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Progress of Monte Carlo methods in nuclear physics using EFT–based NN interaction and in hypernuclear systems.

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Introduction

In this thesis I report the work of my PhD; it treated two different topics, both related by a third one, that is the computational method that I use to solve them. I worked on EFT–theories for nuclear systems and on Hypernuclei. I tried to compute the ground state properties of both systems using Monte Carlo methods.

In the first part of my thesis I briefly describe the Monte Carlo methods that I used: VMC (Variational Monte Carlo), DMC (Diffusion Monte Carlo), AFDMC (Auxiliary Field Diffusion Monte Carlo) and AFQMC (Auxiliary Field Quantum Monte Carlo) algorithms. I also report some new improvements relative to these methods that I tried or suggested: I remember the fixed hypernode extension (§ 2.6.2) for the DMC algorithm, the inclusion of the L^2 term (§ 3.10) and of the exchange term (§ 3.11) into the AFDMC propagator. These last two are based on the same idea used by K. Schmidt to include the spin–orbit term in the AFDMC propagator (§ 3.9). We mainly use the AFDMC algorithm but at the end of the first part I describe also the AFQMC method. This is quite similar in principle to AFDMC, but it was newer used for nuclear systems. Moreover, there are some details that let us hope to be able to overcome with AFQMC some limitations that we find in AFDMC algorithm. However we do not report any result relative to AFQMC algorithm, because we start to implement it in the last months and our code still requires many tests and debug.

In the second part I report our attempt of describing the nucleon–nucleon interaction using EFT–theory within AFDMC method. I explain all our tests to solve the ground state of a nucleus within this method; hence I show also the problems that we found and the attempts that we tried to overcome them before to leave this project.

In the third part I report our work about Hypernuclei; we tried to fit part of the ΛN interaction and to compute the Hypernuclei Λ–hyperon separation energy. Nevertheless we found some good and encouraging results, we noticed that the fixed–phase approximation used in AFDMC algorithm was not so small like assumed. Because of that, in order to obtain interesting results, we need to improve this approximations or to use a better method; hence we looked at AFQMC algorithm aiming to quickly reach good results.

Part I

Monte Carlo Methods

Chapter 1

Variational Monte Carlo

1.1 Why Monte Carlo methods?

The term "Monte Carlo methods" [Kal84, Mal08] indicates all the those stochastic algorithms using the central limit theorem to compute multidimensional integrals. In order to compute numerically a D–dimensional integral with non–stochastic methods (such the Simpson rule, for example) a number of operations (and hence a computational time) that is exponential with the number of dimensions D is required. That is if, we want to estimate the integral with a relative accuracy ϵ, a time proportional to ϵ^{-D} is necessary. Because of the central limit theorem Monte Carlo methods scale as ϵ^{-2}, regardless from the dimensionality.

1.2 Central limit theorem

Let $\{\vec{x}_i\}$ be a sequence of stochastic D–dimensional independent variables distributed with a probability density $\mathscr{P}(\vec{x})$, and $\mathscr{F}(\vec{x})$ a real function. For the function

$$S_N \equiv \frac{1}{N}\sum_{i=1}^{N} \mathscr{F}(\vec{x}_i) \tag{1.1}$$

central limit theorem holds: the probability density S_N in the large N limit can be written as

$$\lim_{N\to+\infty} \mathscr{P}(S_N) = \frac{1}{\sqrt{2\pi\sigma_N^2}} e^{-\frac{(S_N-\langle\mathscr{F}\rangle)^2}{2\sigma_N^2}}, \tag{1.2}$$

where

$$\langle\mathscr{F}\rangle \equiv \int \mathscr{F}(\vec{x})\mathscr{P}(\vec{x})d^Dx, \tag{1.3}$$

$$\langle\mathscr{F}^2\rangle \equiv \int \mathscr{F}^2(\vec{x})\mathscr{P}(\vec{x})d^Dx, \tag{1.4}$$

$$\sigma_N^2 = \frac{\langle\mathscr{F}^2\rangle - \langle\mathscr{F}\rangle^2}{N}. \tag{1.5}$$

In other words S_N is an estimate of $\langle \mathscr{F} \rangle$ ans σ_N is its variance.

Thus we can compute the integral of a generic real function $f(x)$ by means of

$$\int f(\vec{x}) d^D x = \int \frac{f(\vec{x})}{\mathscr{P}(\vec{x})} \mathscr{P}(\vec{x}) d^D x = \int \mathscr{F}(\vec{x}) \mathscr{P}(\vec{x}) d^D x, \tag{1.6}$$

with

$$\mathscr{F}(\vec{x}) \equiv \frac{f(\vec{x})}{\mathscr{P}(\vec{x})}, \tag{1.7}$$

and we can use the central limit theorem Eq(1.2) to write the estimate

$$\int f(\vec{x}) d^D x \simeq S_N \pm \sigma_N. \tag{1.8}$$

The advantage of this procedure is that, according to Eq(1.1), for large N, S_N is spread according to a Gaussian distribution around $\langle \mathscr{F} \rangle$, as from Eq(1.4) with a standard deviation $\sigma_N \propto \frac{1}{\sqrt{N}}$ as in Eq(1.5). The standard deviation decreases as the square root of the number of sampled stochastic variables $\{\vec{x}_i\}$, and it is not dependent from the dimensionality of the integral.

Because of that, the estimation S_N of the integral Eq(1.6) is very efficient for multi–dimensional integrals.

1.3 The idea

With the name Variational Monte Carlo (VMC) method we refer to any algorithm used to stochastically compute the expectation value of an observable $\hat{O}$ on a given wavefunction Ψ_α.

$$O_\alpha \equiv \frac{\langle \Psi_\alpha | \hat{O} | \Psi_\alpha \rangle}{\langle \Psi_\alpha | \Psi_\alpha \rangle} = \frac{\int \Psi_\alpha^\dagger(x) \hat{O} \Psi_\alpha(x) dx}{\int \Psi_\alpha^\dagger(x) \Psi_\alpha(x) dx}. \tag{1.9}$$

Moreover, because of the Riesz theorem, the expectation value of the Hamiltonian obtained by VMC is always an upper bound of the ground state energy:

$$E_\alpha \equiv \frac{\langle \Psi_\alpha | H | \Psi_\alpha \rangle}{\langle \Psi_\alpha | \Psi_\alpha \rangle} = \frac{\int \Psi_\alpha^\dagger(x) H \Psi_\alpha(x) dx}{\int \Psi_\alpha^\dagger(x) \Psi_\alpha(x) dx} \geq E_0. \tag{1.10}$$

If we wanted to study the ground state of a system and we postulated an analytic form of the wavefunction Ψ_α dependent on a set α of variational parameters, we could reach the best description of the ground state within the given ansatz minimizing the energy with respect to the parameters α.

1.4 Markov chains and the Metropolis algorithm

As written in Eq(1.6), in order to compute an integral like Eq(1.9), we need to sample some configuration x from a probability density $\mathscr{P}(x)$. This is in general a not so simple task. There are some efficient and widespread algorithms to

generate uniformly distributed random numbers in a finite size interval. Starting from these sets, it is also possible to obtain a set of random numbers from a normal distribution with the Box–Müller formula. The Metropolis algorithm, based on the Markov chains formalism, allows to sample from a generic distribution. We recall here some fundamentals properties of Markov chains and of the Metropolis algorithm.

A Markov chain is a sequence of stochastic variables converging to a chosen probability density $\mathscr{P}(x)$. A Markov chain is defined as a family $\{x_n\}$ of stochastic variables for which the following properties hold:

- x_i is distributed like a density probability $\mathscr{P}_i(x)$
- $\mathscr{P}_{i+1}(x_{i+1}) = \int \mathscr{W}(x_{i+1} \leftarrow x_i)\mathscr{P}_i(x)\, dx_i$.

where $\mathscr{W}(x_{i+1} \leftarrow x_i)$ is called transition probability.

A Markov chain is called a *stationary* Markov chain when $\mathscr{W}(x_{i+1} \leftarrow x_i)$ is independent from the index i. In this case it is possible to determine all the chain knowing only $\mathscr{P}_1(x)$ and the transition probability $\mathscr{W}$.

Thus we can write

$$\mathscr{P}_k(x_k) = \int \mathscr{W}(x_k \leftarrow x_{k-1}) \dots \mathscr{W}(x_2 \leftarrow x_1)\mathscr{P}_1(x_1)\, dx_{k-1} \dots dx_1, \qquad (1.11)$$

that for a stationary Markov chain simplifies to

$$\mathscr{P}_k(x_k) = \int \mathscr{W}^{k-1}\mathscr{P}_1(x_1)\, dx_{k-1} \dots dx_1. \qquad (1.12)$$

Moreover, if a Markov chain satisfies the detailed balance condition

$$\mathscr{P}_k(x)\mathscr{W}(y \leftarrow x) = \mathscr{P}(y)\mathscr{W}(x \leftarrow y), \qquad (1.13)$$

we can define its limit as:

$$\mathscr{P}_\infty(x) \equiv \lim_{k\to\infty} \mathscr{P}_k(x_k) = \lim_{k\to\infty} \int \mathscr{W}^{k-1}\mathscr{P}_1(x_1)\, dx_{k-1} \dots dx_1. \qquad (1.14)$$

Hereafter we will take into account only stationary Markov chains, and we will assume the following notation

$$\mathscr{P}(x) \equiv \mathscr{P}_\infty(x). \qquad (1.15)$$

As mentioned before, it is not simple to generate a set of stochastic variables distributed like a generic probability density $\mathscr{P}(x)$. Similarly, it is not clear how to generate a new set of stochastic variables x from another one y with a generic transition probability $\mathscr{W}(x \leftarrow y)$.

We assume that it is always possible to split $\mathscr{W}(x \leftarrow y)$ in two terms:

$$\mathscr{W}(x \leftarrow y) \equiv \mathscr{T}(x \leftarrow y)\mathscr{A}(x \leftarrow y), \qquad (1.16)$$

where $\mathscr{T}(x \leftarrow y)$ is a transition probability and $\mathscr{A}(x \leftarrow y)$ is an acceptance probability. We choose a $\mathscr{T}(x \leftarrow y)$ that we are able to apply to x to find y. The idea is that a new set of stochastic variables can be sampled from the old one y simply applying the probability transition $\mathscr{T}(x \leftarrow y)$ to x. Then, using both Eq(1.16) and Eq(1.13), we can find the relation for the acceptance probability $\mathscr{A}(x \leftarrow y)$ that we have to apply after $\mathscr{T}(x \leftarrow y)$:

$$\frac{\mathscr{W}(x \leftarrow y)}{\mathscr{W}(y \leftarrow x)} = \frac{\mathscr{P}(x)}{\mathscr{P}(y)} \qquad \Longrightarrow \qquad \frac{\mathscr{A}(y \leftarrow x)}{\mathscr{A}(x \leftarrow y)} = \frac{\mathscr{P}(y)\mathscr{T}(x \leftarrow y)}{\mathscr{P}(x)\mathscr{T}(y \leftarrow x)}. \tag{1.17}$$

Given the relation in Eq(1.17), we can define

$$\mathscr{A}(x \leftarrow y) = F\left(\frac{\mathscr{P}(x)\mathscr{T}(y \leftarrow x)}{\mathscr{P}(y)\mathscr{T}(x \leftarrow y)}\right) \tag{1.18}$$

where F is any function that satisfies

$$\frac{F(x)}{F(1/x)} = x. \tag{1.19}$$

The standard choice for F is:

$$F(x) \equiv \mathrm{Min}(1, x) \tag{1.20}$$

from which we have

$$\mathscr{A}(x \leftarrow y) = \mathrm{Min}\left(1, \frac{\mathscr{P}(x)\mathscr{T}(y \leftarrow x)}{\mathscr{P}(y)\mathscr{T}(x \leftarrow y)}\right) \tag{1.21}$$

as the acceptance term of Eq(1.16).

The Metropolis[MRR$^+$53] algorithm, called $M(RT)^2$ from the names of the inventors, is a method to sample a generic probability density $\mathscr{P}(x)$.

It proceeds as follows:

1. Start with a set of configurations $\{x_n\}$ (called "walkers") distributed with a probability density $\mathscr{P}_1(x)$. Choose a transition probability $\mathscr{T}(x \leftarrow y)$ convenient to be applied to the configurations.

2. Move each configuration following the chosen probability transition $\mathscr{T}(x \leftarrow y)$; then we "weight" each walker with the acceptance probability $\mathscr{A}(x \leftarrow y)$ of equation Eq(1.21). Iterating this procedure several times only few walkers will have a relevant weight respect to the total population, i.e. our $\mathscr{P}_\infty(x)$ will be represented only by a few configurations. To disallow this disadvantage it is possible to apply $\mathscr{A}(x \leftarrow y)$ simply accepting or rejecting the move according to:

$$\begin{cases} \mathscr{A}(x \leftarrow y) > \varepsilon & \text{accept} \\ \mathscr{A}(x \leftarrow y) < \varepsilon & \text{reject} \end{cases} \tag{1.22}$$

where ε is a random number with $\varepsilon \in [0, 1]$.

3. Iterate the previous points k times, with k big enough to reach the convergence predicted by the properties of the stationary Markov chains, i.e.:

$$\mathscr{P}_k(x) \simeq \mathscr{P}_\infty(x) = \mathscr{P}(x). \tag{1.23}$$

In this way the $\{x_k\}$ configurations will be distributed with a probability density $\mathscr{P}(x)$, as desired.

We want to stress that the more $\mathscr{T}(x \leftarrow y)$ is similar to $\mathscr{W}(x \leftarrow y)$, the more the acceptance probability $\mathscr{A}(x \leftarrow y)$ will be large, and the number of rejected moves will be small like the number of the iterations k needed to reach the convergence. Thus the efficiency of the algorithm will be improved.

Summarizing, to compute an integral with the $M(RT)^2$ algorithm we can proceed as follows. Remembering the equation Eq(1.6), and knowing that $\{x_i\}$ are distributed like a probability density $\mathscr{P}(x)$, with $\mathscr{F}(x) \equiv \frac{f(x)}{\mathscr{P}(x)}$, we can use Eq(1.8) and evaluate

$$\int f(x)dx \simeq S_N \equiv \frac{1}{N}\sum_{i=1}^{N} \mathscr{F}(x_i). \tag{1.24}$$

From equation Eq(1.24) we can see that for a fixed value of N it is possible to reduce the variance, sampling $f(x)$ with a density $\mathscr{P}(x)$ that is "close" to $f(x)$.

1.5 Variational Monte Carlo

The VMC algorithm is simply the application of the previous stochastic method to the idea explained in (§ 1.3).

Now we can see more details about VMC for a simple physical system. For more accurate details we refer to [Kal84, FMNR01, PS77, NU99].

Suppose one wants to study the ground state of a system of N particles neglecting spin or isospin degrees of freedom (or with an Hamiltonian diagonal in spin or isospin space). Under these hypotheses we can compute the integral Eq(1.9) with the method described in the previous section.

We describe the system with a trial wavefunction Ψ_α; typical Ψ_α is written like a product (Slater determinant) of single particle wavefunctions for a Boson (Fermion) system, correlated with a symmetric 2–body Jastrow factor. The integral in Eq(1.10) can be minimized with respect to the parameters α of the trial wavefunction to find a Ψ_α as close as possible to the exact ground state. Then, using the resulting approximation of the wavefunction we are able to compute any other observable by means of Eq(1.24).

Thus to compute

$$O_\alpha \equiv \frac{\langle\Psi_\alpha|O|\Psi_\alpha\rangle}{\langle\Psi_\alpha|\Psi_\alpha\rangle} = \frac{\int \Psi_\alpha^\dagger(x) O \Psi_\alpha(x) dx}{\int \Psi_\alpha^\dagger(x)\Psi_\alpha(x)dx} \tag{1.25}$$

we sample configurations $\{x\}$ from a probability density $\mathscr{P}(x) = \Psi_\alpha^\dagger(x)\Psi_\alpha(x)$, obtaining the estimator for the integral as the sum:

$$O_\alpha = \sum_{\{x\}} \frac{O\Psi_\alpha}{\Psi_\alpha} \tag{1.26}$$

on the sampled configurations x.

In order to implement the $M(RT)^2$ algorithm we have to define a good transition probability $\mathscr{T}(x \leftarrow y)$ as previously described. Starting from a random set of random configurations $\{x\}$ it is possible to evolve that configuration using for $\mathscr{T}(x \leftarrow y)$ a Gaussian centered on y.

$$\mathscr{T}(x \leftarrow y) = \frac{1}{\sqrt{2\pi\sigma}} e^{-\frac{(x-y)^2}{2\sigma}}. \tag{1.27}$$

The width σ of the Gaussian can be tuned to obtain a reasonable acceptance probability and correlation length of the Markov chain, i.e. the best efficiency of the algorithm. An improvement could be obtained including by a drift related to the slope of the wavefunction, i.e. using

$$\mathscr{T}(x \leftarrow y) = \frac{1}{\sqrt{2\pi\sigma}} e^{-\frac{\left(x-y-\sigma\frac{\nabla\Psi_\alpha(y)}{\Psi_\alpha(y)}\right)^2}{2\sigma}}. \tag{1.28}$$

Clearly, the acceptance factor $\mathscr{A}(x \leftarrow y)$ must be computed like in Eq(1.21). This is quite simple, clear and efficient also for system with a lot of particles.

1.6 VMC for nuclei

So far we focused our attention on systems composed of N particles with no internal degrees of freedom, i.e. with a trial wavefunction that is simply a function of the coordinates of the N particles. A good trial wavefunction for such systems can be written as a sum of N_{Det} Slater determinants of single particle wavefunctions ϕ, i.e.

$$\Psi_T = \mathcal{J}_2 \cdot \mathcal{J}_3 \cdot \sum_i^{N_{Det}} c_i \begin{vmatrix} \phi_{i1}(r_1) & \dots & \phi_{iN}(r_1) \\ \vdots & \ddots & \vdots \\ \phi_{i1}(r_N) & \dots & \phi_{iN}(r_N) \end{vmatrix}, \tag{1.29}$$

with a symmetric 2 and 3–body Jastrow factors $\mathcal{J}_2$ and $\mathcal{J}_3$ defined as follows

$$\mathcal{J}_2 = \prod_{i\neq j}^{N} J_2(r_i, r_j), \tag{1.30}$$

$$\mathcal{J}_3 = \prod_{i\neq j\neq k}^{N} J_3(r_i, r_j, r_k). \tag{1.31}$$

Typically, a good choice for J_2 and J_3 could be obtained by solving the two–body and three–body systems.

Now we focus our attention to a typical many–nucleon system. Typically the interaction significantly depends on the relative spin/isospin channel. This

means that in general one should include spin/isospin dependence in the Jastrow factors. The single particle space will be the direct product of the coordinate space $\mathcal{H}_r$, the spin space $\mathcal{H}_\sigma$ and the isospin space $\mathcal{H}_\tau$:

$$\mathcal{H} = \mathcal{H}_r \otimes \mathcal{H}_\sigma \otimes \mathcal{H}_\tau, \tag{1.32}$$

and the one–body wavefunction can be written as a 4–spinor

$$\begin{pmatrix} \phi_{p\uparrow}(r) \\ \phi_{p\downarrow}(r) \\ \phi_{n\uparrow}(r) \\ \phi_{n\downarrow}(r) \end{pmatrix}, \tag{1.33}$$

i.e.

$$\phi_{p\uparrow}(r)\ |p\uparrow\rangle + \phi_{n\uparrow}(r)\ |n\uparrow\rangle + \phi_{p\downarrow}(r)\ |p\downarrow\rangle + \phi_{n\downarrow}(r)\ |n\downarrow\rangle. \tag{1.34}$$

where N (P) is the neutron (proton) component and the arrows indicates the up and down spin projections.

In order to take into account spin/isospin dependent correlations we must use two–body operatorial correlators J_{ij}:

$$J_{ij} = \sum_p^{N_{Op}} j_p(r_{ij})\mathcal{O}_p, \tag{1.35}$$

where $\mathcal{O}_p$ are the N_{Op} two–body spin/isospin operators describing the state dependence of the interaction, and $j_p(r_{ij})$ are radial functions depending on the distance between i and j. It is also possible to add in a similar way three–body correlation terms[Wir81].

Naming $|\Phi\rangle$ the sum over Slater determinants, we define the trial wavefunction as

$$|\Psi_T\rangle = \left[\mathcal{S}\prod_{i<j}(1+J_{ij})\right]\prod_{i<j}J_c(r_{ij})|\Phi\rangle\ . \tag{1.36}$$

where $J_c(r)$ is a "central" Jastrow correlation depending on relative space coordinate only, J_{ij} is the previously defined two–body Jastrow correlation factor and $\mathcal{S}$ is a symmetrization operator enforcing the antisymmetry of the Slater determinant.

We want to point out two things:

- the number of operations necessary to compute the symmetrization operator $\mathcal{S}$ scales as $\left[\frac{N(N-1)}{2}\right]!$ where N is the particle number. So it quickly becomes too expensive to be computed exactly and it can be only stochastically sampled.
- The sum over different Jastrow terms is naturally defined in the product space of single particle sub–spaces, and it cannot be generally rewritten in

a simpler form. Thus it is mandatory to represent the sampled configuration in the full product space of spin/isospin single particles sub–spaces; in other words we can say that our configuration must be represented by a 4^N spinor; similarly the operator in front of our Slater determinant will be a $4^N \times 4^N$ matrix. This exponential scaling limits to small systems the applicability of the method[Pie05].

In nuclear systems, for a VMC calculation[Wir91] it is necessary to use a wavefunction including a spin/isospin dependent Jastrow correlation factor to obtain a reliable wavefunction. Theoretically it is possible not to use explicitly that correlations, but to construct them simply with a sum over a set of different Slater determinant.

Chapter 2

Diffusion Monte Carlo

2.1 The imaginary time Schrödinger equation

Starting from the time dependent Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = H|\psi(t)\rangle \qquad \Longrightarrow \qquad |\psi(t)\rangle = e^{-\frac{iH}{\hbar}(t-t_0)}|\psi(t_0)\rangle \tag{2.1}$$

with an analytic continuation in imaginary time $\tau = it$ we can rewrite Eq(2.1) as

$$-\hbar\frac{\partial}{\partial \tau}|\psi(\tau)\rangle = H|\psi(\tau)\rangle \qquad \Longrightarrow \qquad |\psi(\tau)\rangle = e^{-\frac{H}{\hbar}(\tau-\tau_0)}|\psi(\tau_0)\rangle. \tag{2.2}$$

Expanding the wavefunction on a complete orthonormal set $|\phi_n\rangle$ of wavefunctions of the Hamiltonian H with eigenvalues E_n, at time τ_0 we have that

$$|\psi(\tau_0)\rangle = \sum c_n|\phi_n\rangle \tag{2.3}$$

Thus we can define $|\Psi(\tau)\rangle$ as

$$\begin{aligned} |\Psi(\tau)\rangle &\equiv e^{\frac{E_0}{\hbar}\tau}|\psi(\tau)\rangle = \\ &= e^{\frac{E_0}{\hbar}\tau}e^{-\frac{H}{\hbar}\tau}|\psi(\tau_0)\rangle = \\ &= \sum c_n e^{-\frac{(E_n-E_0)}{\hbar}\tau}|\phi_n\rangle \end{aligned} \tag{2.4}$$

where $e^{E_0\tau/\hbar}$ is a factor that is used to preserve the normalization of the component of the wavefunction along $|\phi_0\rangle$. In the long time limit we have

$$\lim_{\tau\to\infty}|\Psi(\tau)\rangle = c_0|\phi_0\rangle, \tag{2.5}$$

i.e. starting from any wave function $|\psi\rangle$, not orthogonal to the ground state $|\phi_0\rangle$, we can obtain $|\phi_0\rangle$ evolving $|\Psi\rangle$ for a sufficiently long "imaginary" time τ.

Including a completeness on a orthonormal basis $|R'\rangle$ in Eq(2.2) yields:

$$|\Psi(\tau+d\tau)\rangle = e^{-Hd\tau}|\Psi(\tau)\rangle = \int e^{-Hd\tau}|R'\rangle\langle R'|\Psi(\tau)\rangle dR'. \tag{2.6}$$

Projecting on $|R\rangle$ we obtain:

$$\langle R|\Psi(\tau+d\tau)\rangle = \langle R|e^{-Hd\tau}|\Psi(\tau)\rangle = \int \langle R|e^{-Hd\tau}|R'\rangle\langle R'|\Psi(\tau)\rangle dR' \tag{2.7}$$

The propagator $\langle R|e^{-Hd\tau}|R'\rangle$ would be simplified if the Hamiltonian $H = T + V'$ was split in two terms, one T not diagonal and one other V' diagonal in $|R\rangle$. Because T and V' generally do not commute, it is not possible to split the exponential

$$e^{-T\tau}e^{-V'\tau}e^{-(T+V')d\tau} \neq e^{-Td\tau}e^{-V'd\tau}. \tag{2.8}$$

However, in the limit of small $d\tau$ it is possible to use the Trotter-Suzuki formula

$$e^{-(T+V')d\tau} = e^{-\frac{V'd\tau}{2}}e^{-Td\tau}e^{-\frac{V'd\tau}{2}} + \mathcal{O}(d\tau^3) \tag{2.9}$$

and we can still use the previous splitting Eq(2.9) in the limit $|d\tau^3[T,V']| \ll 1$.

Eventually, with Eq(2.9), using two completeness in Eq(2.7) and using the notation $\Psi(R,\tau) \equiv \langle R|\Psi(\tau)\rangle$ e $V'(R) \equiv \langle R|V'|R\rangle$ we have that

$$\begin{aligned}\Psi(R,\tau+d\tau) &\simeq \int \langle R'|e^{-\frac{V'}{2}d\tau}e^{-Td\tau}e^{-\frac{V'}{2}d\tau}|R\rangle\Psi(R',\tau)dR' \\ &\simeq \int e^{-\frac{V'(R')+V'(R)}{2}d\tau}\langle R'|e^{-Td\tau}|R\rangle\Psi(R',\tau)dR'\end{aligned} \tag{2.10}$$

If $T = -\frac{\hbar^2}{2m}\nabla^2$ we have that $\langle R'|e^{-Td\tau}|R\rangle$ is the Green's function of the kinetic term; this Green's function is that of a Fokker-Plank equation for which we already known the analytic form like shown in Eq(2.31).

Thus, calling E_0 the ground state energy, m the mass and $V' = V - E_0$ with V' a generic potential diagonal respect to the coordinates, we have that :

$$\Psi(R,\tau+d\tau) \simeq \int \underbrace{e^{-\left(\frac{V(R')+V(R)}{2}-E_0\right)\frac{d\tau}{\hbar}}}_{G_V(R\leftarrow R',d\tau)} \underbrace{\frac{1}{\left(\frac{2\pi\hbar}{m}d\tau\right)^{\frac{nD}{2}}} \quad e^{-\frac{(R-R')^2}{\frac{2\hbar}{m}d\tau}}}_{G_0(R\leftarrow R',d\tau)} \Psi(R',\tau)dR' \tag{2.11}$$

where D is the number of the spatial dimensions and N is the number of particles.

Now we want to implement the evolution for a time $\tau \to \infty$, in such a way to obtain the ground state $\phi_0(R) = \lim_{\tau\to\infty}\Psi(R,\tau)$. Remembering that Eq(2.11) is valid for small $d\tau$, we can solve the problem iteratively: starting from an arbitrary $\Psi(R,\tau)$, then $\Psi(R,\tau+d\tau)$ is computed and used in Eq(2.11) until convergence is reached. The integral Eq(2.11) can be estimated by means of the standard Monte Carlo procedure.

Remembering Eq(1.6) we define

$$\mathscr{P}(R)_{|\tau} = \Psi(R,\tau), \tag{2.12}$$

$$\mathscr{F}(R)|_{d\tau} = G_V(R \leftarrow R',d\tau)\cdot G_0(R\leftarrow R',d\tau). \tag{2.13}$$

$\mathscr{P}(R)$ is a probability density, so therefore Eq(2.12) requires the condition:

$$\Psi(R,\tau) \geq 0 \qquad \forall\tau, \tag{2.14}$$

i.e. that $V(R)$ is real and that $\Psi(R,\tau)$ is real and positive. This fact limits a naive implementation of the method to the absolute ground state of the Hamiltonian, which is a nodeless function.

The algorithm can be summarized as follows:

1. An initial distribution of walkers is sampled from a trial wavefunction $\Psi(R,\tau_0)$; a sufficiently small time–step $d\tau$ is fixed and a guess E_0 for the ground state energy is made.

2. Each walker is diffused with a Gaussian transition probability:

$$\mathscr{W}(R \leftarrow R') = G_0(R \leftarrow R', d\tau) = \frac{1}{\left(\frac{2\pi\hbar}{m}d\tau\right)^{\frac{nD}{2}}} \quad e^{-\frac{(R-R')^2}{\frac{2\hbar}{m}d\tau}}. \tag{2.15}$$

   This means that new configurations R are generated by means of a purely diffusive dynamics

$$R = R' + \xi \qquad \xi = \sqrt{\sigma}\,\eta \tag{2.16}$$

   where ξ is a stochastic variable with a Gaussian probability density with variance $\sigma^2 = \hbar dt/m$ and zero average using the Box-Müller formula[1].

3. Each of the new N_0 walkers has a weight $G_V(R \leftarrow R', d\tau)$

$$\mathscr{P}_B = e^{-\left(\frac{V(R')+V(R)}{2} - E_0\right)\frac{d\tau}{\hbar}} \tag{2.17}$$

   For each walker a integer number of copies proportional to $\mathscr{P}_B$ are created. The walkers are destroyed if $\mathscr{P}_B = 0$. To have an integer number instead of the factor Eq(2.17) we consider the "branching" factor of the i–th walker defined as

$$m_i = Int\left(e^{-\left(\frac{V(R')+V(R)}{2} - E_0\right)\frac{d\tau}{\hbar}} + \varepsilon\right) \tag{2.18}$$

   with ε a uniform random number in $[0,1]$. The new population is now made up by $N = \sum_{i=1}^{N_0} m_i$ walkers. In order to keep the number of walkers more or less constant during the simulation, the branching probability $\mathscr{P}_B$ can be multiplied by a factor $\frac{N_0}{N}$, thereby redefining the local part of the Green's function G_V. The logarithm of the normalization factor, called growth energy

$$E_{gro} = E_0 - \ln\left(G_V(R \leftarrow R', d\tau)\right)/d\tau \tag{2.19}$$

   can be used to have another estimator for the energy of the system. This procedure gives the distribution of walkers $\Psi(R,\tau+d\tau)$ at time $\tau + d\tau$.

[1] If ε_1 and ε_2 are stochastic variables sampled from a uniform probability density in $[0,1]$, then

$$\eta = \cos(2\pi\varepsilon_2)\sqrt{-2\log(\varepsilon_1)}$$

will be a stochastic variable sampled from a Gaussian probability density with 0 average and unitary variance.

4. When the convergence is reached, i.e. for τ large enough to reach the "infinite" limit Eq(2.5), we can compute expectation values of any observable O:

$$\begin{aligned}\langle O\rangle &= \frac{\langle\phi_0|O|\phi_0\rangle}{\langle\phi_0|\phi_0\rangle} = \lim_{\tau\to\infty}\frac{\langle\Psi(\tau_0)|O|\Psi(\tau)\rangle}{\langle\Psi(\tau_0)|\Psi(\tau)\rangle} \\ &= \lim_{\tau\to\infty}\frac{\int\langle\Psi(\tau_0)|O|R\rangle\langle R|\Psi(\tau)\rangle dR}{\int\langle\Psi(\tau_0)|R\rangle\langle R|\Psi(\tau)\rangle dR}\end{aligned} \tag{2.20}$$

The walkers are already distributed with a probability density $\mathscr{P}(R) = \Psi(R,\tau)$ and thus we have that

$$\langle O\rangle = \frac{\sum_{i=1}^{N}\langle R_i|O|\Psi(\tau_0)\rangle}{\sum_{i=1}^{N}\langle R_i|\Psi(\tau_0)\rangle} = \frac{\sum_{i=1}^{N} O\Psi(R_i,\tau_0)}{\sum_{i=1}^{N}\Psi(R_i,\tau_0)} \tag{2.21}$$

5. The procedure must be iterated until convergence is reached and until a small enough statistical error is reached.

2.2 Fokker-Plank equation

In this technical paragraph we show how to obtain the formula of the Green's function of the Fokker–Plank equation, that we used in the previous paragraph. Moreover we derive also the formula of the Green's function of the Fokker–Plank equation with a diffusive term; this Green's function will be used in the next section.

Consider the following system

$$\begin{cases}\dfrac{\partial}{\partial t}\psi(R,\tau) - A\nabla^2\psi(R,\tau) = 0 \\ \psi(R,0) = \phi(R)\end{cases} \tag{2.22}$$

Using a Fourier transform with respect to R we can write

$$\begin{cases}\dfrac{\partial}{\partial t}\tilde{\psi}(k,\tau) + Ak^2\tilde{\psi}(k,\tau) = 0 \\ \tilde{\psi}(k,0) = \tilde{\phi}(k)\end{cases} \tag{2.23}$$

from which we obtain

$$\tilde{\psi}(k,\tau) = \tilde{\phi}(k)e^{-Ak^2\tau} \tag{2.24}$$

Defining

$$\tilde{g}(k) = (2\pi)^{-\frac{n}{2}}e^{-Ak^2\tau} \tag{2.25}$$

and n as the dimensionality, we can rewrite Eq(2.24) as

$$\tilde{\psi}(k,\tau) = \tilde{\phi}(k)\tilde{g}(k)(2\pi)^{\frac{n}{2}} \tag{2.26}$$

Using the definition of the convolution product

$$\mathscr{F}(\phi * g) = (2\pi)^{\frac{n}{2}}\mathscr{F}(\phi)\mathscr{F}(g) \tag{2.27}$$

we can antitransform obtaining

$$\psi(R,\tau) = [\phi(R',\tau) * g(R',\tau)](R) = \int \phi(R')g(R-R')dR'. \tag{2.28}$$

The inverse transformation of $\tilde{g}(R)$ (a Gaussian) is again a Gaussian with a different variance

$$g(R) = \mathscr{F}^{-1}[\tilde{g}(k)] = \frac{1}{(2\pi)^n}\int e^{-Ak^2\tau}e^{ikR}dk = \frac{1}{(4\pi A\tau)^{\frac{n}{2}}}e^{-\frac{R^2}{4A\tau}}. \tag{2.29}$$

Thus we have

$$\psi(R,\tau) = \frac{1}{(4\pi A\tau)^{\frac{n}{2}}}\int e^{-\frac{(R-R')^2}{4A\tau}}\psi(R',0)dR', \tag{2.30}$$

and the Green's function of the Fokker–Plank equation Eq(2.22) is:

$$G(R \leftarrow R',\tau) = \frac{1}{(4\pi A\tau)^{\frac{n}{2}}}e^{-\frac{(R-R')^2}{4A\tau}}. \tag{2.31}$$

Now consider a system in which the non–local operator includes a gradient

$$\begin{cases} \dfrac{\partial}{\partial t}\psi(R,\tau) - A\nabla^2\psi(R,\tau) + B\nabla\psi(R,\tau) = 0 \\ \psi(R,0) = \phi(R) \end{cases} \tag{2.32}$$

As previously done using the Fourier transform, we obtain from the previous

$$\begin{cases} \dfrac{\partial}{\partial t}\tilde{\psi}(k,\tau) + (Ak^2 + iBk)\tilde{\psi}(k,\tau) = 0 \\ \tilde{\psi}(k,0) = \tilde{\phi}(k) \end{cases} \tag{2.33}$$

and in the end

$$\tilde{\psi}(k,\tau) = \tilde{\phi}(k)e^{-(Ak^2+ikB)\tau}. \tag{2.34}$$

Defining

$$\tilde{g}(k) = (2\pi)^{-\frac{n}{2}}e^{-(Ak^2+ikB)\tau} \tag{2.35}$$

and antitransforming $\tilde{g}(k)$, as for Eq(2.29), but completing the square at the exponent and applying a simple change of variables we obtain a Gaussian centered in 0:

$$g(R) = \frac{1}{(4\pi A\tau)^{\frac{n}{2}}}e^{-\frac{(R-B\tau)^2}{4A\tau}}. \tag{2.36}$$

Thus we have that

$$\psi(R,\tau) = \frac{1}{(4\pi A\tau)^{\frac{n}{2}}}\int e^{-\frac{(R-R'-B\tau)^2}{4A\tau}}\psi(R',0)dR', \tag{2.37}$$

and the Green's function of the Fokker–Plank equation Eq(2.32) is

$$G(R \leftarrow R',\tau) = \frac{1}{(4\pi A\tau)^{\frac{n}{2}}}e^{-\frac{(R-R'-B\tau)^2}{4A\tau}}. \tag{2.38}$$

2.3 Importance sampling

The algorithm described in (§ 2.1) is not very efficient because the branching factor $G_V(R \leftarrow R', d\tau)$ has large fluctuations causing large population fluctuations and statistical correlations of the walkers. But if an approximative trial wavefunction $\varphi(R)$ of the ground state $\phi_0(R)$ is known, then it is possible to dramatically improve the algorithm efficiency.

