Ab Initio Nuclear Structure Theory

Lecture 1: Hamiltonian

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Overview

- **Lecture 1: Hamiltonian**

  Prelude • Many-Body Quantum Mechanics • Nuclear Hamiltonian • Matrix Elements

- **Lecture 2: Correlations**

  Two-Body Problem • Correlations & Unitary Transformations • Similarity Renormalization Group

- **Lecture 3: Light Nuclei**

  Many-Body Problem • Configuration Interaction • No-Core Shell Model • Applications

- **Lecture 4: Beyond Light Nuclei**

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

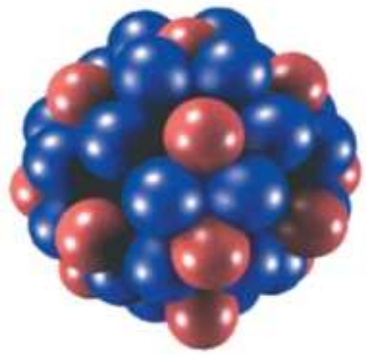
Prelude

Theoretical Context

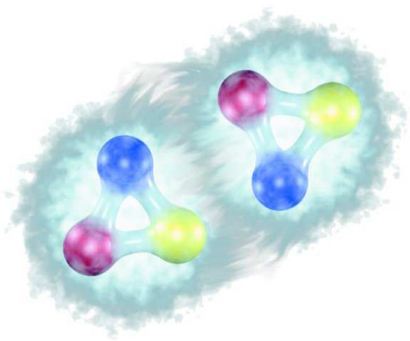
better resolution / more fundamental

Nuclear Structure

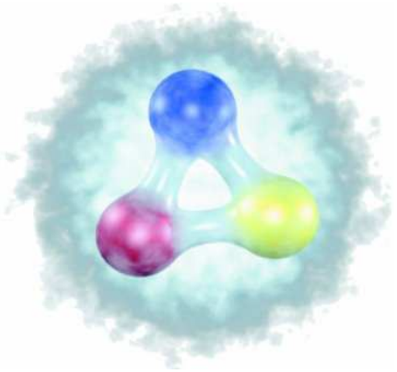
Quantum Chromodynamics



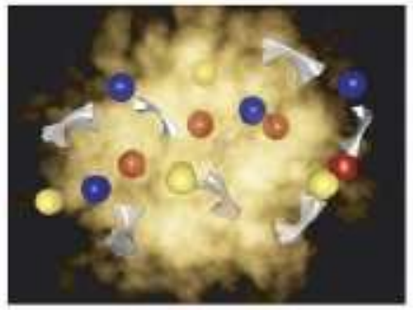
- finite nuclei



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

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  increase of computational resources and developments of algorithms

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- **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

$$\mathrm{H}\ |\Psi_n\rangle = E_n\,|\Psi_n\rangle$$

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

$$|n(l\tfrac{1}{2})jm;\tfrac{1}{2}m_t\rangle = \sum_{m_l,m_s} c\begin{pmatrix} l & 1/2 \\ m_l & m_s \end{pmatrix}\Big| \begin{matrix} j \\ m \end{matrix}\Big) \; |nlm_l\rangle \otimes |\tfrac{1}{2}m_s\rangle \otimes |\tfrac{1}{2}m_t\rangle$$

Many-Body Basis

- **Slater determinants**: antisymmetrized A-body product states

$$|\alpha_1\alpha_2\ldots\alpha_A\rangle = \frac{1}{\sqrt{A!}}\sum_\pi \mathrm{sgn}(\pi)\,\mathrm{P}_\pi\left(|\alpha_1\rangle\otimes|\alpha_2\rangle\otimes\cdots\otimes|\alpha_A\rangle\right)$$

- 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**

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

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

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

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

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

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

- 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

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

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

- 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**

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

- 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

$$|\alpha_1\alpha_2\ldots\alpha_A\rangle = a^\dagger_{\alpha_1} a^\dagger_{\alpha_2} \cdots a^\dagger_{\alpha_A} |0\rangle$$

