron structure
- quarks & gluons
- deconfinement

# New Era of Nuclear Structure Theory

- **QCD at low energies**

improved understanding through lattice simulations & effective field theories



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increase of computational resources and developments of algorithms

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- **quantum many-body methods**

advances in ab initio treatment of the nuclear many-body problem

- **computing and algorithms**

increase of computational resources and developments of algorithms

- **experimental facilities**

amazing perspectives for the exploration of nuclei far-off stability



# The Problem

$$H |\Psi_n\rangle = E_n |\Psi_n\rangle$$

## Assumptions

- use nucleons as effective degrees of freedom
- use non-relativistic framework, relativistic corrections are absorbed in Hamiltonian
- use Hamiltonian formulation, i.e., conventional many-body quantum mechanics
- focus on bound states, though continuum aspects are very interesting

# The Problem

$$H |\Psi_n\rangle = E_n |\Psi_n\rangle$$

What is this many-body Hamiltonian?

nuclear forces, chiral effective field theory, three-body interactions, consistency, convergence,...

What about these many-body states?

many-body quantum mechanics, antisymmetry, second quantisation, many-body basis, truncations,...

How to solve this equation?

ab initio methods, correlations, similarity transformations, large-scale diagonalization, coupled-cluster theory,...

# Many-Body Quantum Mechanics

... a very quick reminder

# Single-Particle Basis

- effective constituents are nucleons characterized by **position, spin and isospin** degrees of freedom

$$|\alpha\rangle = |\text{position}\rangle \otimes |\text{spin}\rangle \otimes |\text{isospin}\rangle$$

- typical **basis choice** for configuration-type bound-state methods

$|\text{position}\rangle = |nlm_l\rangle$       spherical harmonic oscillator or other spherical single-particle potential

$|\text{spin}\rangle = |s = \frac{1}{2}, m_s\rangle$       eigenstates of  $s^2$  and  $s_z$  with  $s=1/2$

$|\text{isospin}\rangle = |t = \frac{1}{2}, m_t\rangle$       eigenstates of  $t^2$  and  $t_3$  with  $t=1/2$

- use **spin-orbit coupling** at the single-particle level

$$|n(l\frac{1}{2})jm; \frac{1}{2}m_t\rangle = \sum_{m_l, m_s} c \left( \begin{array}{cc|c} l & 1/2 & j \\ m_l & m_s & m \end{array} \right) |nlm_l\rangle \otimes |\frac{1}{2}m_s\rangle \otimes |\frac{1}{2}m_t\rangle$$

# Identical Particles & Spin-Statistics Theorem

- **systems of identical particles**: many-body states have to be eigenstates of the transposition operator for any particle pair with eigenvalues  $\pm 1$

$$T_{ij} |\psi\rangle = +1 |\psi\rangle$$

states symmetric under transposition of any pair of particle indices

$$T_{ij} |\psi\rangle = -1 |\psi\rangle$$

states antisymmetric under transposition of any pair of particles

- simple **product states** are not suitable for systems of identical particles

$$|\phi\rangle = |\alpha_1\rangle \otimes |\alpha_2\rangle \otimes \cdots \otimes |\alpha_A\rangle$$

- **spin-statistics theorem** connects transposition symmetry to particle spin:
  - bosons = integer spin = symmetric states
  - fermions = half-integer spin = antisymmetric states

- focus on fermions, i.e., **antisymmetric states in the following**

# Slater Determinants

- antisymmetric states can be constructed via the **antisymmetrization operator**

$$\mathcal{A} = \frac{1}{A!} \sum_{\pi} \text{sgn}(\pi) P_{\pi}$$

sum over all permutations      signum of permutation      permutation operator

- technically it is a **projection operator** onto the antisymmetric A-body Hilbert space and has the same structure as a **general determinant**
- **Slater determinants**: antisymmetrized product states

$$\begin{aligned} |\alpha_1 \alpha_2 \dots \alpha_A\rangle &= \sqrt{A!} \mathcal{A} (|\alpha_1\rangle \otimes |\alpha_2\rangle \otimes \dots \otimes |\alpha_A\rangle) \\ &= \frac{1}{\sqrt{A!}} \sum_{\pi} \text{sgn}(\pi) P_{\pi} (|\alpha_1\rangle \otimes |\alpha_2\rangle \otimes \dots \otimes |\alpha_A\rangle) \end{aligned}$$

- **Pauli principle is a consequence of antisymmetry**: you cannot antisymmetrize a product state that contains two identical single-particle states

# Slater Determinants as Basis

- given a complete single-particle basis  $\{|\alpha\rangle\}$  then the set of Slater determinants formed by all possible combinations of  $A$  different single-particle states is a **complete basis of the antisymmetric A-body Hilbert space**

- resolution of the **identity operator**

$$1 = \sum_{\alpha_1 < \alpha_2 < \dots < \alpha_A} |\alpha_1 \alpha_2 \dots \alpha_A\rangle \langle \alpha_1 \alpha_2 \dots \alpha_A| = \frac{1}{A!} \sum_{\alpha_1, \alpha_2, \dots, \alpha_A} |\alpha_1 \alpha_2 \dots \alpha_A\rangle \langle \alpha_1 \alpha_2 \dots \alpha_A|$$

- careful with **double counting**: Slater determinants that differ only by the order of the single-particle states are identical up to a sign...

- **expansion of general antisymmetric state** in Slater determinant basis

$$|\Psi\rangle = \sum_{\alpha_1 < \alpha_2 < \dots < \alpha_A} C_{\alpha_1 \alpha_2 \dots \alpha_A} |\alpha_1 \alpha_2 \dots \alpha_A\rangle = \sum_i C_i |\{\alpha_1 \alpha_2 \dots \alpha_A\}_i\rangle$$

# Second Quantization: Basics

- define **Fock-space** as direct sum of A-particle Hilbert spaces

$$\mathcal{F} = \mathcal{H}_0 \oplus \mathcal{H}_1 \oplus \mathcal{H}_2 \oplus \cdots \oplus \mathcal{H}_A \oplus \cdots$$

- **vacuum state**: the only state in the zero-particle Hilbert space

$$|0\rangle \in \mathcal{H}_0 \qquad \langle 0|0\rangle = 1 \qquad |0\rangle \neq 0$$

- **creation operators**: add a particle in single-particle state  $|\alpha\rangle$  to an A-body Slater determinant yielding an (A+1)-body Slater determinant

$$a_{\alpha}^{\dagger} |0\rangle = |\alpha\rangle$$

$$a_{\alpha}^{\dagger} |\alpha_1 \alpha_2 \dots \alpha_A\rangle = \begin{cases} |\alpha \alpha_1 \alpha_2 \dots \alpha_A\rangle & ; \alpha \notin \{\alpha_1 \alpha_2 \dots \alpha_A\} \\ 0 & ; \text{otherwise} \end{cases}$$