Introducing the function

$$f(R,\tau) \equiv \Psi(R,\tau)\varphi(R) \tag{2.39}$$

and adding the factor $\varphi(R)$ at both sides of the imaginary time Schrödinger equation Eq(2.2), we obtain

$$-\hbar\frac{\partial}{\partial t}f(R,\tau) = -\frac{\hbar^2}{2m}\nabla^2 f(R,\tau) + \frac{\hbar^2}{m}\nabla\left[v_D(R)f(R,\tau)\right] + \left[E_L(R) - E_0\right]f(R,\tau) \tag{2.40}$$

with

$$v_D(R) = \frac{\nabla\varphi(R)}{\varphi(R)}, \qquad E_L(R) = \frac{H\varphi(R)}{\varphi(R)} \tag{2.41}$$

under the assumption that the potential V is diagonal with respect to the coordinates. Defining

$$K \equiv T + \frac{\hbar^2}{m}\nabla v_D(R) + (E_L(R) - E_0), \tag{2.42}$$

and rewriting Eq(2.41), using the Trotter-Suzuki formula Eq(2.9), we obtain neglecting terms smaller than $d\tau^3$

$$\begin{aligned} f(R,\tau+d\tau) = e^{-\frac{d\tau}{\hbar}K}f(R,\tau) = \int \langle R|e^{-K\frac{d\tau}{\hbar}}|R'\rangle f(R',\tau)dR' = \\ \simeq \int \underbrace{e^{-\frac{d\tau}{\hbar}\left(\frac{E_L(R)+E_L(R')}{2}-E_0\right)}}_{G_B(R\leftarrow R',d\tau)} \underbrace{\langle R|e^{-\frac{d\tau}{\hbar}(T+\frac{\hbar^2}{m}\nabla v_D)}|R'\rangle}_{G_D(R\leftarrow R',d\tau)} f(R',\tau)dR' \end{aligned} \tag{2.43}$$

The analytic form of $G_D(R \leftarrow R', d\tau)$ is not known, unless in the case $\nabla v_D \simeq 0$. In this case Eq(2.40) is a Fokker–Plank equation with a diffusive term, whose Green's function Eq(2.38) is known. Thus, without the branching factor $G_B(R \leftarrow R', d\tau)$, we have that

$$G_D(R \leftarrow R', d\tau) \simeq \tilde{G}_D(R \leftarrow R', d\tau) = \frac{1}{(2\pi\hbar d\tau/m)^{\frac{nD}{2}}} \quad e^{-\frac{\left(R-R'-d\tau\frac{\hbar}{m}v_D(R')\right)^2}{2\hbar d\tau/m}} \tag{2.44}$$

where D is the spacial dimension number and n the number of particles.

Hence we can see that $G_D(R \leftarrow R', d\tau) = \tilde{G}_D(R \leftarrow R', d\tau) + \mathcal{O}[d\tau^2]$. So it is possible to use $\tilde{G}_D(R \leftarrow R', d\tau)$ instead of $G_D(R \leftarrow R', d\tau)$ loosing a term $d\tau^2$.

Now multiplying Eq(2.11) by $\varphi(R)$ we have

$$\begin{aligned} f(R,\tau+d\tau) \equiv \Psi(R,\tau+d\tau)\varphi(R) \simeq \\ \simeq \int G_V(R \leftarrow R', d\tau) G_0(R \leftarrow R', d\tau)\varphi(R)\Psi(R',\tau)dR' \\ \simeq \int G_V(R \leftarrow R', d\tau) G_0(R \leftarrow R', d\tau)\frac{\varphi(R)}{\varphi(R')}\Psi(R',\tau)\varphi(R')dR' \\ \simeq \int G_V(R \leftarrow R', d\tau) G_0(R \leftarrow R', d\tau)\frac{\varphi(R)}{\varphi(R')} f(R',\tau)dR' \end{aligned} \tag{2.45}$$

from which we have the form of $G_D(R \leftarrow R', d\tau)$

$$\begin{aligned} G(R \leftarrow R', d\tau) &= G_V(R \leftarrow R', d\tau) G_0(R \leftarrow R', d\tau)\frac{\varphi(R)}{\varphi(R')} \\ &= G_B(R \leftarrow R', d\tau) \underbrace{\left[\frac{G_V(R \leftarrow R', d\tau) G_0(R \leftarrow R', d\tau)\frac{\varphi(R)}{\varphi(R')}}{G_B(R \leftarrow R', d\tau)}\right]}_{G_D(R \leftarrow R', d\tau)} \end{aligned} \tag{2.46}$$

As seen in the previous paragraph, we want to iteratively solve equation Eq(2.43). The integral Eq(2.43) is computed with a Monte Carlo procedure for which we choose

$$\mathscr{P}(R)|_\tau = f(R,\tau) \tag{2.47}$$

$$\mathscr{F}(R)|_{d\tau} = G_B(R \leftarrow R', d\tau) \cdot G_D(R \leftarrow R', d\tau) \tag{2.48}$$

This means again that we require that the wavefunctions $\varphi(R)$ and $\Psi(R,\tau)$ are positive defined and that $V(R)$ is real. This condition is generally satisfied for the ground state of a Boson system with a real potential $V(R)$.

2.4 DMC algorithm

The summary of the DMC algorithm is so the following:

1. At first a trial wavefunction $\varphi(R)$ is chosen, that is a good approximation of the ground state; a sufficiently small time–step $d\tau$ is taken, a guess for the value of the ground state energy E_0 and a set of N_0 configurations are determined. It is better to choose configurations distributed like $\varphi^2(R)$ because the initial population should be not too far from $\varphi(R) \simeq \phi_0(R)$.

2. A representation of the walkers, initially distributed with a probability density $f(R,\tau)$, is evolved using a transition probability $G_D(R \leftarrow R', d\tau)$. This exact Green's function is not known, but the approximation Eq(2.44) it is good for small $d\tau$:

$$\tilde{G}_D(R \leftarrow R', d\tau) = \frac{1}{(2\pi\hbar d\tau/m)^{\frac{nD}{2}}} \quad e^{-\frac{\left(R-R'-\frac{d\tau\hbar}{m}v_D(R')\right)^2}{2d\tau\hbar/m}} \tag{2.49}$$

3. The walkers are then weighted with the branching factor $G_B(R \leftarrow R', d\tau)$ as defined in Eq(2.43). A number of copies of each walker are made equal to branching factor

$$m_i = Int\left(\frac{N_0}{N}\, e^{-\left(\frac{E_L(R')+E_L(R)}{2}-E_0\right)d\tau/\hbar} + \varepsilon\right) \tag{2.50}$$

with ε a uniform random variable in $[0,1]$, N_0 the target number N of walkers the current number of walkers. Also in this case it is possible to define an estimator of the energy of the ground state extracted from the normalization factor; this is the growth energy E_{gro} like in Eq(2.19):

$$E_{gro} = E_0 - \ln\left(G_B(R \leftarrow R', d\tau)\right)/d\tau \tag{2.51}$$

4. When convergence is reached, i.e. for large τ it is possible to compute expectation values of any observable O for which the ground state is an eigenstate:

$$\begin{aligned}\langle O\rangle &= \frac{\langle\phi_0|O|\phi_0\rangle}{\langle\phi_0|\phi_0\rangle} = \lim_{\tau\to\infty}\frac{\langle\varphi|O|\Psi(\tau)\rangle}{\langle\varphi|\Psi(\tau)\rangle} \\ &= \lim_{\tau\to\infty}\frac{\int\langle\varphi|O|R\rangle\langle R|\Psi(\tau)\rangle dR}{\int\langle\varphi|R\rangle\langle R|\Psi(\tau)\rangle dR} = \lim_{\tau\to\infty}\frac{\int O\varphi(R)\quad\Psi(R,\tau)dR}{\int\varphi(R)\quad\Psi(R,\tau)dR} \\ &= \lim_{\tau\to\infty}\frac{\int\frac{O\varphi(R)}{\varphi(R)}\quad\Psi(R,\tau)\varphi(R)dR}{\int\Psi(R,\tau)\varphi(R)dR}\end{aligned} \tag{2.52}$$

The walkers are now sampled with a probability $\mathscr{P}(R) = f(R,\tau) = \Psi(R,\tau)\varphi(R)$ and thus we can write

$$\langle O\rangle = \sum_{i=1}^{N}\frac{\langle R_i|O|\varphi\rangle}{\langle R_i|\varphi\rangle} = \sum_{i=1}^{N}\frac{O\varphi(R_i)}{\varphi(R_i)} \tag{2.53}$$

We have to note that the first equivalence in Eq(2.52) is true only when $[O,H]=0$, i.e. when the ground state is an eigenstate of O and not only of H. In other cases with Eq(2.53) we compute only the mixed matrix element $\langle\phi_0|O|\varphi\rangle \neq \langle\phi_0|O|\phi_0\rangle$. Thus when $\varphi \simeq \phi_0$ we can estimate the expectation values of that variables computing with VMC $\langle\varphi|O|\varphi\rangle$ and computing

$$\langle O\rangle \simeq 2\langle\phi_0|O|\varphi\rangle - \langle\varphi|O|\varphi\rangle + \mathcal{O}[(\varphi-\phi_0)^2] \tag{2.54}$$

or, if the eigenvalue of O is positive, computing

$$\langle O\rangle \simeq \frac{\left(\langle\phi_0|O|\varphi\rangle\right)^2}{\langle\varphi|O|\varphi\rangle} + \mathcal{O}[(\varphi-\phi_0)^2] \tag{2.55}$$

For more details relative to these observables we refer also to [CB95, BM99, BR04].

5. The procedure must be iterated from point 2, until convergence is reached as for the non importance sampled algorithm.

More details can be found in [NU99, UNR93, Mal08, FMNR01].

2.5 The fixed–node approximation

The constraints imposed by the request that the Monte Carlo procedure samples a given probability density of points in the configuration space, requires that

$$f(R,\tau) = \Psi(R,\tau)\varphi(R) \geq 0 \tag{2.56}$$

This request is automatically fulfilled for the absolute ground state of H. However, if we are interested in computing the properties of a many Fermion system, the corresponding wavefunction is not positive definite, as it occurs for any excited state. In this case the DMC procedure is modified by introducing the so called "fixed–node" approximation[Cep91, Rey82, Mit06, FHN99, TW05].

Within sud approximation, $f(R,\tau)$ has the properties required to be a well defined probability density and can be extended to map a function of the required symmetry.

Eq(2.48) also requires that

$$G(R \leftarrow R', d\tau) = G_B(R \leftarrow R', d\tau) \underbrace{\left[\frac{G_V(R \leftarrow R', d\tau) G_0(R \leftarrow R', d\tau) \frac{\varphi(R)}{\varphi(R')}}{G_B(R \leftarrow R', d\tau)} \right]}_{G_D(R \leftarrow R', d\tau)} \geq 0 \tag{2.57}$$

where $G(R \leftarrow R', d\tau)$ is a probability density.

Now if $V(R)$, $\varphi(R)$ and $\Psi(R,\tau)$ are real functions, we have that $G_B(R \leftarrow R', d\tau) \geq 0$. But also $G_D(R \leftarrow R', d\tau)$ is a transition probability and so $G_D(R \leftarrow R', d\tau) \geq 0$. We have that $G_0(R \leftarrow R', d\tau) \geq 0$ and $G_V(R \leftarrow R', d\tau) \geq 0$ when $V(R)$ is real. With these hypothesis for Eq(2.57) we have that

$$\varphi(R)\varphi(R') \geq 0 \tag{2.58}$$

In order to use the previous algorithm we need to assume that $V(R)$, $\Psi(R,\tau)$ and $\varphi(R)$ are real functions, i.e. that:

- the projected wavefunction has the same sign of $\varphi(R)$, i.e that $\lim_{\tau\to\infty} \Psi(R,\tau) = \chi(R) \neq \phi_0(R)$;
- any walker cannot cross the nodal surface of $\varphi(R)$.

The last requirement is equivalent to add to the Hamiltonian used in the propagator an effective delta term δ_α along the nodal surface[2] α of the trial wavefunction $\varphi(R)$.

In general the problem is transposed into the solution of the following equations

$$\begin{cases} (H + \delta_\alpha)\chi(R) = E_\alpha \chi(R) \\ \chi(R)\varphi(R) \geq 0 \end{cases} \quad \text{with } \lim_{\tau\to\infty} \Psi(R,\tau) = \chi(R) \tag{2.59}$$

[2] $\alpha = \{\forall R | \varphi(R) = 0 \wedge \nabla\varphi(R) \neq 0\}$, i.e. the region where $\varphi(R)$ changes sign.

It is possible to prove that the energy computed is an upper bound to the Fermion ground state, or more generally an upper bound to fundamental state with a given symmetry $\mathcal{A}$.

Let assume that:

- $\varphi(R) \equiv \hat{A}\tilde{\varphi}(R)$ is a a generic real trial wavefunction;
- the operator $\hat{A}$ acts on the wavefunction $\tilde{\varphi}(R)$ in such a way that $\hat{H}$ is invariant respect to the transformation group $\mathcal{G}$ on $\varphi(R) \equiv \hat{A}\tilde{\varphi}(R)$;
- $[\hat{H}, \hat{A}] = 0$ and $\hat{A}$ is a Hermitian ($\hat{A}^\dagger = \hat{A}$) projector (with $\hat{A}\hat{A} = \hat{A}$);
- $\varphi(R) \equiv A\tilde{\varphi}(R)$ belongs to a one–dimensional representation $\mathcal{A}$ of the group $\mathcal{G}$; i.e. $\hat{A}$ projects the component of $\tilde{\varphi}(R)$ that has the symmetry $\mathcal{A}$;
- $\hat{H}$ does not contains itself delta terms;
- E_0 is the energy of the lower eigenstate with symmetry $\mathcal{A}$.

If the Hamiltonian is invariant respect to the action of the symmetry group $\mathcal{G}$, and if $\varphi(R) \equiv \hat{A}\tilde{\varphi}(R)$ transforms like a real one–dimensional representation $\mathcal{A}$ of $\mathcal{G}$, the nodal surface α (i.e. the set of zeros) of the trial wavefunction is unchanged. So it can be $\delta_\alpha \neq 0$ only where $\chi = 0$ or $\hat{A}\chi = 0$.

With these hypothesis we have the following theorem

$$E_0 \leq \frac{\langle \hat{A}\tilde{\varphi}|\hat{H}|\hat{A}\chi\rangle}{\langle \hat{A}\tilde{\varphi}|\hat{A}\chi\rangle} = \frac{\langle \hat{A}\tilde{\varphi}|\hat{H}|\chi\rangle}{\langle \hat{A}\tilde{\varphi}|\chi\rangle} = \frac{\langle \varphi|\hat{H} + \delta_\alpha|\chi\rangle}{\langle \varphi|\chi\rangle} = E_\alpha \tag{2.60}$$

where the equivalence is valid only when the nodal surface $\varphi(R)$ is the same of the true ground state ϕ_0

Finally, a few more observations:

- The trial wavefunction $\varphi(R)$ must have the required symmetry $\mathcal{A}$, otherwise the algorithm projects on the lowest energy component without that symmetry; this fact is particularly important to consider when the procedure is applied to the study of excited states.
- In order to satisfy Eq(2.58) every move of the walker that crosses the the nodal surface α is rejected.
- The wavefunction of a Fermionic system transform like a real one–dimensional representation of the permutation group. In that case A is the operator projecting on the antisymmetric component. The energy so obtained is in that case an upper bound.
- Sometimes the nodal surface is completely defined by the required symmetry. For example, in the case of a polarized Fermionic system, the antisymmetry fixes $D(N-1)$ dimension of the nodal surface. The dimension of the nodal surface is $DN - 1$ (where D are the number of spatial

dimensions and N the number of particles). So in the case $D = 1$ the exact nodal surface is known and we are able to compute the exact energy of the ground state.

- We have to require that $\varphi(R)$ transforms like a one–dimensional real representation of the symmetry group $\mathcal{G}$, that means imposing a stronger condition to satisfy the variational principle. This is because if H is invariant with respect to the group $\mathcal{G}$, $H + \delta_\alpha$ generally is not and we have to consider a subgroup $\mathcal{G}_{FN}$ of $\mathcal{G}$ for which $H + \delta_\alpha$ is invariant, i.e. for which the nodal surface is invariant.

2.6 Fixed–node extensions

We have tested some alleged improvements on the estimate of the upper bound energy in the fixed–node approximation. In fact, for some systems it is not simple to determine by some independent method a nodal surface good enough to reach a required accuracy.

A possible extension can be derived from the fixed–hypernodes approach due to Kalos and Pederiva [PKR$^+$06].

2.6.1 Original fixed–hypernode method

We focus on the ground state of a Fermionic system F with eigenfunction ϕ_F and eigenenergy E_F. The fixed–node DMC algorithm requires that the walkers do not cross the nodal surface of the trial wavefunction in such a way that they can explore only the portion of the configuration space delimited by the nodal surface of the trial wavefunction. In this way we find an energy $E_F^{FN} > E_F$. Considering now a system B of equivalent Bosons the exact energy $E_B^{FN} = E_B$ and the eigenfunction ϕ_B can be obtained. If we take into account the product system of F and B, the wavefunctions will have the following form:

$$\Psi_\pm = \frac{1}{\sqrt{2}} \left[\phi_B(B)\phi_F(F) \pm \phi_B(F)\phi_F(B)\right] \tag{2.61}$$

with eigenvalue $E = E_B + E_F$. Thus it is possible to find an upper bound $E_F^{FHN} = E - E_B$ to the energy of the Fermionic system F, because we can compute the exact E_B. This upper bound is in principle independent of E_F^{FN}. In fact, we can see that the nodal surfaces of $\Psi_\pm$, (so called hypernodal surfaces) are different from those of ϕ_F. In this way, even if we constraint the dynamics of the walkers within a hypernodal pocket, the walkers of the product space can explore also region of the configuration space denied by the nodal surface of ϕ_F in the F space only. This method is called fixed–hypernode. So we could have a different upper bound $E_F^{FN} \neq E_F^{FHN}$ and possibly $E_F^{FHN} < E_F^{FN}$. As we can see in the next section, we "experimentally" obtain $E_F^{FN} = E_F^{FHN}$; anyway we are not able to show a general demonstration for that.

2.6.2 Extension of fixed–hypernode

Consider two different separated systems A and B, symmetric respect to two transformation groups $\mathcal{G}_A$ and $\mathcal{G}_B$ as the representations G_A and G_B. The Hamiltonians are H_A and H_B and the wavefunctions $\phi_A \in \mathcal{H}_A$ and $\phi_B \in \mathcal{H}_B$ with eigenvalues E_A and E_B. Now take into account the sum system with the Hamiltonian $H = H_A \oplus H_B$, $\Psi_0 = \phi_A \oplus \phi_B \in (\mathcal{H}_A \oplus \mathcal{H}_B)$, $G = G_A \oplus G_B$, $\mathcal{G} = \mathcal{G}_A \oplus \mathcal{G}_B$, i.e.

$$H = \begin{pmatrix} H_A & 0 \\ 0 & H_B \end{pmatrix}, \qquad G = \begin{pmatrix} G_A & 0 \\ 0 & G_B \end{pmatrix}, \qquad \Psi_0 = \begin{pmatrix} \phi_A \\ \phi_B \end{pmatrix}. \quad (2.62)$$

The eigenvalue of Ψ_0 is $E = E_A + E_B$ and $E^{FHN} \geq E$ is the fixed–hypernode DMC upperbound (i.e a fixed–node in the extended system). In principle it might be that $E_A^{FN} + E_B^{FN} \neq E^{FHN}$, allowing to have a different upper bound $E_B^{FN} = E^{FHN} - E_A^{FN}$ when we are able to compute the exact $E_A^{FN} = E_A$ (i.e. we known it analytically or when the symmetry representation G_A define the full exact nodal surface of ϕ_A). Anyway, requiring only the symmetry G and using the trial wave function Ψ_0, we have that $E^{FHN} = E_B^{FN} + E_A^{FN}$ because Ψ_0 has the same nodal surface of the wavefunctions of the two systems.

Now assuming $H_A = H_B$, the symmetry operation $\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \notin G$ is also allowed by H but not in G. We can enlarge the group $\mathcal{G}$ to $\mathcal{G}_{ext} = (\mathcal{G}_A \oplus \mathcal{G}_B) + \mathcal{Z}_2$. The Hamiltonian H is degenerated in $\mathcal{Z}_2$, i.e. two different representation exist, corresponding to the two wave functions

$$\Psi_\pm = \frac{1}{\sqrt{2}} \left[\begin{pmatrix} \phi_A \\ \phi_B \end{pmatrix} \pm \begin{pmatrix} \phi_B \\ \phi_A d \end{pmatrix} \right]. \quad (2.63)$$

Generally the hypernodal surface of $\Psi_\pm$ gives different constraint respect to the fixed–node one.

2.6.3 An example

In this section we want to show an example of the previous explained fixed–hypernode approximation, i.e. we compute the energy of a system B with the fixed–node approximation and with the fixed–hypernode approximation. Thus we check if the fixed–hypernode approximation gives a better upper bound relative to the fixed–node one.

We have studied a system of 2 non–interacting particles (1,2) in a 2–dimensional (x,y) anisotropic harmonic potential and $m = \hbar = 1$, $\omega_x = 1$, $\omega_y = 2$:

$$H = -\frac{1}{2}\left(\frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} + \frac{\partial^2}{\partial y_1^2} + \frac{\partial^2}{\partial y_2^2}\right) + \frac{\omega_x^2}{2}\left(x_1^2 + x_2^2\right) + \frac{\omega_y^2}{2}\left(y_1^2 + y_2^2\right). \quad (2.64)$$

The ground state with eigenvalue 3 can be written as

$$\phi_0 = e^{\left(x_1^2 + x_2^2\right)\frac{\omega_x^2}{2}} e^{\left(y_1^2 + y_2^2\right)\frac{\omega_y^2}{2}}. \quad (2.65)$$

Then we have two excited states with eigenvalue 4

$$\phi_1 = x_1\phi_0 \qquad \phi_1' = x_2\phi_0; \tag{2.66}$$

and other two states with eigenvalue 5:

$$\phi_2 = y_1\phi_0 \qquad \phi_2' = y_2\phi_0. \tag{2.67}$$

Here $\mathcal{G}$ is the permutation group. We have only two irreducible non-equivalent representations, the Fermion one and the Boson one. The energy of the Boson state can be computed exactly; for Fermion state the energy depends by the goodness of the nodal surface of the trial wavefunction.

Thus, we take into account an approximated form for the ground state

$$\hat{\phi}_0 = \frac{1}{x_1^2 + x_2^2 + y_1^2 + y_2^2 + 0.1}; \tag{2.68}$$

and for the first excited state:

$$\hat{\phi}_1 = (\sin(2\theta)x_1 + \sin(\theta)y_1)\,\phi_0, \tag{2.69}$$

with θ a variational parameter.

At first we take into account two systems like the previous one:

- a system A with $N = 2$ Bosons in $D = 2$ dimensions;
- a system B with $N = 2$ Fermions in $D = 2$ dimensions;
- the same group symmetry for both systems (the permutation group), but with two different representations : $G_A = \{1\}$ and $G_B = \{1, -1\}$.

We have that $E_A = 3$, $E_B = 4$ and $E = 7$. With the fixed–node DMC algorithm we are able to compute separately $E_A^{FN} = E_A$ and $E_B^{FN} \geq E_B$. With the fixed–node DMC algorithm on the full system, i.e. with the fixed–hypernode DMC, we can compute $E_B^{FHN} = E^{FHN} - E_A \geq E_B$. From the plot of Fig. 2.1 we ca see that $E_B^{FHN} = E_B^{FN}$ independently from the nodal surface, i.e. form the variational parameter θ. We have no explanation for this behavior, for which there is not theoretical prediction.

Now we take into account a quite different system:

- a system A with $N = 2$ Bosons in $D = 2$ dimensions requiring an anti-symmetry respect to the x coordinate;
- a system B with $N = 2$ Fermions in $D = 2$ dimensions;
- now the symmetry group is that of permutations $\mathcal{Z}_2$ and the spatial reflection $\mathcal{P}_x$ (only 2 irreducible nonequivalent representations); For the system A we choose the trivial representation for $\mathcal{Z}_2$ and the non trivial one for $\mathcal{P}_x$; vice versa for the system B. Thus we have $G_A = \{1, -1\}$ and $G_B = \{-1, 1\}$, the energies are $E_A = 4$, $E_B = 4$, and $E = 8$. The symmetry on A fixes the whole nodal surface, and we are able to compute $E_A^{FN} = E_A$. Not the same for the system B for which we are able to compute $E_B^{FN} \geq E_B$.

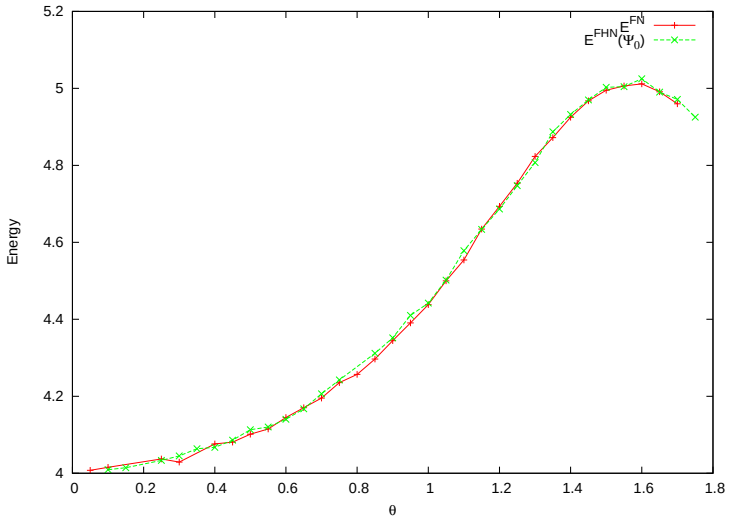

Figure 2.1: The two upper bounds E_B^{FN} and E_B^{FHN} varying a wavefunction variational parameter θ. The exact value is $E_B = 4$.

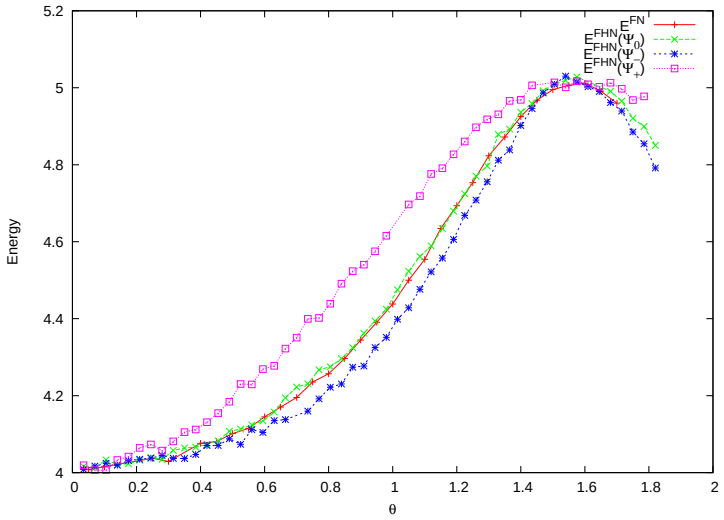

Figure 2.2: Upper bounds E_B^{FN} and the three E_B^{FHN} (using the three different trial wave functions Ψ_0, Ψ_+ and Ψ_-), varying the wavefunction variational parameter θ. The exact value is $E_B = 4$.

As we can see in Fig. 2.2, the upper bound E_B^{FHN} computed with the wave-function Ψ_- is lower than that computed with the fixed node on ϕ_B.

Summarizing, with this extension of the fixed–hypernode algorithm we could obtain a better upper bounds for the Fermion ground state energy with respect to the fixed–node estimation E_B^{FN}. Anyway a better study to understand better when and how much we could improve with this method the fixed node energy could be interesting.

Chapter 3

Auxiliary Field Diffusion Monte Carlo

3.1 Something about the GFMC algorithm

The DMC method introduced in the previous chapter can only be used for systems where the degrees of freedom are the spatial coordinates. For nuclear systems, where we have to take into account spin/isospin degrees of freedom, it is possible to extend the method as explained in (§ 1.6).

We have already discussed in (§ 1.6) the scalability problems related to the size of the spin/isospin space. Moreover in GFMC[Car87, Pie05] we also need to apply to each configuration the propagator of the imaginary time Schrödinger equation. To increase the efficiency of the algorithm, in nuclear systems, a propagator for which the two–body terms are exactly computed is often used. However the gain in efficiency is pretty spoiled by the increased complexity of the calculation. Some additional tricks are used to improve the computability, but despite of that the bigger nuclear systems computed can reach "only" 12 nucleons.

We have to say that for nuclear systems with hard core potentials (like the Argonne $Av18$ potential) GFMC is still the best or at least one of the best available methods[KNG$^+$01]. There is a further shortcoming of GFMC. The propagators that can be sampled must come from local potentials or from spin–orbit terms of the Hamiltonian. This implies that calculations with the Argonne class potentials should be limited to the use of $Av8'$. The inclusion of further terms can be achieved only perturbatively.

3.2 The idea of AFDMC

The starting point is the same of DMC or GFMC algorithms. We assume to have only two body local interactions(i.e. without terms that does not commute with the position other than the kinetic term) and a trial wavefunction made by Slater determinants and at most central correlations (i.e. not operatorial Jastrow correlations).

Focusing our attention to the spin/isospin space, we indicate the single par-

ticle Hilbert spaces with $\mathcal{H}$ with dimension N_S and the space of the full N_{PART} particles system as

$$\mathbb{H} = \bigotimes_{i}^{N_{PART}} \mathcal{H}_i \qquad \text{with} \qquad \dim \mathbb{H} = {N_S}^{N_{PART}} \tag{3.1}$$

Clearly the wavefunction of the ground state lives in $\mathbb{H}$, like the configurations that we have to to sample with GFMC. Let us define also the sum space

$$\mathscr{H} = \bigoplus_{i}^{N_{PART}} \mathcal{H}_i \qquad \text{with} \qquad \dim \mathscr{H} = N_{PART} \cdot N_S \tag{3.2}$$

Now let us suppose to represent in $\mathscr{H}$ the configurations that we have to sample, i.e. in the sum space of single particle spaces. Also suppose to have a propagator for the Schrödinger imaginary time equation Eq(2.2) containing one–body operators only. A propagator like that is closed respect to the sum space $\mathscr{H}$, i.e. we are able to perform simulations representing our operators and sampling our configurations in the space $\mathscr{H}$, whose dimension increases as $4\,N_{PART}$, i.e. linearly with the number of particles. With these hypothesis, the algorithm scales polynomially with the number of nucleons as opposed to the exponential scaling of the GFMC. Anyway we have to remember that our physical propagator contains two–body operators, i.e. terms that do not live in $\mathscr{H}$. But, under the hypothesis of only two–body (central) interaction, we can rewrite our propagator as a sum of quadratic terms:

$$e^{-dt\frac{O^2}{2}}. \tag{3.3}$$

Now we can apply an Hubbard Stratonovich transform, i.e. a Gaussian integration on an auxiliary field x, to rewrite the previous propagator and obtain a propagator containing linear operators only, i.e. one body terms:

$$e^{-dt\frac{O^2}{2}} = \frac{1}{\sqrt{2\pi}} \int dx e^{-\frac{x^2}{2}} e^{-\sqrt{-dt}xO} \tag{3.4}$$

Using this equivalence we can apply the previous idea also to systems with two–body spin/isospin dependent interactions, keeping a polynomial scalability in the particle number. The extra computational cost is that related to the Monte Carlo integration on the auxiliary fields x, from which the name AFDMC comes[Sch99, FSS00].

3.3 Notation and used relations

Let us introduce some technical details and notations for the next development:

- O_i is a generic one body operator in one body space representation.
- $\hat{O}_i$ is the representation in the N–body tensor product space of the one body operator O_i:

$$\hat{O}_i = \mathbb{I}_1 \otimes ... \otimes \mathbb{I}_{i-1} \otimes O_i \otimes \mathbb{I}_{i+1} \otimes ... \otimes \mathbb{I}_N \tag{3.5}$$

- For generic operators (matrix) A, B, $\mathcal{A}$ and $\mathcal{B}$, the following relations are used

$$(A \otimes B) \cdot (\mathcal{A} \otimes \mathcal{B}) = (A \cdot \mathcal{A}) \otimes (B \cdot \mathcal{B}) \tag{3.6}$$

$$A \oplus B = A \otimes \mathbb{I} + \mathbb{I} \otimes B \tag{3.7}$$

$$\sum_i \hat{O}_i = \bigoplus_i O_i \tag{3.8}$$

$$e^{A \oplus B} = e^A \otimes e^B \tag{3.9}$$

$$e^{\sum_i \hat{O}_i} = e^{\oplus_i O_i} = \bigotimes_i e^{O_i} \tag{3.10}$$

- If $V_{ij} = V_{ji}$ is a symmetric matrix, its eigenvalues λ_n are real

$$P_{mi} V_{ij} P^{-1}_{jn} = \lambda_n \delta_{nm}, \tag{3.11}$$

and the eigenvectors matrix satisfies

$$P^T = P^{-1}, \tag{3.12}$$

so it is possible to write V_{ij} as

$$V_{ij} = \sum_k \lambda_k P_{ik} P_{jk}. \tag{3.13}$$

- Let we remember the Hubbard Stratonovich transform

$$e^{-\frac{\lambda}{2} O^2} = \frac{1}{\sqrt{2\pi}} \int dx \; e^{-\frac{x^2}{2}} \; e^{-\sqrt{-\lambda}\, x \, O}. \tag{3.14}$$

- The reason of using the Hubbard Stratonovich transform lays in the following simple observation. Consider a system composed by N particles. Assume that d is the dimension of the single particle space. The space dimension of the complete system is d^N, and a single configuration of the system has to be represented by d^N coefficients. But, if the propagator does not mix different particle states, we can represent the evolution of the wavefunction by $d \cdot N$ coefficients only.

  Let us checkout the conditions under which this is possible. Assume that the propagator has a form as in equation (3.10) and that the starting wavefunction is

$$\Psi = \bigotimes_i c_i \cdot \phi_i, \tag{3.15}$$

where c_i represents a vector of d coefficients. Remembering equation (3.6) we have that

$$\Psi' = e^{\sum_i \hat{O}_i} \cdot \Psi = \left(\bigotimes_i e^{O_i} \right) \cdot \left(\bigotimes_i c_i \cdot \phi_i \right) = \bigotimes_i \left[\left(e^{O_i} \cdot c_i \right) \cdot \phi_i \right]. \tag{3.16}$$

Thus we can represent the new state with only $d \cdot N$ coefficients:

$$c'_i = e^{O_i} \cdot c_i, \qquad \Psi' = e^{\sum_i \hat{O}_i} \cdot \Psi, \qquad \Psi' = \bigotimes_i c'_i \phi_i. \tag{3.17}$$

The fundamental requirement is that the propagator must be a tensor product of single particle operators.