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

$$|\Phi\rangle = |\alpha_1\alpha_2\ldots\alpha_A\rangle = a^\dagger_{\alpha_1} a^\dagger_{\alpha_2} \cdots a^\dagger_{\alpha_A} |0\rangle$$

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

$$|\Phi^p_a\rangle = a^\dagger_{\alpha_p} a_{\alpha_a} |\Phi\rangle$$
$$|\Phi^{pq}_{ab}\rangle = a^\dagger_{\alpha_p} a^\dagger_{\alpha_q} a_{\alpha_b} a_{\alpha_a} |\Phi\rangle$$
$$\vdots$$

index convention: *a*,*b*,*c*,… : hole states, occupied in reference state
p,*q*,*r*,… : 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

$$T = \sum_{\alpha\alpha'} \langle\alpha| t |\alpha'\rangle \, a^\dagger_\alpha a_{\alpha'}$$

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

- **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

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

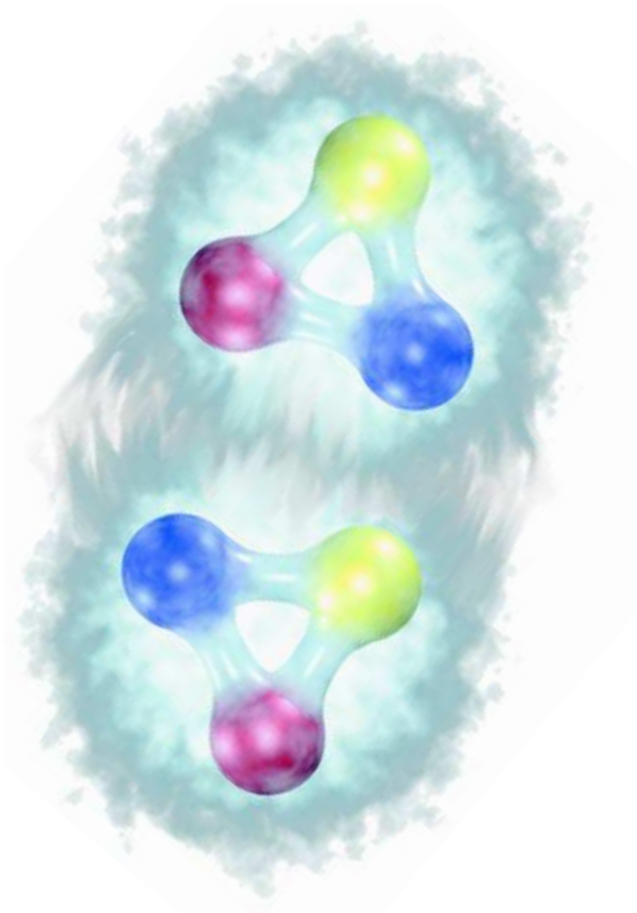
- **intrinsic Hamiltonian** is invariant under translation, rotation, Galilei boost, parity, time evolution, time reversal,...

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

- 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

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

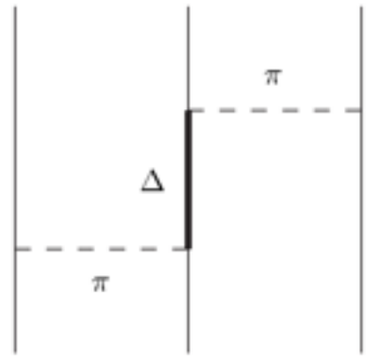
- nuclear interaction is **not fundamental**
- residual force analogous to **van der Waals interaction** between neutral atoms
- **based on QCD** and induced via polarization of quark and gluon distributions of nucleons
- **encapsulates all the complications** of the QCD dynamics and the structure of 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-ran[illegible]erms, local operator form
  - **CD Bonn 2000**: more systematic [illegible]change parametrization including pseudo-scalar, scalar[illegible] inherently nonlocal
- parameters of the NN[illegible] **N phase shifts** up to ~300 MeV and reproduce the[illegible]
- supplemented by **phe[illegible]ological 3N interactions** consisting of a Fujita-M[illegible]zawa-type term plus various hand-picked contributions
- **fit to ground states and spectra of light nuclei**, sometimes up to A≤8