- resulting states are automatically normalized and antisymmetrized
- new single-particle state is added in the first slot, can be moved elsewhere through transpositions



# Second Quantization: Basics

- **annihilation operators**: remove a particle with single-particle state  $|\alpha\rangle$  from an A-body Slater determinant yielding an (A-1)-body Slater determinant

$$a_\alpha |0\rangle = 0$$

$$a_\alpha |\alpha_1 \alpha_2 \dots \alpha_A\rangle = \begin{cases} (-1)^{i-1} |\alpha_1 \alpha_2 \dots \alpha_{i-1} \alpha_{i+1} \dots \alpha_A\rangle & ; \alpha = \alpha_i \\ 0 & ; \text{otherwise} \end{cases}$$

- annihilation operator acts on first slot, need transpositions to get correct single-particle state there
- based on these definitions one can easily show that creation and annihilations operators satisfy **anticommutation relations**

$$\{a_\alpha, a_{\alpha'}\} = 0 \qquad \{a_\alpha^\dagger, a_{\alpha'}^\dagger\} = 0 \qquad \{a_\alpha, a_{\alpha'}^\dagger\} = \delta_{\alpha\alpha'}$$

- complication of handling permutations in "first quantization" are translated to the commutation behaviour of strings of operators

# Second Quantization: States

- Slater determinants can be written as **string of creation operators** acting on vacuum state

$$|\alpha_1 \alpha_2 \dots \alpha_A\rangle = a_{\alpha_1}^\dagger a_{\alpha_2}^\dagger \dots a_{\alpha_A}^\dagger |0\rangle$$

- alternatively one can define an A-body **reference Slater determinant**

$$|\Phi\rangle = |\alpha_1 \alpha_2 \dots \alpha_A\rangle = a_{\alpha_1}^\dagger a_{\alpha_2}^\dagger \dots a_{\alpha_A}^\dagger |0\rangle$$

and construct arbitrary Slater determinants through **particle-hole excitations** on top of the reference state

$$\begin{aligned} |\Phi_a^p\rangle &= a_{\alpha_p}^\dagger a_{\alpha_a} |\Phi\rangle \\ |\Phi_{ab}^{pq}\rangle &= a_{\alpha_p}^\dagger a_{\alpha_q}^\dagger a_{\alpha_b} a_{\alpha_a} |\Phi\rangle \\ &\vdots \end{aligned}$$

**index convention:**  $a, b, c, \dots$  : hole states, occupied in reference state  
 $p, q, r, \dots$  : particle state, unoccupied in reference states

# Second Quantization: Operators

- **operators** can be expressed in terms of creation and annihilation operators as well, e.g., for one-body kinetic energy and two-body interactions:

**'first quantization'**

$$T = \sum_{i=1}^A t_i$$

$$V = \sum_{i < j=1}^A v_{ij}$$

**second quantization**

$$T = \sum_{\alpha\alpha'} \langle \alpha | t | \alpha' \rangle a_{\alpha}^{\dagger} a_{\alpha'}$$

$$V = \frac{1}{4} \sum_{\alpha_1\alpha_2\alpha'_1\alpha'_2} \langle \alpha_1\alpha_2 | v | \alpha'_1\alpha'_2 \rangle a_{\alpha_1}^{\dagger} a_{\alpha_2}^{\dagger} a_{\alpha'_2} a_{\alpha'_1}$$

- **set of one or two-body matrix elements** fully defines the one or two-body operator in Fock space
- second quantization is extremely convenient to **compute matrix elements** of operators with Slater determinants

# Nuclear Hamiltonian

# Nuclear Hamiltonian

- general form of **many-body Hamiltonian** can be split into a center-of-mass and an intrinsic part

$$\begin{aligned} H &= T + V_{NN} + V_{3N} + \dots = T_{\text{cm}} + T_{\text{int}} + V_{NN} + V_{3N} + \dots \\ &= T_{\text{cm}} + H_{\text{int}} \end{aligned}$$

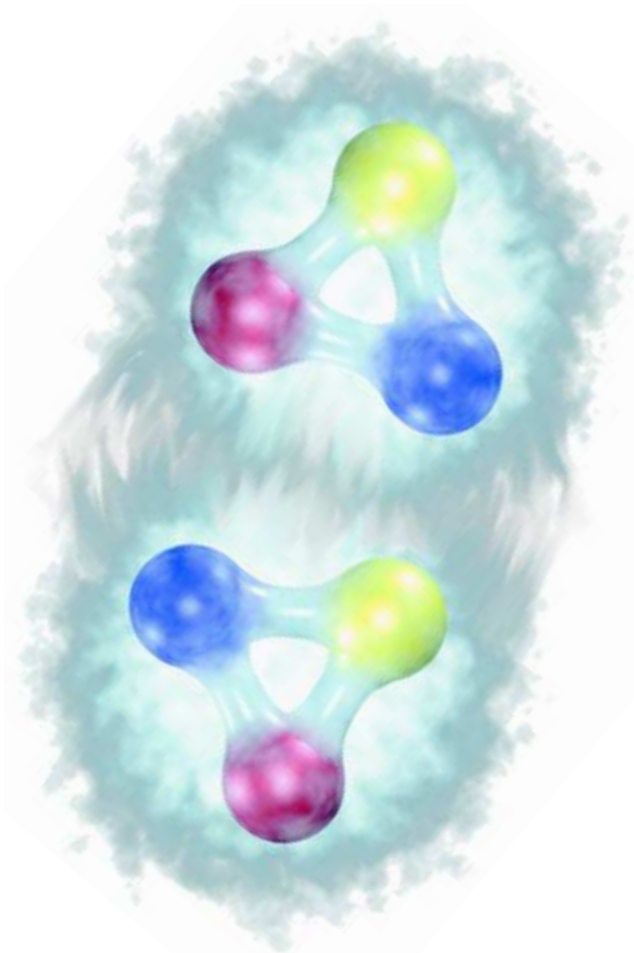
- **intrinsic Hamiltonian** is invariant under translation, rotation, Galilei boost, parity, time evolution, time reversal,...

$$\begin{aligned} H_{\text{int}} &= T_{\text{int}} + V_{NN} + V_{3N} + \dots \\ &= \sum_{i<j}^A \frac{1}{2mA} (\vec{p}_i - \vec{p}_j)^2 + \sum_{i<j}^A v_{NN,ij} + \sum_{i<j<k}^A v_{3N,ijk} + \dots \end{aligned}$$

- these symmetries constrain the possible operator structures that can appear in the interaction terms...

... but how can we really **determine the nuclear interaction** ?