3.4 The propagator

Setting aside the kinetic and one–body terms, that are treatable as in the standard DMC algorithm, let us focus on the role of the two–body operatorial terms on the propagator. Consider a two body potential in the form:

$$V = \frac{1}{2}\sum_{ij} V_{ij}\hat{O}_i \cdot \hat{O}_j, \tag{3.18}$$

and rewrite it using the Eq(3.13) as

$$V = \frac{1}{2}\sum_{k} \lambda_k \left(\sum_i P_{ik}\hat{O}_i\right)^2. \tag{3.19}$$

Now the two body propagator term is

$$e^{-dtV} = e^{-\frac{dt}{2}\sum_k \lambda_k \left(\sum_i P_{ik}\hat{O}_i\right)^2}. \tag{3.20}$$

Neglecting commutators of order $\mathcal{O}(dt^2)$, we can factorize and use the Hubbard Stratonovich transform for each squared operator, obtaining:

$$\begin{aligned} e^{-dtV} &\simeq \prod_k \left(\frac{1}{\sqrt{2\pi}}\int dx_k e^{-\frac{x_k^2}{2}} e^{-\sqrt{-\lambda_k dt}\, x_k \left(\bigoplus_i P_{ik}O_i\right)}\right) \\ &\simeq \prod_k \left(\frac{1}{\sqrt{2\pi}}\int dx_k e^{-\frac{x_k^2}{2}} \left(\bigotimes_i e^{-\sqrt{-\lambda_k dt}\, x_k\, P_{ik}O_i}\right)\right) \\ &\simeq \left(\frac{1}{2\pi}\right)^{\frac{k}{2}} \iint dx_1 ... dx_k\, e^{-\frac{\sum_{j=1}^k x_j^2}{2}} \prod_{j=1}^{k}\left(\bigotimes_i e^{-\sqrt{-\lambda_j dt}\, x_j\, P_{ij}O_i}\right). \end{aligned} \tag{3.21}$$

Limiting ourselves to two operators only, odd terms in the expansion of the exponential give a null contribution to the following integral

$$\begin{aligned} &\iint dxdy\, e^{-\frac{x^2}{2}} e^{-\frac{y^2}{2}} \quad e^{x\sqrt{dt}A}\cdot e^{y\sqrt{dt}B} = \\ &\simeq \int dx e^{-\frac{x^2}{2}} \left(1 + \cancel{x\sqrt{dt}A} + \frac{x^2}{2!}A^2 dt + \cancel{\frac{x^3}{3!}dt\sqrt{dt}A^3} + \mathcal{O}(dt^2)\right) \times \\ &\times \int dy e^{-\frac{y^2}{2}} \left(1 + \cancel{y\sqrt{dt}B} + \frac{y^2}{2!}B^2 dt + \cancel{\frac{y^3}{3!}dt\sqrt{dt}B^3} + \mathcal{O}(dt^2)\right). \end{aligned} \tag{3.22}$$

By adding to the previous expression the following null term

$$0 = \iint dxdy e^{-\frac{x^2}{2}} e^{-\frac{y^2}{2}} \frac{\left(x\sqrt{dt}A\right)\cdot\left(y\sqrt{dt}B\right)}{2!} + \frac{\left(y\sqrt{dt}B\right)\cdot\left(x\sqrt{dt}A\right)}{2!} \tag{3.23}$$

it is possible to complete a square in the expression in parenthesis. Some similar odd terms can be used to complete the cubic terms. Finally we obtain:

$$\begin{aligned}
&\iint dxdy\, e^{-\frac{x^2}{2}} e^{-\frac{y^2}{2}} \quad e^{x\sqrt{dt}A}\cdot e^{y\sqrt{dt}B} = \\
&= \iint dxdy e^{-\frac{x^2}{2}} e^{-\frac{y^2}{2}} \left(1 + \cancel{\left(x\sqrt{dt}A + y\sqrt{dt}B\right)} + \frac{1}{2!}\left(x\sqrt{dt}A + y\sqrt{dt}B\right)^2 + \right. \\
&\quad \left. + \cancel{\frac{1}{3!}\left(x\sqrt{dt}A + y\sqrt{dt}B\right)^3} + \mathcal{O}(dt^2)\right) = \\
&= \iint dxdy\, e^{-\frac{x^2}{2}} e^{-\frac{y^2}{2}} \quad e^{\sqrt{dt}(xA+yB)} \quad + \quad \mathcal{O}(dt^2)
\end{aligned} \tag{3.24}$$

and thus, reconsidering Eq(3.21) combined with Eq(3.24), neglecting terms $\mathcal{O}(dt^2)$, and re–exponentiating we can rewrite the two body propagator Eq(3.21) as

$$\begin{aligned}
e^{-dtV} &\simeq \left(\frac{1}{2\pi}\right)^{\frac{k}{2}} \iint dx_1 ... dx_k\, e^{-\frac{\sum_{j=1}^k x_j^2}{2}} \prod_{j=1}^{k} \left(\bigotimes_i e^{-\sqrt{-\lambda_j dt}\, x_j\, P_{ij} O_i}\right) \\
&\simeq \left(\frac{1}{2\pi}\right)^{\frac{k}{2}} \iint dx_1 ... dx_k\, e^{-\frac{\sum_{j=1}^k x_j^2}{2}} \left(\bigotimes_i e^{-\sum_{j=1}^k \sqrt{-\lambda_j dt}\, x_j\, P_{ij} O_i}\right)
\end{aligned} \tag{3.25}$$

With the previous form, as explained in Eq(3.16) and Eq(3.17), we are able to apply the propagator in a simple way without going out of the sum space $\mathcal{H}$.

3.5 Importance sampling on auxiliary fields

In the previous paragraph we have written the propagator in a suitable form. It would be proper to include also importance sampling like in DMC algorithm. We accomplish that in the same way like in DMC.

We want to show that

$$\int dx e^{-\frac{1}{2}\left(x+\sqrt{-dt\lambda}\langle O\rangle\right)^2} e^{-\frac{1}{2}\langle O^2\rangle \lambda dt} \langle s'|e^{-x\sqrt{-\lambda dt}O}|s\rangle \tag{3.26}$$

is equivalent to

$$\int dx e^{-\frac{1}{2}x^2} \langle s'|e^{-x\sqrt{-\lambda dt}O}|s\rangle \frac{\langle\phi|s'\rangle}{\langle\phi|s\rangle} = \langle s'|e^{-\lambda dt\frac{O^2}{2}}|s\rangle \frac{\langle\phi|s'\rangle}{\langle\phi|s\rangle}. \tag{3.27}$$

If $|s'\rangle$ indicates the new walker configuration, $|s\rangle$ the old one, $|\phi\rangle$ the trial wavefunctions and $e^{-\lambda dt\frac{O^2}{2}}$ the propagator, the previous equation is simply the Green's function expression of the imaginary time Schrödinger equation with importance sampling, as in equation Eq(2.45). In Eq(3.26) we have used for a generic operator θ the notation

$$\langle\theta\rangle = \frac{\langle\phi|\theta|s\rangle}{\langle\phi|s\rangle}. \tag{3.28}$$

Remembering that, because of the definition of s', we have

$$\langle s'|e^{-x\sqrt{-\lambda dt}O}|s\rangle = 1, \tag{3.29}$$

expanding the exponential in Eq(3.26) to order dt we obtain:

$$\begin{aligned}
&\int dx e^{-\frac{1}{2}x^2} e^{\frac{1}{2}\lambda dt(\langle O\rangle)^2} e^{-x\sqrt{-\lambda dt}\langle O\rangle} e^{-\frac{1}{2}\lambda dt\langle O^2\rangle} \cancelto{1}{\langle s'|e^{-x\sqrt{-\lambda dt}O}|s\rangle} \simeq \\
&\int dx e^{-\frac{1}{2}x^2} \left[\left(1+\frac{1}{2}\lambda dt(\langle O\rangle)^2\right)\left(1-x\sqrt{-\lambda dt}\langle O\rangle - \frac{1}{2}dt\lambda(\langle O\rangle)^2\right)\times\right. \\
&\qquad \left.\times\left(1-\frac{1}{2}\langle O^2\rangle dt\lambda\right)\right] + \mathcal{O}(dt^2) \simeq \\
&\int dx e^{-\frac{1}{2}x^2} \left[\cancel{\frac{1}{2}\lambda dt(\langle O\rangle)^2} + \left(1-x\sqrt{-\lambda dt}\langle O\rangle - \cancel{\frac{1}{2}dt\lambda(\langle O\rangle)^2}\right)\right. \\
&\qquad \left.-\frac{1}{2}\langle O^2\rangle dt\lambda\right] + \mathcal{O}(dt^2) \simeq \\
&\int dx e^{-\frac{1}{2}x^2} \frac{\langle\phi\,|1-x\sqrt{-\lambda dt}O - \frac{1}{2}dt\lambda O^2|\,s\rangle}{\langle\phi|s\rangle} \cancelto{1}{\langle s'|e^{-x\sqrt{-\lambda dt}O}|s\rangle} + \mathcal{O}(dt^2) \simeq \\
&\int dx e^{-\frac{1}{2}x^2} \frac{\langle\phi|e^{-x\sqrt{-dt\lambda}O}|s\rangle}{\langle\phi|s\rangle}\langle s'|e^{-x\sqrt{-\lambda dt}O}|s\rangle + \mathcal{O}(dt^2)
\end{aligned} \tag{3.30}$$

that is the same of Eq(3.27).

Now we can directly use Eq(3.26) instead of Eq(3.27) to compute the new configuration s'. The reason is that the ratio $\frac{\langle\phi|s'\rangle}{\langle\phi|s\rangle}$ in Eq(3.27) might fluctuate a lot, and different sampled configurations could give very different weights. Instead if we use Eq(3.26) we have to weight the configuration with the local energy, i.e. with a quantity that is constant if the trial wavefunction is exact, and that otherwise has fluctuations depending on the quality of the wavefunction itself.

Hence we simply sample a normally distributed random Gaussian number g; this will be equal to

$$g = x + \sqrt{-dt\lambda}\langle O\rangle. \tag{3.31}$$

Defining

$$C_{fac} = -\sqrt{-dt\lambda}, \tag{3.32}$$

$$\bar{x} = \sqrt{-dt\lambda}\langle O\rangle = -C_{fac}\langle O\rangle, \tag{3.33}$$

we have that

$$g = x + \bar{x} \Longrightarrow x = g - \bar{x}. \tag{3.34}$$

Thus, to sample a new s' configuration we can use Eq(3.26), i.e. the operator

$$e^{-x\sqrt{-\lambda dt}O} = e^{(g-\bar{x})C_{fac}}, \tag{3.35}$$

and weight the configuration with the local energy

$$e^{-\frac{1}{2}\langle O^2\rangle\lambda dt}. \tag{3.36}$$

3.6 The drift of DMC revisited

In paragraph (§ 2.3) we introduced the concept of importance sampling in the case where auxiliary field or Hubbard Stratonovich transform are not present. We will see that the result of the previous section can be reconciled with the arguments made in the standard DMC case.

For simplicity, consider an Hamiltonian with a kinetic and a central terms only: so the Hamiltonian is something like

$$H = \sum_i \frac{p_i^2}{2m} + V, \tag{3.37}$$

and the propagator will be:

$$\mathcal{P} = e^{-dt/\hbar \sum_i \frac{p_i^2}{2m}} e^{-dt/\hbar V}. \tag{3.38}$$

Now for each particle i we can rewrite the kinetic propagator using an Hubbard Stratonovich transform, i.e. :

$$e^{-dt/\hbar \frac{p_i^2}{2m}} = \frac{1}{\sqrt{2\pi}} \int dx e^{-\frac{x^2}{2}} e^{-\sqrt{-dt/\hbar} x \frac{p_i}{m}} \tag{3.39}$$

It must be notice that while we are not able to apply directly $e^{-dt \frac{p_i^2}{2m}}$ to a configuration $|x\rangle$, we can apply $e^{-\sqrt{-dt} x \frac{p_i}{m}}$. Remembering that $e^{-\frac{i}{\hbar} dp}$ is a translation operator, i.e.:

$$|x'\rangle = e^{-\frac{i}{\hbar} dp} |x\rangle = |x + d\rangle. \tag{3.40}$$

We can apply the previous expression to Eq(3.39) and to Eq(3.38) to obtain

$$\mathcal{P} = \prod_i \frac{1}{\sqrt{2\pi}} \int dx_i e^{-\frac{x_i^2}{2}} e^{-\frac{i}{\hbar}\left(x_i \sqrt{\frac{\hbar dt}{m}}\right) p} \qquad e^{-dt/\hbar V}, \tag{3.41}$$

i.e applying the propagator $\mathcal{P}$ to an old configuration $|R\rangle$ we obtain a new configuration

$$|R'\rangle = \left| R + \left(x_i \sqrt{\frac{dt\hbar}{m}} \right) \right\rangle, \tag{3.42}$$

with a weight

$$e^{-dt/\hbar V}. \tag{3.43}$$

This is exactly the same of the previously obtained equation Eq(2.11).

This perspective is much dearer then that derived by the Fokker–Plank equation because:

- importance sampling for the kinetic term can be derived in a simpler way, like in the previous paragraph, instead of studying the Green's function of a Fokker–Plank equation with a drift term;
- in this way it becomes straightforward to include in the propagator some non–local terms, like explained in the following paragraphs;
- the so called "fixed–phase" approximation in this approach is naturally defined.

3.7 Sign problem

We have seen in the previous chapter how we can deal with the sign problem to study the ground state of Fermion systems using DMC. For the AFDMC the problem is quite more complicated and less clear. In fact, while in DMC we can usually work with real wavefunctions and propagators, AFDMC requires generally complex wavefunctions and complex operators in the propagator. As a consequence, the "fixed node" approximation is no more well defined.

Let us review how this problem is handled in this case.

3.7.1 The fixed–phase approximation I

A first approach might consist of generalizing the "fixed–node" approximation to a sort of "fixed–phase" constraint. Let us focus on a system within an external complex potential but without internal spin or isospin degrees of freedoms. In this way we are able to solve the problem with a DMC algorithm. We can consider an Hamiltonian H

$$H = \frac{p^2}{2m} + V, \tag{3.44}$$

with V diagonal in the coordinates R. Defining

$$\psi(R,\tau) = |\psi(R,\tau)|e^{-i\phi(R,\tau)} \qquad \text{with} \qquad \phi(R,\tau) \in \mathbf{R} \tag{3.45}$$

and requiring taht:

$$\phi(R,\tau) = \phi(R) \tag{3.46}$$

we can rewrite the imaginary time Schrödinger equation as

$$-\hbar\frac{\partial}{\partial\tau}|\psi(R,\tau)|e^{-i\phi(R)} = \hat{H}|\psi(R,\tau)|e^{-i\phi(R)} \tag{3.47}$$

Given that:

$$\nabla^2(|\psi|e^{-i\phi}) = e^{-i\phi}\left(\nabla^2|\psi| - 2i\nabla\phi\nabla|\psi| - i|\psi|\nabla^2\phi - (\nabla\phi)^2|\psi|\right) \tag{3.48}$$

by dividing with the phase factor we can rewrite Eq(3.47)

$$\begin{aligned} -\hbar\frac{\partial}{\partial\tau}|\psi(R,\tau)| &= \left(-\frac{\hbar^2\nabla^2}{2m} + \frac{\hbar^2(\nabla\phi(R))^2}{2m} + \Re\left[V(R)\right]\right)|\psi(R,\tau)| \\ &+i\left[\frac{\hbar^2}{m}\left(\nabla\phi(R)\nabla|\psi(R,\tau)| + \frac{1}{2}|\psi(R,\tau)|\nabla^2\phi(R)\right) + \Im\left[V(R)\right]\right]. \end{aligned} \tag{3.49}$$

Splitting the imaginary and the real part of Eq(3.49), we see that Eq(3.47) is equivalent to the following coupled equations

$$\begin{cases} -\hbar\dfrac{\partial}{\partial\tau}|\psi(R,\tau)| = \left(-\dfrac{\hbar^2\nabla^2}{2m} + \dfrac{\hbar^2(\nabla\phi(R))^2}{2m} + \Re[V]\right)|\psi(R,\tau)| \\ \dfrac{\hbar^2}{m}\left(\nabla\phi(R)\nabla|\psi(R,\tau)| + \dfrac{1}{2}|\psi(R,\tau)|\nabla^2\phi(R)\right) + \Im\left[V(R)\right] = 0 \end{cases} \tag{3.50}$$

Now let us introduce importance sampling adding the factor

$$\varphi(R) = |\varphi(R)|e^{i\phi(R)}, \tag{3.51}$$

i.e. a trial wavefunction with a phase $e^{i\phi(R)}$ in Eq(3.50). We obtain

$$\begin{aligned} &-\hbar\frac{\partial}{\partial\tau}|\psi(R,\tau)|\cancel{e^{-i\phi(R)}}|\varphi(R)|\cancel{e^{i\phi(R)}} = \\ &= |\varphi(R)|\cancel{e^{i\phi(R)}e^{-i\phi(R)}}\left(-\frac{\hbar^2\nabla^2}{2m} + \frac{\hbar^2(\nabla\phi(R))^2}{2m} + V\right)|\psi(R,\tau)|. \end{aligned} \tag{3.52}$$

The following equivalence is satisfied:

$$\begin{aligned} &|\varphi(R)|\left(-\frac{\hbar^2\nabla^2}{2m} + \frac{\hbar^2(\nabla\phi(R))^2}{2m} + V\right)|\psi(R,\tau)| = \\ &= \left(-\frac{\hbar^2\nabla^2}{2m} + \frac{\hbar^2}{m}\nabla\frac{\nabla|\varphi(R)|}{|\varphi(R)|} - \frac{\frac{\hbar^2}{2m}\nabla^2|\varphi(R)|}{|\varphi(R)|} + \frac{\hbar^2(\nabla\phi(R))^2}{2m} + V\right)|\psi(R,\tau)||\varphi(R)|. \end{aligned} \tag{3.53}$$

Hence, defining the operator:

$$\tilde{K}(R) \equiv \left(-\frac{\hbar^2\nabla^2_{|R}}{2m} + \frac{\hbar^2}{m}\nabla_{|R}\frac{\nabla|\varphi(R)|}{|\varphi(R)|} - \frac{\frac{\hbar^2}{2m}\nabla^2_{|R}|\varphi(R)|}{|\varphi(R)|} + \frac{\hbar^2(\nabla\phi(R))^2}{2m} + V(R)\right), \tag{3.54}$$

and a real function:

$$f(R,\tau) \equiv |\psi(R,\tau)||\phi(R)| = \psi(R,\tau)\phi(R), \tag{3.55}$$

we can rewrite Eq(3.52) as:

$$-\hbar\frac{\partial}{\partial\tau}f(R,\tau) = \tilde{K}(R)f(R,\tau) \tag{3.56}$$

So Eq(3.47) plus the fixed–phase condition Eq(3.46), i.e. Eq(3.50), is equivalent to:

$$\begin{cases} -\hbar\dfrac{\partial}{\partial\tau}f(R,\tau) = \tilde{K}(R)f(R,\tau) \\ \dfrac{\hbar^2}{m}\left(\nabla\phi(R)\nabla|\psi(R,\tau)| + \dfrac{1}{2}|\psi(R,\tau)|\nabla^2\phi(R)\right) + \Im\left[V(R)\right] = 0 \end{cases} \tag{3.57}$$

with $f(R,\tau)$ defined as in Eq(3.55) and $\tilde{K}$ as in Eq(3.54). We can finally see that Eq(3.57) can be rewritten multiplying by $|\psi(R,\tau)|$

$$\nabla\frac{|\psi(R,\tau)|^2(\nabla\phi(R))}{2} + \Im[V(R)]|\psi(R,\tau)| = 0 \tag{3.58}$$

The spectrum of Eq(3.57) is not the same of the original Schrödinger equation, because the Hilbert space is limited to $\psi(R,\tau)$ with a time–independent phase $e^{-i\phi(R)}$.

To obtain an upper bound of the ground state both equations of Eq(3.57) must be satisfied. Instead, what is usually done is simply to solve the first equation, loosing the upper bound properties of the energy.

We can consider most complex cases, i.e. when a magnetic field B is present. In this case a vector potential appears:

$$A(R) = \frac{B}{2}(-y, x, 0), \tag{3.59}$$

with a generic potential $V(R)$ diagonal in R. The Hamiltonian assumes this form:

$$\begin{aligned} H =& \frac{\Pi^2}{2} + V(r) \qquad \text{with} \qquad \Pi = -i\nabla - A(r) \\ =& \frac{-\nabla^2}{2} + \left[\frac{A^2(R)}{2} + V(R)\right] + \frac{i}{2}\left[\nabla A(r) + 2A(R)\nabla\right] \end{aligned} \tag{3.60}$$

Now we consider the eigenvalue equations:

$$\begin{aligned} &H\psi(R) = E\psi(R) \\ &H|\psi(R)|e^{i\phi(R)} = E|\psi(R)|e^{i\phi(R)}. \end{aligned} \tag{3.61}$$

The Hamiltonian act on the wavefunction as follows:

$$\begin{aligned} H\left(|\psi|e^{i\phi}\right) = e^{i\phi}\Bigg\{&\left[-\frac{\nabla^2}{2} + \frac{(\nabla\phi)^2}{2} + \frac{A^2}{2} + V + A(\nabla\phi)\right] \\ &+ i\left[(\nabla\phi)\nabla + \frac{(\nabla^2\phi)}{2} + \frac{(\nabla A)}{2} + A\nabla\right]\Bigg\}|\psi| \end{aligned} \tag{3.62}$$

Hence, we can decouple the imaginary and the real part, because the eigenvalue is real. Eq(3.61) becomes:

$$\begin{cases} \left[-\dfrac{\nabla^2}{2} + \dfrac{1}{2}\left((\nabla\phi) + A\right)^2 + V\right]|\psi| = E|\psi| \\ \\ \left[(\nabla\phi)\nabla + \dfrac{(\nabla^2\phi)}{2} + \dfrac{(\nabla A)}{2} + A\nabla\right]|\psi| = 0 \end{cases} \tag{3.63}$$

Multiplying by $2|\psi|$ the second equation we obtain

$$\nabla\left[|\psi|^2\left((\nabla\phi) + A\right)\right] = 0. \tag{3.64}$$

In order to solve Eq(3.63) it is possible to solve the first equation choosing a trial wavefunction assuring that Eq(3.64) is satisfied for each ψ obtained from the first equation only. Doing so we satisfied the variational principle[OCM93].

As we have seen, either implementing a "fixed–phase" approximation is not so simple, because we have to solve a system of two coupled differential equations or to search a very precise trial wavefunction, the evolution which satisfies the other equation. Because of that, in AFDMC a rougher fixed–phase approximation is used, similar in the idea to the "constrained path" approximation used in GFMC.

3.7.2 The constrained–path approximation

Consider now a complex wavefunction, as in the previous section, with a real central potential. To apply our DMC algorithm we have to satisfy Eq(2.47) and

Eq(2.48), as is done in the fixed–node approximation.

To satisfy Eq(2.48), we can redefine the drift $v_D(R)$ of Eq(2.41)

$$v_D(R) = \frac{\nabla \Re(\varphi(R))}{\Re(\varphi(R))}, \tag{3.65}$$

so that $\tilde{G}_D(R \leftarrow R', d\tau)$ will be positive defined. In the same way we can require that $v_D(R)$ is real to keep the R coordinates real.

As for the fixed–node algorithm Eq(2.58), we require

$$\frac{\Re(\varphi(R'))}{\Re(\varphi(R))} > 0 \tag{3.66}$$

rejecting the move if the new walker does not satisfy the previous.

Thus, remembering Eq(2.57), Eq(2.43) and assuming that $\tilde{G}_D(R \leftarrow R', d\tau) \simeq G_D(R \leftarrow R', d\tau)$ we can write $G_B(R \leftarrow R', d\tau)$ as follows:

$$\begin{aligned} G_B(R \leftarrow R', d\tau) &\simeq \frac{G_V(R \leftarrow R', d\tau) G_0(R \leftarrow R', d\tau)}{\tilde{G}_D(R \leftarrow R', d\tau)} \frac{\varphi(R)}{\varphi(R')} \\ &\simeq e^{-\left(\frac{V(R)+V(R')}{2}\right)\frac{d\tau}{\hbar}} e^{-\left(2\sigma\eta+\sigma^2 v_D(R')\right)\frac{v_D(R')}{2}} \frac{\Re(\varphi(R))}{\Re(\varphi(R'))} \end{aligned} \tag{3.67}$$

and we can use this factor for the branching step.

The expectation of an observable O could now be computed as

$$\langle O \rangle = \sum_{i=1}^{N} \frac{O \Re(\varphi(R_i))}{\Re(\varphi(R_i))}. \tag{3.68}$$

In this approach there is no sound justification for several assumptions. The situation becomes worse, more complicated and less clear, when we have to take into account the effects of a complex potential. Hence for more accurate and systematic description we refer to [CGOZ99, ZCG97].

The "constrained–path" approach is derived from that used in GFMC. Moreover, in GFMC the propagator is implemented using the *exact* two–body propagator, very good trial wavefunctions and no auxiliary filed integrations. The lack of all these conditions makes the constrained path a bad choice for AFDMC.

3.7.3 The fixed–phase approximation II

Instead of the previous constrained path approximation, we use a suitable version of the fixed–phase approximation. It can be derived like in the previous paragraph. Considering a complex wavefunction and a real central potential.

In order to satisfy Eq(2.48), we define the drift $v_D(R)$ as in Eq(2.41)

$$v_D(R) = \frac{\nabla|\varphi(R)|}{|\varphi(R)|} = \Re\left(\frac{\nabla\varphi(R)}{\varphi(R)}\right) \tag{3.69}$$

so that $\tilde{G}_D(R \leftarrow R', d\tau)$ is positive defined

With this choice the branching term $G_B(R \leftarrow R', d\tau)$ must be corrected as

$$G_B(R \leftarrow R', d\tau) = \frac{|\varphi(R')|}{|\varphi(R)|}\frac{\varphi(R)}{\varphi(R')} \times \\ \times \exp\left[-\left(\frac{-\frac{\hbar^2}{2m}\frac{\nabla^2|\varphi(R)|}{|\varphi(R)|} + \frac{V\varphi(R)}{\varphi(R)} - \frac{\hbar^2}{2m}\frac{\nabla^2|\varphi(R')|}{|\varphi(R')|} + \frac{V\varphi(R')}{\varphi(R')}}{2} - E_0\right)\frac{d\tau}{\hbar}\right] \tag{3.70}$$

Now, as before, we can write:

$$\varphi(R) = |\varphi(R)|e^{i\phi(R)} \tag{3.71}$$

with $\phi(R)$ a real function. From this we derive:

$$\frac{|\varphi(R')|}{|\varphi(R)|}\frac{\varphi(R)}{\varphi(R')} = e^{i\left[\phi(R)-\phi(R')\right]} \tag{3.72}$$

The fixed–phase approximation requires that $f(R,\tau)$ has zero phase, i.e. that the phase of $\Psi^*(R,\tau)$ is the same of $\varphi(R)$ in order to satisfy Eq(2.47).

We have to take into account only the real part of $G_B(R \leftarrow R', d\tau)$ Eq(3.70). To keep the normalization of the Green's function we multiply it by

$$1 - \frac{\hbar}{2m}(\nabla\phi(R))^2 d\tau. \tag{3.73}$$

This factor can be included directly in the branching term $G_B(R \leftarrow R', d\tau)$ (3.70) using the following relation

$$\Re\left(\frac{\nabla^2\varphi(R)}{\varphi(R)}\right) = \frac{\nabla^2|\varphi(R)|}{|\varphi(R)|} - (\nabla\phi(R))^2. \tag{3.74}$$

This means to compute the kinetic energy as $\Re\left(\frac{\nabla^2\varphi(R)}{\varphi(R)}\right)$ instead of $\frac{\nabla^2|\varphi(R)|}{|\varphi(R)|}$. The full branching factor will then be

$$G_B(R \leftarrow R'.d\tau) = \\ = \exp\left[-\left(\frac{-\frac{\hbar^2}{2m}\Re\left(\frac{\nabla^2\varphi(R)}{\varphi(R)}\right) + \frac{V\varphi(R)}{\varphi(R)} - \frac{\hbar^2}{2m}\Re\left(\frac{\nabla^2\varphi(R')}{\varphi(R')}\right) + \frac{V\varphi(R')}{\varphi(R')}}{2} - E_0\right)\frac{d\tau}{\hbar}\right]. \tag{3.75}$$

The expectation value of an observable O can be computed by means of

$$\langle O\rangle = \sum_{i=1}^{N} \Re\left(\frac{O\varphi(R_i)}{\varphi(R_i)}\right). \tag{3.76}$$

This approach has derivation similar to that of the constrained–path. However, in this context we reach the same result in a clear and simpler way. Moreover, all this derivations are clearly extensible to operators other than the kinetic

energy and it becomes clearer why it works quite well respect to the constrained–path approximation.

Eventually, the procedure consists of taking into account equation Eq(3.26) directly, i.e. the propagator with the importance sampling for a generic quadratic operator linearized with an integration on auxiliary fields.

The expression that has to be positive defined, i.e. the weight of our configuration, is simply the exponential of the mixed expectation value of the squared operator, that is of the local energy. So we approximate Eq(3.26) using $\Re\left(\frac{1}{2}\langle O^2\rangle\lambda\right)$ (the local energy) instead of $\frac{1}{2}\langle O^2\rangle\lambda$.

We want to point out two facts that justify this constraint:

- if we have a good trial wavefunction, the local energy is already a good approximation of the ground state energy. The weight will be more or less constant and with a neglected phase that will be as small as the trial wavefunction is close to the exact one.
- the weight is a function of the eigenvalue of the ground state, so it will not only be real but also constant. As a consequence we will have small fluctuations in the weight, i.e. a smaller statistical noise.

This is fine for every spin/isospin operator, but we have to keep care to apply this method to the kinetic term. In fact the drift so computed for the auxiliary filed could generally be complex, but we are not able to apply a complex translation. So we keep simply the real part of the drift like in Eq(3.69).

3.8 Algorithm

Now we can briefly summarize the algorithm structure:

- We start with a trial wavefunction written like a sum of Slater determinants of single particle wavefunctions. A central Jastrow correlation can be used.
- We choose a sufficiently small time step and a sufficiently large number of walkers as for the DMC algorithm.
- For each configuration we can sample the new coordinates with a drift in the same way as in DMC. For the drift, we keep only its real part.
- For each configuration, i.e. for each set of coordinates, we have to diagonalize the 2–body potential Eq(3.18) and we obtain in this way the operators that have to act on each one–particle spinor. Then we can apply the propagator related to each of that operators with the importance sampling following the procedure explained in (§ 3.5).
- We have now to compute the weight of each configuration using the local energy, the factor will be
$$e^{-dt(\langle H\rangle - E_0)}$$
because of the use of the importance sampling and of the drift in auxiliary fields like in (§ 3.5).

- We impose our constraint weighting 0 the walker for which the real part of the trial wavefunction change sign.

- When the projection on the ground state is reached, we can compute on each walker the mixed estimators of those observables that we want to study. We average these with the previous weight, in the same way as we do for DMC.

- After having "branched" the walkers with their weight like in DMC, we can go back to the third point and iterate the algorithm.

3.9 Spin–orbit terms

We have seen how to include into the propagator local terms in the Hamiltonian, the kinetic term, and 2–body spin/isospin dependent terms but local in the coordinates. Now let us look how it is possible to include a spin–orbit term. The derivation is initially due to K.E.Schmidt, and it is unpublished so far.

With Greek indexes we indicate Cartesian components $\{x, y, z\}$. A is the number of nucleons with mass m. Latin index are summed on particle number A.

We consider an Hamiltonian with a spin–orbit interaction like that.

$$\begin{aligned} H =& \sum_{j,\beta} \frac{\left(p_j^\beta\right)^2}{2m} + \sum_{i<j} \frac{1}{4\hbar} \sum_\alpha L_{jk}^\alpha \sigma_{jk}^\alpha \left(v(r_{ij}) + \sum_\delta \tau_j^\delta \tau_k^\delta v_\tau(r_{ij}) \right) \\ =& \sum_{j,\beta} \frac{\left(p_j^\beta\right)^2}{2m} + \sum_{i<j} \frac{1}{4\hbar} \sum_{\alpha\beta\gamma} \epsilon_{\alpha\beta\gamma}\, r_{jk}^\beta\, p_{jk}^\gamma \left(\sigma_j^\alpha + \sigma_k^\alpha\right) \left(v(r_{ij}) + \sum_\delta \tau_j^\delta \tau_k^\delta v_\tau(r_{ij}) \right) \end{aligned} \tag{3.77}$$

Subtracting the center of mass kinetic energy from the previous formula, we obtain

$$H = \sum_{i<j,\alpha,\beta} \left[\frac{\left(p_{ij}^\beta\right)^2}{\frac{3}{2}mA} + p_{ij}^\beta \left(\sum_{\gamma,\delta} \epsilon_{\beta\gamma\delta} \left(\sigma_i^\gamma + \sigma_j^\gamma\right) r_{ij}^\delta \right) \left(\frac{1}{3} V(r_{ij}) + \tau_i^\alpha \tau_j^\alpha V_\tau(r_{ij}) \right) \right] \tag{3.78}$$

where

$$p_{ij} = \frac{p_i - p_j}{2}, \tag{3.79}$$

$$r_{ij} = r_i - r_j. \tag{3.80}$$

From here on, we do the following assumptions to simplify the notation

$$p \rightarrow \frac{p}{\sqrt{\frac{3}{2}mA}}, \tag{3.81}$$

$$V \rightarrow V\sqrt{\frac{3}{2}mA}\frac{1}{2\hbar}, \tag{3.82}$$

$$V_\tau \rightarrow V_\tau\sqrt{\frac{3}{2}mA}\frac{1}{2\hbar}. \tag{3.83}$$

Defining

$$\theta_{ij}^{\beta} = \sum_{\gamma\delta}\epsilon_{\beta\gamma\delta}\sigma_i^\gamma r_{ij}^\delta, \tag{3.84}$$

and performing the necessary algebraic steps, we rewrite Eq(3.78) as:

$$\begin{aligned} H = \sum_{i\neq j,\alpha\beta}\frac{1}{2}\left(p_{ij}^\beta + \theta_{ij}^\beta\left(\frac{1}{3}V(r_{ij}) + \tau_i^\alpha\tau_j^\alpha V_\tau(r_{ij})\right)\right)^2 \\ -\frac{1}{2}\left(\theta_{ij}^\beta\left(\frac{1}{3}V(r_{ij}) + \tau_i^\alpha\tau_j^\alpha V_\tau(r_{ij})\right)\right)^2. \end{aligned} \tag{3.85}$$

In the previous expression quadratic operators appear and we can recast the propagator e^{-Hdt} used in AFDMC algorithm by means the Hubbard Stratonovich transform

$$\begin{aligned} \prod_{i\neq j,\alpha\beta}\int_d x_{ij}^{\alpha\beta}\exp\left[-\frac{\left(x_{ij}^{\alpha\beta}\right)^2}{2}\right]\exp\left[-\sqrt{-dt}p_{ij}^\beta x_{ij}^{\alpha\beta}\right]\times \\ \exp\left[-\sqrt{-dt}\theta_{ij}^\beta x_{ij}^{\alpha\beta}\frac{V(r_{ij})}{3}\right]\exp\left[-\sqrt{-dt}\theta_{ij}^\beta x_{ij}^{\alpha\beta}V_\tau(r_{ij})\tau_i^\alpha\tau_j^\alpha\right]\times \\ \exp\left[\frac{dt}{2}\left(\sum_{\gamma\delta}\left(\sigma_i^\gamma+\sigma_j^\gamma\right)r_{ij}^\delta\epsilon_{\beta\gamma\delta}\right)^2\times \right. \\ \left.\left(\frac{V(r_{ij})}{9}+\frac{2V(r_{ij})V_\tau(r_{ij})}{3}\tau_i^\alpha\tau_j^\alpha+V_\tau^2(r_{ij})\right)\right]. \end{aligned} \tag{3.86}$$

In this way the momentum operators are separated from the other ones. The last exponential contains no auxiliary fields x, but only two body central operators; we are able to treat those terms in a standard way with an Hubbard Stratonovich transform. The third exponential is a simple one–body term. The problem is in the fourth exponential. In fact that term contains non–commuting two body terms, but still an integration on auxiliary fields x:

$$-\sqrt{-dt}\theta_{ij}^\beta x_{ij}^{\alpha\beta}V_\tau(r_{ij})\tau_i^\alpha\tau_j^\alpha. \tag{3.87}$$

In principle could apply one more Hubbard Stratonovich transform. This is not so simple because we should rewrite Eq(3.87) as a sum of square operator

$$\theta_{ij}^\beta\tau_i^\alpha\tau_j^\alpha = \frac{1}{4}\left[\left(\theta_{ij}^\beta\tau_i^\alpha+\tau_j^\alpha\right)^2-\left(\theta_{ij}^\beta\tau_i^\alpha-\tau_j^\alpha\right)^2\right] \tag{3.88}$$

making sure that:

$$\left[\theta_{ij}^{\beta}\tau_i^{\alpha}\ ,\ \tau_j^{\alpha}\right] = 0 \qquad \text{for } i \neq j. \tag{3.89}$$

If the previous commutator is not zero we are introducing an error of order $\sqrt{dt}$ when splitting the exponential containing the operator on particle i and operator on particle j respectively. This error is under control only for a single small dt iteration, but not for the large number of iterations needed to reach the limit $t \to \infty$; in this case we are out of the convergence radius.