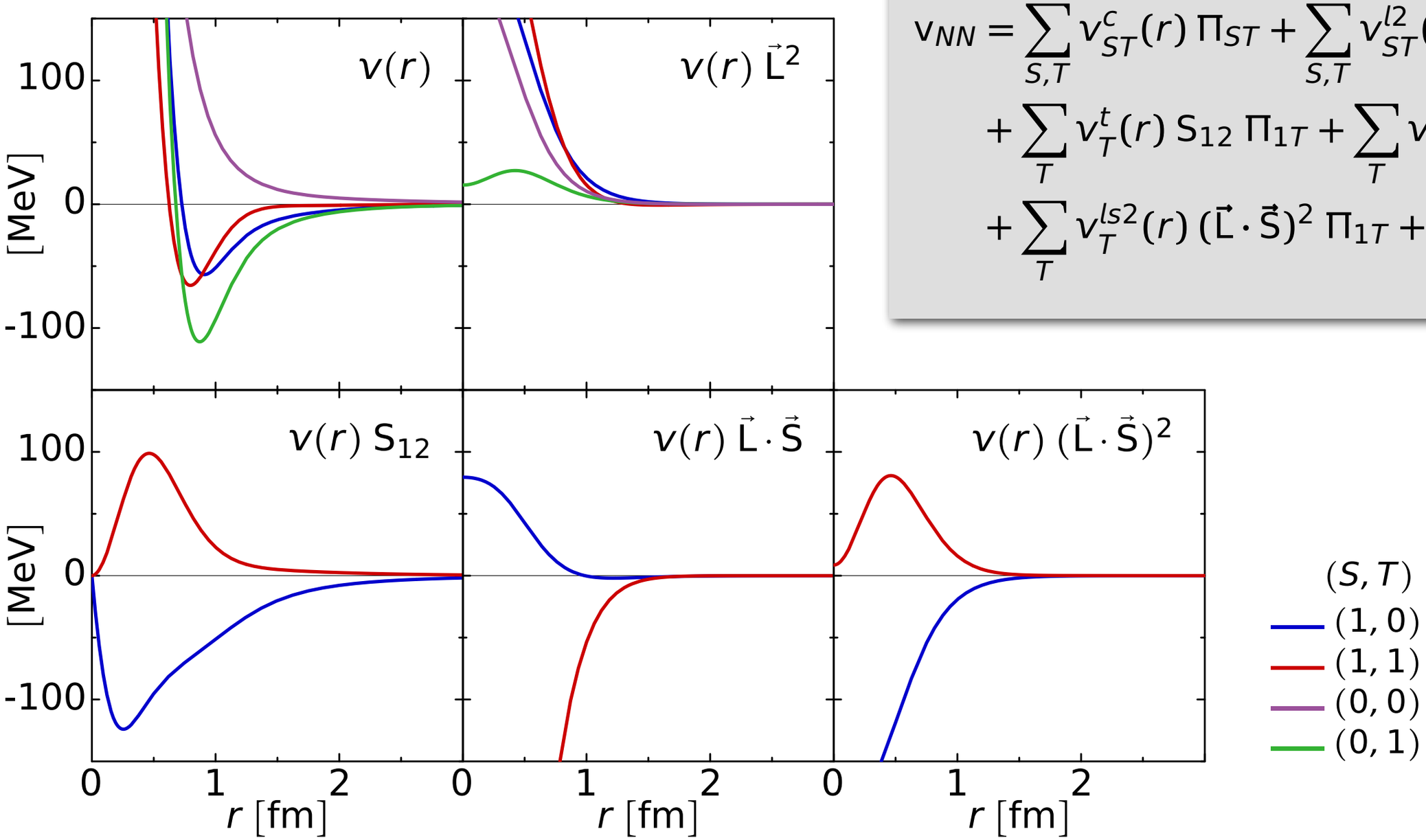
no consistency
no systematics
no connection to QCD