# Nature of the Nuclear Interaction



~ 1.6fm

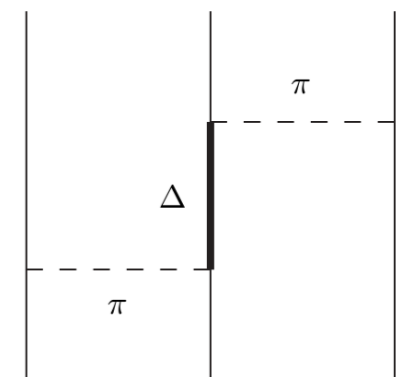
$$\rho_0^{-1/3} = 1.8\text{fm}$$

- nuclear interaction is **not fundamental**
- residual force analogous to **van der Waals interaction** between neutral atoms
- **based on QCD** and induced via polarization of quark and gluon distributions of nucleons
- **encapsulates all the complications** of the QCD dynamics and the structure of nucleons
- acts only if the nucleons overlap, i.e. at **short ranges**
- irreducible **three-nucleon interactions** are important

# Yesterday... from Phenomenology

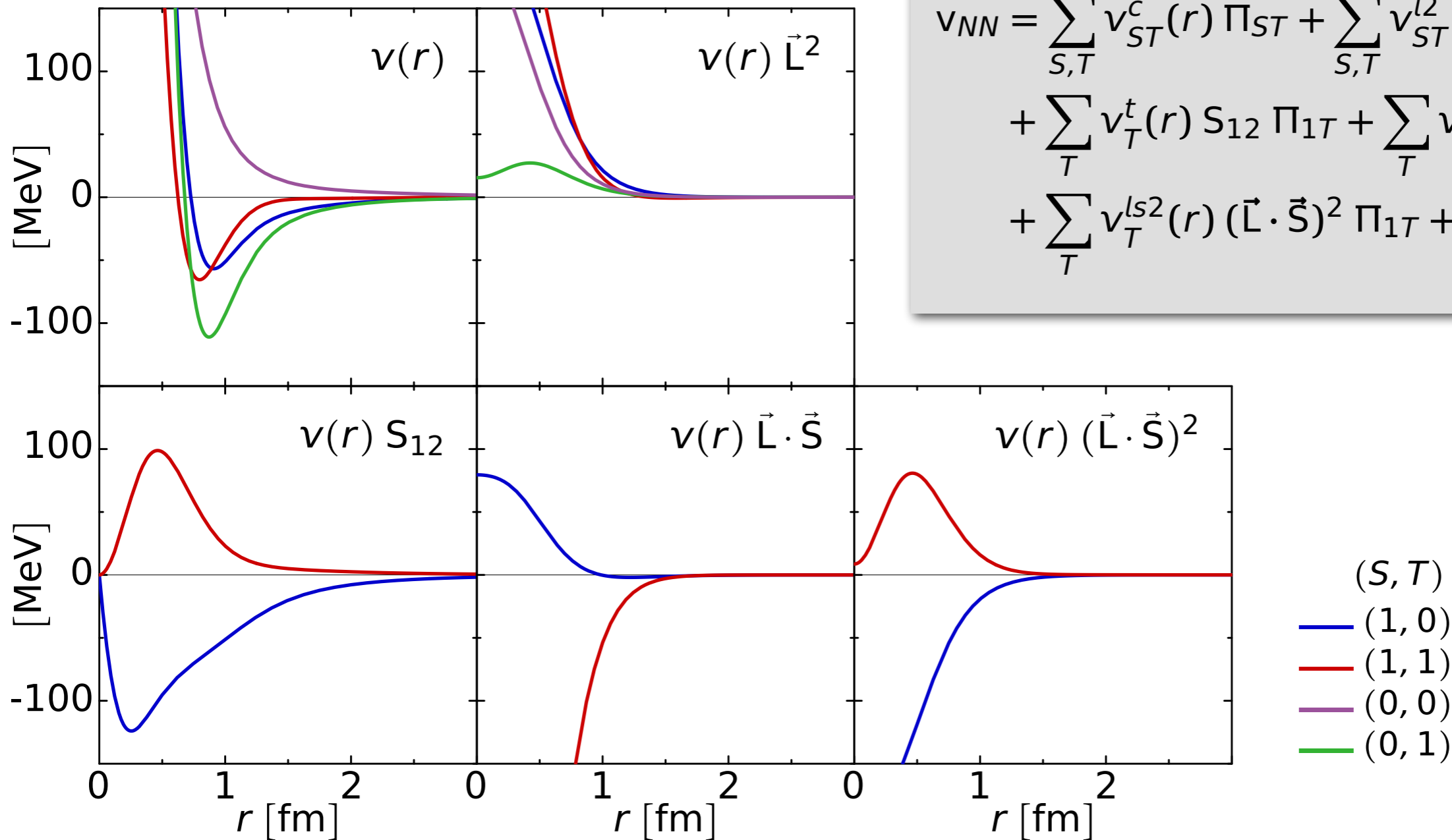
Wiringa, Machleidt,...

- until 2005: **high-precision phenomenological NN interactions** were state-of-the-art in ab initio nuclear structure theory
  - **Argonne V18**: long-range one-pion exchange plus phenomenological parametrization of medium- and short-range terms, local operator form
  - **CD Bonn 2000**: more systematic one meson-exchange parametrization including pseudo-scalar, scalar and vector mesons, inherently nonlocal
- parameters of the NN potential ( $\sim 40$ ) **fit to NN phase shifts** up to  $\sim 300$  MeV and reproduce them with high accuracy
- supplemented by **phenomenological 3N interactions** consisting of a Fujita-Miyazawa-type term plus various hand-picked contributions
- **fit to ground states and spectra of light nuclei**, sometimes up to  $A \leq 8$



# Argonne V18 Potential

Wiringa, et al., PRC 51, 38 (1995)