Because of Eq(3.89), we can apply yet one more integration on auxiliary fields y and z on the fourth exponential term of the propagator:

$$\begin{aligned}
&\prod_{i\neq j,\alpha\beta} \exp\left[-\sqrt{-dt}\theta_{ij}^{\beta}x_{ij}^{\alpha\beta}V_\tau(r_{ij})\tau_i^{\alpha}\tau_j^{\alpha}\right] = \\
&= \prod_{i\neq j,\alpha\beta} \iint dz_{ij}^{\alpha\beta}dy_{ij}^{\alpha\beta} \exp\left[-\frac{\left(y_{ij}^{\alpha\beta}\right)^2+\left(z_{ij}^{\alpha\beta}\right)^2}{2}\right] \times \\
&\qquad \exp\left[-\sqrt{-\sqrt{-dt}x_{ij}^{\alpha\beta}\frac{V_\tau(r_{ij})}{2}}\left(y_{ij}^{\alpha\beta}+\imath z_{ij}^{\alpha\beta}\right)\theta_{ij}^{\beta}\tau_i^{\alpha}\right] \times \\
&\qquad \exp\left[-\sqrt{-\sqrt{-dt}x_{ij}^{\alpha\beta}\frac{V_\tau(r_{ij})}{2}}\left(y_{ij}^{\alpha\beta}-\imath z_{ij}^{\alpha\beta}\right)\tau_i^{\alpha}\right]
\end{aligned} \tag{3.90}$$

Hence to write the full propagator it is possible to make use of the identity

$$\left(\sum_{\gamma\delta}\left(\sigma_i^{\gamma}+\sigma_j^{\gamma}\right)r_{ij}^{\delta}\epsilon_{\beta\gamma\delta}\right)^2 = 4 + 2\sum_{\beta\gamma}\sigma_i^{\beta}\sigma_j^{\gamma}\left(\delta_{\beta\gamma}-\hat{r}_{ij}^{\beta}\hat{r}_{ij}^{\gamma}\right) \tag{3.91}$$

and, in order to simplify the notation, we define the following Hermitian matrix, eigenvalues and eigenvectors

$$T_{ij} = dt\tfrac{8}{3}V(r_{ij})V_\tau(r_{ij}) \tag{3.92}$$

$$S_{i\beta,j\gamma} = 2dt\left(\tfrac{1}{3}V(r_{ij})^2+3V_\tau(r_{ij})^2\right)\left(\delta_{\beta\gamma}-\hat{r}_{ij}^{\beta}\hat{r}_{ij}^{\gamma}\right) \tag{3.93}$$

$$\mathscr{T}_{i\beta,j\gamma} = \tfrac{4}{3}dtV(r_{ij})V_\tau(r_{ij})\left(\delta_{\beta\gamma}-\hat{r}_{ij}^{\beta}\hat{r}_{ij}^{\gamma}\right) \tag{3.94}$$

$$T_{ij} = Q_{ik}^{T}\lambda_k^{T}Q_{jk}^{T} \tag{3.95}$$

$$\mathscr{T}_{i\beta,j\gamma} = Q_{i\beta,k\delta}^{\mathscr{T}}\lambda_{k\delta}^{\mathscr{T}}Q_{j\gamma,k\delta}^{\mathscr{T}} \tag{3.96}$$

$$S_{i\beta,j\gamma} = Q_{i\beta,k\delta}^{S}\lambda_{k\delta}^{S}Q_{j\gamma,k\delta}^{S} \tag{3.97}$$

Eventually the propagator is:

$$\begin{aligned}
&\prod_i \int dx\, dy\, dz\, dq^T\, dq^S\, dq^{\mathscr{T}} \exp\left[-\frac{1}{2}\sum_{j\alpha\beta}\left(\left(x_{ij}^{\alpha\beta}\right)^2+\left(y_{ij}^{\alpha\beta}\right)^2+\left(z_{ij}^{\alpha\beta}\right)^2\right)\right]\times\\
&\exp\left[-\frac{1}{2}\sum_{j\delta}\left(q_{j\delta}^S\right)^2\right]\exp\left[-\frac{1}{2}\sum_{j\alpha}\left(q_{j\alpha}^T\right)^2\right]\exp\left[-\frac{1}{2}\sum_{j\alpha\delta}\left(q_{j\alpha\delta}^{\mathscr{T}}\right)^2\right]\times\\
&\exp\left[2dt\sum_j\frac{V(r_{ij})^2}{3}+3V_\tau(r_{ij})^2\right]\times\\
&\exp\sum_\beta p_i^\beta\left[-\frac{\sqrt{-dt}}{2}\sum_{j\alpha}\left(x_{ij}^{\alpha\beta}-x_{ji}^{\alpha\beta}\right)\right]\times\\
&\exp\sum_\gamma \sigma_i^\gamma\left[-\sum_{j\delta}\left(\sqrt{\lambda_{j\delta}^S}q_{j\delta}^S Q_{i\gamma,j\delta}^S+\sum_{\alpha\beta}\sqrt{-dt}x_{ij}^{\alpha\beta}\epsilon_{\beta\gamma\delta}r_{ij}^\delta\right)\right]\times\\
&\exp\sum_\alpha \tau_i^\alpha\left[-\sum_j\left[\sqrt{\lambda_j^T}q_{j\alpha}^T Q_{ij}^T+\sum_\beta\sqrt{-\sqrt{-dt}x_{ij}^{\alpha\beta}\frac{V_\tau(r_{ij})}{2}}\left(y_{ij}^{\alpha\beta}-\imath z_{ij}^{\alpha\beta}\right)\right]\right]\times\\
&\exp\sum_{\alpha\gamma}\sigma_i^\gamma\tau_i^\alpha\left[-\sum_{j\delta}\left(P_{i\gamma,j\delta}^{\mathscr{T}}q_{j\delta\alpha}^{\mathscr{T}}\sqrt{\lambda_{j\delta}^{\mathscr{T}}}\right)\right.\\
&\qquad\left.-\sum_{j\delta\beta}\left(\sqrt{-\sqrt{-dt}x_{ij}^{\alpha\beta}\frac{V_\tau(r_{ij})}{2}}\left(y_{ij}^{\alpha\beta}+\imath z_{ij}^{\alpha\beta}\right)\epsilon_{\beta\gamma\delta}r_{ij}^\delta\right)\right]
\end{aligned}\tag{3.98}$$

where the sums on j are intended on $j \neq i$.

Then we can apply the importance sampling in the standard way, namely sampling with a drift and weighting with the local energy. For the fields q the method is exactly the standard one, while it is quite different for y and z fields because of the double Gaussian integration. If we label with g a Gaussian distribution centered in 0 with variance 1, we have that

$$x_{ij}^{\alpha\beta} = g_{ij}^{\alpha\beta} - \bar{x}_{ij}^{\alpha\beta} \tag{3.99}$$

$$y_{ij}^{\alpha\beta} = \tilde{g}_{ij}^{\alpha\beta} - \bar{y}_{ij}^{\alpha\beta} \tag{3.100}$$

$$z_{ij}^{\alpha\beta} = \bar{g}_{ij}^{\alpha\beta} - \bar{z}_{ij}^{\alpha\beta} \tag{3.101}$$

$$\bar{x}_{ij}^{\alpha\beta} = \sqrt{-dt}\left\langle p_{ij}^\beta + \theta_{ij}^\beta\left(\tfrac{V(r_{ij})}{3}+V_\tau(r_{ij})\tau_i^\alpha\tau_j^\alpha\right)\right\rangle \tag{3.102}$$

$$\bar{y}_{ij}^{\alpha\beta} = \left\langle\sqrt{-\sqrt{dt}x_{ij}^{\alpha\beta}\tfrac{V_\tau(r_{ij})}{2}}\left(\tau_j^\alpha+\tau_i^\alpha\textstyle\sum_{\delta\gamma}\sigma_i^\gamma\epsilon_{\beta\gamma\delta}r_{ij}^\delta\right)\right\rangle \tag{3.103}$$

$$\bar{z}_{ij}^{\alpha\beta} = -\imath\left\langle\sqrt{-\sqrt{dt}x_{ij}^{\alpha\beta}\tfrac{V_\tau(r_{ij})}{2}}\left(\tau_j^\alpha-\tau_i^\alpha\textstyle\sum_{\delta\gamma}\sigma_i^\gamma\epsilon_{\beta\gamma\delta}r_{ij}^\delta\right)\right\rangle \tag{3.104}$$

where for a generig operator Ω we assume the following definition of the notation

$\langle\Omega\rangle$:

$$\langle\Omega\rangle = \frac{\langle\{r,S,T\}\,|\Omega|\,\Psi_T\rangle}{\langle\{r,S,T\}|\Psi_T\rangle} \tag{3.105}$$

At the end it is necessary to restore the standard notation of Eq(3.83), reintroducing the physical constants. Notice that in this way we have $27N^2 - 12N$ auxiliary fields instead of the $18N$ of the AFDMC without spin orbit terms.

We have to notice that we can apply the fourth term of Eq(3.98), only when its coefficient is a purely imaginary term. Only in that case that term of the propagator is a translation operator, i.e. we have a real shift. So we have to use for the propagator a term like this

$$\exp\sum_{\beta} p_i^{\beta}\left[-\frac{\sqrt{-dt}}{2}\sum_{j\alpha}\Re\left(x_{ij}^{\alpha\beta}-x_{ji}^{\alpha\beta}\right)\right] \tag{3.106}$$

3.10 L^2 terms

On the same idea of the spin–orbit term, we have tried to include a L^2 term into the propagator.

Like in the previous section we assume that Greek indexes indicate $\{x,y,z\}$ labels, A is the number of nucleons with mass m and Latin index are summed on particle number A. We consider an Hamiltonian with a L^2 term interaction like

$$H = \sum_{i,\beta}\frac{\left(p_i^{\beta}\right)^2}{2m} + \sum_{i<j}\frac{1}{4\hbar^2}V(r_{ij})\sum_{\alpha}\left(L_{jk}^{\alpha}\right)^2 \tag{3.107}$$

where

$$L_{ij}^{\alpha} = \sum_{\beta\gamma}\epsilon_{\alpha\beta\gamma}r_{ij}^{\beta}\,2p_{ij}^{\gamma} \tag{3.108}$$

$$p_{ij} = \frac{p_i - p_j}{2} \tag{3.109}$$

$$r_{ij} = r_i - r_j \tag{3.110}$$

Once more, subtracting the center of mass kinetic energy from the previous formula, we obtain

$$H = \sum_{i<j,\alpha}\left[\frac{\left(p_{ij}^{\alpha}\right)^2}{\frac{1}{2}mA} + \frac{V(r_{ij})}{\hbar^2}\sum_{\beta\gamma\beta'\gamma'}\epsilon_{\alpha\beta\gamma}\epsilon_{\alpha\beta'\gamma'}\,r_{ij}^{\beta}\,p_{ij}^{\gamma}\,r_{ij}^{\beta'}\,p_{ij}^{\gamma'}\right]. \tag{3.111}$$

But we have that:

$$\epsilon_{\alpha\beta\gamma}\epsilon_{\alpha\beta'\gamma'} = \epsilon_{\alpha\beta\gamma}\left(\delta_{\beta\beta'}\delta_{\gamma\gamma'} - \delta_{\beta\gamma'}\delta_{\gamma\beta'}\right) \tag{3.112}$$

and so we can rewrite Eq(3.111) as

$$H = \sum_{i<j,\alpha}\left\{\frac{\left(p_{ij}^{\alpha}\right)^2}{\frac{1}{2}mA} + \frac{V(r_{ij})}{\hbar^2}\sum_{\beta\gamma}\epsilon_{\alpha\beta\gamma}\left[\left(r_{ij}^{\beta}\,p_{ij}^{\gamma}\right)^2 - r_{ij}^{\beta}\,p_{ij}^{\gamma}\,r_{ij}^{\gamma}\,p_{ij}^{\beta}\right]\right\} \tag{3.113}$$

Taking into account the commutation relation and that $\beta \neq \gamma$ because of the $\epsilon_{\alpha\beta\gamma}$ factor, we have that

$$r^\beta \; p^\gamma \; r^\gamma \; p^\beta = r^\beta \; p^\beta \; p^\gamma \; r^\gamma. \tag{3.114}$$

We can then rewrite the previous term as:

$$\frac{1}{4}\left[\left(r^\beta p^\beta + p^\gamma r^\gamma\right)^2 - \left(r^\beta p^\beta - p^\gamma r^\gamma\right)^2\right], \tag{3.115}$$

with

$$\left[r^\beta p^\beta \; , \; p^\gamma r^\gamma\right] = 0 \qquad \text{for } \beta \neq \gamma. \tag{3.116}$$

Eq(3.116) is important because it permits to split the exponential without making an error of order $\sqrt{dt}$ in the propagation due to commutators, as explained for equation Eq(3.89).

So we can write the propagator $e^{-dt(H-E_0)}$ as

$$\begin{aligned}
\prod_i \int dx\; dy\; dz\; dk \exp\left[-\frac{1}{2}\left(\sum_{j\alpha}\left(x_{ij}^\alpha\right)^2 + \sum_{j\beta\gamma}\left(y_{ij}^{\beta\gamma}\right)^2 + \left(z_{ij}^{\beta\gamma}\right)^2 + \left(k_{ij}^{\beta\gamma}\right)^2\right)\right] \times \\
\exp\left[-\sum_{j\alpha}\sqrt{\frac{-dt}{mA/2}}p_{ij}^\alpha x_{ij}^\alpha\right] \times \\
\exp\left[-\sum_{j\alpha\beta\gamma}\sqrt{\epsilon_{\alpha\beta\gamma}}\sqrt{-dt\frac{V(r_{ij})}{\hbar^2}}r_{ij}^\beta p_{ij}^\gamma y_{ij}^{\beta\gamma}\right] \times \\
\exp\left[\sum_{j\alpha\beta\gamma}\sqrt{\epsilon_{\alpha\beta\gamma}}\frac{\imath}{2}\sqrt{-dt\frac{V(r_{ij})}{\hbar^2}}\left(r_{ij}^\beta p_{ij}^\beta + p_{ij}^\gamma r_{ij}^\gamma\right)z_{ij}^{\beta\gamma}\right] \times \\
\exp\left[-\sum_{j\alpha\beta\gamma}\sqrt{\epsilon_{\alpha\beta\gamma}}\frac{1}{2}\sqrt{-dt\frac{V(r_{ij})}{\hbar^2}}\left(r_{ij}^\beta p_{ij}^\beta - p_{ij}^\gamma r_{ij}^\gamma\right)k_{ij}^{\beta\gamma}\right]
\end{aligned} \tag{3.117}$$

where we have introduced the auxiliary fields x, y, z and k. Because of Eq(3.116) we can split the last two exponentials and we obtain a propagator that only contains $r_{ij}^\beta p_{ij}^\gamma$ or $r_{ij}^\beta p_{ij}^\beta$ operators. We can do one more Hubbard Stratonovich integration to split r from p. Details on importance sampling and approximation due to the "phase" (i.e. to keep a real drift) are qualitatively the same of (§ 3.9).

Notice that in nuclear potentials also two–body terms of the form

$$L^2\left(\sigma_i \cdot \sigma_j\right) \tag{3.118}$$

$$L^2\left(\tau_i \cdot \tau_j\right) \tag{3.119}$$

$$L^2\left(\sigma_i \cdot \sigma_j\right)\left(\tau_i \cdot \tau_j\right) \tag{3.120}$$

are presents. I was not able to rewrite terms like that in a way in which it is possible to have a relation like Eq(3.116) or Eq(3.89), necessary to use the

second Hubbard Stratonovich transform. So, at this stage of the work, those terms cannot be used in the propagator of AFDMC.

Anyway, we can observe that the general approach based on splitting each momentum operator from the others can fruitfully be used in GFMC algorithm. When we split momentum operators, in GFMC we can treat the other terms directly even if they are not quadratic, by means of integration on some auxiliary fields probably we can include non–local terms in GFMC propagator.

3.11 Exchange term between particles with different masses

A standard nuclear Hamiltonian can in principle contain terms that mix isospin components, i.e. exchange terms that mix neutron and proton states. Fortunately the mass of the two particle is more or less the same and so we can assume the same mass for both states.

Treating exchange term exactly is a bit tricky, because we do not know in principle which mass to use to diffuse the coordinate of a walker that is in a neutron–proton mixed state. We could solve the problem in the following way.

Let us call the proton and nucleon masses m and M respectively.

The kinetic propagator would have the form

$$\prod_i e^{-\frac{dt}{2m}P_i^2 O_i} = \prod_i e^{-\frac{dt}{4m}(P_i^2+O_i)^2} e^{-\frac{dt}{4m}P_i^4} e^{-\frac{dt}{4m}O_i^2}, \tag{3.121}$$

where O_i is a diagonal matrix like

$$O_i = \begin{pmatrix} 1 & 0 \\ 0 & m/M \end{pmatrix} \tag{3.122}$$

Now we can apply the Hubbard Stratonovich transform, focusing only on one particle i:

$$\int dxdydz \frac{1}{(2\pi)^{3/2}} e^{-\frac{x^2+y^3+z^2}{2}} e^{-\sqrt{-\frac{dt}{2m}}x(P_i^2+O_i)} e^{-\sqrt{-\frac{dt}{2m}}yP_i^2} e^{-\sqrt{-\frac{dt}{2m}}zO_i} \tag{3.123}$$

Because it holds

$$[O_i, P_i] = 0 \tag{3.124}$$

we can rewrite the previous equation exchanging some terms, keeping the integral correct up to terms linear in dt. This conclusion is important as shown for equations Eq(3.89) and Eq(3.116). Rewriting Eq(3.123) we obtain:

$$\int dxdydz \frac{1}{(2\pi)^{3/2}} e^{-\frac{x^2+y^3+z^2}{2}} e^{-\sqrt{-\frac{dt}{2m}}(x+y)P_i^2} e^{-\sqrt{-\frac{dt}{2m}}(x+z)O_i} \tag{3.125}$$

and now we can apply a further Hubbard Stratonovich transform obtaining

$$\int dxdydzdk \frac{1}{(2\pi)^2} e^{-\frac{x^2+y^3+z^2+k^2}{2}} e^{-\sqrt{-\sqrt{-\frac{2dt}{m}}(x+y)}kP_i} e^{-\sqrt{-\frac{dt}{2m}}(x+z)O_i} \tag{3.126}$$

Now we are able to use this propagator, also with importance sampling in the same way like we have done in (§ 3.9) and followings.

Probably, if the masses are nearly the same, it is more computationally efficient to rewrite the kinetic term like:

$$T = \sum_i \frac{P_i^2}{2m} - \frac{M-m}{2M} \sum_i \frac{P_i^2}{2m} \theta_i \tag{3.127}$$

$$\theta_i = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \tag{3.128}$$

In this way it is only necessary to compute the double Hubbard Stratonovich transform on the last factor, that has a quite small $\frac{M-m}{2M}$ coefficient.

This approach could be implemented also in GFMC, so it could be possible to take into account these mass corrections also into the propagator and not only perturbatively.

3.12 Estimation of the accuracy if the fixed–phase approximation of AFDMC

The fixed phase approximation introduces a systematic, uncontrolled error on the estimates of interest. Here I report the results of an extensive exploration of these effects recently performed on the ground states of light nuclei.

The test consist of comparing our results to very accurate results of GFMC calculations by S. Pieper, using the Argonne $Av1'$, $Av4'$ and $Av6'$ potentials[Pie05, WSS95, WP02, PW01, PPPW97].

We particularly focus our attention on Helium isotopes, namely ^{4}He, ^{6}He and ^{8}He. For ^{4}He we use as importance function an antisymmetrized wavefunction on spin/isospin states with a single radial function compounded by a Hartree Fock calculation with Skyrme interaction. Then we use a central Jastrow factor that is simply the function obtained solving the 2–body problem with the central part of the potential. To find the better wavefunction we weight this Jastrow with a prefactor called "quencher".

For ^{6}He and ^{8}He we use the same approach, but we have two different orbitals with an appropriate combination of Slater determinants in order to have the good quantum numbers.

In the best hypothesis, we will have that for any trial wavefunction in input we are able to project to the exact ground state energy. We also have to remember that it is necessary to check the bias due to the finite size population of walkers and to the finite size time step of the propagator; i.e. we have to extrapolate into the limit $dt \to 0$ and $N_w \to \infty$, or to verify that this extrapolation is less than the statistical error.

We use three different algorithms, theoretically equivalent except for the behaviors of the fixed–phase approximation and of the extrapolation for small time steps and big number of walkers:

- the "drift" AFDMC algorithm, i.e. the standard AFDMC with the drift as previously explained. For simplicity in this paragraph we call this "drift" algorithm.

- the "Carlson" AFDMC algorithm. Starting from Eq(3.27) for each of the sampled walkers we can create two walkers. We generate the first one with a stochastic variable x sampled like in Eq(3.27), and the second using the stochastic variable $-x$. Doing so we obtain a double population but we removed the noise due to the odd terms of the auxiliary field integral. However, we have to keep the number of walker constant. So for each pair of new walkers we randomly choose one of them, with probability proportional to the branching factor. Then we assume for the weight of this walker the average of the two previous branching factors. We stress that the propagator does not include in the weights the local energy as in the "drift" AFDMC. The consequence is a larger fluctuation in the population. Anyway, we can observe that the propagator is correct up to order $\mathcal{O}(dt^2)$, like in the previous algorithm, and that the stochastic noise on odd auxiliary field terms is eliminated with the trick of the double sampling.

- the "Schmidt" AFDMC algorithm. We try this hybrid algorithm to unify the major peculiarities of the previous two. We take into account the Green's function of the previous "Carlson" AFDMC algorithm, but instead of sampling the auxiliary fields like that Green's function, we sample them from that of the drift algorithm. Then we need to apply a corrective weight factor that is the ratio of the two different Green's function.

3.12.1 ^{4}He

We report in the following three different plots of the energy values obtained with the three different potentials $Av1'$, $Av4'$ and $Av6'$ for ^{4}He. The value of Pieper corrected without the electromagnetic contribution is also plotted.

The results, obtained with the three different methods, are reported with and without the Jastrow factor. For a fixed node DMC algorithm we see that the result is independent on the Jastrow factor, because it does not change the nodal surface. Because of the fixed–phase approximations this is no longer true.

We also tried to change also the size of the orbital (the parameter named $rmax$ in the following) in order to resize the orbital by simply rescaling the radial coordinate. For the following plots the Hartree Fock orbital length is fixed to 20fm. So we plot the energy as function of the variational parameter $rmax$, with and without the Jastrow term, and with the three different algorithms and potentials.

As we can see from Fig. 3.1, Fig. 3.2 and Fig. 3.3, we have a quite good result only for the central potential (Fig. 3.1). For values of $rmax$ too far from the optimal one we have a larger extrapolation coefficient in time step and walkers number. however, the extrapolated values are all in agreement with the expected answer. We can notice that the drift AFDMC algorithm has the worse extrapolation behavior when we have a bad wavefunction. This trend is amplified with $Av4'$ and $Av6'$ potentials.

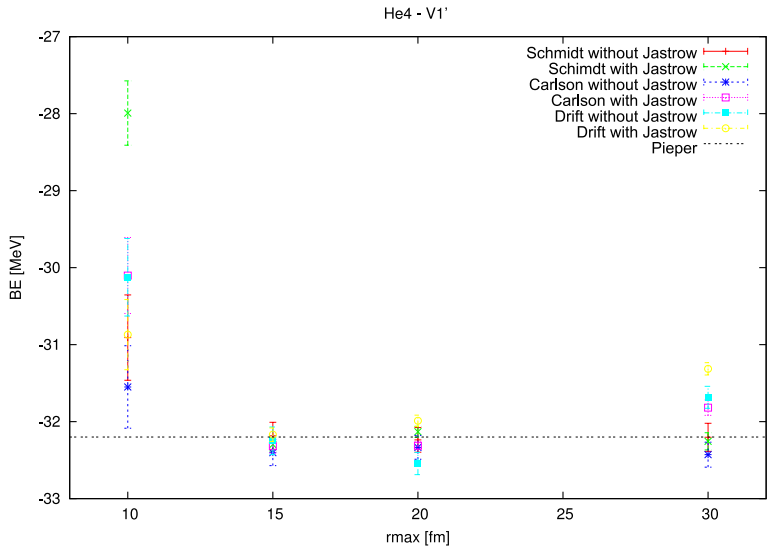

Figure 3.1: ^{4}He binding energy with $Av1'$.

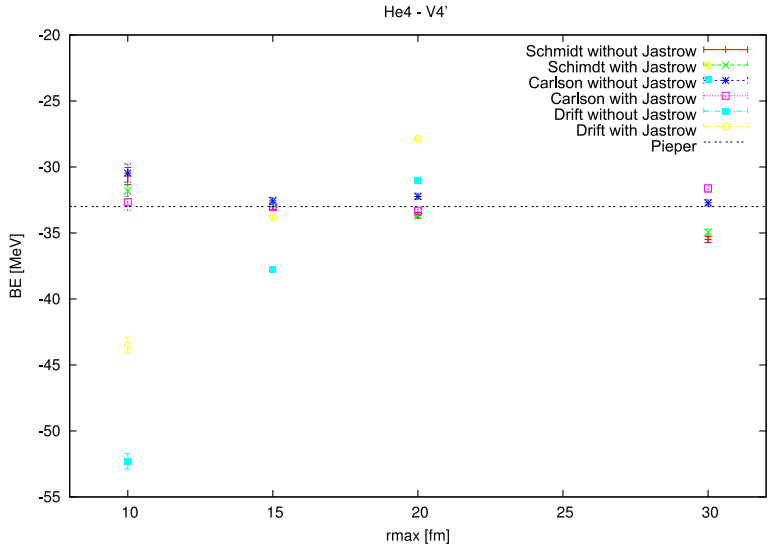

Figure 3.2: ^{4}He binding energy with $Av4'$.

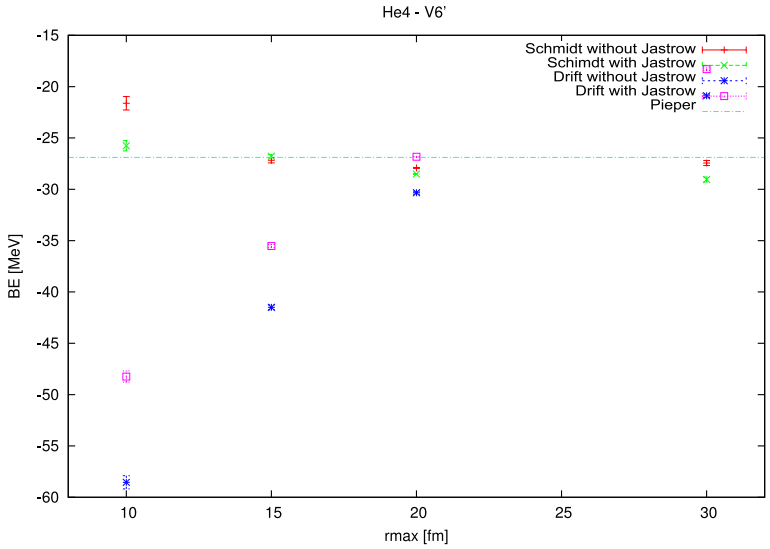

Figure 3.3: ^{4}He binding energy with $Av6'$.

In the last plot Fig. 3.3 there are no points relative to the "Carlson" algorithm because we were not able to reach a good stable value; we are not able to explain why this algorithm is so unstable with $Av6'$; we can probably argue that the presence of a big tensor term into the potential brings some troubles to the sign problem.

Now we can summarize our results and conclusions:

- The "Schmidt" algorithm (and the "Carlson" one for $Av1'$ and $Av4'$) is better than the "drift" one because of:

  1. the small time step and walker number extrapolation;
  2. the dependence in the variational parameters of the wavefunction (Jastrow and size of the orbitals "rmax") is negligible after extrapolation for $N_w \to \infty$ and $dt \to 0$; that is not so for the "drift" algorithm.

- With the "drift" algorithm it is possible to obtain good results (see Tab. 3.1), when the trial wavefunction is accurately chosen. For small nuclei, where we have a comparison with GFMC we are able to fine the trial wavefunction to obtain the correct numbers.

  As we can see from the plot, we were able to obtain these results by accurately tuning the trial wavefunction in such a way to reproduce the expected energy. As we can see from the plots with different Jastrow or orbital size of the trial wavefunction, the results are so different that we are

	BE [MeV]	error [MeV]	Pieper [MeV]
^{4}He	-26.81	0.08	-26.89
^{6}He	-25.05	0.05	-25.80
^{8}He	-24.03	0.08	-23.73
^{15}O	-89.90	0.1	
^{16}O	-105.4	0.1	
^{17}O	-104.4	0.1	
^{39}Ca	-261.2	0.4	
^{40}Ca	-279.4	0.4	

Table 3.1: Energy of some nuclei with the $Av6'$ potential computed with the "drift" algorithm and compared with Pieper GFMC calculations where available.

not able to be predictive. This means that the method is not good to fit a potential or to do calculations for which we do not have any comparison. Relatively to the second part of this thesis (EFT for nuclei) we can say that it is very hard to find good results. This is because we have a bad trial wavefunction, no comparative calculations, and also a bigger sign problem respect to the standard nuclear AFDMC with Argonne potential, due to the big vacuum and self–energy terms.

- The previous problem is overcome by the "Schmidt" algorithm. However, the results are far from the results of Pieper. For example for ^{4}He we obtain a BE of about 1MeV too big. That error is too high to allow its application to Hypernuclear systems, where we have to compute the difference in the binding energy between the nucleus and the relative hypernucleus. In fact, for ${}^{5}_{\Lambda}$He , for example, we have an estimated error of about 2MeV where the energy that we want to compute is 3.12MeV. The problem becomes harder if we have also to fit the potential. Moreover take into account that ^{4}He is the simpler system, because of its closed shell, its relatively good trial wavefunction and fast in computation.

3.12.2 Perspectives

In the previous paragraph we have stressed limits and problems of the AFDMC algorithm as we have used and implemented. Then now we try to plan how we could try to solve or overcome these problems. It is possible both to improve the algorithm, and to choose a better wavefunction.

In fact the accuracy of the fixed–phase approximation depends on the quality of the trial wavefunction; if we have a wavefunction closer to the exact one, the approximation will be improved. For nuclei and hypernuclei, for example, we could try to obtain a better trial wave function. A possibility consist of performing VMC calculations, trying to expand the wavefunction on a series of Slater determinants. Minimizing the energy we can find better one–body wavefunc-

tions and include effectively spin/isospin correlations. We plan to implement this idea soon. But while it is theoretically possible in this way to find a trial wavefunction arbitrarily close to the exact one, we have to check if it is possible to obtain a sufficiently good trial wavefunction to make usable the fixed–phase approximation using a not too large computable number of Slater determinants.

Concerning possible improvements of the method, we could try to develop a better implementation of the fixed–phase approximation or a similar constraint. We already explored some alternatives attempts as explained in the previous paragraph. Other improvements might be possible. A different approach might be be that of using a different algorithm, the Auxiliary Field Quantum Monte Carlo (AFQMC), which will be described in the next chapter. It looks like this algorithm has a lower bias due to the fixed–phase approximation.

Chapter 4

Auxiliary Field Quantum Monte Carlo

The Auxiliary Field Quantum Monte Carlo (AFQMC) algorithm was developed by S. Zhang [STBZ04, PZ04, ASKZ06, ASZK06]. By means of this method it is possible to study the ground state of a system with a generic two body interaction.

4.1 The basic idea

Consider an Hamiltonian containing one and two body terms:

$$H = H_1 + H_2 = H_1 + \frac{1}{2}O^2, \tag{4.1}$$

where H_2 can be rewritten as the square of one body terms. So, like in DMC, we can compute the ground state Ψ_0 by evolving a starting trial wavefunction Ψ_T in imaginary time

$$\begin{aligned} \Psi_0 &= \lim_{t\to\infty} e^{-t(H-E_0)}\Psi_T = \lim_{t\to\infty} e^{-t(H_1-E_0+\frac{O^2}{2})}\Psi_T \\ &= \lim_{t\to\infty}\lim_{M\to\infty}\left(e^{-\frac{t}{M}(H-E_0)}e^{-\frac{t}{M}\frac{O^2}{2}}\right)^M \Psi_T. \end{aligned} \tag{4.2}$$

Choosing a sufficiently high t to reach the convergence and defining $dt = \frac{t}{M}$ sufficiently small to make negligible the contributions of order $\mathcal{O}(dt^2)$ due to $[H_1, O]$ terms, we can apply the propagator

$$\mathcal{P} = e^{-dt(H-E_0)}e^{-dt\frac{O^2}{2}} \tag{4.3}$$

M times to the starting trial wavefunction Ψ_T and obtain a sampling of the ground state Ψ_0.

If we rewrite $e^{-dt\frac{O^2}{2}}$ using a Gaussian integration on an auxiliary field (an Hubbard Stratonovich transform), we obtain a propagator that contains only one body operators:

$$\mathcal{P} = \frac{1}{\sqrt{2\pi}}\int e^{-dt(H-E_0)}e^{-\frac{x^2}{2}}e^{-\sqrt{dt}xO} \tag{4.4}$$

In principle Ψ_0 lives in an Hilbert space $\mathbb{H}$ that is the product space of single particle Hilbert spaces $\mathcal{H}$ of the N_{PART} particles of the studied systems:

$$\mathbb{H} = \bigotimes_{i}^{N_{PART}} \mathcal{H}_i \qquad \dim \mathbb{H} = {N_S}^{N_{PART}} \tag{4.5}$$

If $\mathcal{H}$ are spaces of finite size with dimension N_S, the dimension of $\mathbb{H}$ will be ${N_S}^{N_{PART}}$. That is, the space dimension (and so also the computational cost to find Ψ_0) increases exponentially with the number of particles in the system. This is necessary when we use a generic trial wavefunction Ψ_T and a propagator written as in Eq(4.3).

On the other hand if we take into account a trial wavefunction Ψ_T that is simply the sum of Slater determinants of single particles wavefunctions, we can represent it in the sum of single particle spaces:

$$\mathscr{H} = \bigoplus_{i}^{N_S} \mathcal{H}_i \qquad \dim \mathscr{H} = N_{PART} \cdot N_S \tag{4.6}$$

where $\mathscr{H}$ has only dimension $N_{PART} \cdot N_S$ instead of ${N_S}^{N_{PART}}$ like $\mathbb{H}$. Now a propagator $\mathcal{P}$ like that of Eq(4.3) is not closed onto the space $\mathscr{H}$, and so applying that $\mathcal{P}$ to that Ψ_T we obtain an object that is in general out of $\mathscr{H}$ and that belongs to $\mathbb{H}$. Conversely if we use the propagator $\mathcal{P}$ of equation Eq(4.4) we can work only in the $\mathscr{H}$ space because that $\mathcal{P}$ is closed onto $\mathscr{H}$.

This is the fundamental point of that algorithm that allows to have a polynomial scalability with the number of particles.

It must be stressed that in order to do that we use an Hilbert space $\mathcal{H}$ for the single particle space that has a finite dimension N_S. Typically the single particle space is infinite–dimensional. The necessity of truncating the Hilbert space to a finite dimension is a limitation of the method. Clearly increasing N_S it is possible to reach a better results, at the price of an increased computational cost. A good compromise consist of choosing different Hilbert spaces $\mathcal{H}$ (i.e. single particle basis sets) with increasing N_S until the convergence is reached. With different basis sets we can have slower or faster convergence with the number N_S of basis elements considered. Another thing to take into account is that with this method it is possible to include any type of two body interaction, at a difference with DMC. Anyway, differently from DMC, it is not possible to include three or more body terms even if they are local.

4.2 Single particle space $\mathcal{H}$

As said in the previous section, it is important to use a good single particle space to choose a basis set for which the algorithm has a fast convergence with N_S. Because of that, being interested in finite size systems and focusing our attention to nuclear systems, the single particle space is written as the following direct product:

$$\mathcal{H} = \mathcal{H}_\sigma \otimes \mathcal{H}_\tau \otimes \mathcal{H}_L \otimes \mathcal{H}_r \tag{4.7}$$

where

$$\mathcal{H}_\sigma \quad \text{is the spin space} \tag{4.8}$$
$$\mathcal{H}_\tau \quad \text{is the isospin space} \tag{4.9}$$
$$\mathcal{H}_L \quad \text{is the angular momentum space} \tag{4.10}$$
$$\mathcal{H}_r \quad \text{is the radial space} \tag{4.11}$$

Each space will be spanned by a suitable basis set. For the spin and isospin spaces we choose the 2 eigenstates of σ_z and τ_z respectively. For the angular momentum space we choose the spherical harmonics Y_m^l. For the radial space we can choose an arbitrary tabulated set of orthonormal orbitals. We choose $\mathcal{H}_L \otimes \mathcal{H}_r$ because we are interested to finite size systems. For the uniform nuclear matter case a different basis set might be chosen.