Argonne V18 Potential

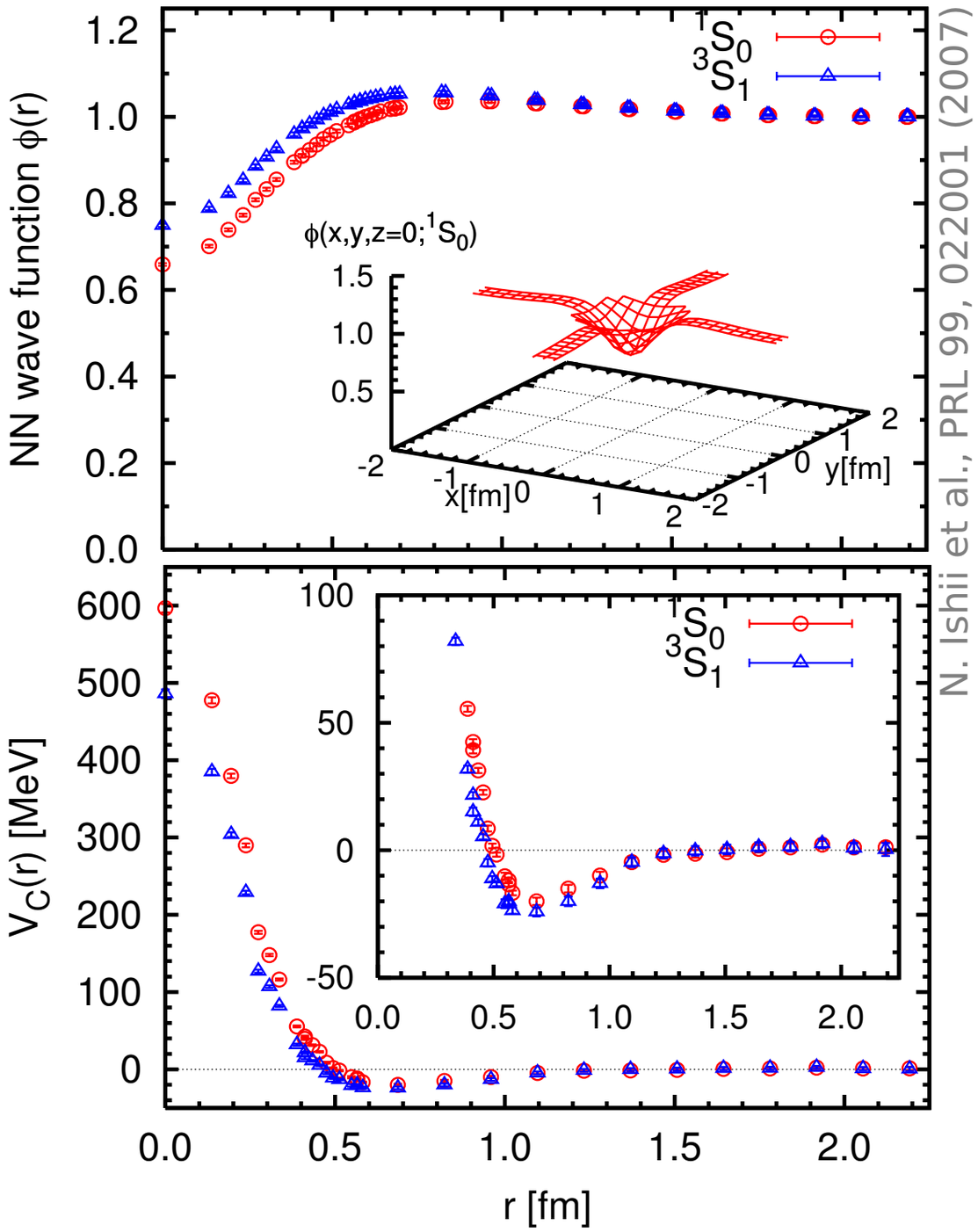
Wiringa, et al., PRC 51, 38 (1995)

$$v_{NN} = \sum_{S,T} v^c_{ST}(r)\,\Pi_{ST} + \sum_{S,T} v^{l2}_{ST}(r)\,\vec{L}^2\,\Pi_{ST} + \sum_{T} v^t_T(r)\,S_{12}\,\Pi_{1T} + \sum_{T} v^{ls}_T(r)\,(\vec{L}\cdot\vec{S})\,\Pi_{1T} + \sum_{T} v^{ls2}_T(r)\,(\vec{L}\cdot\vec{S})^2\,\Pi_{1T} + \ldots$$