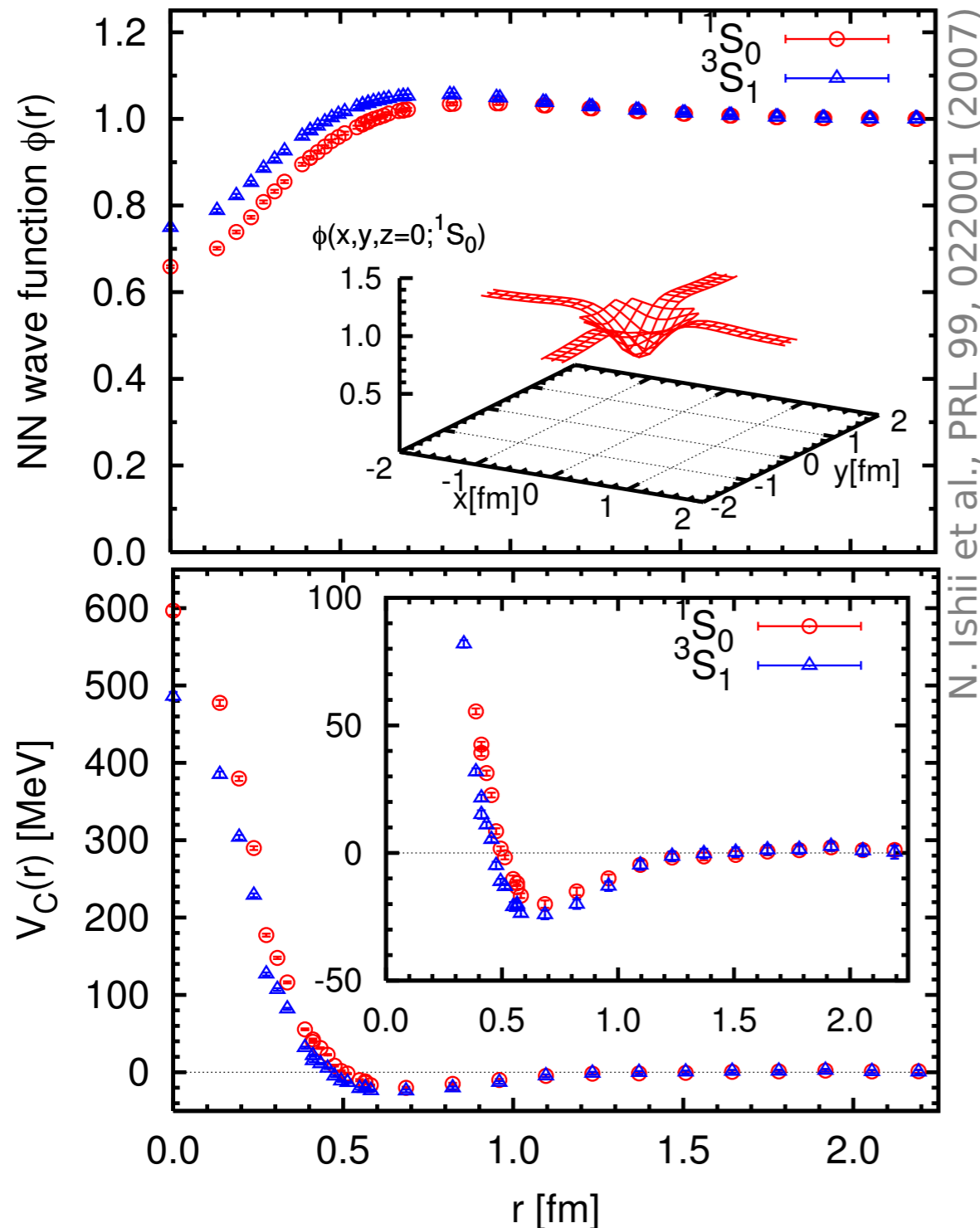


$$\begin{aligned}
 v_{NN} = & \sum_{S,T} v_{ST}^c(r) \Pi_{ST} + \sum_{S,T} v_{ST}^{l^2}(r) \vec{L}^2 \Pi_{ST} \\
 & + \sum_T v_T^t(r) S_{12} \Pi_{1T} + \sum_T v_T^{ls}(r) (\vec{L}\cdot\vec{S}) \Pi_{1T} \\
 & + \sum_T v_T^{ls^2}(r) (\vec{L}\cdot\vec{S})^2 \Pi_{1T} + \dots
 \end{aligned}$$



# Tomorrow... from Lattice QCD

Hatsuda, Aoki, Ishii, Beane, Savage, Bedaque,...



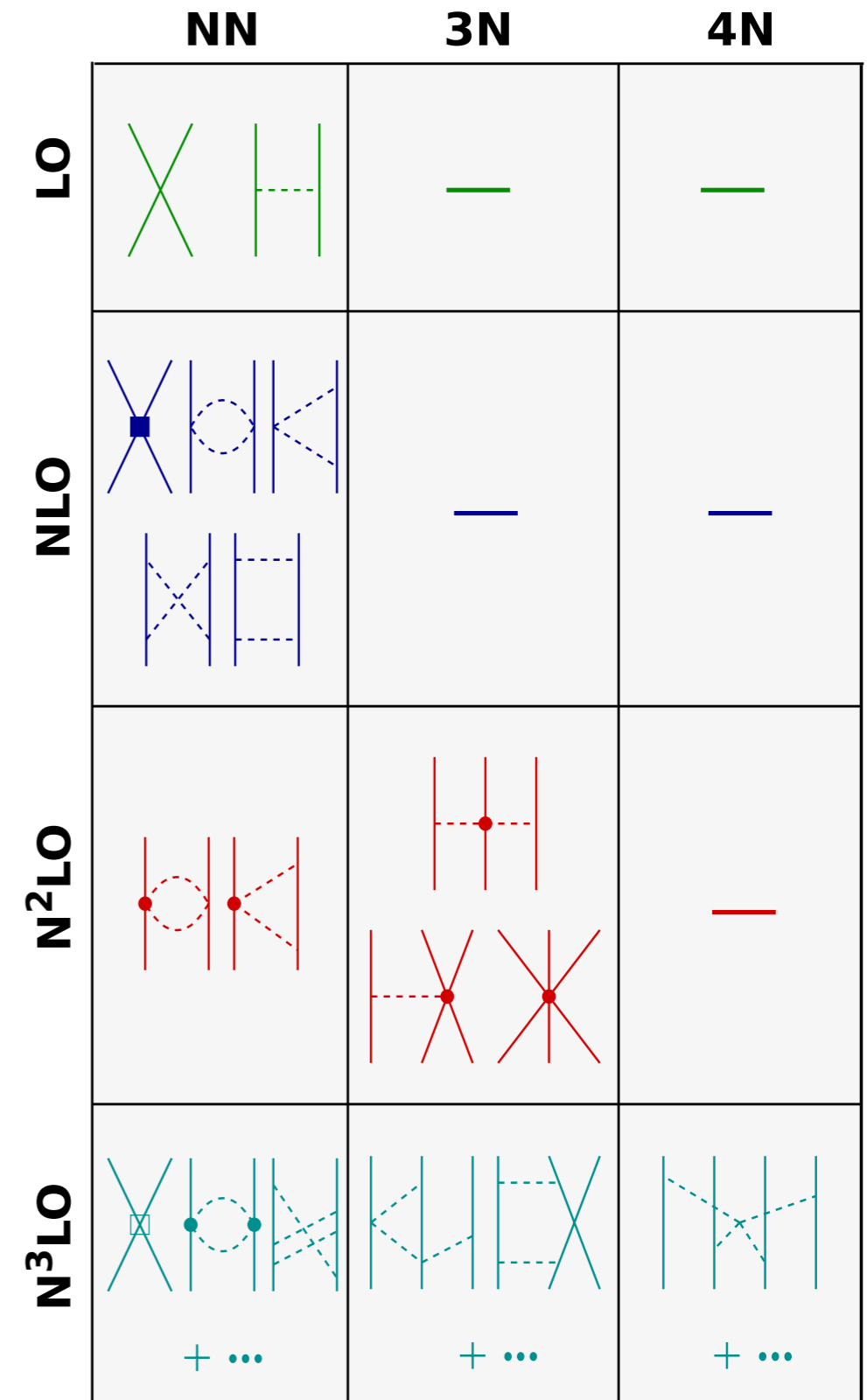
N. Ishii et al., PRL 99, 022001 (2007)