A single particle basis element can then be written as:

$$|i\rangle = |\chi_{\sigma\tau}\rangle \otimes \left|Y_{mi}^{li}\right\rangle \otimes |f_i\rangle\,, \tag{4.12}$$

with

$$|\chi_{\sigma\tau}\rangle \quad \in \mathcal{H}_\sigma \otimes \mathcal{H}_\tau, \tag{4.13}$$
$$\left|Y_{mi}^{li}\right\rangle \quad \in \mathcal{H}_L, \tag{4.14}$$
$$|f_i\rangle \quad \in \mathcal{H}_r. \tag{4.15}$$

4.3 Matrix elements

To apply the algorithm to a generic system with a generic Hamiltonian:

$$H = H_1 + H_2 = \sum_{il} U_{il} c_i^\dagger c_l + \frac{1}{2} \sum_{ijkl} c_i^\dagger c_j^\dagger c_k c_l V_{ijkl} \tag{4.16}$$

we have to compute all the one body U_{il} and two–body V_{ijkl} matrix elements.

We remember here some properties

$$\begin{aligned} V_{ijkl} &= \langle ij\,|V|\,lk\rangle \\ &= \iint dxdy\; i^*(x) l(x) j^*(y) k(y) V(x,y) \end{aligned} \tag{4.17}$$

$$V^\dagger(x,y) = V(y,x) \tag{4.18}$$

$$\begin{aligned} V_{jilk} &= \langle ji\,|V|\,kl\rangle \\ &= \iint dxdy\; j^*(x) k(x) i^*(y) l(y) V(x,y) = \\ &= \iint dxdy\; i^*(x) l(x) j^*(y) k(y) V(y,x) = \\ &= \iint dxdy\; i^*(x) l(x) j^*(y) k(y) V^\dagger(x,y) = \\ &= V_{ijkl}^* \end{aligned} \tag{4.19}$$

It is important to be able to efficiently compute the V_{ijkl} matrix elements, although they need to be computed only once. In principle the matrix elements require a "bad" 6–dimensional integration. Taking into account the properties of the potential and choosing an appropriate basis set for the single particle space, it is possible to reduce it to a simpler 2–dimensional integral. For a potential like Argonne $Av4'$ we can compute those matrix elements as follows:

$$\begin{aligned}&\langle ij\,|V|\,kl\rangle = \delta_{li,ll}\delta_{mi,ml}\delta_{lj,lk}\delta_{mj,mk}\times \\ &\times \iint dr dr' r^2 r'^2 f_i^*(r) f_j^*(r') f_l(r) f_k(r')\,\langle \chi_i\chi_j\,|V(r,r')|\,\chi_l\chi_k\rangle\,,\end{aligned} \tag{4.20}$$

using only a 2–dimensional integral.

As we can see in (§ 4.4), it is also necessary to compute some matrix elements coming from the kinetic terms. Assuming the standard definitions of the spherical coordinates:

$$x = r\sin\theta\cos\phi \tag{4.21}$$

$$y = r\sin\phi\sin\theta \tag{4.22}$$

$$z = r\cos\theta \tag{4.23}$$

$$\text{with} \qquad \theta\in[0,\pi] \qquad \phi\in[0,2\pi) \tag{4.24}$$

we have that

$$-\frac{\hbar^2}{2m}\left\langle i\left|\nabla^2\right|j\right\rangle = -\frac{\hbar^2}{2m}\delta_{li,lj}\delta_{mi,mj}\,\langle\chi_i|\chi_j\rangle\left\langle f_i\left|\frac{\partial^2}{\partial r^2}+\frac{2}{r}\frac{\partial}{\partial r}-\frac{l(l+1)}{r^2}\right|f_j\right\rangle, \tag{4.25}$$

and

$$\begin{aligned}\left\langle i\left|\frac{\partial}{\partial x}\right|j\right\rangle &= \left\langle f_i\,Y^{li}_{mi}\chi_i\left|\frac{\partial}{\partial x}\right|f_j\,Y^{lj}_{mj}\chi_j\right\rangle = \\ &= \int dr r^2 f_i^*(r)\left[a_x f_j'(r)+\frac{b_x}{r}f_j(r)\right]\langle\chi_i|\chi_j\rangle\,,\end{aligned} \tag{4.26}$$

with these definitions:

$$a_x = \iint d\theta\,d\phi\sin\theta\;Y^{*l1}_{m1}(\theta,\phi)\sin\theta\cos\phi Y^{l2}_{m2}(\theta,\phi) \tag{4.27}$$

$$b_x = \iint d\theta\,d\phi\;\sin\theta\;Y^{*l1}_{m1}(\theta,\phi)\left(-\frac{\sin\phi}{\sin\theta}\frac{\partial}{\partial\phi}+\cos\phi\cos\theta\frac{\partial}{\partial\theta}\right)Y^{l2}_{m2}(\theta,\phi) \tag{4.28}$$

$$a_y = \iint d\theta\,d\phi\sin\theta\;Y^{*l1}_{m1}(\theta,\phi)\sin\theta\sin\phi Y^{l2}_{m2}(\theta,\phi) \tag{4.29}$$

$$b_y = \iint d\theta\,d\phi\;\sin\theta\;Y^{*l1}_{m1}(\theta,\phi)\left(\frac{\cos\phi}{\sin\theta}\frac{\partial}{\partial\phi}+\sin\phi\cos\theta\frac{\partial}{\partial\theta}\right)Y^{l2}_{m2}(\theta,\phi) \tag{4.30}$$

$$a_z = \iint d\theta\,d\phi\sin\theta\;Y^{*l1}_{m1}(\theta,\phi)\cos\theta Y^{l2}_{m2}(\theta,\phi) \tag{4.31}$$

$$b_z = \iint d\theta\,d\phi\;\sin\theta\;Y^{*l1}_{m1}(\theta,\phi)\left(-\sin\theta\frac{\partial}{\partial\theta}\right)Y^{l2}_{m2}(\theta,\phi). \tag{4.32}$$

Eq(4.25) and Eq(4.26) are useful, because in that way it is possible to reduce to a 2–dimensional(or 1–dimensional) integral a generic matrix element (for which computation it is required in principle a 6–dimension integral).

Thus in presence of a generic 2–body potential that only depends on the distance between two particles, times a more complicated operator (spin–orbit, tensor etc.) it is possible to pre–compute some constants like in Eq(4.27) and following formulas.

This distinction is important, because it is necessary to pre–compute all the 1-body and 2–body matrix elements. They are ${N_S}^4$. and an integral in 2–dimension is very fast to compute in an accurate way (using a Simpson rule), while for a 6–dimensional integral it is better to use a Monte Carlo method that anyway require to much time to compute all the ${N_S}^4$ elements.

4.4 Center of mass corrections

In order to study finite size systems, we have to remove the center of mass contribution to the kinetic energy. So if the momentum of the center of mass is

$$P^\beta = \sum_i p_i^\beta M = m \cdot N_{PART} \tag{4.33}$$

its kinetic contribution to the energy (in first quantization) is written as

$$\begin{aligned} K_{cm} = \frac{P^2}{2M} &= -\frac{\hbar^2}{2M} \sum_{\beta=x,y,z} \left[\sum_{i,j} \partial_{\beta i} \partial_{\beta j} \right]^2 \\ &= -\frac{\hbar^2}{2M} \sum_{\beta=x,y,z} \left[\sum_i \partial_{\beta i}^2 - \sum_{i \neq j} \partial_{\beta i} \partial_{\beta j} \right]. \end{aligned} \tag{4.34}$$

Rewriting in second quantization we can divide it in a 1–body term and another 2–body one:

$$K_{cm} = \sum_{ij} T_{ij}^{cm} c_i^\dagger c_j + \sum_{ijkl} V_{ijkl}^{cm} c_i^\dagger c_j^\dagger c_k c_l, \tag{4.35}$$

where

$$T_{ij}^{cm} = -\frac{\hbar^2}{2M} \left\langle i \left| \nabla^2 \right| j \right\rangle, \tag{4.36}$$

and

$$V_{ijkl}^{cm} = \frac{\hbar^2}{2M} \left\langle ij \left| \nabla_k \cdot \nabla_l \right| kl \right\rangle. \tag{4.37}$$

This last matrix element can be rewritten in a simpler way

$$\begin{aligned} \left\langle ij \left| \nabla_k \cdot \nabla_l \right| kl \right\rangle &= \left\langle Y_{mi}^{li} f_i Y_{mj}^{lj} f_j \left| \nabla_k \cdot \nabla_l \right| Y_{mk}^{lk} f_k Y_{ml}^{ll} f_l \right\rangle = \\ &= \frac{\hbar^2}{2M} \sum_{\beta=x,y,x} \left\langle Y_{mi}^{li} f_i \left| \partial_\beta \right| Y_{ml}^{ll} f_l \right\rangle \left\langle Y_{mj}^{lj} f_j \left| \partial_\beta \right| Y_{mk}^{lk} f_k \right\rangle \end{aligned} \tag{4.38}$$

Therefore, the Hamiltonian of a system with kinetic term T and a two–body interaction V can be rewritten, separating one–body and two–body contributions:

$$\begin{aligned} H &= K + V - K_{cm} \\ &= \sum_{ij} (T_{ij} - T_{ij}^{cm}) c_i^\dagger c_j + \frac{1}{2} \sum_{ijkl} (V_{ijkl} - V_{ijkl}^{cm}) c_i^\dagger c_j^\dagger c_k c_l, \end{aligned} \tag{4.39}$$

being

$$T_{ij} - T_{ij}^{cm} = -\frac{\hbar^2}{2m\frac{N_{PART}}{N_{PART}-1}}\langle i|\nabla^2|j\rangle. \tag{4.40}$$

4.5 The propagator

Now we remember Eq(4.1). We want to write the two–body term of the potential as the square of a one–body operator. Now to do that, remembering the properties of V in (§ 4.3), we define this $\left({N_S}^2 \times {N_S}^2\right)$ Hermitian matrix

$$\mathcal{V}_{(il)(jk)} = V_{ijkl} \tag{4.41}$$

$$\mathcal{V}_{(il)(jk)} = \mathcal{V}^*_{(jk)(il)} \tag{4.42}$$

$$\mathcal{V} = \mathcal{V}^\dagger \tag{4.43}$$

Because of its Hermiticity it is possible to diagonalize it with a matrix P satisfying the relation:

$$\left(P^{-1}\right)_{\alpha(il)} = P^*_{(il)\alpha}. \tag{4.44}$$

It is also possible to rewrite $\mathcal{V}$ like:

$$\mathcal{V}_{(il)(jk)} = \sum_\alpha P_{(il)\alpha}\lambda_\alpha P^*_{(jk)\alpha}, \tag{4.45}$$

where λ_α are the eigenvalues of $\mathcal{V}$ that are real again because of Hermiticity.

The generic two–body term of the Hamiltonian has the form:

$$H_2 = \frac{1}{2}\sum_{ijkl} c_i^\dagger c_j^\dagger c_k c_l V_{ijkl} \tag{4.46}$$

Taking into account a system composed by Fermions we can rewrite the previous formula applying the standard anticommutation rules

$$c_i^\dagger c_j^\dagger c_k c_l V_{ijkl} = \mathcal{V}_{(il)(jk)} c_i^\dagger c_l c_j^\dagger c_k - \mathcal{V}_{(il)(jk)} c_i^\dagger c_k \delta_{jl} \tag{4.47}$$

We now define the single body operators

$$\rho_\alpha = \sum_{il} P_{(il)\alpha} c_i^\dagger c_l; \tag{4.48}$$

$$\tilde{\rho}_\alpha = \sum_{il} P^*_{(il)\alpha} c_i^\dagger c_l; \tag{4.49}$$

$$\eta_\alpha = -\frac{1}{4}\sum_{ik} c_i^\dagger c_k \left[\sum_j \left(P_{(ij)\alpha}P^*_{(jk)\alpha} + P_{(jk)\alpha}P^*_{(ij)\alpha}\right)\right]; \tag{4.50}$$

$$\Omega_0 = \sum_\alpha \lambda_\alpha \eta_\alpha = -\frac{1}{4}\sum_{ik} c_i^\dagger c_k \left[\sum_j \left(\mathcal{V}_{(ij)(jk)} + \mathcal{V}_{(jk)(ij)}\right)\right]. \tag{4.51}$$

We can see that

$$\rho_\alpha \tilde{\rho}_\alpha = \sum_{ijkl} P_{(il)\alpha} c_i^\dagger c_l P^*_{(jk)\alpha} c_j^\dagger c_k, \tag{4.52}$$

$$\begin{aligned} \tilde{\rho}_\alpha \rho_\alpha &= \sum_{ijkl} P^*_{(jk)\alpha} c_j^\dagger c_k P_{(il)\alpha} c_i^\dagger c_l = \\ &= \sum_{ijkl} P_{(il)\alpha} c_i^\dagger c_l P^*_{(jk)\alpha} c_j^\dagger c_k + P_{(il)\alpha} \left(c_j^\dagger c_l \delta_{ik} - c_i^\dagger c_k \delta_{jl} \right) P^*_{(jk)\alpha}, \end{aligned} \tag{4.53}$$

$$\left[(\rho_\alpha + \tilde{\rho}_\alpha)^2 - (\rho_\alpha - \tilde{\rho}_\alpha)^2 \right] = 2 \left[\rho_\alpha \tilde{\rho}_\alpha + \tilde{\rho}_\alpha \rho_\alpha \right]. \tag{4.54}$$

Finally the two–body Hamiltonian reads

$$\begin{aligned} H_2 &= \frac{1}{2} \sum_{ijkl} c_i^\dagger c_j^\dagger c_k c_l V_{ijkl} = \\ &= \Omega_0 + \frac{1}{2} \sum_\alpha \frac{\lambda_\alpha}{4} \left[(\rho_\alpha + \tilde{\rho}_\alpha)^2 - (\rho_\alpha - \tilde{\rho}_\alpha)^2 \right]. \end{aligned} \tag{4.55}$$

Now defining

$$H_1' = H_1 + \Omega_0; \tag{4.56}$$

$$H_2' = -\frac{1}{2} \sum_\gamma \Omega_\gamma^2; \tag{4.57}$$

with

$$\Omega_\gamma = \begin{cases} \dfrac{\imath \sqrt{\lambda_\alpha}}{2} (\rho_\alpha + \tilde{\rho}_\alpha) & \text{for } \gamma = 2\alpha - 1 \\ \dfrac{\sqrt{\lambda_\alpha}}{2} (\rho_\alpha - \tilde{\rho}_\alpha) & \text{for } \gamma = 2\alpha \end{cases} \tag{4.58}$$

we can rewrite the Hamiltonian as a sum of single body operators and the square of single body operators:

$$\begin{aligned} H = H_1 + H_2 &= H_1 + \frac{1}{2} \sum_{ijkl} c_i^\dagger c_j^\dagger c_k c_l V_{ijkl} = \\ &= H_1 + \Omega_0 + \frac{1}{2} \sum_\alpha \frac{\lambda_\alpha}{4} \left[(\rho_\alpha + \tilde{\rho}_\alpha)^2 - (\rho_\alpha - \tilde{\rho}_\alpha)^2 \right] \\ &= H_1 + \Omega_0 - \frac{1}{2} \sum_\gamma \Omega_\gamma^2 \\ &= H_1' + H_2', \end{aligned} \tag{4.59}$$

obtaining an equation similar to Eq(4.1).

Now we can come back to the propagator of equations Eq(4.3) and Eq(4.4) using the relations previously shown:

$$
\begin{aligned}
& e^{-dt(H-E_0)} = e^{-dtH_1'} e^{-dtH_2'} + \mathcal{O}(dt^2) = \\
& = e^{-dt(H_1'-E_0)} e^{dt\sum_\gamma \frac{\Omega_\gamma^2}{2}} + \mathcal{O}(dt^2) = \\
& = e^{-dt(H_1'-E_0)} \prod_\gamma e^{dt\frac{\Omega_\gamma^2}{2}} + \mathcal{O}(dt^2) = \\
& = \frac{1}{(2\pi)^{N_S^2}} e^{-dt(H_1'-E_0)} \prod_\gamma \int dx_\gamma \exp\left(-\frac{x_\gamma^2}{2}\right) \exp\left(-\sqrt{dt}\,\Omega_\gamma\, x_\gamma\right) + \mathcal{O}(dt^2) = \\
& = \frac{1}{(2\pi)^{N_S^2}} e^{-dt(H_1'-E_0)} \int \{dx_\gamma\} \exp\left(-\sum_\gamma \frac{x_\gamma^2}{2}\right) \exp\left(-\sqrt{dt}\,\sum_\gamma \Omega_\gamma\, x_\gamma\right) + \mathcal{O}(dt^2) = \\
& = \frac{1}{(2\pi)^{N_S^2}} \int \{dx_\gamma\} \exp\left(-\sum_\gamma \frac{x_\gamma^2}{2}\right) \exp\left(-dtH_1' - \sqrt{dt}\,\sum_\gamma \Omega_\gamma\, x_\gamma\right) + \mathcal{O}(dt^2) = \\
& = \frac{1}{(2\pi)^{N_S^2}} \int \{dx_\gamma\} e^{-\sum_\gamma \frac{x_\gamma^2}{2}}\, \Xi + \mathcal{O}(dt^2)
\end{aligned}
\tag{4.60}
$$

where Ξ is defined as

$$
\Xi = \exp\left(-dt(H_1' - E_0) - \frac{\sqrt{dt}}{2}\,\sum_\gamma \Omega_\gamma\, x_\gamma\right). \tag{4.61}
$$

Now, like noted in [ASZK06], it is more efficient to "shift" the Ω_γ operators using the (probably not too) bad description of the system given by the trial wavefunction Ψ_T. Technically it is important because in this way it is possible to improve the accuracy of the method, reducing the noise on the auxiliary field sampling and eventually improving the "phase" approximation used to overcome the sign problem.

Hence from each Ω_γ operator we remove a sort of "mean field" term

$$
\tilde{\Omega}_\gamma = \Omega_\gamma - \langle \Psi_T \left|\Omega_\gamma\right| \Psi_T \rangle, \tag{4.62}
$$

redefining in an equivalent way the one and two–body terms of the Hamiltonian

$$
H_2'' = -\frac{1}{2}\sum_\gamma \tilde{\Omega}_\gamma^2, \tag{4.63}
$$

$$
H_1'' = H_1 + \Omega_0 + \sum_\gamma \frac{\langle \Psi_T \left|\Omega_\gamma\right| \Psi_T \rangle^2}{2} - \langle \Psi_T \left|\Omega_\gamma\right| \Psi_T \rangle\, \Omega_\gamma, \tag{4.64}
$$

$$
H = H_1' + H_2' = H_1'' + H_2''. \tag{4.65}
$$

The following expression of the propagator is then obtained

$$
\tilde{\Xi} = \exp\left(-dt(H_1'' - E_0) - \sqrt{dt}\,\sum_\gamma \tilde{\Omega}_\gamma\, x_\gamma\right), \tag{4.66}
$$

$$
\begin{aligned}
e^{-dt(H-E_0)} &= \frac{1}{(2\pi)^{N_S^2}} \int \{dx_\gamma\} e^{-\sum_\gamma \frac{x_\gamma^2}{2}} \, \tilde{\Xi} + \mathcal{O}(dt^2) = \\
&= \frac{1}{(2\pi)^{N_S^2}} \int \{dx_\gamma\} e^{-\sum_\gamma \frac{x_\gamma^2}{2}} \, e^{-dt(H_1''-E_0)} e^{-\sqrt{dt} \, \sum_\gamma \tilde{\Omega}_\gamma \, x_\gamma} + \mathcal{O}(dt^2).
\end{aligned}
\tag{4.67}
$$

4.6 Importance sampling

Taking into account the evolution equation Eq(4.2), iterate several times the propagator to a wavefunction $|\omega_t\rangle$ gives the ground state:

$$
|\omega_{t+dt}\rangle = e^{-dt(H-E_0)} \, |\omega_t\rangle \, . \tag{4.68}
$$

Clearly, for $t = 0$ we have that:

$$
|\omega_0\rangle = |\Psi_T\rangle \, . \tag{4.69}
$$

The wavefunction $|\omega_{t+dt}\rangle$ in equation Eq(4.68) lives in the full product space, that is

$$
|\omega\rangle \quad \in \quad \bigotimes_{N_{PART}} \mathcal{H}, \tag{4.70}
$$

where $\mathcal{H}$ is the single particle Hilbert space. We want to represent our configurations like combinations of Slater determinant of single particle wavefunctions. It is possible in the limit of $N_W \to \infty$

$$
|\omega\rangle = \sum_i^{N_W} |v_i\rangle \, , \tag{4.71}
$$

where N_W is the number of walkers, i.e. the number of configurations that we sample, and $|v_i\rangle$ is a configuration that lives in the direct sum of single particle Hilbert spaces, i.e. that is written is a Slater determinant of single particle wavefunctions:

$$
|v\rangle \quad \in \quad \bigoplus_{N_{PART}} \mathcal{H}. \tag{4.72}
$$

So we can rewrite

$$
|\omega_{t+dt}\rangle = \sum_i^{N_W} |v_{i,t+dt}\rangle = \sum_i^{N_W} e^{-dt(H-E_0)} \, |v_{i,t}\rangle \, , \tag{4.73}
$$

defining for each i

$$
|v_{t+dt}\rangle = e^{-dt(H-E_0)} \, |v_t\rangle \, . \tag{4.74}
$$

Using the propagator in Eq(4.67) we have:

$$
\begin{aligned}
|v_{t+dt}\rangle &= e^{-dt(H-E_0)} \, |v_t\rangle \\
&= \frac{1}{(2\pi)^{N_S^2}} \int \{dx_\gamma\} e^{-\sum_\gamma \frac{x_\gamma^2}{2}} \, e^{-dt(H_1''-E_0)} e^{-\sqrt{dt} \, \sum_\gamma \tilde{\Omega}_\gamma \, x_\gamma} \, |v_t\rangle \, .
\end{aligned}
\tag{4.75}
$$

With the aim of sampling in a more efficient way the auxiliary variables x_γ we choose to multiply both terms of the previous equation by $\langle\Psi_T|v_{t+dt}\rangle$, defining

$$|u\rangle = |v\rangle \langle\Psi_T|v\rangle \tag{4.76}$$

and sampling $|u\rangle$ configurations instead of $|v\rangle$ we obtain from Eq(4.75) the following expression:

$$|u_{t+dt}\rangle = \frac{1}{(2\pi)^{N_S^2}} \int \{dx_\gamma\} e^{-\sum_\gamma \frac{x_\gamma^2}{2}} \; e^{-dt(H_1''-E_0)} e^{-\sqrt{dt}\;\sum_\gamma \tilde{\Omega}_\gamma\; x_\gamma} \; |u_t\rangle \; \frac{\langle\Psi_T|v_{t+dt}\rangle}{\langle\Psi_T|v_t\rangle} \tag{4.77}$$

Now using the definition of $|u\rangle$ we can rewrite the relation used in the previous equation in a better form:

$$\begin{aligned}
\frac{\langle\Psi_T|v_{t+dt}\rangle}{\langle\Psi_T|v_t\rangle} &= \frac{\left\langle\Psi_T\left|e^{-(H-E_0)dt}\right|v_t\right\rangle}{\langle\Psi_T|v_t\rangle} = \frac{\left\langle\Psi_T\left|e^{-(H-E_0)dt}\right|u_t\right\rangle}{\langle\Psi_T|u_t\rangle} = \\
&\simeq \frac{\langle\Psi_T\left|1-(H-E_0)dt\right|u_t\rangle}{\langle\Psi_T|u_t\rangle} = \\
&\simeq \frac{\langle\Psi_T\left|1-(H_1''+H_2''-E_0)dt\right|u_t\rangle}{\langle\Psi_T|u_t\rangle} = \\
&\simeq \frac{\left\langle\Psi_T\left|1-(H_1''-E_0-\frac{1}{2}\sum_\gamma\tilde{\Omega}_\gamma^2)dt\right|u_t\right\rangle}{\langle\Psi_T|u_t\rangle}.
\end{aligned} \tag{4.78}$$

Considering that:

- in Eq(4.77) odd terms in x_γ give zero contribution because of the Gaussian integral;
- the equivalence $\int e^{-x^2/2}dx = \int e^{-x^2/2}x^2dx$ holds;
- terms $\mathcal{O}(dt^2)$ are neglected;

it is possible to use instead of Eq(4.78) the alternative form:

$$\frac{\left\langle\Psi_T\left|1-\left(\sqrt{dt}\sum_\gamma x_\gamma\tilde{\Omega}_\gamma\right)+\frac{1}{2}\left(\sqrt{dt}\sum_\gamma x_\gamma\tilde{\Omega}_\gamma\right)^2\right|e^{-dt(H_1''-E_0)}u_t\right\rangle}{\langle\Psi_T|u_t\rangle}. \tag{4.79}$$

Defining for a generic operator $\mathcal{Q}$ the following notation:

$$\langle\langle\mathcal{Q}\rangle\rangle = \frac{\left\langle\Psi_T\left|\mathcal{Q}\right|e^{-dt(H_1''-E_0)}u_t\right\rangle}{\langle\Psi_T|u_t\rangle}, \tag{4.80}$$

we can rewrite Eq(4.79) as:

$$\langle\langle 1\rangle\rangle - \sqrt{dt}\langle\langle\sum_\gamma x_\gamma\tilde{\Omega}_\gamma\rangle\rangle + \frac{dt}{2}\langle\langle\left(\sum_\gamma x_\gamma\tilde{\Omega}_\gamma\right)^2\rangle\rangle. \tag{4.81}$$

Now it is possible to see that Eq(4.77) is equivalent to

$$|u_{t+dt}\rangle = \frac{1}{(2\pi)^{N_S^2}} \int \{dx_\gamma\} e^{-\sum_\gamma \frac{\left(x_\gamma^2 + \sqrt{dt}\langle\langle\tilde{\Omega}_\gamma\rangle\rangle\right)}{2}} \; e^{-dt(H_1'' - E_0)} e^{-\sqrt{dt}\;\sum_\gamma \tilde{\Omega}_\gamma\; x_\gamma} \,|u_t\rangle\, e^{dt\frac{\langle\langle\sum_\gamma \tilde{\Omega}_\gamma^2\rangle\rangle}{2}} \tag{4.82}$$

neglecting again $\mathcal{O}(dt^2)$ terms.

Now we have that

$$e^{dt\frac{\langle\langle\sum_\gamma \tilde{\Omega}_\gamma^2\rangle\rangle}{2}} = e^{-dt\frac{\langle\Psi_T|H-E_0|u_t\rangle}{\langle\Psi_T|u_t\rangle}} + \mathcal{O}(dt^2) \simeq e^{-dt(E_{LOC}-E_0)} + \mathcal{O}(dt^2) \tag{4.83}$$

with

$$E_{LOC} = \frac{\langle\Psi_T\,|H|\,u_t\rangle}{\langle\Psi_T|u_t\rangle}$$

It is important to note that in the limit of an exact trial wavefunction, the previous term must be closer to 1 with 0 imaginary part, so it can be a good choice to use it as a weight factor, i.e. like a branching factor.

So the structure of the algorithm is the following:

1. consider an initial configuration (walker) $|u_t\rangle$;
2. compute a set $\{\eta_\gamma\}$ of random numbers with a Gaussian probability distribution centered in 0 with variance 1. and compute $\langle\langle\tilde{\Omega}_\gamma\rangle\rangle$ so that $x_\gamma = \eta_\gamma - \sqrt{dt}\langle\langle\tilde{\Omega}_\gamma\rangle\rangle$;
3. apply the propagator $e^{-dt(H_1''-E_0)}e^{-\sqrt{dt}\sum_\gamma \tilde{\Omega}_\gamma\, x_\gamma}$ to the configuration $|u_t\rangle$ obtaining the new configuration $|u_{t+dt}\rangle$;
4. compute the local energy and weight (i.e. branch) the new configuration $|u_{t+dt}\rangle$ with the weight $e^{-dt(E_{LOC}-E_0)}$;
5. return to the point 2. with the new configurations and go on until the projection to the ground state is reached.

4.7 Sign problem

For many–Fermion systems the algorithm is not as simple as described in the previous section. In fact the branching factor $e^{-dt(E_{LOC}-E_0)}$ should always be a positive weight, while generally it can generally be complex. To overcome this problem the following restraint on the weight is made:

$$e^{-dt(\Re[E_{LOC}]-E_0)} \cdot \max\left[0, \cos\left(phase\left[\frac{\langle\Psi_T|u_{t+dt}\rangle}{\langle\Psi_T|u_t\rangle}\right]\right)\right]. \tag{4.84}$$

4.8 Algorithm structure

We conclude briefly by summarizing the whole algorithm:

1. Choose the single particle space $\mathcal{H}$, like shown in (§ 4.2).

2. Compute all the matrix elements, as in (§ 4.3).
3. Find a good trial wavefunction Ψ_T, written as a sum of Slater determinant of single particle wavefunctions defined in $\mathcal{H}$.
4. Now it is possible to compute all $\tilde{\Omega}_\gamma$ operators needed in the propagator.
5. Choose a set $\{u_0\}$ of N_w starting configurations.
6. Compute a new configuration set $\{u_{t+dt}\}$ from the previous $\{u_t\}$. This is achieved by choosing a set $\{\eta_\gamma\}$ of random numbers with a Gaussian propability distribution centered in 0 with variance 1, and applying the propagator $e^{-dt(H_1'-E_0)}e^{-\sqrt{dt}\sum_\gamma \tilde{\Omega}_\gamma\, x_\gamma}$ with $x_\gamma = \eta_\gamma - \sqrt{dt}\langle\langle\tilde{\Omega}_\gamma\rangle\rangle$ to the configurations $\{|u_t\rangle\}$.
7. Compute all the observables to be estimated and weight them with the factor Eq(4.84).
8. Compute the branching factor Eq(4.84) and create a number of copies of each configuration proportional to the branching factor, keeping the number of configurations more or less constant.
9. Go back to the point 6 iterating the procedure like for other DMC methods.

4.9 Considerations

As mentioned at the end of the previous chapter, we looked at the AFQMC algorithm to overcome the limitations of the AFDMC related to the the fixed–phase approximation. Let us discuss this assertion, and stress differences between AFDMC and AFQMC algorithms.

DMC is very accurate, tested and used for electron systems. Nevertheless the extension of DMC to nuclear systems (i.e. AFDMC) is not trivial as we have seen in the previous chapter. Moreover a further approximation (fixed–phase) must be used. The AFQMC algorithm described in this chapter is, at present, well tested and used only for electron systems. But to use it for nucleon systems we do not have to extend the algorithm. The fixed–phase approximation must be used in the same way both for electron systems than in nuclear systems. Moreover the trick in Eq(4.62) makes possible to include part of the two–body terms of the propagator in a sort of one–body "mean field" term. In this way, as shown in [ASZK06], it is possible to drastically reduce the bias due to the fixed–phase approximation. It is not possible to use the same procedure in the AFDMC algorithm, because of the excessive computational cost needed to compute this mean field term.

Hence, we expect to obtain reasonable results with the AFQMC algorithm also for nuclear systems.

Apart from the discussion concerning the fixed–phase approximation we also want to stress the capability of AFQMC of including any two–body potential. While in AFDMC we are limited to use only local potentials or some non–local

ones (spin–orbit etc.) at the cost of increasing the complexity of the calculation, with AFQMC we can use any arbitrary two–body potentials. But unfortunately with AFQMC is not possible to use any three–body force. While with AFDMC we can use three body potentials containing at most a two–body operators (i.e. two–body spin/isospin dependent terms), whit AFQMC we cannot include any there–body term.

We also have to note that with AFQMC we have to cut the size of the single particle Hilbert space, i.e. we have a further (variational) approximation on top of the fixed–phase one. So for each calculation we need to choose a single basis and to consider only a finite set of elements; we must do several runs considering an increasing number of elements of single particle states to find the asymptotic trend. We believe that this is not a big limitation of the algorithm; many currently employed methods based on exact diagonalization like No Core Shell Model or the Hyperspherical Harmonic method suffer of the same limitation. Moreover

- we can use any one–body basis set, choosing the one allowing us to faster reach the asymptotic limit;
- we can use a bigger number of basis element than with exact diagonalization methods, because of the polynomial scalability of AFQMC, compared to the exponential one of exact diagonalization methods.

The last note is about the impossibility of using even a simple Jastrow factor in the trial wavefunction within AFQMC. Thus, all correlations must be effectively described only by an appropriate combination of uncorrelated Slater determinants. Looking at the results showed at the end of the previous chapter, we expect that for nuclear systems this is not a relevant limitation: central Jastrow factors seem to give no relevant contribution in AFDMC calculations.

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Part II

Effective Field Theory in nuclear physics

Chapter 5

Introduction

This is the starting work of my PhD; this project remained uncompleted because of technical problems possibly related to the "fixed–phase" approximation. Anyway, the idea of this project is very interesting and promising; we hope to be able to reopen this project in a near future whit better numerical methods or reasonable and useful approximations allowing for the solution of the problem.

The study of nuclei is still an open problem in theoretical physics because of:

- *The absence of a single exact nuclear potential, derived from prime principles.* There are many phenomenological nuclear potentials (e.g. Argonne, Illinois, Urbana, Skyrme) realistic for the two body sector and at densities typical of nuclei. Properties at supersaturation densities (relevant in astrophysics) and effects of n–body ($n > 2$) interactions are not well–known and predicted. Nuclear potentials derived from Effective Field Theories (EFT) were recent developed (e.g. CD-Bonn, Nijmegen). They are written starting from QCD symmetries, thereby adding more theoretical basis to phenomenological potentials and a systematic way to order and add new terms.

  Nevertheless, Effective parameters must still be fitted on experimental data and cannot be derived directly from QCD simulations yet.

- *The absence of a sufficiently accurate method to calculate nuclei and nuclear matter properties.* Mean field methods (like Hartree–Fock) are too much model dependent, despite the feasibility of the computation also for large systems. Hamiltonian diagonalization methods (e.g. No Core Shell Model) could be accurately applied only to few body systems, because of the high number of basis elements to be considered to reach convergence. Accurate Variational Monte Carlo methods (VMC) have been used up to $n \leq 12$. The increase of the number of nucleons is computationally expensive, because of the exponential growth of the number of spin–isospin states. Green's Function Monte Carlo (GFMC), starting from very accurate variational wavefunctions, could give good results within the constrained path approximation and nonlocal potential terms. Systems stud-

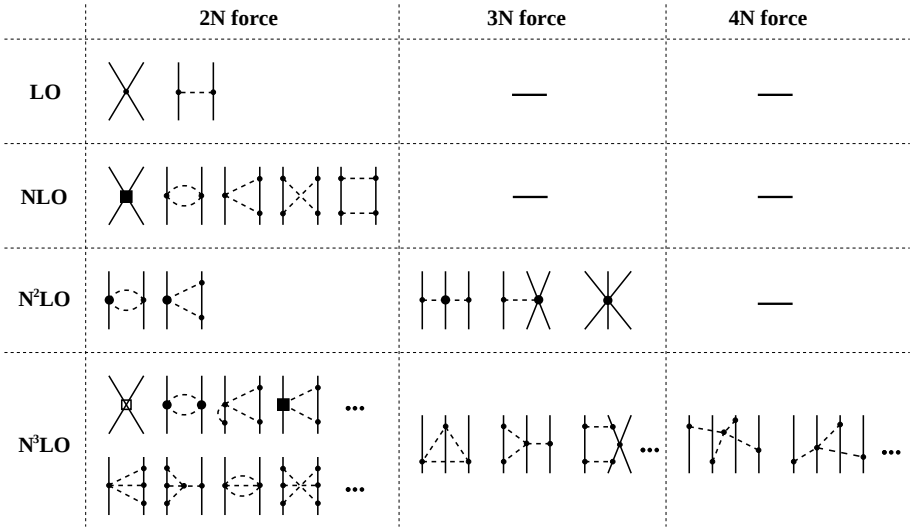

Figure 5.1: EFT diagrams at different orders and corresponding 2–body, 3–body and more nucleon–nucleon potential terms. Solid and dashed lines denote nucleons and pions, respectively. Solid dots, filled circles and filled squares and crossed squares refer to different chiral order vertices. Figure from [Epe10].

ied so far are limited to $n \leq 12$ for the same reasons that limit VMC calculations. Auxiliary Field Diffusion Monte Carlo method (AFDMC) open the possibility to study heavier nuclei than GFMC (^{40}Ca, for example) or nuclear matter (now up to $n = 114$). Because of its promising behavior we chose this method to try to solve harder problems, like that of nucleons within EFT, even if there are still some difficulties to include not local and three body potential terms. Unfortunately we have seen in (§ 3.12) that the method as we have implemented it, and the poor quality of the wavefunctions used are not sufficiently accurate for this problem.

This is the preamble. The final goal is to have an accurate computational method to solve the nuclear problem as described by a realistic and good theory. So we assumed that the AFDMC method is right one. The recent EFT developments suggest that it could be very promising to use them as our theoretical background. So, we simply tried to solve nuclear EFT using the AFDMC method.