Tomorrow... from Lattice QCD

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

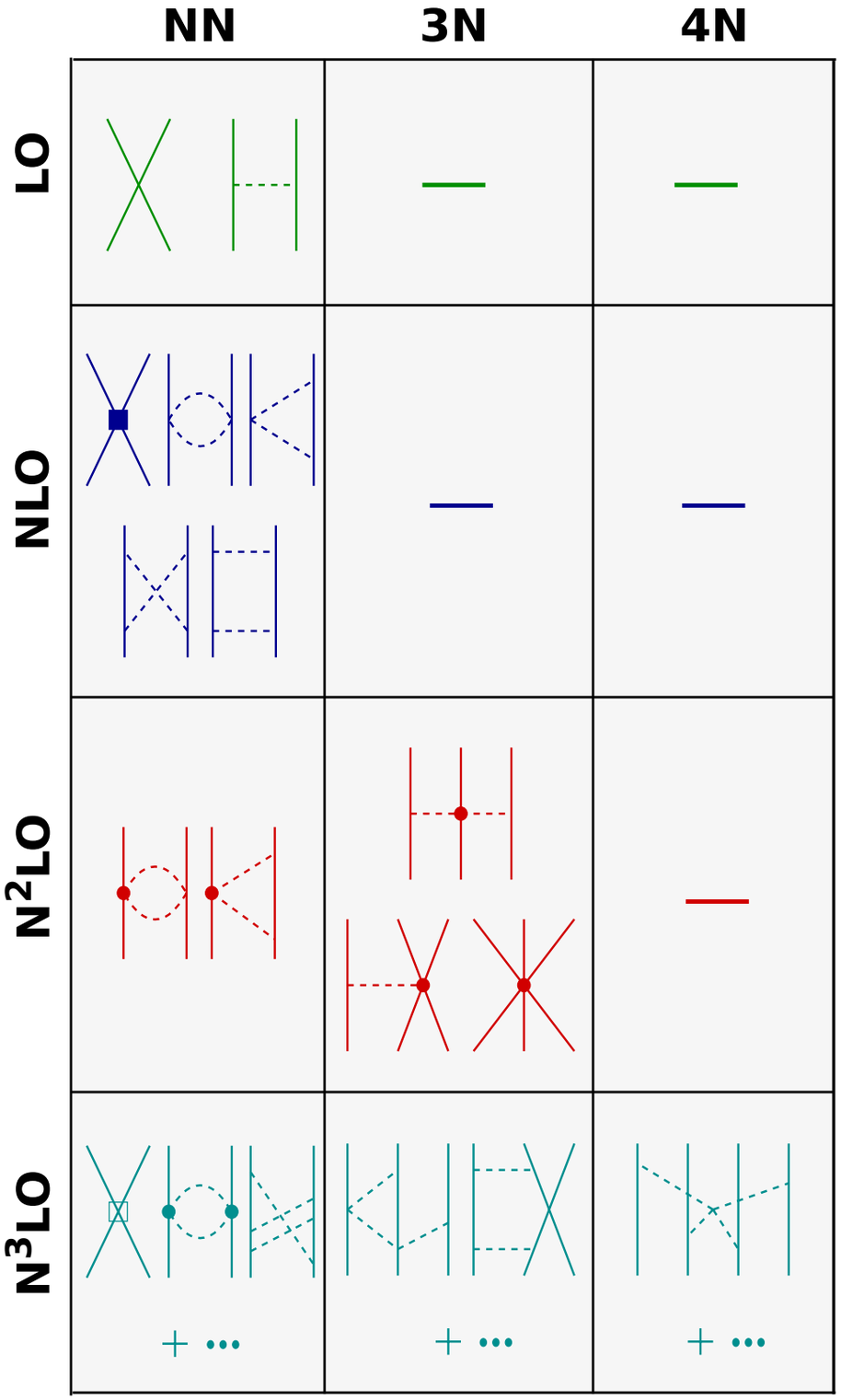


- first attempts towards construction of nuclear interactions directly from **lattice QCD simulations**
- compute relative **two-nucleon wave function** on the lattice
- **invert Schrödinger equation** to extract effective two-nucleon potential
- only **schematic results** so far (unphysical masses and 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 (π,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