- first attempts towards construction of nuclear interactions directly from **lattice QCD simulations**
- compute relative **two-nucleon wave function** on the lattice
- **invert Schrödinger equation** to extract effective two-nucleon potential
- only **schematic results** so far (unphysical masses and mass dependence, model dependence,...)
- **alternatives**: phase-shifts or low-energy constants from lattice QCD

# Today... from Chiral EFT

Weinberg, van Kolck, Machleidt, Entem, Meißner, Epelbaum, Krebs, Bernard,...

- low-energy **effective field theory** for relevant degrees of freedom ( $\pi, N$ ) based on symmetries of QCD
- explicit long-range **pion dynamics**
- unresolved short-range physics absorbed in **contact terms**, low-energy constants fit to experiment
- systematic expansion in a small parameter with power counting enable **controlled improvements** and **error quantification**
- hierarchy of **consistent NN, 3N, 4N,...** interactions
- consistent **electromagnetic and weak operators** can be constructed in the same framework

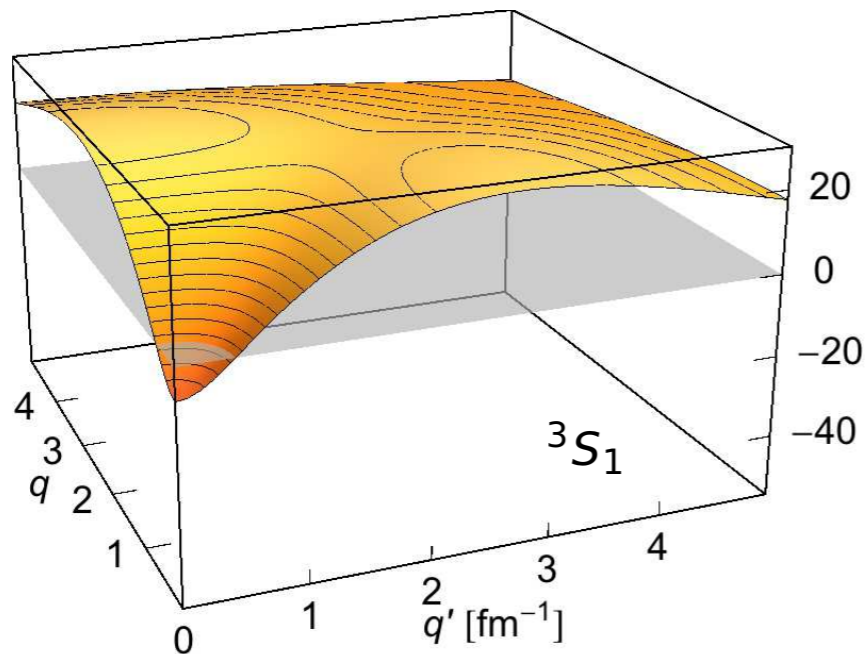


# Momentum-Space Matrix Elements

$$\langle q(LS)JM; TM_T | v_{NN} | q'(L'S)JM; TM_T \rangle$$

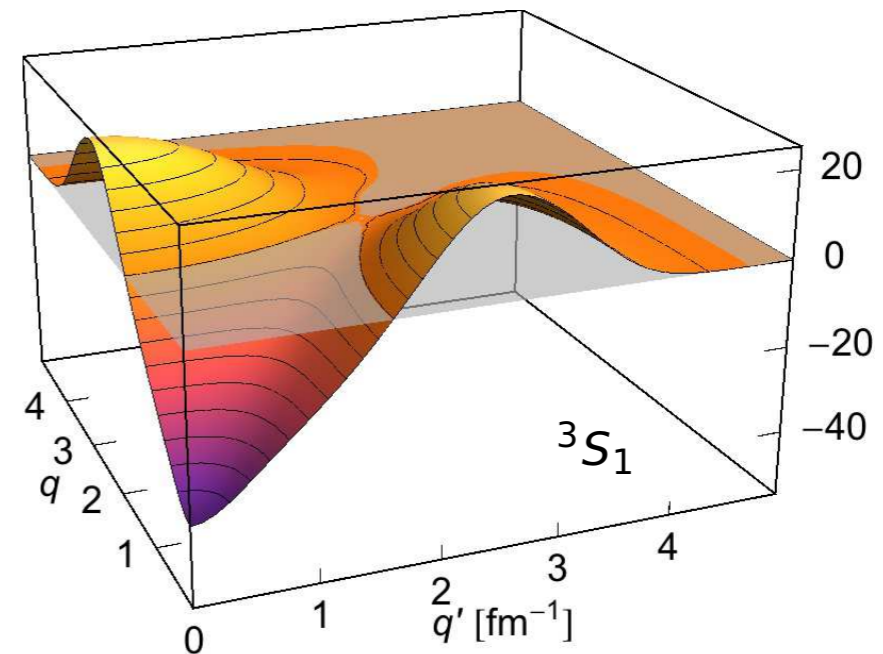
**Argonne V18**

J=1  
L=0  
L'=0  
S=1  
T=0

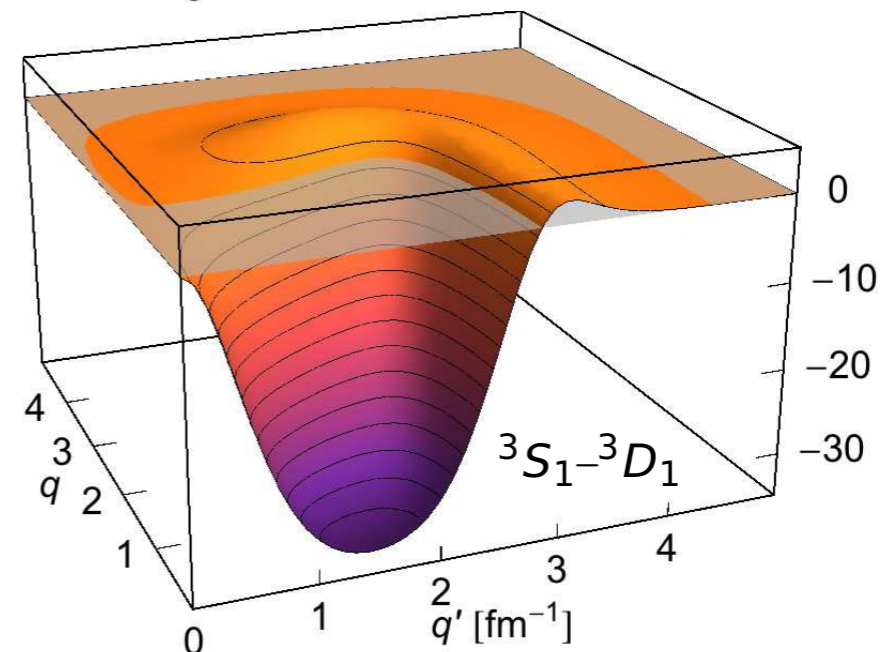
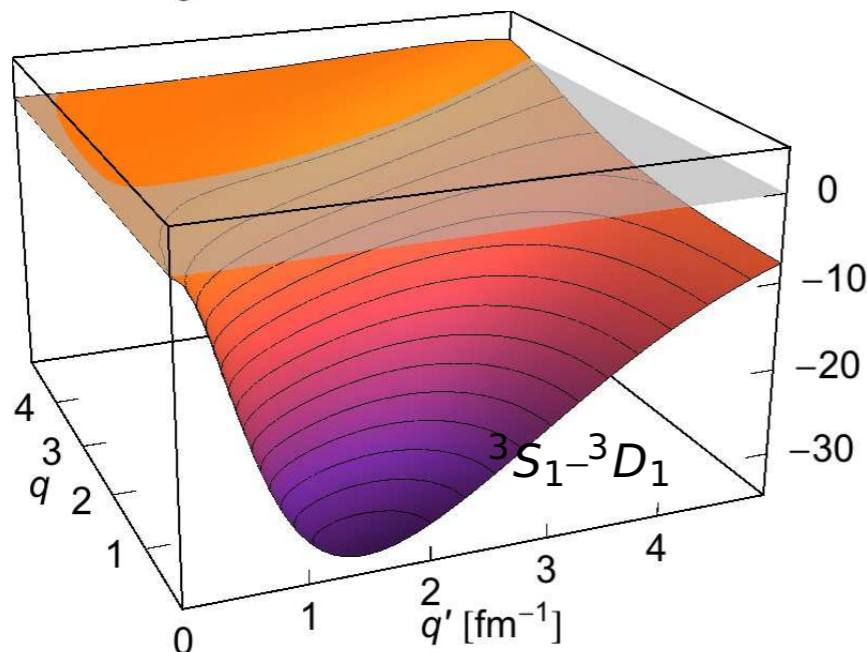


**chiral NN**

(N3LO, E&M, 500 MeV)



J=1  
L=0  
L'=2  
S=1  
T=0



# Matrix Elements

# Partial-Wave Matrix Elements

- **relative partial-wave matrix elements** of NN and 3N interaction are **universal input** for many-body calculations
- selection of **relevant partial-wave bases** in two and three-body space with all  $M$  quantum numbers suppressed:

two-body relative momentum:  $|q (LS) JT\rangle$

two-body relative HO:  $|N (LS) JT\rangle$

three-body Jacobi momentum:  $|\pi_1 \pi_2; [(L_1 S_1) J_1, (L_2 \frac{1}{2}) J_2] J_{12}; (T_1 \frac{1}{2}) T_{12}\rangle$

three-body Jacobi HO:  $|N_1 N_2; [(L_1 S_1) J_1, (L_2 \frac{1}{2}) J_2] J_{12}; (T_1 \frac{1}{2}) T_{12}\rangle$

antisym. three-body Jacobi HO:  $|E_{12} i J_{12}^\pi T_{12}\rangle$



