Effective Field Theories and Quantum Monte Carlo in Nuculear Physics.

P. Armani[1,2] S. Gandolfi[2,4] P. Faccioli[1,2] and F. Pederiva[1,3]

[1] *Dipartimento di Fisica dell'Universitá di Trento, via Sommarive 14, 38050 Povo, Trento, Italy*
[2] *INFN, Gruppo Collegato di Trento, via Sommarive 14, 38050 Povo, Trento, Italy*
[3] *INFM DEMOCRITOS National Simulation Center, via Beirut 2-4, 34014 Trieste, Italy Trieste*
[4] *S.I.S.S.A., via Beirut 2-4, 34014 Trieste, Italy*

1. The Nuclear Problem

The study of nuclei and nuclear matter is still an open problem in theoretical physic because of:

- The absence of an unique exact nuclear potential, derived from first principles.

  There are a lot **phenomenological** nuclear potential (es. Argonne, Illinois, Urbana, Skyrme) very realistic for two body sector and at density typical of nuclei. Higher density behavior (relevant in astrophysics) and n-body ($n > 2$) terms are not well–known.

  Nuclear potentials derived from **Effective Field Theories** (EFT) were recent developed (es. CD-Bonn, Nijmegen); they are written starting from QCD symmetries adding more fundamental basis to phenomenological potentials and a systematic way to order and add new terms. Effective parameters must be otherwise fitted on experimental data and not derived (at now) directly from QCD simulations. Therefore the knowledge of n–body contributions is still limited by the lack of experimenta input. For this reasons they suffer anyway of the same experimental limits about the n-body ($n > 2$) sectors.

- The absence of a sufficient accurate method to calculate nuclei and nuclear matter properties. **Mean field** methods (like Hartree–Fock) are too much model potential dependent, despite the computation is feasible. Hamiltonian diagonalization methods (es. **No Core Shell Model**) could be applied only to few body problems ($n \leq 12$), because of the high number of basis functions to be considered to reach convergence. Accurate **Variational Monte Carlo** methods (VMC) has been used up to $n \leq 12$. Increasing the number of nucleons is very hard, because of the exponential growth of spin–isospin states. **Green Function Monte Carlo** (GFMC), starting from very accurate variational wave functions, gives accurate results although affected by constrained path approximation and nonlocal potential terms. My systems worked out so far are limited to $n \leq 12$ for the same reason as VMC method. **Auxiliary Field Diffusion Monte Carlo** (AFDMC) method[1] open the possibility to study nuclei heavier than GFMC (^{40}Ca, for example [2]) or nuclear matter (now up to $n = 114$ [3]). The trick is to consider not the total product spin–isospin space, but only the sum of single particle spaces, and to rewrite two body terms in one body ones using Hubbard–Stratonovich transformation. There are still some difficulties with including nonlocal potential terms; moreover very accurate spin–isospin correlation dependent trial wave function couldn't be used. Because of this restriction, for some systems Fixed–Phase or Constrained Path approximations are not accurate enough compared to GFMC.

2. Effective Field Theories

At present it is impossible to study nuclear systems starting directly from QCD because of its non–perturbative character. Lattice QCD simulations are also prohibitive because of their enormous computational cost.
Limiting the study to a specified system and energy regime (es. fundamental state of nuclei), not all degrees of freedom (es. quark and gluon) are fundamental for the system dynamic.
Effective Field Theories helps to construct an equivalent effective Lagrangian

- including only few relevant effective degrees of freedom (es. baryons and lighter mesons);
- ordering in a perturbative series the Lagrangian terms (in principle infinite);
- preserving the fundamental symmetries.

At momentum lower than $M \sim 1$GeV QCD is intrinsically non perturbative. M is order of nucleon mass M_N. The typical momenta Q exchanged between nucleons in small nuclei are order of the size of small nuclei, i.e. $Q \sim m_\pi \simeq 138$MeV. Therefore it is possible to consider two energy scales:

- **low energy** scale, involving only relevant degrees of freedom (nucleons, pions,...) with momentum $Q < M$.
- **high energy** scale, including degrees of freedom that are omitted; their effects are included in effective theory by a counterterms series. This contains in principle an infinite number of therms. Observing that $\frac{Q}{M} < 1$, it's possible to order these terms in a perturbative series, considering only a finite number of terms for a specified precision.

