Nuclear Dynamics and Cold Atoms: Computational Many-Body Physics

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Introduction

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- Contribute to the development of code that will perform Monte Carlo simulations on large nuclei ($40 - 200+$ nucleons) to obtain observables such as ground state energy and density distribution.

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Quantum Monte Carlo

Idea: Use imaginary time evolution to project out the ground state wavefunction of a many-body system.

$$\lim_{\tau \to \infty} \mathrm{e}^{-\tau \hat{H}} \psi_0 = \psi$$

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Break into components:

$$\mathrm{e}^{-\Delta\tau \hat{H}} \approx \mathrm{e}^{\frac{-\Delta\tau \hat{T}}{2}} \mathrm{e}^{-\Delta\tau \hat{V}} \mathrm{e}^{\frac{-\Delta\tau \hat{T}}{2}}$$

Quantum Monte Carlo

Ket evolution:

$$\mathrm{e}^{-\tau\hat{H}}\left|\psi_0\right\rangle = \ldots \left(\mathrm{e}^{\frac{-\Delta\tau\hat{T}}{2}}\mathrm{e}^{-\Delta\tau\hat{V}}\mathrm{e}^{\frac{-\Delta\tau\hat{T}}{2}}\right)\left(\mathrm{e}^{\frac{-\Delta\tau\hat{T}}{2}}\mathrm{e}^{-\Delta\tau\hat{V}}\mathrm{e}^{\frac{-\Delta\tau\hat{T}}{2}}\right)\left|\psi_0\right\rangle$$

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If ϕ is a Slater Determinant and $\hat{A}$ is a one-body operator, then $\mathrm{e}^{-\tau\hat{A}}\phi$ is also a Slater Determinant.

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$$e^{-\tau\hat{H}}|\psi_0\rangle = \ldots \left(e^{\frac{-\Delta\tau\hat{T}}{2}} e^{-\Delta\tau\hat{V}} e^{\frac{-\Delta\tau\hat{T}}{2}}\right)\left(e^{\frac{-\Delta\tau\hat{T}}{2}} e^{-\Delta\tau\hat{V}} e^{\frac{-\Delta\tau\hat{T}}{2}}\right)|\psi_0\rangle$$

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If ϕ is a Slater Determinant and $\hat{A}$ is a one-body operator, then $e^{-\tau\hat{A}}\phi$ is also a Slater Determinant.

But $\hat{V}$ is a two-body operator...

$\hat{V}$

Potential Interaction:

$$\hat{V} = \sum_{i<j} V(r_{ij})$$

After second quantization:

$$\hat{V} = \sum_{i,j,k,l} V_{ijkl}\, a_i^\dagger a_j^\dagger a_l a_k = \sum_{i,j,k,l} V_{ijkl} \left(a_i^\dagger a_k\right) \left(a_j^\dagger a_l\right)$$

$$\hat{V} = \sum_i \hat{n}_\uparrow(i) \hat{n}_\downarrow(i)$$

Hubbard-Stratonovich Transformation

$\mathrm{e}^{-\Delta\tau\hat{V}}\,|\phi\rangle = \mathrm{e}^{-\Delta\tau\sum_i \hat{n}_\uparrow(i)\hat{n}_\downarrow(i)}\,|\phi\rangle$ is hard.

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Obtain multi-dimensional product:

$$\prod_n^N \prod_i dx_n dx_i \rho(x)\hat{O}(x)$$

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Monte Carlo method: randomly sample across parameter space

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Solution: define an effective Hamiltonian, $\hat{H}_{ev} = \hat{V}_{ev} + \hat{T}$, that does not have a sign problem.

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In the previous slides, $\hat{H} = \hat{H}_{ev}$ and $\hat{V} = \hat{V}_{ev}$.