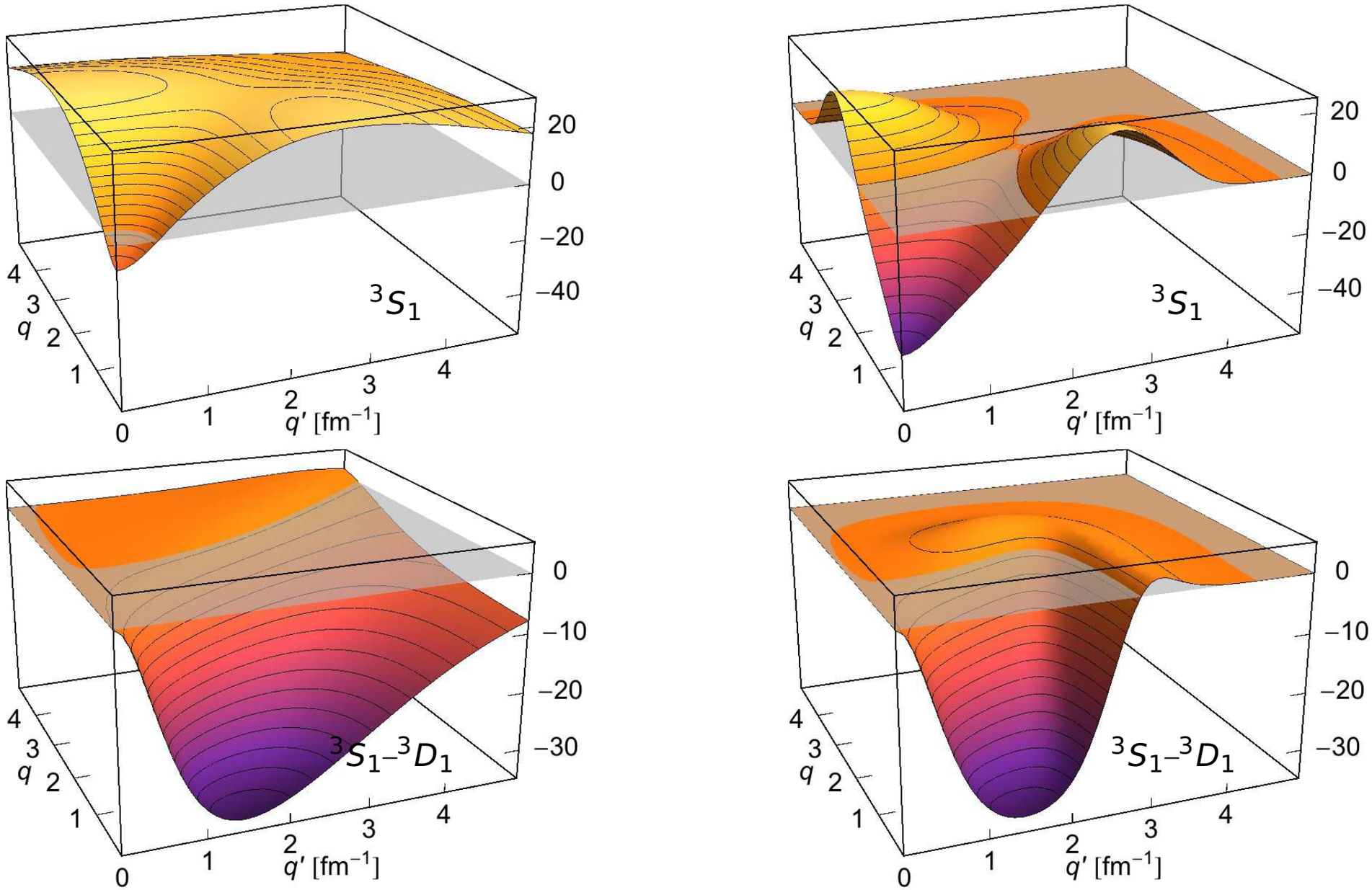
Momentum-Space Matrix Elements

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

Argonne V18

chiral NN
(N3LO, E&M, 500 MeV)