Moreover a **regularization cut–off** must be introduced for momentum larger than Q, removing ultraviolet divergences and the high energy physic already described by the counterterms.

The **Lagrangian used** in this work (that can be systematically improved at higher orders in perturbative series expansion) is the fallowing[4, 5]:

$$\begin{aligned}\mathscr{L}_0 = &-\frac{1}{2}\left[(\vec{\nabla}\pi_i)^2 - (\partial_0\pi_i)^2 + m_\pi^2\pi_i^2\right] + N^\dagger\left[i\partial_0 - \frac{1}{8f_\pi^2}\epsilon_{ijk}\tau_i\pi_j\partial_0\pi_k - M_0\right]N \\ &- \frac{g_A}{2f_\pi}N^\dagger\tau_i\sigma_j\nabla_j\pi_i N - \frac{1}{2}C\left(N^\dagger N\right)\left(N^\dagger N\right) - \frac{1}{2}C_I\left(N^\dagger\tau_i N\right)\left(N^\dagger\tau_i N\right)\end{aligned}$$

3. Regularization and Effective Parameters

Starting from the previous Lagrangian $\mathscr{L}_0$ it's necessary:

- to fix a **regularization** scheme, with a **cut–off** Λ on momenta Q.
- to determine all **effective parameters** that depends on regularization schema and cut–off Λ.
- to have an **Hamiltonian formalism** to use Monte Carlo methods.

The **cut–off** Λ is implemented representing the pion fields on a periodic lattice with step $a \simeq 2$fm. Consistently, a discrete definition of derivative is required: we use three point formula.
About effective parameters we can say that

- at this order m_π correspond to the physical pion mass (the mean of π^+, π^- and π^0 masses)
- M_0 is the nucleon bare mass. The difference between the physical mass M_N is the eigenenergy due to interaction energy between the single nucleon and the pion fields.
- g_A is the axial vector coupling of nucleon and f_π is the pion decay constant.
- C and C_I are the effective coefficients parameters of counterterms.

Another very good but fundamental approximation, is to consider **the nucleons number constant**. With these assumptions, the Hamiltonian is the following:

$$\begin{aligned}H &= H_\pi + H_{\pi N} + H_N \\ H_\pi &= \frac{1}{2}a^3\sum_{\vec{l}}\Pi_{\pi_i}^2(\vec{l}) + \frac{1}{2}a^3\sum_{\vec{l},\vec{n}}\pi_i(\vec{l})\ K_{\vec{l}\vec{n}}\ \pi_i(\vec{n}) \\ H_{\pi N} &= \frac{g_a}{2f_\pi}\sum_{m=1}^{A}\tau_i\sigma_j\frac{\pi_i(\lfloor a^{-1}\vec{x}_m\rfloor + \hat{j}) - \pi_i(\lfloor a^{-1}\vec{x}_m\rfloor - \hat{j})}{2a} \\ H_N &= AM_0 + \frac{1}{2}\sum_{m=1}^{A}\sum_{\substack{n=1\\ n\neq m}}^{A}\delta_a(\vec{x}_m - \vec{x}_n)(C + C_I\vec{\tau}_m\cdot\vec{\tau}_n) \\ K_{\vec{l}\vec{n}} &= \left(m_\pi^2 + \frac{1}{a^2}\frac{3}{2}\right)\delta_{\vec{l}\vec{n}} - \frac{1}{2a^2}\sum_{\vec{\mu}=\hat{x},\hat{y},\hat{z}}\delta_{\vec{l},\vec{n}+2\vec{\mu}}\end{aligned}$$

4. Methods

In order to compute the energy of the ground state of the previous Hamiltonian, three methods are used:

- **Variational Monte Carlo**. The problem is well posed and an upper bound of the exact energy is obtained . Jastrow spin–isospin dependent correlations are used to have a better wave function. Otherwise, with a non central Jastrow (i.e. spin–isospin dependent) it's possible to treat only few body nuclear systems, because the entire spin–isospin product space is to be considered, which dimension increase exponentially as 4^n respect to the nucleon number n.
- **Green Function Monte Carlo**. The idea is to start from a variational wave function and evolve it in imaginary time in order to project on the fundamental state. But, because of the intrinsic complex nature of the Hamiltonian, the problem is not well posed, and an approximation like **constrained path**[6] or **fixed–phase** is necessary to compute a positive defined transition function. With a real Hamiltonian it is possible to use the **fixed–node** approximation, obtaining an upper bound to the energy. Otherwise the upper bound property is not guaranteed however, if the trial wave function is very good, the approximation is under control. So it is necessary to have a good variational wave function, using a Jastrow spin–isospin dependent correlation function and limiting the method to the study of few body systems. Moreover nonlocal terms (coming at higher order in EFT) are not easy to included.
- **Auxiliary Field Diffusion Monte Carlo**. The idea is the same as that one of GFMC, but the two body terms in the propagator are rewritten into a one body term using the **Hubbard–Stratonovich** transformation and including auxiliary fields. The goal of AFDMC method is to reduce the configuration space to be considered from the product space (dimension 4^n) to the sum of one body spaces (dimension $4n$), making possible to treat many nucleons systems. Otherwise operatorial Jastrow correlations (i.e. non local or spin–isospin dependent), can not be included into the trial wave function. So a poorer trial wave function is used Consequently it might became problematic to correctly describe the system and to limit fixed–phase or constrained path approximations.

5. Toy Model

As a first step, **pions vacuum** was studied. The Hamiltonian is only $H_0 = H_\pi$. For this system the exact ground state wave function was been found:

$$\Psi_0 = \exp\left[-\frac{1}{2}a^3\sum_{\vec{i},\vec{j},\alpha}\pi_{\vec{i}}^\alpha\ E_{\vec{i}\vec{j}}\ \pi_{\vec{j}}^\alpha\right]$$

This is important, because the pion fields vacuum energy V_0 is several orders larger than typical nucleon binding energy.
As a second step a system with only one nucleon into the pion fields is considered. A simpler interaction term is used:

$$\tilde{H}_{\pi N} = \frac{g_a}{2f_\pi}\sum_\alpha\frac{\pi^\alpha_{(\lfloor a^{-1}\vec{x}_m\rfloor + \hat{j})} - \pi^\alpha_{(\lfloor a^{-1}\vec{x}_m\rfloor - \hat{j})}}{2a}$$

For this system with Hamiltonian $\tilde{H} = H_\pi + \tilde{H}_{\pi N}$ the exact ground state was found:

$$\tilde{\Psi} = \exp\left[-\frac{1}{2}a^3\sum_{\vec{i},\vec{j},\alpha}\tilde{\pi}_{\vec{i}}^\alpha\ E_{\vec{i}\vec{j}}\ \tilde{\pi}_{\vec{j}}^\alpha\right]$$

with

$$\tilde{\pi}_{\vec{i}}^\alpha = \pi_{\vec{i}}^\alpha - \frac{g_A}{2f_\pi}\sum_{\vec{j},\beta}\partial_\beta\Delta(\vec{j})\delta_a(a\vec{j} - \vec{x}_n)$$

The difference between the smallest eigenvalues of H_0 and $\tilde{H}$ is the nucleon eigenenergy of the toy model.