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Addition of protons requires trial wave functions based on the harmonic oscillator.

$$\Psi_n(x, y, z) = N H_{n_x}(x) H_{n_y}(y) H_{n_z}(z) \mathrm{e}^{-r^2/2r_0^2}; \quad r_0^2 = \frac{\hbar}{m\omega}$$

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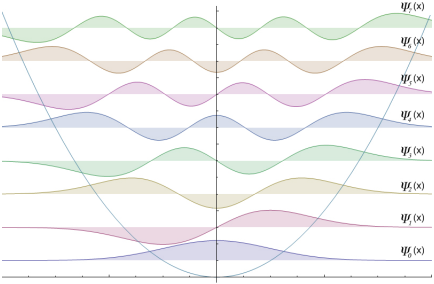

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Evolution potential = sum of three Yukawa interactions (in the form $V = -g^2 \frac{e^{-mr}}{r}$:

$$V_{ev} = \frac{V_\pi M_\pi^2}{k^2 + M_\pi^2} + \frac{V_\sigma M_\sigma^2}{k^2 + M_\sigma^2} + \frac{V_\omega M_\omega^2}{k^2 + M_\omega^2}$$

π = parameters for pion exchange
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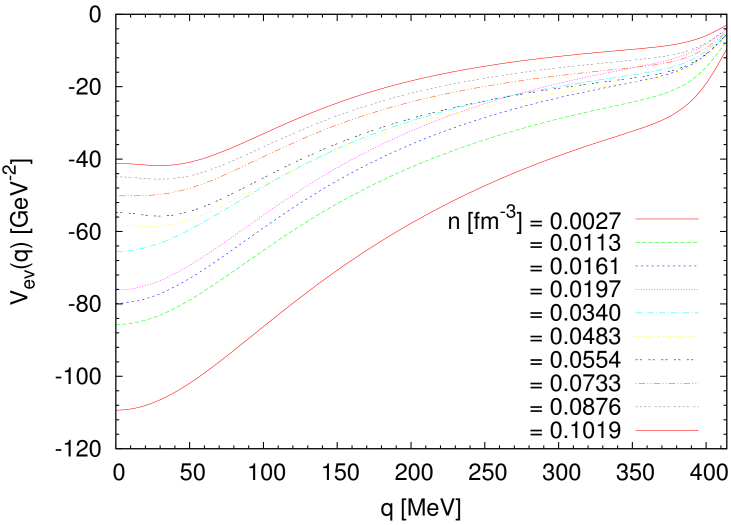
Parameters are fit to minimize phase shifts.

Potentials at Fixed Densities



New Potential Parameters

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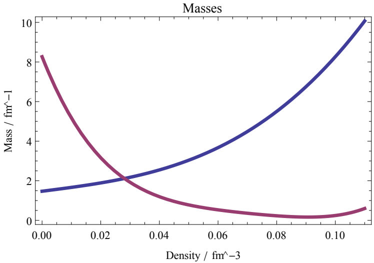
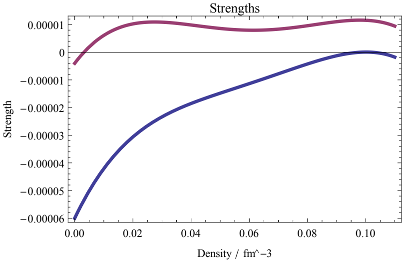
Recalculate parameters and fit to polynomial functions, allowing for fast calculation of V_{ev} at any given k and r.





Blue = σ parameters, purple = ω parameters

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Isospin Dependent Interactions

Some interaction components from chiral effective field theory have isospin dependence.

Ex: one-pion exchange component

$$V_{1\pi} = \frac{g_A^2}{4f_\pi^2}\vec{\tau}_1 \cdot \vec{\tau}_2 \frac{\vec{\sigma}_1 \cdot \vec{q}\,\vec{\sigma}_2 \cdot \vec{q}}{q^2 + m_\pi^2}$$

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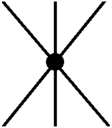
Other interactions are not present in neutron matter.

Ex. three-body contact term



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- Jeremy Holt
- Aurel Bulgac

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