- lots of **transformations** between the different bases are needed in practice
- **exception**: Quantum Monte Carlo methods working in coordinate representation need local operator form

# Symmetries and Matrix Elements

- relative partial-wave matrix elements make **maximum use of the symmetries** of the nuclear interaction
- consider, e.g., the relative two-body matrix elements in HO basis

$$\langle N (LS) JM; TM_T | v_{NN} | N' (L'S') J'M'; T'M'_T \rangle$$

- the matrix elements of the NN interaction
  - ... do not connect different  $J$
  - ... do not connect different  $M$  and are independent of  $M$
  - ... do not connect different parities
  - ... do not connect different  $S$
  - ... do not connect different  $T$
  - ... do not connect different  $M_T$

$$\Rightarrow \langle N (LS) J; TM_T | v_{NN} | N' (L'S) J; TM_T \rangle$$

- relative matrix elements are **efficient and simple to compute**

# Transformation to Single-Particle Basis

- most many-body calculations need **matrix elements with single-particle quantum numbers** (cf. second quantization)

$$\begin{aligned} \langle \alpha_1 \alpha_2 | v_{NN} | \alpha'_1 \alpha'_2 \rangle &= \\ &= \langle n_1 l_1 j_1 m_1 m_{t1}, n_2 l_2 j_2 m_2 m_{t2} | v_{NN} | n'_1 l'_1 j'_1 m'_1 m'_{t1}, n'_2 l'_2 j'_2 m'_2 m'_{t2} \rangle \end{aligned}$$

- obtained from relative HO matrix elements via **Moshinsky-transformation**

$$\begin{aligned} \langle n_1 l_1 j_1, n_2 l_2 j_2; JT | v_{NN} | n'_1 l'_1 j'_1, n'_2 l'_2 j'_2; JT \rangle &= \\ &= \sqrt{(2j_1 + 1)(2j_2 + 1)(2j'_1 + 1)(2j'_2 + 1)} \sum_{\lambda S T} \sum_{\lambda' S' T'} \langle \lambda S T | v_{NN} | \lambda' S' T' \rangle \\ &\times \langle l_1 l_2 j_1 j_2 | \lambda S T \rangle \langle l'_1 l'_2 j'_1 j'_2 | \lambda' S' T' \rangle \\ &\times \langle N \Lambda, \nu \lambda | n'_1 l'_1, n'_2 l'_2; L' \rangle \\ &\times (2j_1 + 1)(2S + 1)(2L + 1)(2L' + 1) (-1)^{L+L'} \{1 - (-1)^{\lambda+S+T}\} \\ &\times \langle \nu(\lambda S) j T | v_{NN} | \nu'(\lambda' S') j T \rangle \end{aligned}$$

**this analytic transformation from relative to single-particle matrix elements only exists for the harmonic oscillator basis**