6. Trial Wave Function

Starting from the toy model, the trial wave function was determined.
With the true pion–nucleon interaction $H_{\pi N}$ it is not possible to find the one–nucleon ground state as for the toy model, but fallowing the same structure a pion–nucleon$_m$ correlation with the operator θ_m was included:

$$\Theta_m = \exp\left[-\frac{1}{2}\frac{g_T}{2f_\pi}a^3\sum_{\vec{i},\vec{j},\alpha,\beta}\pi_{\vec{i}}^\alpha\ E_{\vec{i}\vec{j}}\partial_\beta\Delta(\vec{j} - \lfloor a^{-1}\vec{x}_m\rfloor)\sigma_\beta\tau_\alpha\right]$$

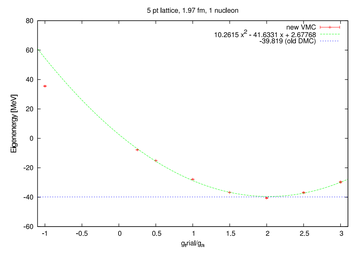
Two body nucleon–nucleon correlations are included with other Jastrow spin–isospin dependent terms, paying attention to symmetrize operators to preserve the antisymmetry of the uncorrelated wave function [7].
Calling $|\chi\rangle$ the antisymmetric uncorrelated nucleon wave function, the final form of the trial wave function:

$$|\Psi_T\rangle = \Psi_0\left[\mathscr{S}\prod_{m>n}(1 + \tau_\alpha(m)\tau_\alpha(n)f_\tau(r_{mn}))\right]\prod_{m>n}f_c(r_{mn})\ \prod_w\Theta_w|\chi\rangle$$

The correlation functions $f_c(r_{mn})$ and $f_\tau(r_{mn})$ and the parameter g_T og Θ_M must be determined variationally, minimizing the energy of the system.

7. Effective and Variational Parameters

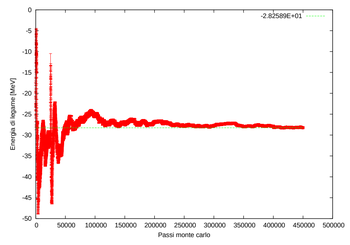
As a first step the nucleon eigenenergy is computed by DMC. Variational parameter g_T is fixed by minimizing the variational nucleon eigenenergy (see figure).



The remnant two effective field theory coefficients have to be fixed fitting the binding energy of two few nucleons systems (es. ^{3}He and ^{2}H).

8. Results, problems and future developments

The AFDMC algorithm does not work for two nucleon system, because of too poor correlation in trial wave function. So, in order to fit C and C_I parameters on a few nucleon system we try to use VMC and GFMC methods. Probably for a high precision result, also $NN\pi$ correlations must be included. For some systems the AFDMC algorithm results stable and scale linearly with nucleon number. In figure is plotted the AFDMC energy evolution for ^{4}He, with two arbitrary coefficients C and C_I.



References

[1] S. Schmidt, K.E. Fantoni. *Phys. Lett. B*, 446:99–103, 1999.

[2] F. Gandolfi, S. Pederiva and S Beccara. Monte carlo calculation for the neutron-rich ca isotopes. *Eu. Phys. J. A*, 32(2), 2006.

[3] A. Sarsa, S. Fantoni, K. E. Schmidt, and F. Pederiva. Neutron matter at zero temperature with auxiliary field diffusion monte carlo. *Phys. Rev.*, C68:024308, 2003.

[4] C. Ordonez, L. Ray, and U. van Kolck. The two-nucleon potential from chiral lagrangians. *Phys. Rev.*, C53:2086–2105, 1996.

[5] Bugra Borasoy, Evgeny Epelbaum, Hermann Krebs, Dean Lee, and Ulf-G. Meissner. Lattice simulations for light nuclei: Chiral effective field theory at leading order. *Eur. Phys. J.*, A31:105–123, 2007.

[6] J. Carlson, J. E. Gubernatis, G. Ortiz, and Shiwei Zhang. Issues and observations on applications of the constrained-path monte carlo method to many-fermion systems. *Phys. Rev. B*, 59(20):12788–12798, May 1999.

[7] Robert B. Wiringa. Variational calculations of few-body nuclei. *Phys. Rev.*, C43:1585–1598, 1991.