But why EFT? These are the main advantages:

- *The possibility of having a theoretical tool to build a systematically improvable Lagrangian starting from symmetry principles.* We can roughly say that EFT is obtained by selecting the relevant degrees of freedom and writing the most general Lagrangian allowed by the fundamental symmetries. If we have a way to cast these infinite terms in an ordered series, we can choose and take into account only the most relevant terms, obtaining a systematically and arbitrarily improvable Lagrangian. Fig. 5 could be

very useful to display this property.

- *The possibility of taking into account also the dynamic effects of the EFT degrees of freedom.* If we take into account a standard phenomenological potential like Argonne $Av18$ we have a potential between nucleons and no more. The same happens if we take into account a nucleon potential derived by an EFT. This is a good approximation but it is still possible to have some effects due to excitations of nucleons, to the meson exchange and so on. It is not simple at all to introduce these corrections in a systematic approach like EFT. The alternative is to exploit EFT in a direct way. Assuming pions the only relevant degrees of freedom after the nucleons, if we integrate out the pion fields we obtain a potential quite similar to the standard ones. Instead, if we take into account the dynamic effects due to the pion fields, i.e. if we are able to solve the problem explicitly including the pion field, we could have a richer and realistic description of the nuclear interaction. This includes directly effects that in standard potentials are equivalent to a sort of "density–dependence" and "energy–dependence". We do not know how large these corrections are. A calculation of these effects should in any case be very interesting, in order to assess their importance.

A further observation is in order. If we take into account a standard nucleon potential, and if we try to solve it using the AFDMC method, we have to introduce auxiliary fields to describe the interaction. Moreover, the nucleon–nucleon interaction is described by the exchanged meson fields. So, why do not include directly these physical fields instead of the auxiliary fields of the AFDMC method? If we are able to do a calculation with AFDMC auxiliary fields, would it not be possible to perform a calculation with physical exchanged meson fields? This is a point of view that should be further pursued.

Chapter 6

Effective Field Theories

The following sections are intended only as a short and very introductory summary. We remand to [Epe08, Lee09, Pic98, BBH$^+$00, Bor07] to a better, clearer and more detailed description.

6.1 Preliminary

The dream of the nuclear theorist is to solve the nuclear systems starting directly from the elementary particles and their fundamental interactions. This is so far impossible to achieve attacking the study of nuclear systems starting directly from QCD, because it is strongly limited by its non–perturbative character. Also lattice QCD simulations are prohibitive because of their enormous computational cost. On the other hand, if we limit our interest to the study of a specified system and energy regime (e.g. fundamental state of nuclei), not all degrees of freedom (like quarks and gluons) are necessary to realistically describe the system dynamic.

Effective Field Theories help to construct an equivalent effective Lagrangian:

- including only the relevant effective degrees of freedom (e.g. baryons and lighter exchanged 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 not perturbative. M is order of nucleon mass M_N. The typical momenta Q exchanged between nucleons in small nuclei are order of their size, i.e. $Q \sim m_\pi \simeq 138$MeV. It is thus possible to consider two energy scales:

- low energy scale, involving only relevant degrees of freedom (nucleons, pions,...) with momentum $Q < M$. We have to study a nuclear system, that

is compounds of nucleons, and so we have to take into account the nucleon degrees of freedom. Moreover, we have to consider other exchanged mesons or excited states of the nucleons. The contribution of these terms is suppressed with the inverse of their masses for the exchanged mesons, or with the inverse of the difference with the nucleon mass for the nucleon excitation. So, we can simply take into account nucleonic and pionic degrees of freedom. At higher orders also the Δ excitation becomes relevant, at such degrees of freedom as other exchanged mesons like ρ or ω.

- high energy scale, involving degrees of freedom that are omitted. The effects are included in effective theory by a counterterms series, in principle infinite. Considering that $\frac{Q}{M} < 1$, it is possible to order these terms in a perturbative series, considering only a finite number of terms for a given precision.

On top of the selection of the relevant degrees of freedom, a regularization cut–off must be introduced for momentum larger than Q, removing ultraviolet divergences and the high energy physics that will be described by the added counterterms.

6.2 The Lagrangian

As previously mentioned, we take into account only nucleonic and pionic degrees of freedom. In following formulas we include also the Δ excitation, even if we do not use it in our calculations.

Using stereographic coordinates we can define the covariant pion derivative as

$$D^a_\mu \equiv \mathcal{D}^{-1} \frac{\partial_\mu \pi^a}{2 f_\pi} \ , \tag{6.1}$$

with $f_\pi \simeq 92$ MeV the pion decay constant and

$$\mathcal{D} \equiv 1 + \frac{\boldsymbol{\pi}^2}{4 f_\pi^2} \ , \tag{6.2}$$

where $\boldsymbol{\pi}$ is the pion isovector. Chiral covariant objects, including D, the nucleon N and the delta–isobar Δ fields, transform under axial chiral rotation (the spontaneously broken part of the $SU(2)_L \times SU(2)_R$ chiral symmetry) as a $\boldsymbol{\pi}$–dependent isospin rotation (the unbroken subgroup). Therefore, an isospin invariant Lagrangian built out of covariant objects will automatically satisfy the full $SU(2)_L \times SU(2)_R$ chiral symmetry.

For a generic chiral–covariant field with isospin I, $\psi^{(I)}$, its covariant derivative is defined as

$$\mathscr{D}_\mu \psi^{(I)} \equiv \left(\partial_\mu + \boldsymbol{t}^{(I)} \cdot \boldsymbol{E}_\mu \right) \psi^{(I)} \ , \tag{6.3}$$

where

$$\boldsymbol{E}_\mu \equiv i \frac{\boldsymbol{\pi}}{f_\pi} \times \boldsymbol{D}_\mu \ . \tag{6.4}$$

For an isovector with Cartesian indices like $\boldsymbol{D}_\nu$, it is conventional to write the covariant derivative as

$$\mathscr{D}_\mu \boldsymbol{D}_\nu \equiv \partial_\mu \boldsymbol{D}_\nu + i \boldsymbol{E}_\mu \times \boldsymbol{D}_\nu \ . \tag{6.5}$$

In the same way we can define a covariant derivative for nucleon and Δ–isobars

$$\mathscr{D}_\mu N = \left(\partial_\mu + \boldsymbol{\tau}\cdot\boldsymbol{E}_\mu\right) N \,, \tag{6.6}$$

$$\mathscr{D}_\mu \Delta = \left(\partial_\mu + \boldsymbol{\tau}^{(3/2)}\cdot\boldsymbol{E}_\mu\right) \Delta \,, \tag{6.7}$$

Now we can write the most general chiral Lagrangian using the fields N, Δ, D and their covariant derivatives. Ordering the terms of this Lagrangian respect to the momentum, i.e. using the Weinberg chiral index[Wei90, Wei91], we can obtain the lowest order Lagrangian.

Using Weinberg's ν index, or chiral index, the leading chiral Lagrangian[OnRvK94, OnRvK96, vK94] is

$$\begin{aligned}\mathscr{L}_0 =& -\frac{1}{2}\mathcal{D}^{-2}\partial_\mu\pi_i\partial^\mu\pi_i - \frac{1}{2}\mathcal{D}^{-1}m_\pi^2\pi_i^2 + N^\dagger\left[i\partial_0 - \frac{\mathcal{D}^{-1}}{f_\pi^2}\epsilon_{ijk}\tau_i\pi_j\partial_0\pi_k - M_0\right]N \\ &- \frac{g_A}{f_\pi}N^\dagger\tau_i\sigma_j\nabla_j\pi_i N - \frac{1}{2}C\left(N^\dagger N\right)\left(N^\dagger N\right) - \frac{1}{2}C_I\left(N^\dagger\tau_i N\right)\left(N^\dagger\tau_i N\right) \\ &+ \Delta^\dagger\left[i\partial_0 - \frac{\mathcal{D}^{-1}}{f_\pi^2}\epsilon_{ijk}\tau_i^{(3/2)}\pi_j\partial_0\pi_k - m_\Delta\right]\Delta \\ &- \frac{h_A}{f_\pi}\left[N^\dagger T_i S_j\nabla_j\pi_i\Delta + \text{H.c.}\right] + \ldots\end{aligned} \tag{6.8}$$

where g_a is the nucleon axial charge, M_0 the nucleon bare mass, m_π the pion mass and m_Δ the Δ mass. At the leading chiral order we have that m_π is the physical pion mass. The 2×4 transition operators S and T coupling N and Δ fields, are defined as:

$$S_i S_j^\dagger = \tfrac{1}{3}\left(2\delta_{ij} - \imath\epsilon_{ijk}\sigma_k\right) \tag{6.9}$$

$$T_i T_j^\dagger = \tfrac{1}{6}\left(\delta_{ij} - \imath\epsilon_{ijk}\tau_k\right). \tag{6.10}$$

We must remember that this Lagrangian must be also regularized choosing a cut–off to high momenta, in such a way to remove the ultraviolet divergences. The remaining constants in $\mathscr{L}_0$, like M_0 e m_Δ, are regularization dependent and must be properly tuned.

If we want, we can also find the next order terms in the chiral expansion:

$$\begin{aligned}\mathscr{L}_1 =& -\frac{B_1}{2f_\pi^2}\mathcal{D}^{-2}N^\dagger N\left(\partial_\mu\pi_i\partial^\mu\pi_i\right) - \frac{B_2}{2f_\pi^2}\mathcal{D}^{-2}\epsilon_{ijk}\epsilon_{abc}N^\dagger\sigma_k\tau_c N\nabla_i\pi_a\nabla_j\pi_b \\ &- \frac{B_3}{2f_\pi^2}m_\pi^2\mathcal{D}^{-1}N^\dagger N\pi_i^2 + \ldots\end{aligned} \tag{6.11}$$

However it is sensible to start using the leading order Lagrangian only, therefore taking into account only nucleons and pions. So, we consider the following

Lagrangian:

$$\begin{aligned}\mathscr{L}_0 = &-\frac{1}{2}\left[(\vec{\nabla}\pi_i)^2 - (\partial_0\pi_i)^2 + m_\pi^2\pi_i^2\right] + N^\dagger\left[i\partial_0 - \frac{1}{8f_\pi^2}\epsilon_{ijk}\tau_i\pi_j\partial_0\pi_k - M_0\right]N \\ &- \frac{g_A}{2f_\pi}N^\dagger\tau_i\sigma_j\nabla_j\pi_i N - \frac{1}{2}C\left(N^\dagger N\right)\left(N^\dagger N\right) - \frac{1}{2}C_I\left(N^\dagger\tau_i N\right)\left(N^\dagger\tau_i N\right).\end{aligned} \tag{6.12}$$

Notice that in our approach we also introduce the nucleon kinetic term because this is required to apply the standard DMC algorithm. We are allowed to do that because this term is second order.

$$\mathscr{L}_k = N^\dagger\frac{\nabla^2}{2M_0}N. \tag{6.13}$$

Now we have to find the corresponding Hamiltonian. We define the conjugate fields

$$\Pi_N(\vec{x}) = \frac{\delta\mathscr{L}}{\delta\partial_0 N} = iN^\dagger(\vec{x}), \tag{6.14}$$

$$\Pi_{N^\dagger}(\vec{x}) = \frac{\delta\mathscr{L}}{\delta\partial_0 N^\dagger} = 0, \tag{6.15}$$

$$\Pi_\pi(\vec{x}) = \frac{\delta\mathscr{L}}{\delta\partial_0\pi_k} = \partial_0\pi_k(\vec{x}) - \frac{1}{8f_\pi^2}\epsilon_{ijk}\pi_j N^\dagger\tau_i N, \tag{6.16}$$

obtaining

$$H = \int\left[\Pi_N(\vec{x})\partial_0 N(\vec{x}) + \Pi_\pi(\vec{x})\partial_0\pi(\vec{x}) - \mathscr{L}(\vec{x})\right]d\vec{x}. \tag{6.17}$$

We can rewrite the previous expression of the Hamiltonian as a sum of three terms:

$$H = H_\pi + H_N + H_{\pi N} \tag{6.18}$$

where

$$H_\pi = \frac{1}{2}\int\Pi_\pi^2(\vec{x}) + \left(\vec{\nabla}\pi(\vec{x})\right)^2 + m_\pi^2\pi^2(\vec{x})d\vec{x} \tag{6.19}$$

is the pion–field Hamiltonian,

$$H_{\pi N} = \frac{g_a}{2f_\pi}\int N^\dagger(\vec{x})\sigma_j\tau_i\nabla_j\pi_i(\vec{x})N(\vec{x})d\vec{x} \tag{6.20}$$

is the pion–nucleon interaction, and

$$\begin{aligned}H_N = &\int N^\dagger(\vec{x})\left(M_0 - \frac{\nabla^2}{2M_0}\right)N(\vec{x})d\vec{x} \\ &+ \frac{1}{2}C\int\int\delta(\vec{x}-\vec{y})N^\dagger(\vec{x})N(\vec{x})N^\dagger(\vec{y})N(\vec{y})d\vec{x}d\vec{y} \\ &+ \frac{1}{2}C_I\int\int\delta(\vec{x}-\vec{y})N^\dagger(\vec{x})\tau_i N(\vec{x})N^\dagger(\vec{y})\tau_i N(\vec{y})d\vec{x}d\vec{y}\end{aligned} \tag{6.21}$$

is the nucleonic Hamiltonian.

The previous Hamiltonian is quantized with the canonical commutation rules

$$[\Pi_N(\vec{x},t), N(\vec{y},t)]_+ = -i\delta^3(\vec{x}-\vec{y}) \tag{6.22}$$
$$[\Pi_N(\vec{x},t), \Pi_N(\vec{y},t)]_+ = 0 \tag{6.23}$$
$$[N(\vec{x},t), N(\vec{y},t)]_+ = 0 \tag{6.24}$$

$$[\Pi_\pi(\vec{x},t), \pi(\vec{y},t)] = -i\delta^3(\vec{x}-\vec{y}) \tag{6.25}$$
$$[\Pi_\pi(\vec{x},t), \Pi_\pi(\vec{y},t)] = 0 \tag{6.26}$$
$$[\pi(\vec{x},t), \pi(\vec{y},t)] = 0 \tag{6.27}$$

So the Hilbert space $\mathscr{H}$ is the composition of the nucleon and pion Fock space:

$$\mathscr{H} = \mathscr{F}_\pi \otimes \mathscr{F}_N, \tag{6.28}$$

where:

$$\begin{aligned} \mathscr{F}_N &= \overset{\infty}{\underset{i=0}{\otimes}} \mathcal{A}\mathscr{H}_N^i, \\ \mathscr{F}_\pi &= \overset{\infty}{\underset{i=0}{\otimes}} \mathcal{S}\mathscr{H}_\pi^i, \end{aligned} \tag{6.29}$$

and $\mathscr{H}_\pi^i$ ($\mathscr{H}_N^i$) is the i pion (nucleon) Hilbert space. $\mathcal{S}$ and $\mathcal{A}$ are the symmetrization and antisymmetrization operators respectively.

For the moment we are interested only in the low energy regime, consistently with the fact that we are retaining only the leading order of the Lagrangian. In this regime it is safe to assume that the baryon number is conserved. This implies that instead of considering the full nucleon Fock space $\mathscr{F}_N$ we are allowed to take into account only $\mathcal{A}\mathscr{H}_N^i$, where i is the number of nucleons in our system.

This simple assumption is technically very crucial and important because it greatly simplifies the problem and its solution. Thus, instead of the Hilbert space of Eq(6.28), we simply take into account

$$\mathscr{H} = \mathscr{F}_\pi \otimes \mathcal{A}\mathscr{H}_N^A. \tag{6.30}$$

Moreover, we have to stress that the dynamic term of the pion fields, i.e. the $\partial_0\pi$ terms in the Lagrangian $\mathcal{L}_0$ of equation Eq(6.12), is usually neglected. With this assumption it is possible to integrate out the pion fields and to derive in an easy way a nucleon potential. However, important effects might be neglected. We discuss this approximation in the next chapter.

6.3 Regularization and Effective Parameters

Starting from the Lagrangian $\mathscr{L}_0$ a few steps are in order to further develop an algorithmic approach:

- Fix a regularization scheme, with a cut–off Λ on momenta Q.
- Determine all effective parameters that depend on regularization scheme and cut–off Λ.

- Seek an Hamiltonian formalism to use Monte Carlo methods with the chosen regularization scheme.

About the effective parameters, we can say that:

- At this order m_π corresponds to the physical pion mass (the average 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. So we can set M_0 requiring that the difference between the ground state energy of one nucleon and the system with no nucleons is equal to the physical nucleon mass M_N.
- g_A is the axial vector coupling of nucleon and f_π is the pion decay constant. They are known from experimental data.
- C and C_I are the effective coefficients parameters of the counterterms. They are regularization dependent, so we need to set them reproducing some experimental or previously computed theoretical data.

We choose to set the cut–off Λ representing the pion fields on a periodic lattice with step $a \simeq 2$fm. This choice must be consistent with the degrees of freedom that we take into account and that we omit. This defines an energy range

$$\frac{m_\pi}{M} < \frac{\Lambda}{M} < \frac{m_\Delta - M_N}{M} < 1 \tag{6.31}$$

We do not need to regularize nucleon fields too, because we have already assumed that the baryon number is conserved, i.e. we can deal with nucleons by introducing a simple standard wavefunction. So, we describe the pion fields on a periodic cubic lattice. We assume a cubic box of size L, discretized in n_l points per dimension, with step of size a so that $L = N_l\, a$. Consistently, a discrete definition of derivative on pion fields is required. We choose the 3 points formula:

$$\nabla_x \pi(\vec{l}) \equiv \frac{\pi(\vec{l} + \hat{x}) - \pi(\vec{l} - \hat{x})}{2a} \tag{6.32}$$

with $\vec{l} + n_l \vec{i} \equiv \vec{l}$ and $\vec{i} \in \mathbb{Z}^3$. Assuming periodic boundary conditions and using the notation $\pi(\vec{l})$ instead of $\pi(a\vec{l})$, we can rewrite the Hamiltonian H_π Eq(6.19) as:

$$H_\pi = \frac{1}{2} a^3 \sum_{\vec{l}} \Pi_\pi^2(\vec{l}) + \frac{1}{2} a^3 \sum_{\vec{l},\vec{n}} \pi(\vec{l})\; K_{\vec{l}\vec{n}}\; \pi(\vec{n}), \tag{6.33}$$

with

$$K_{\vec{l}\vec{n}} = \left(m_\pi^2 + \frac{1}{a^2} \frac{3}{2} \right) \delta_{\vec{l}\vec{n}} - \frac{1}{2a^2} \sum_{\vec{\mu}=\hat{x},\hat{y},\hat{z}} \delta_{\vec{l},\vec{n}+2\vec{\mu}} \tag{6.34}$$

$$\vec{l} \in \left\{ \forall \vec{l} \in \mathbb{Z}^3 | 0 \le l_i < n_l \right\}. \tag{6.35}$$

Now, in rewriting the other Hamiltonian terms, we have to regularize the nucleon contact terms, i.e. to choose a regularization for the δ function. We choose it

consistently with the lattice regularization, i.e.

$$\delta_a(\vec{k}) \equiv \begin{cases} \dfrac{1}{a^3} & \text{if} \quad |k_x| < \dfrac{a}{2}, \quad |k_x| < \dfrac{a}{2}, \quad |k_x| < \dfrac{a}{2} \\ 0 & \text{otherwise} \end{cases} \tag{6.36}$$

With these assumptions the nucleon part of the hamiltonian becomes:

$$H_N = AM_0 - \sum_{m=1}^{A} \frac{\nabla_m^2}{2M_0} + \frac{1}{2} \sum_{m=1}^{A} \sum_{\substack{n=1 \\ n \neq m}}^{A} \delta_a(\vec{x}_m - \vec{x}_n)(C + C_I \vec{\tau}_m \cdot \vec{\tau}_n). \tag{6.37}$$

Now we can rewrite the nucleon–pion term Eq(6.20) as

$$\frac{g_a}{2f_\pi} \int \int N^\dagger(\vec{x}) \sigma_j \tau_i \nabla_j \pi_i(\vec{y}) N(\vec{x}) \delta(\vec{x} - \vec{y}) d\vec{x} d\vec{y}. \tag{6.38}$$

Because of the definition of our regularization

$$\int \delta(\vec{x}) d\vec{x} \quad \longrightarrow \quad a^3 \sum_{\vec{k}} \delta_a(\vec{k}), \tag{6.39}$$

we can finally write

$$\begin{aligned} H_{\pi N} &= \frac{g_a}{2f_\pi} \sum_{m=1}^{A} a^3 \sum_{\vec{k}} \tau_i \sigma_j \nabla_j \pi_i(\vec{k}) \delta_a(\vec{k} - x_m) \\ &= \frac{g_a}{2f_\pi} \sum_{m=1}^{A} \tau_i \sigma_j \nabla_j \pi_i(\lfloor a^{-1} \vec{x}_m \rfloor) \\ &= \frac{g_a}{2f_\pi} \sum_{m=1}^{A} \tau_i \sigma_j \frac{\pi_i(\lfloor a^{-1} \vec{x}_m \rfloor + \hat{j}) - \pi_i(\lfloor a^{-1} \vec{x}_m \rfloor - \hat{j})}{2a}, \end{aligned} \tag{6.40}$$

where A is the nucleon number of the system. In the previous formula we have used the notation $\lfloor \vec{x} \rfloor$ defined as

$$\lfloor \vec{x} \rfloor \equiv (\lfloor x_x \rfloor, \lfloor x_y \rfloor, \lfloor x_z \rfloor) \tag{6.41}$$

$$\lfloor x \rfloor \equiv \text{nearest integer to } x \tag{6.42}$$

We want to stress that in order to avoid the nucleon–nucleon self interaction, only terms with $m \neq n$ must be considered in Eq(6.37).

6.4 The pion vacuum

Because of the presence of the $\partial_0 \pi$ term even, the 0–nucleon system is not trivial, because the energy of the vacuum pion field alone is not zero. As we can see, the vacuum energy could be very large with respect to the typical nuclear binding energy. So, it is very important to know the correct value of the vacuum energy and its wavefunction in such a way that it can be subtracted exactly from AFDMC estimates in order to compute the nucleon energy.

Let us now derive the pion vacuum wavefunction, first in the continuum case then in the discrete one.

We take into account H_π of Eq(6.19). Because of the commutation relations Eq(6.27), it is possible to define a set of eigenfunction for the operator $\hat{\pi}(\vec{x})$

$$\hat{\pi}(\vec{x})|\pi(\vec{x})\rangle = \pi(\vec{x})|\pi(\vec{x})\rangle, \tag{6.43}$$

with the normalization condition

$$\begin{aligned} &\langle\pi(\vec{x})|\pi'(\vec{x})\rangle = \delta\left(\pi(\vec{x}) - \pi'(\vec{x})\right), \\ &\int \mathcal{D}\pi(\vec{x})|\pi(\vec{x})\rangle\langle\pi(\vec{x})| = 1. \end{aligned} \tag{6.44}$$

We can define the operator $\hat{\Pi}(\vec{x})$, the conjugate of $\hat{\pi}(\vec{x})$, as the functional derivative of $\pi(\vec{x})$

$$\hat{\Pi}(\vec{x}) = -i\frac{\delta}{\delta\pi(\vec{x})}. \tag{6.45}$$

The functional wavefunction will be

$$\Psi\left[\pi(\vec{x})\right] = \langle\pi(\vec{x})|\Psi\rangle, \tag{6.46}$$

and it must satisfy the Schrödinger equation:

$$\begin{aligned} i\frac{\partial}{\partial t}\Psi\left[\pi(\vec{x})\right] &= H_\pi\left[\pi(\vec{x})\right] \\ &= \frac{1}{2}\int\left(-i\frac{\delta^2}{\delta\pi(\vec{x})^2} + \left(\vec{\nabla}\pi(\vec{x})\right)^2 + m_\pi^2\pi^2(\vec{x})\right)\Psi\left[\pi(\vec{x})\right]d\vec{x}. \end{aligned} \tag{6.47}$$

For the free theory (without nucleons) $\Psi_0\left[\pi(\vec{x})\right]$ is the fundamental eigenstate when the expectation value of the annihilation operator $\hat{a}_{\vec{k}}$ is zero:

$$\hat{a}_{\vec{p}}(t) = \int \frac{d\vec{x}}{(2\pi)^3 w_{\vec{p}}}\,\pi(x)\,i\overset{\leftrightarrow}{\partial}_0\,e^{i(\vec{p}\vec{x} - w_{\vec{p}}t)}, \tag{6.48}$$

where

$$w_{\vec{p}} = \sqrt{\vec{p}^2 + m_\pi^2}, \tag{6.49}$$

and

$$A\overset{\leftrightarrow}{\partial}_0 B \equiv A\partial_0 B - B\partial_0 A. \tag{6.50}$$

We remember Eq(6.27) and Eq(6.45), and then we rewrite Eq(6.48) as:

$$\hat{a}_{\vec{p}}(t)\Psi_0\left[\pi(\vec{x})\right] = \int \frac{d\vec{x}}{(2\pi)^3 w_{\vec{p}}}\,e^{i(\vec{p}\vec{x} - w_{\vec{p}}t)}\left(w_{\vec{p}}\pi(\vec{x}) + \frac{\delta}{\delta\pi(\vec{x})}\right)\,\Psi_0\left[\pi(\vec{x})\right] = 0. \tag{6.51}$$

Trying to use the following functional in Eq(6.51)

$$\Psi_0\left[\pi(\vec{x})\right] = e^{-\frac{1}{2}\int\pi(\vec{x})E(\vec{x},\vec{y})\pi(\vec{y})d\vec{x}d\vec{y}} \tag{6.52}$$

we can obtain

$$\int e^{i\vec{x}\vec{p}}\left(w_{\vec{p}}\pi(\vec{x}) - \int E(\vec{x},\vec{y})\pi(\vec{y})d\vec{y}\right)d\vec{x} = 0 \tag{6.53}$$

Using the Fourier transform to solve the previous equation, we can obtain the following relation for the kernel $E(\vec{x},\vec{y})$:

$$E(\vec{x},\vec{y}) = \int \frac{d\vec{p}}{(2\pi)^3} e^{i\vec{p}(\vec{x}-\vec{y})} w_{\vec{p}}. \tag{6.54}$$

The vacuum energy E_0 will be the eigenvalue of the equation $H_\pi \Psi_0[\pi(\vec{x})] = E_0 \Psi_0[\pi(\vec{x})]$:

$$E_0 = \frac{1}{2}E(0,0) = \frac{\delta^3(0)}{2}\int \frac{d\vec{p}}{(2\pi)^3}\, w_{\vec{p}} \tag{6.55}$$

In the continuum, i.e. without a high momentum cut–off, the previous expression is divergent if we do not use the normal order.

In the discretized case, the fields are regularized on the lattice. We take into account the Hamiltonian H_π of Eq(6.33) with the derivative definition $\vec{\nabla}\pi(\vec{k})$ of Eq(6.32) . We also assume periodic boundary conditions for a lattice $n_l \times n_l \times n_l$ of step a, with side $L = n_l a$ and volume $V = L^3$.

Remembering the following relations where $\vec{k}$ and $\vec{l}$ satisfy Eq(6.35):

$$\vec{x} \longrightarrow a\vec{l}, \qquad \vec{p} \longrightarrow \frac{2\pi}{a\, n_l}\vec{k} \tag{6.56}$$

$$f(\vec{x}) = f(a\vec{l}) \longrightarrow f_{\vec{l}}, \qquad \tilde{f}(\vec{p}) = \tilde{f}\left(\frac{2\pi}{a\, n_l}\vec{k}\right) \longrightarrow \tilde{f}_{\vec{k}} \tag{6.57}$$

the discrete Fourier transform and antitransform are defined on the continuous and discrete space in this way:

$$\tilde{f}(\vec{p}) = \int_V f(\vec{x}) e^{-i\vec{x}\vec{p}} d\vec{x} \qquad \longrightarrow \qquad \tilde{f}_{\vec{k}} = \sum_{\vec{l}} f_{\vec{l}}\, e^{-i\frac{2\pi}{n_l}\vec{l}\vec{k}}, \tag{6.58}$$

$$f(\vec{x}) = \frac{1}{(2\pi)^3}\int_{\tilde{V}} \tilde{f}(\vec{p}) e^{i\vec{x}\vec{p}} d\vec{p} \qquad \longrightarrow \qquad f_{\vec{l}} = \frac{1}{n_l^3}\sum_{\vec{k}} \tilde{f}_{\vec{k}}\, e^{i\frac{2\pi}{n_l}\vec{l}\vec{k}}. \tag{6.59}$$

The following relations are also satisfied:

$$\frac{1}{(2\pi)^3}\int_V e^{i\vec{x}\vec{p}} d\vec{p} = \delta(\vec{x}) \qquad \longrightarrow \qquad \frac{1}{n_l^3}\sum_{\vec{k}} e^{i\frac{2\pi}{n_l}\vec{k}\vec{l}} = \delta_{\vec{l},0}. \tag{6.60}$$

As for the continuum case Eq(6.52), we can define a vacuum functional as

$$\Psi_0\left[\pi(\vec{l})\right] = \exp\left[-\frac{1}{2}a^3 \sum_{\vec{l}\vec{n}} \pi(\vec{l}) E_{\vec{l}\vec{n}} \pi(\vec{n})\right], \tag{6.61}$$

with

$$E_{\vec{l}\vec{n}} = \frac{1}{n_l^3}\sum_{\vec{k}} e^{i\frac{2\pi}{n_l}\vec{k}(\vec{l}-\vec{n})} w_{\vec{k}}. \tag{6.62}$$

The vacuum energy E_0 will be the eigenvalue of $H_\pi \Psi_0 \left[\pi(\vec{l})\right] = E_0 \Psi_0 \left[\pi(\vec{l})\right]$:

$$\frac{1}{2}a^3 \left[\sum_{\vec{i}} E_{\vec{i}\vec{i}} + \sum_{\vec{l}\vec{n}} \left(K_{\vec{l}\vec{n}} - \sum_{\vec{i}} E_{\vec{i}\vec{l}} E_{\vec{i}\vec{n}} \right) \pi(\vec{l})\pi(\vec{n}) \right] \Psi_0 \left[\pi(\vec{l})\right] = E_0 \Psi_0 \left[\pi(\vec{l})\right] \tag{6.63}$$

from which we have

$$K_{\vec{l}\vec{n}} = \sum_{\vec{i}} E_{\vec{i}\vec{l}} E_{\vec{i}\vec{n}}. \tag{6.64}$$

Now using Eq(6.62) we can rewrite the previous expression as:

$$n_l^6 \; K_{\vec{l}\vec{n}} = \sum_{\vec{k}\vec{i}\vec{j}} w_{\vec{i}} \; w_{\vec{j}} \; e^{i\frac{2\pi}{n_l}\vec{i}(\vec{k}-\vec{l})} \; e^{i\frac{2\pi}{n_l}\vec{j}(\vec{k}-\vec{n})}. \tag{6.65}$$

Using the identity Eq(6.60) on $\vec{k}$ we obtain the condition $\vec{i} = -\vec{j}$. So we can write:

$$n_l^3 \; K_{\vec{l}\vec{n}} = \sum_{\vec{i}} w_{\vec{i}}^2 \; e^{i\frac{2\pi}{n_l}\vec{i}(\vec{n}-\vec{l})}. \tag{6.66}$$

Using Eq(6.59) to antitransform the previous, we obtain

$$\begin{aligned}
\sum_{\vec{n}\vec{l}\vec{k}} w_{\vec{k}}^2 \; e^{i\frac{2\pi}{n_l}\vec{n}(\vec{k}-\vec{i})} \; e^{-i\frac{2\pi}{n_l}\vec{l}(\vec{k}+\vec{j})} &= n_l^3 \sum_{\vec{n}\vec{l}} K_{\vec{l}\vec{n}} e^{-i\frac{2\pi}{n_l}\vec{l}\vec{j}} \; e^{-i\frac{2\pi}{n_l}\vec{n}\vec{i}} \\
\sum_{\vec{n}\vec{k}} w_{\vec{k}}^2 \; e^{i\frac{2\pi}{n_l}\vec{n}(\vec{k}-\vec{i})} \delta_{\vec{k},-\vec{j}} &= \sum_{\vec{n}\vec{l}} K_{\vec{l}\vec{n}} e^{-i\frac{2\pi}{n_l}\vec{l}\vec{j}} \; e^{-i\frac{2\pi}{n_l}\vec{n}\vec{i}} \\
n_l^3 \sum_{\vec{k}} w_{\vec{k}}^2 \; \delta_{\vec{k},\vec{i}} \delta_{\vec{k},-\vec{j}} &= \sum_{\vec{n}\vec{l}} K_{\vec{l}\vec{n}} e^{-i\frac{2\pi}{n_l}\vec{l}\vec{j}} \; e^{-i\frac{2\pi}{n_l}\vec{n}\vec{i}} \\
n_l^3 w_{\vec{i}}^2 \; \delta_{\vec{i},-\vec{j}} &= \sum_{\vec{n}\vec{l}} K_{\vec{l}\vec{n}} e^{-i\frac{2\pi}{n_l}\vec{l}\vec{j}} \; e^{-i\frac{2\pi}{n_l}\vec{n}\vec{i}},
\end{aligned} \tag{6.67}$$

from which

$$w_{\vec{i}}^2 = \sum_{\vec{n}} K_{0\vec{n}} e^{-i\frac{2\pi}{n_l}\vec{n}\vec{i}}. \tag{6.68}$$

Remembering the definition $K_{\vec{l}\vec{n}}$ Eq(6.34), because of the periodic boundary conditions, we have that:

$$\begin{aligned}
w_{\vec{k}}^2 &= \sum_{\vec{n}} \left[\left(m_\pi^2 + \frac{1}{a^2}\frac{3}{2} \right) \delta_{0\vec{n}} - \frac{1}{2a^2} \sum_{\vec{\mu}=\hat{x},\hat{y},\hat{z}} \delta_{0,\vec{n}+2\vec{\mu}} \right] e^{-i\frac{2\pi}{n_l}\vec{n}\vec{k}} \\
&= m_\pi^2 - \frac{1}{2a^2} \sum_{\vec{\mu}=\hat{x},\hat{y},\hat{z}} \left[\frac{e^{-i\frac{2\pi}{n_l}\vec{k}2\vec{\mu}} + e^{+i\frac{2\pi}{n_l}\vec{k}2\vec{\mu}}}{2} - 1 \right] \\
&= m_\pi^2 - \frac{1}{2a^2} \sum_{\vec{\mu}=\hat{x},\hat{y},\hat{z}} \left[\cos\left(\frac{4\pi}{n_l}\vec{k}\vec{\mu} \right) - 1 \right] \\
&= m_\pi^2 + \frac{1}{a^2} \sum_{\vec{\mu}=\hat{x},\hat{y},\hat{z}} \sin^2\left(\frac{2\pi}{n_l}\vec{k}\vec{\mu} \right).
\end{aligned} \tag{6.69}$$

Using Eq(6.56) we can see that the previous expression becomes in the continuum limit:

$$\frac{1}{a^2}\sum_{\vec{\mu}=\hat{x},\hat{y},\hat{z}}\sin^2\left(\frac{2\pi}{n_l}\vec{k}\vec{\mu}\right)=\frac{1}{a^2}\sum_{\vec{\mu}=\hat{x},\hat{y},\hat{z}}\sin^2\left(a\vec{p}\vec{\mu}\right)\quad\underset{a\to 0}{\longrightarrow}\quad\frac{1}{a^2}\sum_{\vec{\mu}=\hat{x},\hat{y},\hat{z}}\left(a\vec{p}\vec{\mu}\right)^2=\vec{p}^2 \tag{6.70}$$

i.e. we obtain again the expression Eq(6.49) for $w_{\vec{k}}$

$$w_{\vec{p}}^2\quad\underset{a\to 0}{\longrightarrow}\quad m_\pi^2+\vec{p}^2. \tag{6.71}$$

Taking into account Eq(6.63), Eq(6.64) and Eq(6.62) we have that the vacuum energy for the lattice is

$$E_0=\frac{1}{2}\sum_{\vec{i}}E_{\vec{i}\vec{i}}=\frac{1}{2}n_l\frac{1}{n_l}\sum_{\vec{k}}w_{\vec{k}}=\frac{1}{2}\sum_{\vec{k}}\sqrt{m_\pi^2+\frac{1}{a^2}\sum_{\vec{\mu}=\hat{x},\hat{y},\hat{z}}\sin^2\left(\frac{2\pi}{n_l}\vec{k}\vec{\mu}\right)}. \tag{6.72}$$

6.5 Nucleon–pion correlations

Consider a system made by only one nucleon. Similarly to what happens to the pion vacuum, because of the presence of the $\partial_0\pi$ term, we have a non trivial correlation between nucleon and pion. This means that we have to compute the ground state of one nucleon inside the pion lattice. The ground state energy will be the sum of the pion vacuum energy plus, the physical nucleon mass. In this way we can determine the nucleon bare mass. Let us call (improperly) self–energy of the nucleon the difference between its physical mass and the real one. As for the pion vacuum energy, we can see that the nucleon self–energy is much larger than the typical nucleon binding energy. Thus, we have to compute its value and to accurately describe the nucleon–pion correlation that allows us to perform an accurate AFDMC calculation.