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



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: $|\pi_1\pi_2;[(L_1S_1)J_1,(L_2\tfrac{1}{2})J_2]J_{12};(T_1\tfrac{1}{2})\,T_{12}\rangle$

  three-body Jacobi HO: $|N_1N_2;[(L_1S_1)J_1,(L_2\tfrac{1}{2})J_2]J_{12};(T_1\tfrac{1}{2})\,T_{12}\rangle$

  antisym. three-body Jacobi HO: $|E_{12}\,i\,J^\pi_{12}\,T_{12}\rangle$

- 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

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

- 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

$$\Rightarrow \quad \langle N\,(LS)\,J;TM_T|\,\mathrm{v}_{NN}\,|N'\,(L'S)\,J;TM_T\rangle$$

- 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)

$$\langle \alpha_1 \alpha_2 | \mathrm{v}_{NN} | \alpha_1' \alpha_2' \rangle =$$
$$= \langle n_1 l_1 j_1 m_1 m_{t1}, n_2 l_2 j_2 m_2 m_{t2} | \mathrm{v}_{NN} | n_1' l_1' j_1' m_1' m_{t1}', n_2' l_2' j_2' m_2' m_{t2}' \rangle$$

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

$$\langle n_1 l_1 j_1, n_2 l_2 j_2; JT | \mathrm{v}_{NN} | n_1' l_1' j_1', n_2' l_2' j_2'; JT \rangle =$$
$$= \sqrt{(2j_1+1)(2j_2+1)(2j_1'+1)(2j_2'+1)} \sum \sum \sum \sum \sum$$
$$\times \begin{Bmatrix} l_1 & l_2 & L \\ s & s & S \\ j_1 & j_2 & J \end{Bmatrix} \begin{Bmatrix} & & \\ & & \\ & & \end{Bmatrix}$$
$$\times \langle\langle N\Lambda, \nu\lambda | n_1 l_1, n_2 l_2; L \rangle\rangle \langle\langle N\Lambda, \nu'\lambda' | n_1' l_1', n_2' l_2'; L' \rangle\rangle$$
$$\times (2J+1)(2S+1)(2L+1)(2L'+1)\,(-1)^{L+L'}\,\{1-(-1)^{\lambda+S+T}\}$$
$$\times \langle \nu(\lambda S) j T | \mathrm{v}_{NN} | \nu'(\lambda' S) j T \rangle$$

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

$$\begin{aligned} \mathrm{H} = \mathrm{H}_{\mathrm{cm}} + \mathrm{H}_{\mathrm{int}} &= \mathrm{T}_{\mathrm{cm}} + \mathrm{T}_{\mathrm{int}} + \mathrm{V}_{\mathrm{NN}} \\ &= \frac{1}{2M}\vec{\mathrm{P}}^2_{\mathrm{cm}} + \frac{1}{2\mu}\vec{\mathrm{q}}^2 + \mathrm{V}_{\mathrm{NN}} \end{aligned}$$

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

$$|\,\psi\,\rangle = |\,\Phi_{\mathrm{cm}}\,\rangle \otimes |\,\phi_{\mathrm{int}}\,\rangle$$

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

$$\mathrm{H}_{\mathrm{int}}\,|\,\phi_{\mathrm{int}}\,\rangle = E\,|\,\phi_{\mathrm{int}}\,\rangle$$

Solving the Two-Body Problem

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

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

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

- **symmetries** simplify the problem dramatically:
  - H_{int} does not connect/mix different J, M, S, T, M_T and parity π
  - 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^π 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**