# Matrix Element Machinery

- beneath any ab initio many-body method there is a **machinery for computing, transforming and storing matrix elements** of all operators entering the calculation

compute and store relative two-body HO matrix elements of NN interaction

compute and store Jacobi three-body HO matrix elements of 3N interaction

perform unitary transformations of the two- and three-body relative matrix elements (e.g. Similarity Renormalization Group)

transform to single-particle JT-coupled two-body HO matrix elements and store

transform to single-particle JT-coupled three-body HO matrix elements and store

● ● ●  
same for 4N with four-body matrix elements



# Two-Body Problem

# Solving the Two-Body Problem

- **simplest ab initio problem**: the only two-nucleon bound state, the deuteron
- start from **Hamiltonian in two-body space**, change to center of mass and intrinsic coordinates

$$\begin{aligned} H &= H_{\text{cm}} + H_{\text{int}} = T_{\text{cm}} + T_{\text{int}} + V_{\text{NN}} \\ &= \frac{1}{2M} \vec{p}_{\text{cm}}^2 + \frac{1}{2\mu} \vec{q}^2 + V_{\text{NN}} \end{aligned}$$

- **separate** two-body state into center of mass and intrinsic part

$$|\psi\rangle = |\phi_{\text{cm}}\rangle \otimes |\phi_{\text{int}}\rangle$$

- solve **eigenvalue problem for intrinsic part** (effective one-body problem)

$$H_{\text{int}} |\phi_{\text{int}}\rangle = E |\phi_{\text{int}}\rangle$$

# Solving the Two-Body Problem

- expand eigenstates in a **relative partial-wave HO basis**

$$|\phi_{\text{int}}\rangle = \sum_{NLSJMTM_T} C_{NLSJMTM_T} |N(LS)JM; TM_T\rangle$$

$$|N(LS)JM; TM_T\rangle = \sum_{M_L M_S} c \left( \begin{matrix} L & S \\ M_L & M_S \end{matrix} \middle| \begin{matrix} J \\ M \end{matrix} \right) |NLM_L\rangle \otimes |SM_S\rangle \otimes |TM_T\rangle$$

- **symmetries** simplify the problem dramatically:
  - $H_{\text{int}}$  does not connect/mix different  $J, M, S, T, M_T$  and parity  $\pi$
  - angular mom. coupling only allows  $J=L+1, L, L-1$  for  $S=1$  or  $J=L$  for  $S=0$
  - total antisymmetry requires  $L+S+T=\text{odd}$
- for given  $J^\pi$  at most two sets of angular-spin-isospin quantum numbers contribute to the expansion

# Deuteron Problem

- assume  $J^\pi = 1^+$  for the **deuteron ground state**, then the basis expansion reduces to

$$|\phi_{\text{int}}, J^\pi = 1^+\rangle = \sum_N C_N^{(0)} |N(01) 1M; 00\rangle + \sum_N C_N^{(2)} |N(21) 1M; 00\rangle$$

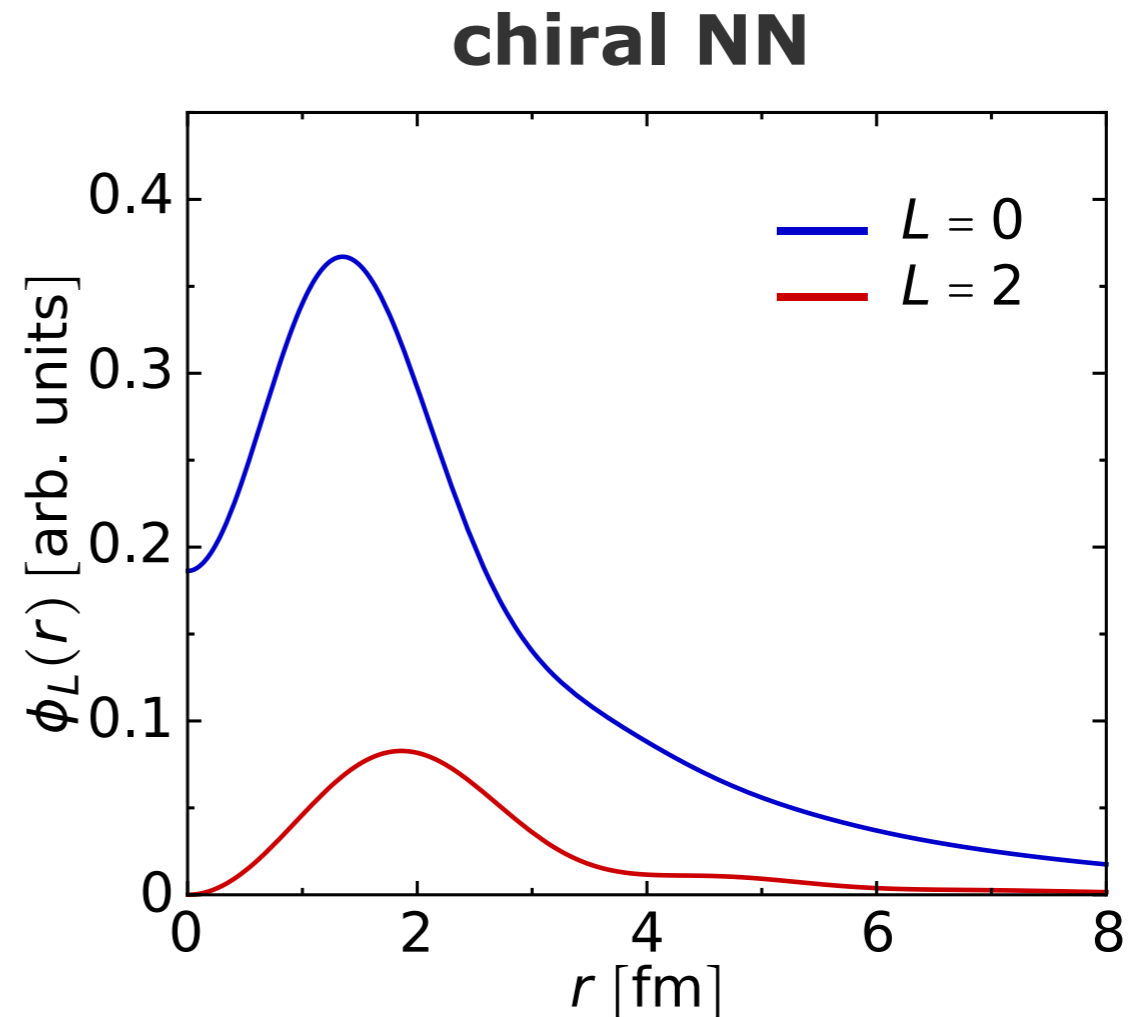
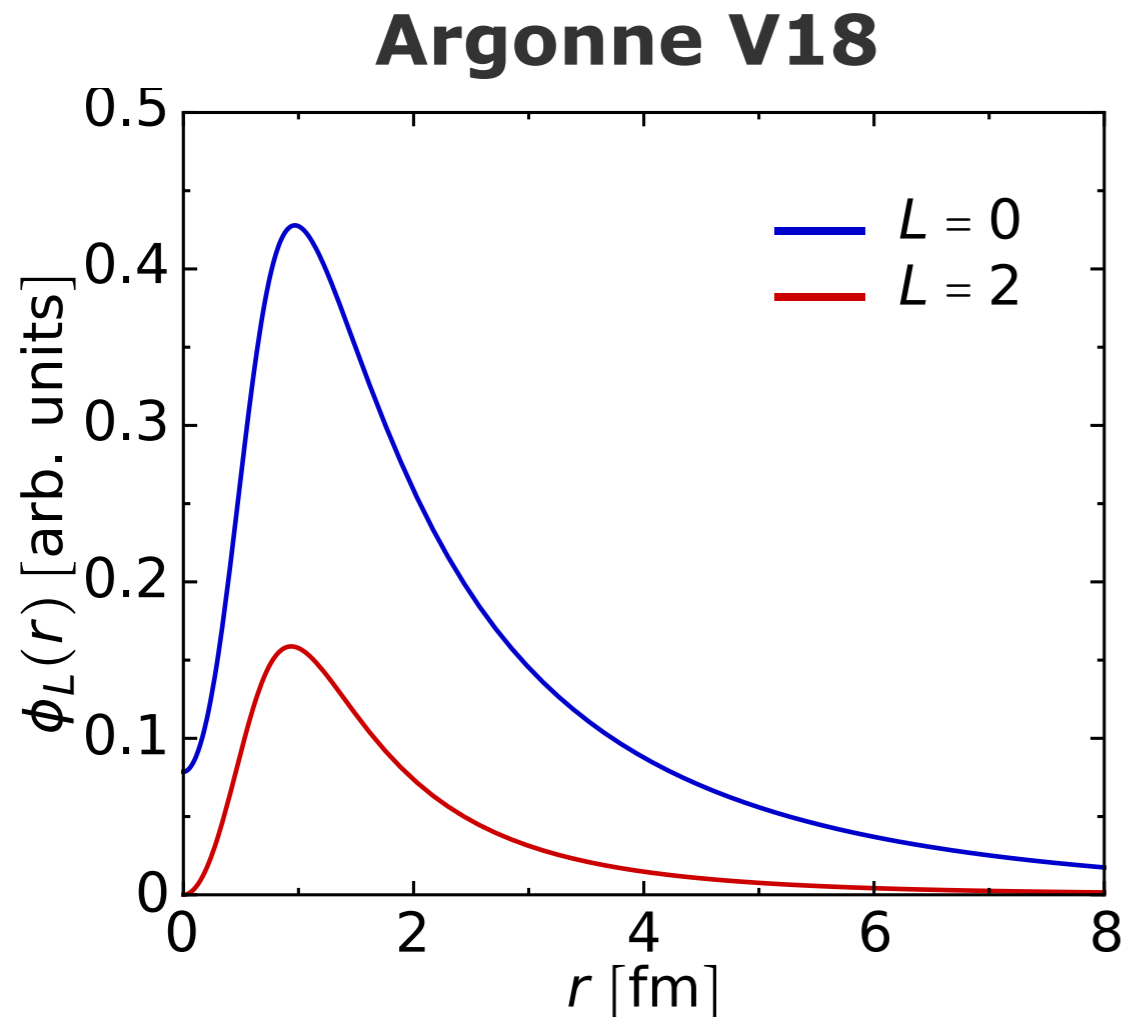
- inserting into Schrödinger equation and multiplying with basis bra leads to **matrix eigenvalue problem**