As we will see, we cannot analytically solve the one–nucleon problem, so the exact nucleon–pion correlation is not known. However, we can still accurately compute the nucleon self–energy.

To study this nucleon–pion correlation, we forget the nucleon kinetic term. So we start from a simple toy model and then we will try to improve it.

6.5.1 Yukawa model

We start taking into account only one species of pions and the following simplified Hamiltonian:

$$H=H_\pi+H_{\pi N} \tag{6.73}$$

$$H_\pi=\frac{1}{2}\int\Pi_\pi^2(\vec{x})+\left(\vec{\nabla}\pi(\vec{x})\right)^2+m_\pi^2\pi^2(\vec{x})d\vec{x} \tag{6.74}$$

$$H_{\pi N}=\frac{g_a}{2f_\pi}\int N^\dagger(\vec{x})\pi(\vec{x})N(\vec{x})d\vec{x}. \tag{6.75}$$

We can rewrite Eq(6.74) by integrating by parts:

$$H_\pi = \frac{1}{2}\int \Pi_\pi^2(\vec{x}) - \pi(\vec{x})\nabla^2\pi(\vec{x}) + m_\pi^2\pi^2(\vec{x})d\vec{x}, \tag{6.76}$$

and Eq(6.75) assuming a constant nucleon number:

$$H_{\pi N} = \frac{g_a}{2f_\pi}\sum_{n=1}^{A}\int \pi(\vec{x})\delta(\vec{x}-\vec{x}_n)d\vec{x} = \frac{g_a}{2f_\pi}\sum_{n=1}^{A}\pi(\vec{x}_n). \tag{6.77}$$

We define $\Delta(\vec{x})$ as the fundamental solution of

$$(-\nabla^2 + m_\pi^2)\Delta(\vec{x}) = \delta(\vec{x}) \qquad \Longrightarrow \qquad \Delta(\vec{x}) = \frac{e^{-m_\pi|\vec{x}|}}{|\vec{x}|}. \tag{6.78}$$

We can also define the fields $\pi(\vec{x})$ and $\Pi_\pi(\vec{x})$ as:

$$\Pi_\pi(\vec{x}) \;\rightarrow\; \Pi'_\pi(\vec{x}) \equiv \Pi_\pi(\vec{x}), \tag{6.79}$$

$$\pi(\vec{x}) \;\rightarrow\; \pi'(\vec{x}) \equiv \pi(\vec{x}) + \frac{g_a}{2f_\pi}\sum_{n=1}^{A}\int \Delta(\vec{x}-\vec{z})\delta(\vec{z}-\vec{x}_n)d\vec{z}. \tag{6.80}$$

The non interacting Hamiltonian for the new fields is

$$\begin{aligned} H_\pi =& \frac{1}{2}\int \Pi_\pi^{'2}(\vec{x})d\vec{x} \quad + \frac{1}{2}\int \left(\pi'(\vec{x}) - \frac{g_a}{2f_\pi}\sum_{n=1}^{A}\int \Delta(\vec{x}-\vec{z})\delta(\vec{z}-\vec{x}_n)d\vec{z}\right)\times \\ & \times \left(-\nabla^2\pi(\vec{x}) + m_\pi^2\right)\left(\pi'(\vec{x}) - \frac{g_a}{2f_\pi}\sum_{m=1}^{A}\int \Delta(\vec{x}-\vec{y})\delta(\vec{y}-\vec{x}_m)d\vec{y}\right)d\vec{x} \end{aligned} \tag{6.81}$$

Integrating by parts, because of the properties of $\delta(\vec{x})$ and of the definition of $\Delta(\vec{x})$ Eq(6.78), we can write:

$$H_\pi = H'_\pi \; - \frac{g_a}{2f_\pi}\sum_{n=1}^{A}\pi(\vec{x}_n) \; - \frac{g_a^2}{8f_\pi^2}\sum_{m=1}^{A}\sum_{n=1}^{A}\Delta(\vec{x}_m - \vec{x}_n) \tag{6.82}$$

with

$$H'_\pi = \frac{1}{2}\int \Pi_\pi^{'2}(\vec{x}) + \left[\nabla^2\pi'(\vec{x})\right]^2 + m_\pi^2\pi^{'2}(\vec{x})d\vec{x}. \tag{6.83}$$

The second term of Eq(6.82) cancels with the interaction term of Eq(6.73)):

$$H = H'_\pi - \frac{g_a^2}{8f_\pi^2}\sum_{m=1}^{A}\sum_{n=1}^{A}\Delta(\vec{x}_m - \vec{x}_n). \tag{6.84}$$

With the new fields, we have that the Hamiltonian differs from the free one only by a constant V_0 . This is the energy interaction of the nucleons with the pion fields:

$$V_0 = -\frac{g_a^2}{8f_\pi^2}\sum_{m=1}^{A}\sum_{n=1}^{A}\Delta(\vec{x}_m - \vec{x}_n) = -\frac{g_a^2}{8f_\pi^2}\sum_{m=1}^{A}\sum_{n=1}^{A}\frac{e^{-m_\pi|\vec{x}_m-\vec{x}_n|}}{|\vec{x}_m-\vec{x}_n|}. \tag{6.85}$$

Therefore, for this toy model we have that the nucleon bare mass M_0 is equal to $M_0 = M_N - M_A$, with $M_A = V_0$ where V_0 is computed for $A = 1$.

We can write also the ground state of the system; we remember Eq(6.52), Eq(6.54) and then we apply the same transformations Eq(6.80) and Eq(6.79), obtaining

$$\Psi_0\left[\pi'(\vec{x}), \vec{x}_n\right] = \exp\left[-\frac{1}{2}\int\left(\pi'(\vec{x}) - \frac{g_a}{2f_\pi}\sum_{n=1}^{A}\Delta(\vec{x}-\vec{x}_n)\right)E(\vec{x},\vec{y})\times \right. \\ \left. \times\left(\pi'(\vec{y}) - \frac{g_a}{2f_\pi}\sum_{m=1}^{A}\Delta(\vec{y}-\vec{y}_m)\right)d\vec{x}d\vec{y}\right]. \tag{6.86}$$

Now we can do the same on the discrete lattice, with the same assumptions of the previous paragraph. The free pion Hamiltonian H_π Eq(6.33) will be

$$H_\pi = \frac{1}{2}a^3\sum_{\vec{l}}\Pi_\pi^2(\vec{l}) + \frac{1}{2}a^3\sum_{\vec{l},\vec{n}}\pi(\vec{l})\,K_{\vec{l}\vec{n}}\,\pi(\vec{n}), \tag{6.87}$$

while the interaction term $H_{\pi N}$ becomes:

$$H_{\pi N} = \frac{g_a}{2f_\pi}\sum_{n=1}^{A}\sum_{\vec{l}}\pi(\vec{l})\delta_a(a\vec{l}-\vec{x}_n) = \frac{g_a}{2f_\pi}\sum_{n=1}^{A}\pi(\lfloor a^{-1}\vec{x}_n\rfloor). \tag{6.88}$$

Now we can define a discretized version of $\Delta(\vec{x})$, consistently with the discrete derivative Eq(6.32):

$$(-\nabla^2 + m_\pi^2)\Delta(\vec{n}) = \delta_a(\vec{n}), \tag{6.89}$$

$$\Delta(\vec{n}) = \frac{1}{a^3 n_l^3}\sum_{\vec{l}}\frac{e^{\frac{2\pi}{n_l}\vec{l}\vec{n}}}{m_\pi^2 + \frac{1}{a^2}\sum\limits_{\vec{\mu}=\hat{x},\hat{y},\hat{z}}\sin^2\left(\frac{2\pi}{n_l}\vec{l}\vec{\mu}\right)} \\ = \frac{1}{a^3 n_l^3}\sum_{\vec{l}}\frac{\cos\left(\frac{2\pi}{n_l}\vec{l}\vec{n}\right)}{m_\pi^2 + \frac{1}{a^2}\sum\limits_{\vec{\mu}=\hat{x},\hat{y},\hat{z}}\sin^2\left(\frac{2\pi}{n_l}\vec{l}\vec{\mu}\right)}. \tag{6.90}$$

The fields $\pi(\vec{n})$ and $\Pi_\pi(\vec{n})$ are defined as:

$$\Pi_\pi(\vec{n}) \;\rightarrow\; \Pi'_\pi(\vec{n}) \equiv \Pi_\pi(\vec{n}), \tag{6.91}$$

$$\pi(\vec{n}) \;\rightarrow\; \pi'(\vec{n}) \equiv \pi(\vec{n}) + \frac{g_a}{2f_\pi}\sum_{n=1}^{A}\sum_{\vec{l}}\Delta(\vec{l})\delta_a(a\vec{l}-\vec{x}_n). \tag{6.92}$$

As for the continuum case we write the free Hamiltonian using the new fields definition obtaining:

$$H = H'_\pi - \frac{g_a^2}{8f_\pi^2}\sum_{m=1}^{A}\sum_{n=1}^{A}\Delta(\lfloor a^{-1}(\vec{x}_n - \vec{x}_m)\rfloor), \tag{6.93}$$

with

$$H'_\pi = \frac{1}{2}a^3 \sum_{\vec{l}} \Pi'^2_\pi(\vec{l}) + \frac{1}{2}a^3 \sum_{\vec{l},\vec{n}} \pi'(\vec{l})\, K_{\vec{l}\vec{n}}\, \pi'(\vec{n}). \tag{6.94}$$

The interaction of the nucleons with the pion field will be:

$$\begin{aligned} V_0 &= -\frac{g_a^2}{8f_\pi^2} \sum_{m=1}^{A}\sum_{n=1}^{A} \Delta(\lfloor a^{-1}(\vec{x}_n - \vec{x}_m)\rfloor) \\ &= -\frac{g_a^2}{8f_\pi^2} \frac{1}{a^3 n_l^3} \sum_{m=1}^{A}\sum_{\substack{n=1 \\ n\neq m}}^{A}\sum_{\vec{k}} \frac{\cos\left(\frac{2\pi}{n_l}\vec{k}\left(\lfloor a^{-1}(\vec{x}_n - \vec{x}_m)\rfloor\right)\right)}{m_\pi^2 + \frac{1}{a^2}\sum_{\vec{\mu}=\hat{x},\hat{y},\hat{z}} \sin^2\left(\frac{2\pi}{n_l}\vec{k}\vec{\mu}\right)}. \end{aligned} \tag{6.95}$$

As from Eq(6.61) , we can write the ground state wavefunction:

$$\begin{aligned} \Psi_0\left[\pi'(\vec{l}), \vec{x}_n\right] = \exp\Bigg[-\frac{1}{2}a^3 \sum_{\vec{l}\vec{n}} \left(\pi'(\vec{l}) - \frac{g_a}{2f_\pi}\sum_{i=1}^{A}\Delta(\vec{l} - \lfloor a^{-1}\vec{x}_i\rfloor)\right) \times \\ \times E_{\vec{l}\vec{n}} \left(\pi'(\vec{n}) - \frac{g_a}{2f_\pi}\sum_{j=1}^{A}\Delta(\vec{n} - \lfloor a^{-1}\vec{x}_j\rfloor)\right)\Bigg]. \end{aligned} \tag{6.96}$$

In this way we have obtained the ground state energy and the wavefunction of a A nucleon system, taking into account only the H_π and the Yukawa $H_{\pi N}$ terms of the Hamiltonian, both in the continuum that in the lattice case.

6.5.2 Derivative coupling model

We try now to further improve the previous model. We still have to take into account only one type of pions, and we consider the Hamiltonian:

$$H = H_\pi + H_{\pi N}, \tag{6.97}$$

$$\begin{aligned} H_\pi &= \frac{1}{2}\int \Pi^2_\pi(\vec{x}) + \left(\vec{\nabla}\pi(\vec{x})\right)^2 + m_\pi^2\pi^2(\vec{x})d\vec{x} \\ &= \frac{1}{2}\int \Pi^2_\pi(\vec{x}) - \pi(\vec{x})\nabla^2\pi(\vec{x}) + m_\pi^2\pi^2(\vec{x})d\vec{x}, \end{aligned} \tag{6.98}$$

$$\begin{aligned} H_{\pi N} &= \frac{g_a}{2f_\pi}\int N^\dagger(\vec{x})\partial_z\pi(\vec{x})N(\vec{x})d\vec{x} \\ &= \frac{g_a}{2f_\pi}\sum_{n=1}^{A}\int \partial_z\pi(\vec{x})\delta(\vec{x} - \vec{x}_n)d\vec{x} = \frac{g_a}{2f_\pi}\sum_{n=1}^{A}\partial_z\pi(\vec{x}_n). \end{aligned} \tag{6.99}$$

We define $\Delta(\vec{x})$ as in Eq(6.78) and the pion fields $\pi(\vec{x})$ and $\Pi_\pi(\vec{x})$ as

$$\Pi_\pi(\vec{x}) \;\rightarrow\; \Pi'_\pi(\vec{x}) \equiv \Pi_\pi(\vec{x}), \tag{6.100}$$

$$\pi(\vec{x}) \;\rightarrow\; \pi'(\vec{x}) \equiv \pi(\vec{x}) - \frac{g_a}{2f_\pi}\sum_{n=1}^{A}\int \partial_z\Delta(\vec{x} - \vec{z})\delta(\vec{z} - \vec{x}_n)d\vec{z}. \tag{6.101}$$

The free Hamiltonian can be rewritten as

$$H_\pi = \frac{1}{2}\int \Pi_\pi'^2(\vec{x})d\vec{x} \quad + \frac{1}{2}\int \left(\pi'(\vec{x}) + \frac{g_a}{2f_\pi}\sum_{n=1}^{A}\int \partial_z\Delta(\vec{x}-\vec{z})\delta(\vec{z}-\vec{x}_n)d\vec{z}\right)\times$$
$$\times\left(-\nabla^2\pi(\vec{x}) + m_\pi^2\right)\left(\pi'(\vec{x}) + \frac{g_a}{2f_\pi}\sum_{m=1}^{A}\int \partial_z\Delta(\vec{x}-\vec{y})\delta(\vec{y}-\vec{x}_m)d\vec{y}\right)d\vec{x}. \tag{6.102}$$

Integrating by parts, because of the properties of $\delta(\vec{x})$ and because of the definition of $\Delta(\vec{x})$, we have that

$$H_\pi = H'_\pi \; - \frac{g_a}{2f_\pi}\sum_{n=1}^{A}\pi(\vec{x}_n) \; + \frac{g_a^2}{8f_\pi^2}\sum_{m=1}^{A}\sum_{n=1}^{A}\partial_z^2\Delta(\vec{x}_m-\vec{x}_n) \tag{6.103}$$

with H'_π as in Eq(6.83). So we have

$$H = H_\pi + H_{\pi N} = H'_\pi \; + \frac{g_a^2}{8f_\pi^2}\sum_{m=1}^{A}\sum_{n=1}^{A}\partial_z^2\Delta(\vec{x}_m-\vec{x}_n) = H'_\pi + V_0. \tag{6.104}$$

The ground state will have eigenvalue $E_0 + V_0$. Its wavefunction will be

$$\Psi_0\left[\pi'(\vec{x}), \vec{x}_n\right] = \exp\left[-\frac{1}{2}\int\left(\pi'(\vec{x}) + \frac{g_a}{2f_\pi}\sum_{n=1}^{A}\partial_z\Delta(\vec{x}-\vec{x}_n)\right)E(\vec{x},\vec{y})\times\right.$$
$$\left.\times\left(\pi'(\vec{y}) + \frac{g_a}{2f_\pi}\sum_{m=1}^{A}\partial_z\Delta(\vec{y}-\vec{y}_m)\right)d\vec{x}d\vec{y}\right]. \tag{6.105}$$

Now we try to do the same for the discrete case. With the derivative definition Eq(6.32), with $\Delta(\vec{n})$ defined as in Eq(6.90) and with the following Hamiltonian $H = H_\pi + H_{\pi N}$:

$$H_\pi = \frac{1}{2}a^3\sum_{\vec{l}}\Pi_\pi^2(\vec{l}) + \frac{1}{2}a^3\sum_{\vec{l},\vec{n}}\pi(\vec{l})\; K_{\vec{l}\vec{n}}\; \pi(\vec{n}), \tag{6.106}$$

$$\begin{aligned} H_{\pi N} &= \frac{g_a}{2f_\pi}\sum_{n=1}^{A}\sum_{\vec{l}}\partial_z\pi(\vec{l})\delta_a(a\vec{l}-\vec{x}_n) \\ &= \frac{g_a}{2f_\pi}\sum_{n=1}^{A}\partial_z\pi(\lfloor a^{-1}\vec{x}_n\rfloor) \\ &= \frac{g_a}{2f_\pi}\sum_{n=1}^{A}\frac{\pi(\lfloor a^{-1}\vec{x}_n\rfloor+\hat{z}) - \pi(\lfloor a^{-1}\vec{x}_n\rfloor-\hat{z})}{2a}, \end{aligned} \tag{6.107}$$

we can define, as for the Yukawa toy–model:

$$\Pi_\pi(\vec{n}) \;\rightarrow\; \Pi'_\pi(\vec{n}) \equiv \Pi_\pi(\vec{n}) \tag{6.108}$$

$$\begin{aligned}\pi(\vec{n}) \;\rightarrow\; \pi'(\vec{n}) &\equiv \pi(\vec{n}) - \frac{g_a}{2f_\pi}\sum_{n=1}^{A}\sum_{\vec{l}}\partial_z\Delta(\vec{l})\delta_a(a\vec{l}-\vec{x}_n) \\ &= \pi(\vec{n}) - \frac{g_a}{2f_\pi}\sum_{n=1}^{A}\sum_{\vec{l}}\frac{\Delta(\vec{l}+\hat{z})-\Delta(\vec{l}-\hat{z})}{2a}\delta_a(a\vec{l}-\vec{x}_n).\end{aligned} \tag{6.109}$$

Now using the previous relations to rewrite the Hamiltonian, we have

$$H_\pi = H'_\pi \; -\frac{g_a}{2f_\pi}\sum_{i=1}^{A}\partial_z\pi(\lfloor a^{-1}\vec{x}_i\rfloor) + \frac{g_a^2}{8f_\pi^2}\sum_{i=1}^{A}\sum_{j=1}^{A}\partial_z^2\Delta(\lfloor a^{-1}\vec{x}_i - a^{-1}\vec{x}_j\rfloor) \tag{6.110}$$

with H'_π as from Eq(6.94). As we can see, also in this case the second term is removed by the interaction term $H_{\pi N}$ of the full Hamiltonian $H = H_\pi + H_{\pi N}$:

$$H = H'_\pi \; + \frac{g_a^2}{8f_\pi^2}\sum_{i=1}^{A}\sum_{j=1}^{A}\partial_z^2\Delta(\lfloor a^{-1}\vec{x}_i - a^{-1}\vec{x}_j\rfloor) = H'_\pi + V_0 \tag{6.111}$$

Now using the notation $\Delta(\vec{n}_i - \vec{n}_j) = \Delta(\lfloor a^{-1}\vec{x}_i - a^{-1}\vec{x}_j\rfloor)$, we have

$$\begin{aligned}\partial_z\Delta(\vec{n}_i-\vec{n}_j) &= \frac{\Delta(\vec{n}_i-\vec{n}_j+\hat{z})-\Delta(\vec{n}_i-\vec{n}_j-\hat{z})}{2a} \\ &= \frac{1}{2a^4n_l^3}\sum_{\vec{l}}\frac{\cos\left(\frac{2\pi}{n_l}\vec{l}(\vec{n}_i-\vec{n}_j+\hat{z})\right)-\cos\left(\frac{2\pi}{n_l}\vec{l}(\vec{n}_i-\vec{n}_j-\hat{z})\right)}{m_\pi^2+\frac{1}{a^2}\sum\limits_{\vec{\mu}=\hat{x},\hat{y},\hat{z}}\sin^2\left(\frac{2\pi}{n_l}\vec{l}\vec{\mu}\right)} \\ &= -\frac{1}{a^4n_l^3}\sum_{\vec{l}}\frac{\sin\left(\frac{2\pi}{n_l}\vec{l}\hat{z}\right)\cos\left(\frac{2\pi}{n_l}\vec{l}(\vec{n}_i-\vec{n}_j)\right)}{m_\pi^2+\frac{1}{a^2}\sum\limits_{\vec{\mu}=\hat{x},\hat{y},\hat{z}}\sin^2\left(\frac{2\pi}{n_l}\vec{l}\vec{\mu}\right)}\end{aligned} \tag{6.112}$$

$$\begin{aligned}\partial_z^2\Delta(\vec{n}_i-\vec{n}_j) &= \frac{\partial_z\Delta(\vec{n}_i-\vec{n}_j+\hat{z})-\partial_z\Delta(\vec{n}_i-\vec{n}_j-\hat{z})}{2a} \\ &= -\frac{1}{a^5n_l^3}\sum_{\vec{l}}\frac{\sin^2\left(\frac{2\pi}{n_l}\vec{l}\hat{z}\right)\cos\left(\frac{2\pi}{n_l}\vec{l}(\vec{n}_i-\vec{n}_j)\right)}{m_\pi^2+\frac{1}{a^2}\sum\limits_{\vec{\mu}=\hat{x},\hat{y},\hat{z}}\sin^2\left(\frac{2\pi}{n_l}\vec{l}\vec{\mu}\right)}\end{aligned} \tag{6.113}$$

We obtain the expression of V_0 for the lattice

$$V_0 = -\frac{g_a^2}{8f_\pi^2}\frac{1}{a^5n_l^3}\sum_{i=1}^{A}\sum_{j=1}^{A}\sum_{\vec{l}}\frac{\sin^2\left(\frac{2\pi}{n_l}\vec{l}\hat{z}\right)\cos\left(\frac{2\pi}{n_l}\vec{l}(\lfloor a^{-1}\vec{x}_i - a^{-1}\vec{x}_j\rfloor)\right)}{m_\pi^2+\frac{1}{a^2}\sum\limits_{\vec{\mu}=\hat{x},\hat{y},\hat{z}}\sin^2\left(\frac{2\pi}{n_l}\vec{l}\vec{\mu}\right)} \tag{6.114}$$

and the ground state wavefunction

$$\Psi_0\left[\pi'(\vec{l}),\vec{x}_n\right] = \exp\left[-\frac{1}{2}a^3\sum_{\vec{l}\vec{n}}\left(\pi'(\vec{l})+\frac{g_a}{2f_\pi}\sum_{i=1}^{A}\partial_z\Delta(\vec{l}-\lfloor a^{-1}\vec{x}_i\rfloor)\right)\times\right.$$
$$\left.\times E_{\vec{l}\vec{n}}\left(\pi'(\vec{n})+\frac{g_a}{2f_\pi}\sum_{j=1}^{A}\partial_z\Delta(\vec{n}-\lfloor a^{-1}\vec{x}_j\rfloor)\right)\right]$$
$$= \exp\left[-\frac{1}{2}a^3\sum_{\vec{l}\vec{n}}\left(\pi'(\vec{l})+\frac{g_a}{2f_\pi}\sum_{i=1}^{A}\frac{\Delta(\vec{l}-\lfloor a^{-1}\vec{x}_i\rfloor+\hat{z})-\Delta(\vec{l}-\lfloor a^{-1}\vec{x}_i\rfloor-\hat{z})}{2a}\right)\times\right.$$
$$\left.\times E_{\vec{l}\vec{n}}\left(\pi'(\vec{n})+\frac{g_a}{2f_\pi}\sum_{j=1}^{A}\frac{\Delta(\vec{n}-\lfloor a^{-1}\vec{x}_j\rfloor+\hat{z})-\Delta(\vec{n}-\lfloor a^{-1}\vec{x}_j\rfloor-\hat{z})}{2a}\right)\right] \tag{6.115}$$

In this way we have obtained the ground state energy and the wavefunction of a A nucleon system, taking into account only the H_π and the derivative toy–model $H_{\pi N}$ terms of the Hamiltonian, both on the continuum and on the lattice case.

6.5.3 Spin-Isospin dependent coupling

Now we try to use the exact $H_{\pi N}$ term as in the previous two paragraphs. The full pion–nucleon coupling is:

$$\begin{aligned} H_{\pi N} &= \frac{g_a}{2f_\pi}\int N^\dagger(\vec{x})\sigma_j\tau_i\nabla_j\pi_i(\vec{x})N(\vec{x})d\vec{x} \\ &= \frac{g_a}{2f_\pi}\sum_{n=1}^{A}\sigma_{nj}\tau_{ni}\nabla_j\pi_i(\vec{x}_n). \end{aligned} \tag{6.116}$$

We take into account the Hamiltonian $H = H_\pi + H_{\pi N}$, excluding the nucleon–nucleon part. As in the previous paragraphs we can define

$$\Pi_{\pi_i}(\vec{x}) \;\rightarrow\; \Pi'_{\pi_i}(\vec{x}) \equiv \Pi_{\pi_i}(\vec{x}), \tag{6.117}$$

$$\begin{aligned} \pi_i(\vec{x}) \;\rightarrow\; \pi'_i(\vec{x}) &\equiv \pi_i(\vec{x}) - \frac{g_a}{2f_\pi}\int N^\dagger(\vec{z})\sigma_j\tau_i\nabla_j\Delta(\vec{x}-\vec{z})N(\vec{z})d\vec{z} \\ &= \pi_i(\vec{x}) - \frac{g_a}{2f_\pi}\sum_{n=1}^{A}\sigma_{nj}\tau_{ni}\nabla_j\Delta(\vec{x}-\vec{x}_n), \end{aligned} \tag{6.118}$$

with $\Delta(\vec{x})$ defined as in Eq(6.78).

Once more we rewrite the Hamiltonian with the new fields:

$$H = H'_\pi \; + \frac{g_a^2}{8f_\pi^2}\sum_{m=1}^{A}\sum_{n=1}^{A}\sigma_{mj}\sigma_{nj'}\tau_{mi}\tau_{ni}\nabla_j\nabla_{j'}\Delta(\vec{x}_m-\vec{x}_n). \tag{6.119}$$

Because of the properties of $\Delta(\vec{x})$, we have that:

$$\nabla_j \nabla_{j'} \Delta(\vec{x}) = \delta_{j'j} \nabla_j^2 \Delta(\vec{x}), \tag{6.120}$$

and consequently Eq(6.119) becomes:

$$H = H'_\pi \ + \frac{g_a^2}{8 f_\pi^2} \sum_{m=1}^{A} \sum_{n=1}^{A} \sigma_{mj} \sigma_{nj} \tau_{mi} \tau_{ni} \nabla_j^2 \Delta(\vec{x}_m - \vec{x}_n). \tag{6.121}$$

In the case $A = 1$ because of the properties of the σ matrices, we have that $\tau_i^2 = \sigma_i^2 = 1$. We can then simplify Eq(6.121) obtaining:

$$H = H'_\pi \ + 9 \frac{g_a^2}{8 f_\pi^2} \nabla_j^2 \Delta(0) = H'_\pi \ + \ V_0. \tag{6.122}$$

We might state that an analytic solution was also found for the case $A = 1$. However, this is not the case. Consider the ground state wavefunction to which we now also add the nucleon spin/isospin component $\chi(s,t)$:

$$\Psi_0 \left[\pi_i(\vec{x}), s, t\right] = e^{-\frac{1}{2} \int \pi_i(\vec{x}) E(\vec{x},\vec{y}) \pi_i(\vec{y}) d\vec{x} d\vec{y}} \ \chi(s,t). \tag{6.123}$$

Using Eq(6.118) we can rewrite

$$\begin{aligned} &\Psi_0 \left[\pi_i(\vec{x}), x_n, s_n, t_n\right] = \\ &\quad = \exp\left[-\frac{1}{2} \int \left(\pi'_i(\vec{x}) + \frac{g_a}{2 f_\pi} \sum_{n=1}^{A} \sigma_{nj} \tau_{ni} \nabla_j \Delta(\vec{x} - \vec{x}_n) \right) E(\vec{x}, \vec{y}) \times \right. \\ &\quad \left. \times \left(\pi'_i(\vec{y}) + \frac{g_a}{2 f_\pi} \sum_{m=1}^{A} \sigma_{mj} \tau_{mi} \nabla_j \Delta(\vec{y} - \vec{y}_m) \right) d\vec{x} d\vec{y} \right] \ \chi(s_n, t_n) \end{aligned} \tag{6.124}$$

and even for one nucleon, we have that:

$$H \Psi_0 \left[\pi_i(\vec{x}), x_n, s_n, t_n\right] \neq (E_0 + V_0) \Psi_0 \left[\pi_i(\vec{x}), x_n, s_n, t_n\right] \tag{6.125}$$

i.e. Ψ_0 is not an eigenfunction of H'_π because of the presence of non–commuting spin/isopsin operators.
Nevertheless, a variational wavefunction of the form described in Eq(6.124) might still be a better approximation those derived in the previous simplified models for ADFMC calculation.

Let us now derive the discrete formulation of the wavefunction. The Hamiltonian will be

$$\begin{aligned} H_{\pi N} &= \frac{g_a}{2 f_\pi} \sum_{n=1}^{A} \sum_{\vec{l}} \sigma_{nj} \tau_{ni} \nabla_j \pi_i(\vec{l}) \delta_a(a\vec{l} - \vec{x}_n) \\ &= \frac{g_a}{2 f_\pi} \sum_{n=1}^{A} \sigma_{nj} \tau_{ni} \nabla_j \pi_i(\lfloor a^{-1} \vec{x}_n \rfloor) \\ &= \frac{g_a}{2 f_\pi} \sum_{n=1}^{A} \sigma_{nj} \tau_{ni} \frac{\pi_i(\lfloor a^{-1} \vec{x}_n \rfloor + \hat{j}) - \pi_i(\lfloor a^{-1} \vec{x}_n \rfloor - \hat{j})}{2a}, \end{aligned} \tag{6.126}$$

and the new fields:

$$\Pi_{\pi_i}(\vec{n}) \;\rightarrow\; \Pi'_{\pi_i}(\vec{n}) \equiv \Pi_{\pi_i}(\vec{n}) \tag{6.127}$$

$$\begin{aligned}\pi_i(\vec{n}) \;\rightarrow\; \pi'_i(\vec{n}) &\equiv \pi_i(\vec{n}) - \frac{g_a}{2f_\pi}\sum_{n=1}^{A}\sum_{\vec{l}}\sigma_{nj}\tau_{ni}\nabla_j\Delta_i(\vec{l})\delta_a(a\vec{l}-\vec{x}_n) \\ &= \pi_i(\vec{n}) - \frac{g_a}{2f_\pi}\sum_{n=1}^{A}\sum_{\vec{l}}\sigma_{nj}\tau_{ni}\frac{\Delta_i(\vec{l}+\hat{j})-\Delta_i(\vec{l}-\hat{j})}{2a}\delta_a(a\vec{l}-\vec{x}_n).\end{aligned} \tag{6.128}$$

The wavefunction can be written as:

$$\begin{aligned}&\Psi_0\left[\pi'_i(\vec{l}),\vec{x}_n,s_n,t_n\right] = \\ &= \exp\left[-\frac{1}{2}a^3\sum_{\vec{l}\vec{n}}\left(\pi'_i(\vec{l})+\frac{g_a}{2f_\pi}\sum_{k=1}^{A}\sigma_{kj}\tau_{ki}\nabla_j\Delta_i(\vec{l}-\lfloor a^{-1}\vec{x}_k\rfloor)\right)\times\right. \\ &\left.\times\, E_{\vec{l}\vec{n}}\left(\pi'_i(\vec{n})+\frac{g_a}{2f_\pi}\sum_{l=1}^{A}\sigma_{lj}\tau_{li}\nabla_j\Delta_i(\vec{n}-\lfloor a^{-1}\vec{x}_l\rfloor)\right)\right]\chi(s_n,t_n) \\ &= \exp\left[-\frac{1}{2}a^3\sum_{\vec{l}\vec{n}}\left(\pi'_i(\vec{l})+\frac{g_a}{2f_\pi}\sum_{k=1}^{A}\sigma_{kj}\tau_{ki}\frac{\Delta_i(\vec{l}-\lfloor a^{-1}\vec{x}_k\rfloor+\hat{j})-\Delta_i(\vec{l}-\lfloor a^{-1}\vec{x}_k\rfloor-\hat{j})}{2a}\right)\times\right. \\ &\left.\times\, E_{\vec{l}\vec{n}}\left(\pi'_i(\vec{n})+\frac{g_a}{2f_\pi}\sum_{l=1}^{A}\sigma_{lj}\tau_{li}\frac{\Delta_i(\vec{n}-\lfloor a^{-1}\vec{x}_l\rfloor+\hat{j})-\Delta_i(\vec{n}-\lfloor a^{-1}\vec{x}_l\rfloor-\hat{j})}{2a}\right)\right]\chi(s_n,t_n).\end{aligned} \tag{6.129}$$

6.6 Wave Functions

In order to be able to perform efficient AFDMC calculations we need a good trial wavefunction for the ground state. We have seen that for the pion vacuum system we known the exact wavefunction Ψ_0 Eq(6.61). For the one nucleon system we can only have an approximate wavefunction as Eq(6.129) or those of the previous simpler models. For many–nucleon systems we eventually have to take into account some nucleon–nucleon correlations.

We can thus define a one–body operator for a nucleon–pion correlator. We use a spin/isospin independent θ'_m:

$$\Theta'_m = \exp\left[-\frac{1}{2}\frac{g_T}{2f_\pi}a^3\sum_{\vec{i},\vec{j},\alpha}\pi^\alpha_{\vec{i}}\,E_{\vec{i}\vec{j}}\,\partial_\beta\Delta(\vec{j}-\lfloor a^{-1}\vec{x}_m\rfloor)\right], \tag{6.130}$$

or a θ_m that contains spin/isospin operators:

$$\Theta_m = \exp\left[-\frac{1}{2}\frac{g_T}{2f_\pi}a^3\sum_{\vec{i},\vec{j},\alpha,\beta}\pi^\alpha_{\vec{i}}\,E_{\vec{i}\vec{j}}\,\partial_\beta\Delta(\vec{j}-\lfloor a^{-1}\vec{x}_m\rfloor)\sigma_\beta\tau_\alpha\right], \tag{6.131}$$

with $\partial_\beta \Delta$ defined as in Eq(6.112) and g_T a variational parameter. Two body nucleon–nucleon correlations could be included with other spin/isospin dependent Jastrow terms, taking care to symmetrize the operators to preserve the antisymmetry of the uncorrelated wavefunction. Calling $|\chi\rangle$ the antisymmetric uncorrelated nucleon wavefunction (i.e. a sum of Slater determinant of single particle wavefunctions), the final trial wavefunction becomes

$$|\Psi_T\rangle = \Psi_0 \left[\mathscr{S} \prod_{m>n} (1 + \tau_\alpha(m)\tau_\alpha(n) f_\tau(r_{mn})) \right] \prod_{m>n} f_c(r_{mn}) \prod_w \Theta_w |\chi\rangle \tag{6.132}$$

where Ψ_0 is the pion vacuum wavefunction of Eq(6.61). The correlation functions $f_c(r_{mn})$ and $f_\tau(r_{mn})$ and the parameter g_T of Θ_m have to be determined variationally, minimizing the energy of the system.

Chapter 7

AFDMC within EFT

7.1 Assumptions

In the first part of this thesis we have seen the technical details of the AFDMC method. In the previous chapter we have shown the basics of EFT to define our nuclear system. Now we try to solve this problem with the AFDMC method.

We start with the leading order EFT as defined by the Hamiltonian described in (§ 6.3). We have already chosen our degrees of freedom (nucleons ad pions), our regularization scheme and our cut–off $a \simeq$ fm . In order to study a nucleus like ^{4}He it is customary[BEK$^+$07] to choose a pion field box with $L \simeq$ 10fm, i.e. with 5 lattice site per dimension. Other parameters and constants used in simulations are reported in Tab. 7.1.

$\hbar$	1	
$\hbar c$	197.33	fm MeV
a	1.9733	fm
n_l	5	
L	9.8663	fm
m_π	138.08	MeV
M_N	938.92	MeV
g_a	1.26	
f_π	92	MeV

Table 7.1: Used parameters

Now we have to set three effective parameters in our Hamiltonian: the bare nucleon mass M_0 and the two contact interaction terms C and C_I. Moreover we have also to set the variational parameter we use in the trial wavefunction of AFDMC algorithm.