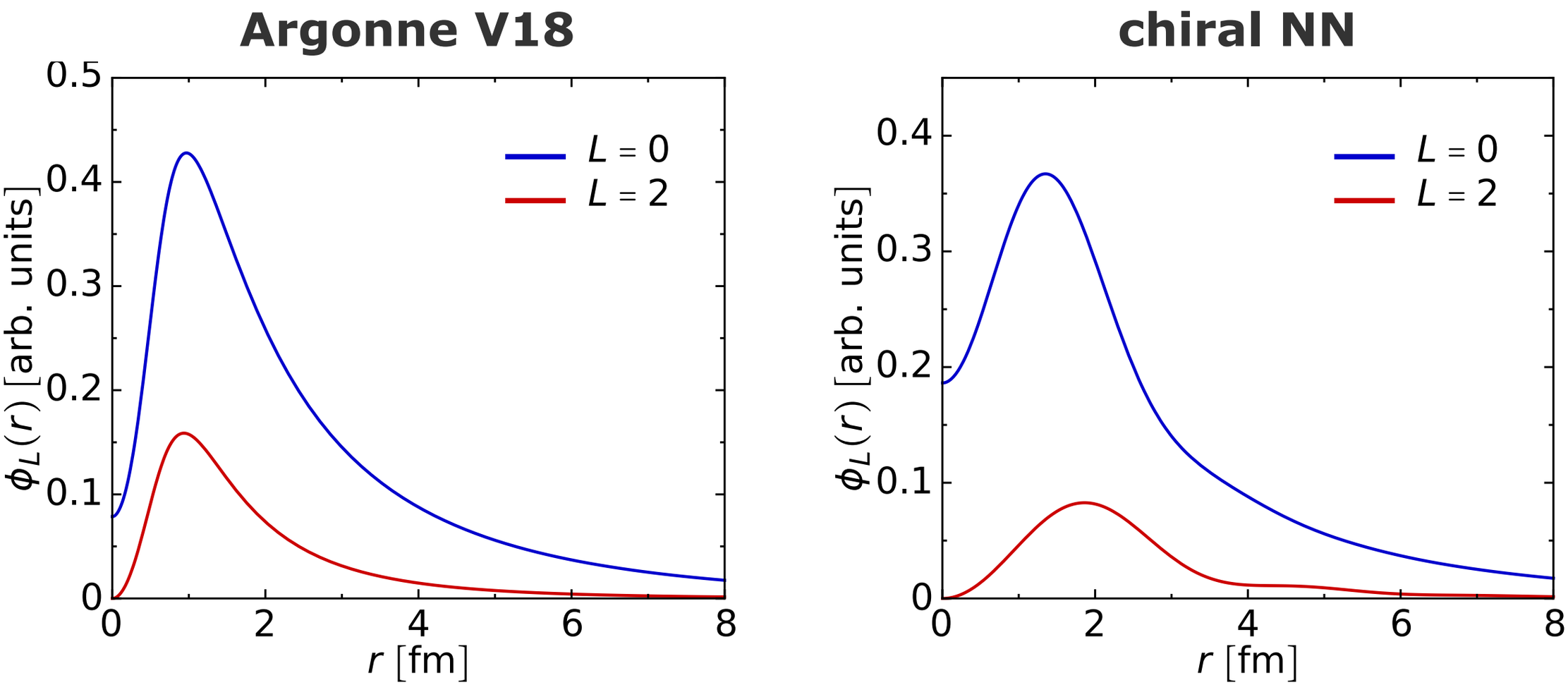
$$\left(\begin{array}{c|c} \langle N'(01)\ldots|\,\mathrm{H}_{\text{int}}\,|N(01)\ldots\rangle & \langle N'(01)\ldots|\,\mathrm{H}_{\text{int}}\,|N(21)\ldots\rangle \\ \hline \langle N'(21)\ldots|\,\mathrm{H}_{\text{int}}\,|N(01)\ldots\rangle & \langle N'(21)\ldots| \end{array}\right) \left(\begin{array}{c} C_N^{(0)} \\ \hline C_N^{(2)} \end{array}\right) \left(\begin{array}{c} C_{N'}^{(0)} \\ \hline C_{N'}^{(2)} \end{array}\right)$$

- eigenvectors yi… …icients and eigenvalues the energies

- **truncate … …ces to $N \le N_{\text{max}}$** and choose N_{max} large enough so that observables are converged, i.e., do not depend on N_{max} anymore

simplest possible Jacobi-NCSM calculation

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