$$\begin{pmatrix} \langle N'(01)\dots | H_{\text{int}} | N(01)\dots \rangle & \langle N'(01)\dots | H_{\text{int}} | N(21)\dots \rangle \\ \langle N'(21)\dots | H_{\text{int}} | N(01)\dots \rangle & \langle N'(21)\dots | H_{\text{int}} | N(21)\dots \rangle \end{pmatrix} \begin{pmatrix} C_{N'}^{(0)} \\ C_{N'}^{(2)} \end{pmatrix} = E \begin{pmatrix} C_{N'}^{(0)} \\ C_{N'}^{(2)} \end{pmatrix}$$

**simplest possible Jacobi-NCSM calculation**

- eigenvectors with coefficients and eigenvalues the energies
- **truncate** basis to  $N \leq N_{\text{max}}$  and choose  $N_{\text{max}}$  large enough so that observables are converged, i.e., do not depend on  $N_{\text{max}}$  anymore

# Deuteron Solution



- deuteron wave function show two characteristics that are **signatures of correlations** in the two-body system:
  - suppression at small distances due to short-range repulsion
  - $L=2$  admixture generated by tensor part of the NN interaction

# Correlations & Unitary Transformations

# Correlations

**correlations:  
everything beyond the independent  
particle picture**

- many-body eigenstates of independent-particle models described by one-body Hamiltonians are **Slater determinants**
- thus, a single Slater determinant **does not describe correlations**
- but Slater determinants are a basis of the antisym. A-body Hilbert space, so any state can be expanded in Slater determinants
- to describe **short-range correlations**, a superposition of many Slater determinants is necessary

# Why Unitary Transformations ?

realistic nuclear interactions generate strong short-range correlations in many-body states

## Unitary Transformations

- adapt Hamiltonian to truncated low-energy model space
- improve convergence of many-body calculations
- preserve the physics of the initial Hamiltonian and all observables

many-body methods rely on truncated Hilbert spaces  
not capable of describing these correlations



# Unitary Transformations

- unitary transformations **conserve the spectrum** of the Hamiltonian, with a unitary operator  $U$  we get

$$\begin{aligned} H|\psi\rangle &= E|\psi\rangle & 1 &= U^\dagger U = U U^\dagger \\ U^\dagger H U U^\dagger |\psi\rangle &= E U^\dagger |\psi\rangle & \text{with} & \tilde{H} = U^\dagger H U \\ \tilde{H}|\tilde{\psi}\rangle &= E|\tilde{\psi}\rangle & |\tilde{\psi}\rangle &= U^\dagger |\psi\rangle \end{aligned}$$



- for **other observables** defined via matrix elements of an operator  $A$  with the eigenstates we obtain

$$\langle\psi|A|\psi'\rangle = \langle\psi|U U^\dagger A U U^\dagger |\psi'\rangle = \langle\tilde{\psi}|\tilde{A}|\tilde{\psi}'\rangle$$

**unitary transformations conserve all observables as long as the Hamiltonian and all other operators are transformed consistently**

# Overview

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