Nuclear many-particle Hamiltonian (in coordinate representation)

$$H = \sum_{i=1}^{A} \frac{-\hbar^2}{2m} \nabla_i^2 + \frac{1}{2} \sum_{i,j=1}^{Z} v_{ij}^{(2)Coul} + \frac{1}{2} \sum_{i,j=1}^{A} v_{ij}^{(2)nucl} + \frac{1}{6} \sum_{i,j,k=1}^{A} v_{ijk}^{(3)nucl}$$

Formal structure $H = T^{(1)} + V^{(2)} + V^{(3)}$

- kinetic energy of all nucleons (1-body operator)
- 2-body Coulomb interactions between protons
- 2-body and 3-body strong nuclear interactions

many-particle Schrödinger equation (in coordinate representation)

$$(H - E_n)\Psi_n(x_1, x_2, ..., x_A) = 0$$
 with $x = (\vec{r}, s_z, t_z)$

Nuclear many-particle Hamiltonian (in occupation number representation)

Creation operators for nucleon states: \hat{c}_i^{\dagger}

$$\hat{H} = \sum_{i,j=1}^{\infty} \langle i|t|j \rangle \hat{c}_{i}^{\dagger} \hat{c}_{j} + \frac{1}{2} \sum_{i,j,k,l=1}^{\infty} \langle ij|V^{(2)}|kl \rangle \hat{c}_{i}^{\dagger} \hat{c}_{j}^{\dagger} \hat{c}_{l} \hat{c}_{k}$$
$$+ \frac{1}{6} \sum_{i,j,k,l,m,n=1}^{\infty} \langle ijk|V^{(3)}|lmn \rangle \hat{c}_{i}^{\dagger} \hat{c}_{j}^{\dagger} \hat{c}_{k}^{\dagger} \hat{c}_{n} \hat{c}_{m} \hat{c}_{l}$$

Nuclear many-particle state vectors (occupation number rep.)

Basic building blocks: set of Slater determinants for A nucleons (anti-symmetrized products of single-particle wave functions)

These correspond to the state vectors in occupation number rep.

$$\Phi_{n_1,\dots,n_{\infty}}(1,\dots,A) = (\hat{c}_1^{\dagger})^{n_1} (\hat{c}_2^{\dagger})^{n_2} \dots (\hat{c}_{\infty}^{\dagger})^{n_{\infty}} |0\rangle$$
with $n_k = 0$ or 1 and $\sum_{k=1}^{\infty} n_k = A$

Theorem: the most general state vector of a many-body system can be written as an infinite superposition of Slater determinants

$$\Psi(1,...,A;t) = \sum_{n_1,...,n_\infty=0}^{1} f(n_1,...,n_\infty;t) \Phi_{n_1,...,n_\infty}(1,...,A)$$

Numerical solution of nuclear many-particle problem

Need to truncate infinite set of Slater determinants.

"Ab-initio" methods use of the order of 10⁵ to 10⁶ Slater determinants.

Need largest available supercomputers (Livermore, ORNL, ...)

Use quasi-particle transformation to "particle" states (above Fermi level) and "hole" states (below Fermi level); state vector for ground state becomes "quasi-particle" vacuum.

Then use Wick's theorem to simplify matrix elements of creation and annihilation operators.

Microscopic theories of nuclear structure



"Ab-initio" calculations for light nuclei

- Green's function Monte Carlo method
- "No-core" shell model (no inert core, many-body theory for all nucleons)
- Coupled-cluster theory (based on Goldstone's "linked cluster expansion")

Green's function Monte Carlo calculations for light nuclei using Argonne v18 + 3-body interaction Ref: Pieper, Wiringa & Carlson, Phys. Rev. C 70, 054325 (2004)

first step: variational Monte Carlo (VMC) calculation to find an optimal many-body trial wave function for a given state. The trial WF contains variational parameters that are adjusted to minimize the energy expectation value, which is evaluated by METROPOLIS Monte Carlo integration.

second step: the trial wave function (antisymmetric by explicit construction) is used as input to a Green's function Monte Carlo (GFMC) algorithm which projects out the lowest energy eigenstate by a propagation in imaginary time.

See figure next page!

NOTE: inclusion of 3-body N-N interaction (labeled IL2, red-yellow) improves agreement between theory and exp. data!



No-core shell model

Ref: Navratil, Gueorguiev, Vary, Ormand and Nogga, Phys. Rev. Lett. 99, 042501 (2007)



Coupled-cluster theory Ref: Hagen, Papenbrock, Dean, and Hjorth-Jensen Phys. Rev. Lett. 101, 092502 (2008)

TABLE I. CCSD results for various nuclei from a chiral nucleon-nucleon potential at order NNNLO. E/A and V/A: ground-state and potential energy per nucleon, respectively. $\Delta E/A$: difference to the experimental ground-state energy (theoretical mass table evaluations for ⁴⁸Ni). *R* and *R*_{exp} are the computed and measured charge radius.

Nucleus	E/A	V/A	$\Delta E/A$	<i>R</i>	<i>R</i> _{exp}
	[MeV]	[MeV]	[MeV]	[fm]	[fm]
${}^{4}\text{He}$ ${}^{16}\text{O}$	-5.99	-22.75	1.08	1.86	1.64
	-6.72	-30.69	1.25	2.71	2.74
⁴⁰ Ca	-7.72	-36.40	0.84	3.24	3.48
⁴⁸ Ca ⁴⁸ Ni	$-7.40 \\ -6.02$	-37.97 - 36.04	1.27 1.21	3.22 3.50	3.47