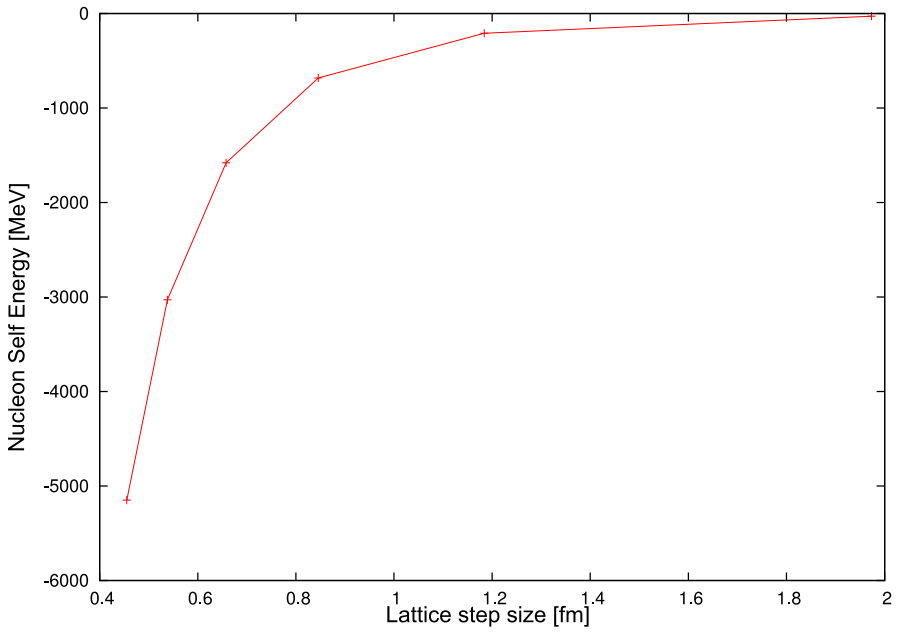

Figure 7.1: Nucleon eigenenergy $M_N - M_0$ for the derivative toy–model for a lattice with $L = 5.92$ fm as function of the lattice size a.

At first we have to find M_0, i.e. to solve the one nucleon system and to find the better one nucleon trial wavefunction. Then we need to find the two contact interaction terms C and C_I, reproducing the binding energy of two different nucleon systems. If we had been able to do that, then we could made some predictive calculations for other nuclei, eventually improved the EFT Hamiltonian at next orders, or included others degrees of freedom as the Δ.

Note that with the previous assumptions we obtain a vacuum pion energy equal to

$$E_0 = 34.4633\text{GeV} \tag{7.1}$$

From the computational point of view, it is important to realize that this value is several orders of magnitude larger than the energies we are interested in. Fluctuations that are very small compared to this value and that might come from an inaccurate description of the pion vacuum would eventually prevent the computation of any quantity with a meaningful accuracy. Therefore, it is of extreme importance to include the exact pion vacuum wavefunction Ψ_0 in order to prevent the occurence of such statistical fluctuations. If we want to eventually improve our EFT decreasing the lattice size and increasing the lattice points, we have to keep care of the diverging value of the vacuum energy.

We can do a similar discussion for the nucleon eigenenergy. For a qualitative study, we consider one of the previous simplified models. Nucleon self–energy as function of the pion lattice size are shown in Fig. 7.1. We can argue that

in the case of a lattice step not too much smaller than those we use ($a \simeq 2$ fm), we might not be able to perform an AFDMC calculation without an exact description of the nucleon–pion correlation. Without it, the statistical noise related to this self–energy is some order of magnitudes bigger of the typical nuclear binding energies, and so it hides the signal that we want to compute.

7.2 AFDMC details

In this paragraph we analyze some technical details of the AFDMC implementation.

The variables that we have to sample are the nucleon coordinates, their spin and isospin states, and the value of the pion field for each lattice site for all the three pion species. So, to better understand the Monte Carlo implementation, let us think each lattice pion site as a sort of "particle", for which we have a "kinetic" term (i.e. the Π_π^2 term) and a sort of "position", i.e. the value of the field in that site.

So we can rewrite our Hamiltonian as

$$H = T_N + T_\pi + V_C + V_{\sigma\tau} + V_\tau, \tag{7.2}$$

with

$$T_N = -\sum_{m=1}^{A} \frac{\nabla_m^2}{2M_0}, \tag{7.3}$$

$$T_\pi = \frac{1}{2} a^3 \sum_{\vec{l}} \Pi_{\pi_i}^2(\vec{l}), \tag{7.4}$$

$$V_c = AM_0 + \frac{1}{2} a^3 \sum_{\vec{l},\vec{n}} \pi_i(\vec{l})\, K_{\vec{l}\vec{n}}\, \pi_i(\vec{n}) + \frac{1}{2} \sum_{m=1}^{A} \sum_{\substack{n=1 \\ n\neq m}}^{A} C\delta_a(\vec{x}_m - \vec{x}_n), \tag{7.5}$$

$$V_{\tau\sigma} = H_{\pi N} = \frac{g_a}{2f_\pi} \sum_{m=1}^{A} \tau_i \sigma_j \frac{\pi_i(\lfloor a^{-1}\vec{x}_m \rfloor + \hat{j}) - \pi_i(\lfloor a^{-1}\vec{x}_m \rfloor - \hat{j})}{2a}, \tag{7.6}$$

$$V_\tau = \frac{1}{2} \sum_{m=1}^{A} \sum_{\substack{n=1 \\ n\neq m}}^{A} C_I(\vec{\tau}_m \cdot \vec{\tau}_n)\delta_a(\vec{x}_m - \vec{x}_n). \tag{7.7}$$

In the AFDMC algorithm the kinetic contribution to the nucleon dynamics is given in terms of the standard drifted Gaussian propagator. We can say the same for the propagator corresponding to T_π. For each lattice site we have to sample the pion field value with a drifted Gaussian as for the positions of nucleons.

The term V_c is simply a central potential term, while $V_{\sigma\tau}$ contains a one–body spin/isospin operator. The propagator of both of them can be included in the standard DMC without any difficulty.

The propagator of the remaining V_τ contact term, because of the presence of the two–body isospin operator, requires the use of the Hubbard Stratonovich

transform, i.e. the inclusion of other auxiliary fields.

The trial wavefunction will be simply a function of nucleon positions and spin/isospin one–body states, and of the pion field values of each lattice site for all the three pion families. We can think of using a trial wavefunction like that in Eq(6.132). Anyway to be able to use AFDMC method, we have to neglect the two–body isospin dependent term. It might be used in a VMC or GFMC calculation taking into account the full spin/isospin product space. We also want to stress the fact that the spin/isospin operators in the nucleon–pion correlator Θ_m are only one–body operators, so they can be in principle used also in a AFDMC calculation. However, in order to compute, for example, the nucleon kinetic term, we have to write the derivative of $|\Psi_T\rangle$ with respect to a nucleon coordinate. Because of the presence of non commuting operators in Θ_m, it is impossible to write an analytic form for the derivative of $|\Psi_T\rangle$. It is anyway possible to compute it numerically. This numerical calculation is very expensive if done at any Monte Carlo step for each nucleon and lattice site.

7.3 Nucleon bare mass

As said before, at first we have to compute the nucleon bare mass. We do a AFDMC calculation for the one nucleon system, using for the nucleon correlator the spin/isospin independent operator Θ'_m. We start choosing $M_0 = M_N$, i.e. a bare mass equal to the physical mass. Computing the energy ground state value of this system, we have to obtain an overbound equal to M_N respect to the pion vacuum energy. Clearly with $M_0 = M_N$ we obtain a shift respect to this ansatz. So we add this shift to M_0 and we make a new AFDMC calculation. We iterate this procedure several times until we reach the convergence.

Finally, after the extrapolation for $dt \to 0$ and $n_w \to \infty$ as shown in the plots, we obtain the following values for the nucleon self–energy

$$M_A = M_N - M_0 = -(39.82 \pm 0.05) MeV \tag{7.8}$$

and the nucleon bare mass

$$M_0 = (978.74 \pm 0.05) MeV \tag{7.9}$$

7.4 Variational parameters

In order to improve the calculation of the previous paragraph, and also to reduce the statistical noise and the computational cost related to the the self–energy, we attempt to refine the trial wavefunction.

We try to study the one–nucleon system, at first using Θ'_m as the nucleon–pion correlator and changing the g_T parameter of Θ'_m.

Then we try also to include one–body spin/isospin correlations using the correlator Θ_m. In this case we are able to obtain a very accurate result for the variational parameter $g_T = 2g_a$, as shown in Fig. 7.4. In fact we are able

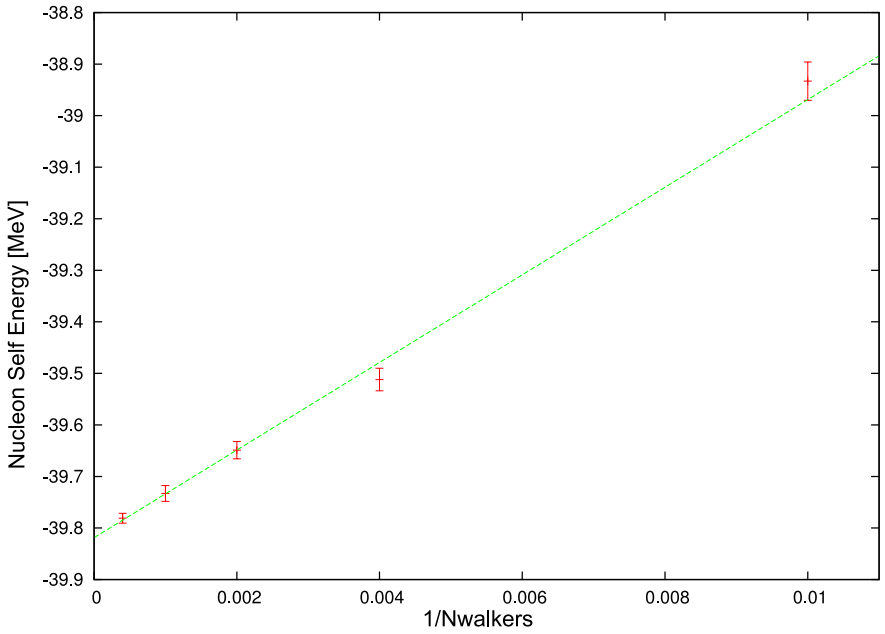

Figure 7.2: Nucleon self–energy $M_N - M_0$ as function of the inverse of the number of walkers used in the AFDMC algorithm.

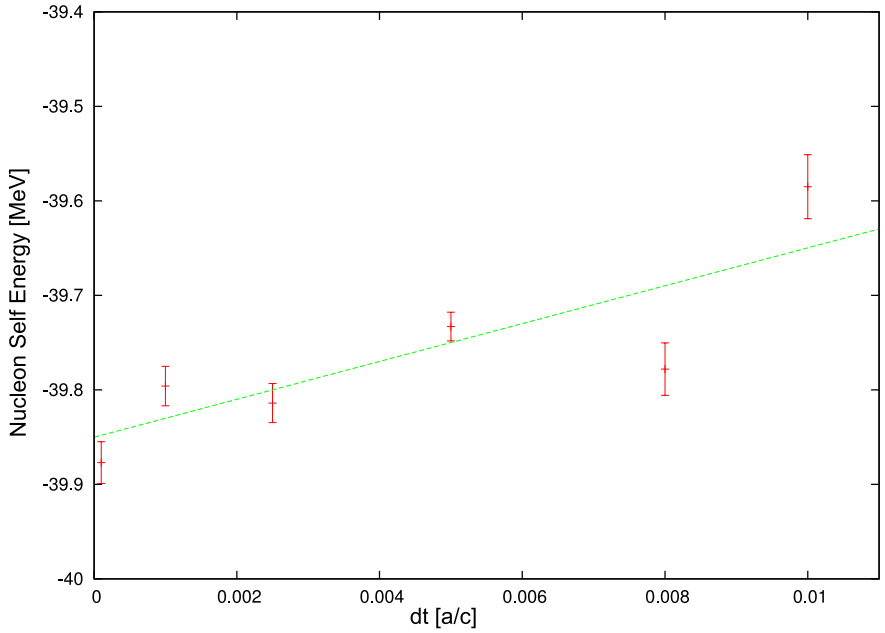

Figure 7.3: Nucleon self–energy $M_N - M_0$ as function of the AFDMC time step dt used in the propagator.

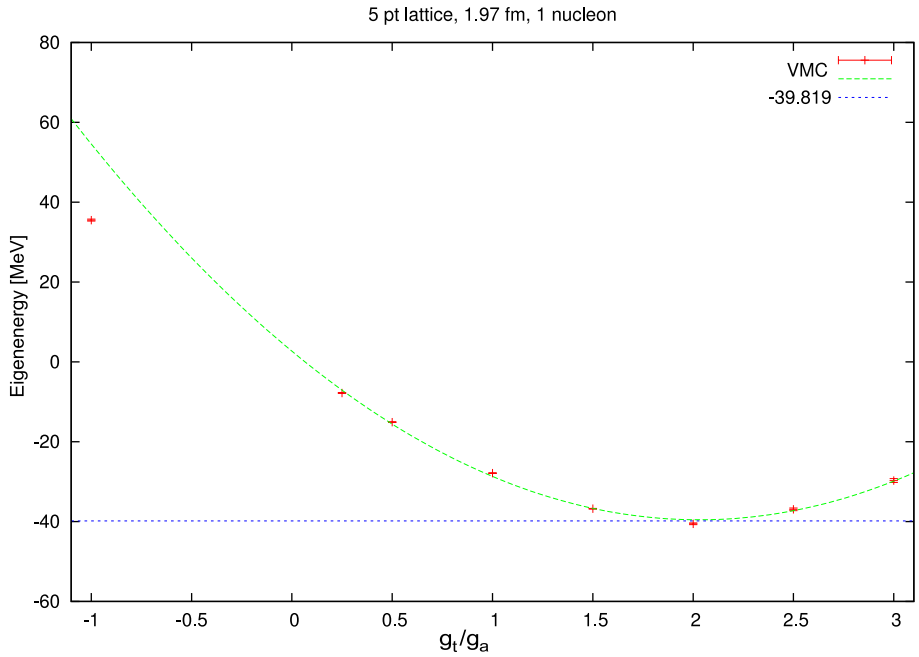

Figure 7.4: Nucleon self–energy computed with the AFDMC algorithm (-39.819 MeV) and with VMC algorithm as function of the variational parameter g_T/g_a of the trial wavefunction.

to obtain with VMC the same result of AFDMC, with a very small statistical variance.

In other words, this wave function is very close to that of the exact ground state. However, as explained before, this wavefunction is very expensive to be computed because derivatives can be calculated only numerically. Thus for AFDMC calculations it is better to use only the correlator Θ'_m with $g_T = 2g_a$.

7.5 C and C_I parameter fit

We have determined the nucleon bare mass M_0. Now we have to set other two parameters in the Hamiltonian, i.e. the coefficients of the nucleon contact interaction term. To do that, to avoid bias due to the finite size of the pion box and the many–body effects, we initially try to solve the $^1S_0$ and $^3S_1$ 2–nucleon states in the box. The solution is known from [BBPnS04]. We made several attempts to solve this problem, i.e. to fit C and C_I, within AFDMC. We have tried to use different trial wavefunctions and approximations, but the statistical noise and the instabilities of the fixed–phase approximation do not allow to be so accurate to find C and C_I (see Fig. 7.5 and Fig. 7.6).

We tried to do other calculations for ^{4}He, ^{8}He ^{16}O with a chosen value of C and C_I coefficients. For these systems, the AFDMC calculation are stable (see

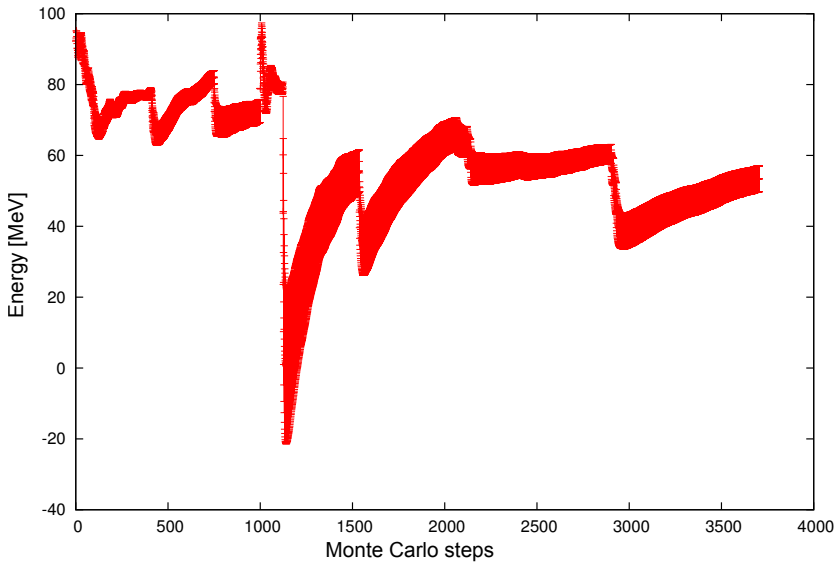

Figure 7.5: Example of the estimate of the energy for the two–nucleon system as function of the Monte Carlo steps of an AFDMC simulation. It is possible to notice anomalus jumps, that evidence the instability of the algorithm. In Fig. 7.6 it is shown a calculation with more samples.

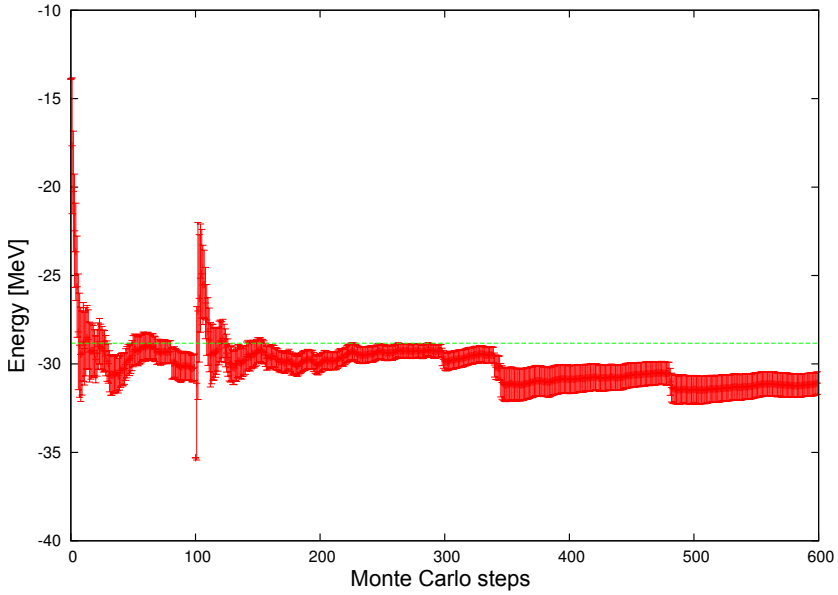

Figure 7.6: Example of the estimate of the energy for the two–nucleon system as function of the Monte Carlo steps of the AFDMC simulation. It is possible to notice that also increasing statistic with respect to Fig. 7.5, the instabilities do not leave AFDMC to reach a stable value.

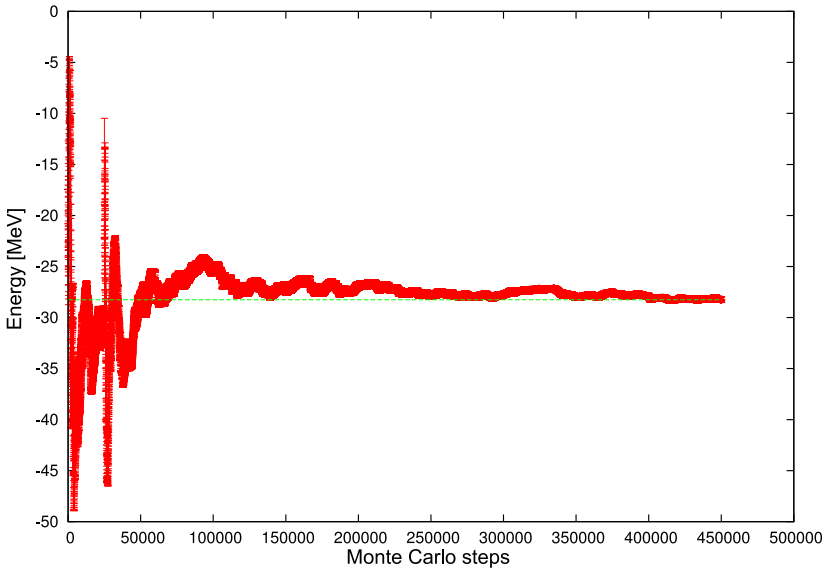

Figure 7.7: Estimate of the energy of ^{4}He as function of the Monte Carlo steps of an AFDMC simulation. We set arbitrarily $C = -3.62 \cdot 10^{-5}\text{MeV}^{-2}$ and $C_I = -2.28 \cdot 10^{-6}\text{MeV}^{-2}$.

Fig. 7.7). However we have a too poor Lagrangian and too many nucleons to be able to remove spurious many–body effects or to compare our calculation with other ones.

Moreover, C and C_I are strictly regularization dependent, and we cannot use the same coefficients computed in other works.

Chapter 8

EFT with istantaneous pion fields

An attempt to solve the EFT problem, though in an approximate way, consist of neglecting the dynamic term $\partial_0\pi$, in the hope that C and C_I coefficients must be the same also taking into account the $\partial_0\pi$ term. This work was done in collaboration with Bingwei Long at ECT*.

8.1 2–body potential

As said before, if we neglect the $\partial_0\pi$ term of the EFT Lagrangian, i.e. if we consider instantaneous the pion meson exchange between nucleons, we are able to integrate out the pion field and to write a nucleon potential.

So we take into account the Hamiltonian as defined in (§ 6.3). We use the same regularization and the same conventions of the previous chapter. As mentioned before, the problem is simplified by removing the Π_π^2 term in H_π. In this way the pion vacuum energy is zero, as the nucleon self energy. The drawback is the exclusion of all retardation effect and correlations induced by the pion dynamics.

In order to write a nucleon–nucleon potential we consider a 2–nucleon system. We choose to work in momentum space. The momentum eigenstates of a single nucleon are normalized as orthonormal

$$\langle \vec{p}\,'\,\sigma'\,\tau'|\vec{p}\,\sigma\,\tau\rangle = \delta_{\vec{p}\,'\,\vec{p}}\,\delta_{\sigma'\sigma}\delta_{\tau'\tau}\,. \tag{8.1}$$

Since the normalization in spin and isospin space is trivial, we focus on momentum space. In the center of mass frame, with $\vec{p}$ $(-\vec{p})$ and $\vec{p}\,'$ $(-\vec{p}\,')$ the initial and final momentum of the nucleon 1 (2), the normalization is

$$\langle \vec{p}\,', -\vec{p}\,'|\vec{p}, -\vec{p}\rangle = \delta_{\vec{p}\,'\,\vec{p}}\,. \tag{8.2}$$

The free Hamiltonian for the two-nucleon system is

$$H_0 = \frac{\vec{p}_1^{\,2}}{2m_N} + \frac{\vec{p}_2^{\,2}}{2m_N}\,. \tag{8.3}$$

So,

$$\langle \vec{p}', -\vec{p}' | H_0 | \vec{p}, -\vec{p} \rangle = \frac{\vec{p}^{\,2}}{m_N} \delta_{\vec{p}'\,\vec{p}} \,. \tag{8.4}$$

In order to simplify the notation, from now on, $|\vec{p}\rangle \equiv |\vec{p}, -\vec{p}\rangle$. The contact interactions have matrix elements as follows

$$\langle \vec{p}' | V_{ct} | \vec{p} \rangle = L^{-3} \mathcal{F}(\vec{q}) \left(C + C_I \vec{\tau}_1 \cdot \vec{\tau}_2 \right) , \tag{8.5}$$

where $\vec{q} \equiv \vec{p}' - \vec{p}$ and $\mathcal{F}(\vec{q})$ is simply the Fourier transform of our δ_α regularization:

$$\begin{aligned} \mathcal{F}(\vec{q}) \equiv & \int_{L^3} d^3x \, \delta_a(\vec{x}) e^{-i\vec{q}\cdot\vec{x}} \\ = & \prod_{z=1}^{3} \frac{\sin(q_z a/2)}{q_z a/2} \,. \end{aligned}$$

Note that $\mathcal{F}(\vec{q}) = \mathcal{F}(-\vec{q})$. The OPE (one pion exchange) potential in momentum space reads

$$\langle \vec{p}' | V^{OPE} | \vec{p} \rangle = -L^{-3} \left(\frac{g_A}{2 f_\pi} \right)^2 \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 \, \mathcal{F}^2(\vec{q}) \, \frac{\left(\sum_{z=1}^{3} \sigma_1^z \frac{\sin q_z a}{a} \right) \left(\sum_{z=1}^{3} \sigma_2^z \frac{\sin q_z a}{a} \right)}{m_\pi^2 + \sum_{z=1}^{3} \sin^2(q_z a)/a^2} \,. \tag{8.6}$$

It is easy to see that both $\langle \vec{p}' | V_{ct} | \vec{p} \rangle$ and $\langle \vec{p}' | V^{OPE} | \vec{p} \rangle$ have the correct dimension, L^{-1}. Now we can compute the matrix element of H between orthonormal momentum eigenstates,

$$\begin{aligned} \langle \vec{p}' | H | \vec{p} \rangle = & \frac{\vec{p}^{\,2}}{m_N} \delta_{\vec{p}'\vec{p}} + L^{-3} \mathcal{F}(\vec{q}) \left(C + C_I \vec{\tau}_1 \cdot \vec{\tau}_2 \right) + \\ & - L^{-3} \left(\frac{g_A}{2 f_\pi} \right)^2 \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 \, \mathcal{F}^2(\vec{q}) \, \frac{\left(\sum_{z=1}^{3} \sigma_1^z \frac{\sin q_z a}{a} \right) \left(\sum_{z=1}^{3} \sigma_2^z \frac{\sin q_z a}{a} \right)}{m_\pi^2 + \sum_{z=1}^{3} \sin^2(q_z a)/a^2} \end{aligned} \tag{8.7}$$

8.2 Hamiltonian diagonalization and fit of effective parameters

In the previous paragraphs we have written the nucleon potential and the 2–body matrix element of our EFT theory at leading order in the approximation of instantaneous pions. Now we want to solve the two body problem. So we have to find the ground state wavefunction and eigenvalue for the triplet ${}^3S_1$ and the ${}^1S_0$ two-nucleon states. We have to diagonalize Eq(8.7) to find the minimum eigenstate and eigenvalue.

We choose a discretized momentum basis set consistent with the lattice regularization. We need to take into account a finite number of basis elements so we choose the smallest momentum states. We consider up to 13 momentum states per dimension, i.e. up to 2197 total states for ${}^1S_0$ and 6591 for ${}^3S_1$. At first we compute all the matrix elements between these states, both for ${}^3S_1$ and ${}^1S_0$. Then we choose to use the Lanczos algorithm to numerically diagonalize the matrix to find the lowest energy solution.

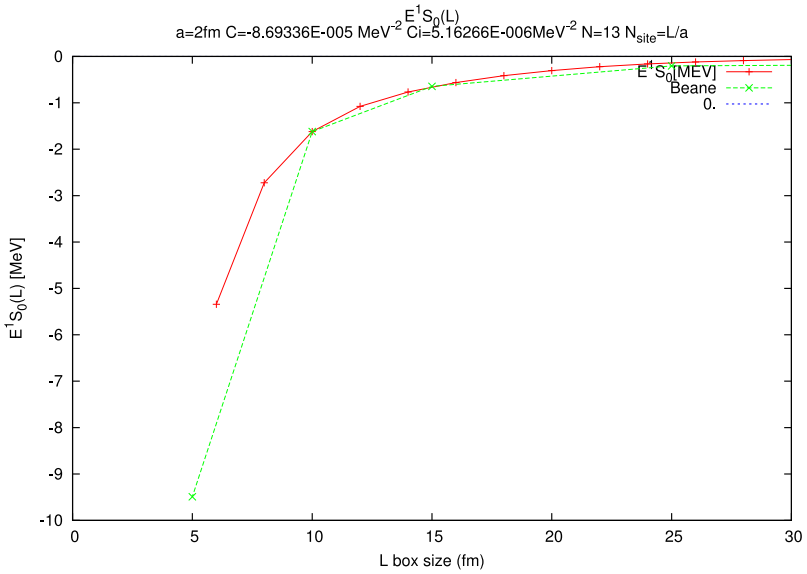

Figure 8.1: Plot of exact diagonalization results(red) compared to the results of Beane et al.(green) for the ${}^1S_0$ state. Results are in good agreement, but for the smallest box size. A possible reason is that EFT is not so accurate to describe a 2–neutron system in a so small box.

As in the previous chapter, we have to fix the coefficients C and C_I of the contact terms. The energy levels of the two nucleon system in a box is known from [BBPnS04]. In this work Beane et al. compute the corrections due to the finite size effects and periodic boundary conditions of the two nucleon system. So we fix this coefficients in a way to reproduce the data of Beane for the previously defined lattice, i.e. with $a = 2$ fm and $L = 10$ fm. Finally we obtain

$$C = -8.69 \cdot 10^{-5} \text{MeV}^{-2} \tag{8.8}$$

$$C_I = 5.16 \cdot 10^{-6} \text{MeV}^{-2} \tag{8.9}$$

We check our calculations with that of Beane, studying the dependence of the ground state energy on the size of the box L (as shown in Fig. 8.2 and Fig. 8.1) and making sure to have reached the convergence in the number of basis elements considered for the diagonalization. This last result is shown in Fig. 8.3 where N indicates the number of momentum elements considered for each dimension.

8.3 Another AFDMC attempt

With the previous diagonalization method we have determined the two effective parameters and also the nucleon potential derived from our EFT. Now we can use these information to do several things:

- Use the AFDMC with the potential that we have obtained. This is not

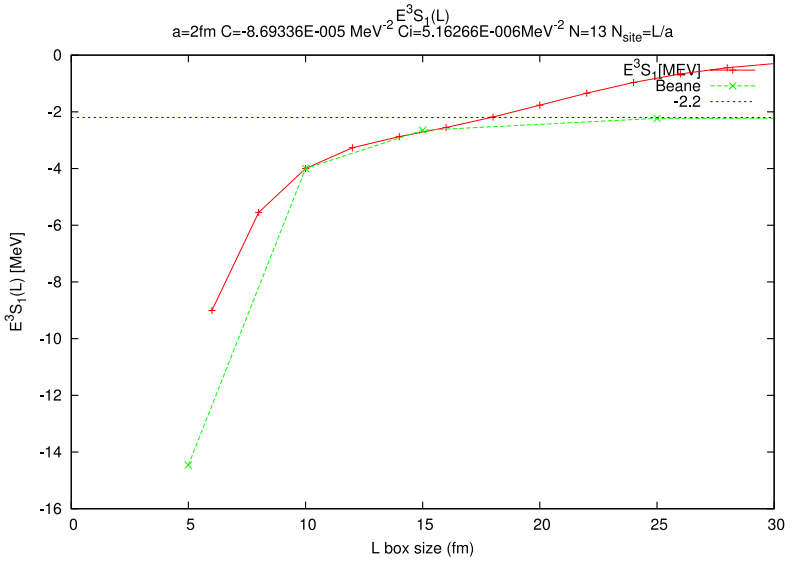

Figure 8.2: Plot of exact diagonalization results(red) compared to the results of Beane et al.(green) for the ${}^3S_1$ state. A good agreement with Beane's calculations is found up to box with size $L \simeq 17$ fm. Disagreements for larger L are due to the too few number of states considered to diagonalize the Hamiltonian, i.e. using a basis cut to $N = 13$ the convergence $N \to \infty$ is not reached for box larger than $L = 17$ fm.

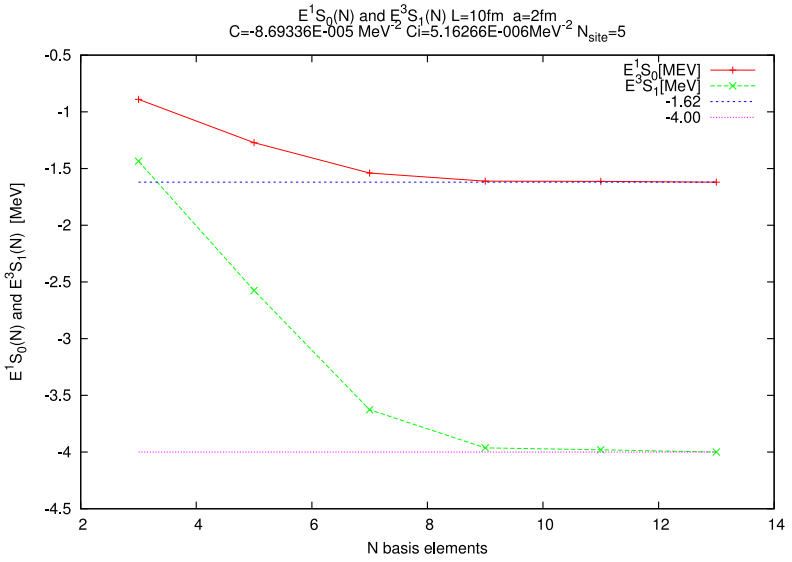

Figure 8.3: Convergence of the binding energy for both ${}^1S_0$ than ${}^3S_1$ states as function of the considered number of basis elements. We assume a box large $L = 10$ fm with a lattice of size $a = 2$ fm. The convergence is reached using $N \geq 9$ basis elements.

useful and without any interest. In fact we have obtained a poor potential that has nothing more than a standard phenomenological one. We do not have any dynamic correlation inside. Moreover there is a bias related to the presence of the lattice, of it is symmetry and of the finite size and boundary conditions of the box. We cannot learn nothing new about the physic system or the interaction.

- Use the AFDMC EFT approach like in the previous chapter, i.e. using instead of the potential the Hamiltonian with the explicit presence of the pion fields. From the physical point of view we do not have any improvement respect to the previous point. From a technical point of view, it could be interesting to see how the auxiliary fields of AFDMC are directly related to the pion fields.

- Use the previous used diagonalization method to study other nuclei. This is not possible because of the exponential explosion of the number of state to be considered, i.e. of the matrix size to be diagonalized.

- As said before we can hope that the coefficients C and C_I so determined are not so far from that one of the Hamiltonian that includes the $\partial_0\pi$ terms in H_π, i.e. without the approximation of instantaneous pions. So we tried to compute with the method explained in the previous chapter the binding energy of ^{4}He system; we obtain a too deep binding energy (~ 125MeV). We tried also the 2–nucleon $^1S_0$ and $^3S_1$ states finding again the already discussed AFDMC instability of these two systems.

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Part III

Hypernuclei

Chapter 9

Introduction

In this part of the thesis we want to use our AFDMC knowledge to solve the ground state of hypernuclei. We plan also to perform a calculation for neutron matter in the presence of hyperons. In this chapter we summarize the knowledge and the experimental and theoretical interest to hypernuclear systems.

9.1 Hyperons and hypernuclei

Hyperons are barion with non zero strangeness. In table Tab. 9.1 we show all the hyperon types and their principal properties. As we can see they have

Hyperon	Composition	Mass [MeV]	Lifetime [s]	Decay modes
Λ	uds	1115.683(6)	$2.60 \cdot 10^{-10}$	$p_+ + \pi_-$, $n + \pi_-$
Σ_+	uus	1189.37(0.7)	$8.018 \cdot 10^{-11}$	$p_+ + \pi_0$, $n + \pi_+$
Σ_0	uds	1192.642(24)	$7.4 \cdot 10^{-20}$	$\Lambda + \gamma$
Σ_-	dds	1197.449(30)	$1.479 \cdot 10^{-10}$	$n + \pi_-$
Ξ_0	uss	1314.83(20)	$2.90 \cdot 10^{-10}$	$\Lambda + \pi_0$
Ξ_-	dss	1321.31(13)	$1.639 \cdot 10^{-10}$	$\Lambda + \pi_-$
Ω_-	sss	1672.45(29)	$8.21 \cdot 10^{-11}$	$\Lambda + K_-$, $\Xi_0 + \pi_-$
				$\Xi_- + \pi_0$

Table 9.1: Hyperon types and properties[ADA$^+$08].

a mass quite bigger than a nucleon and a lifetime characteristic of a weak decay. We want to study systems made up by hyperons and nucleons, so we are interested to known the interaction between hyperons themselves and hyperons and nucleons. In presence of accurate experimental results on nucleon–hyperon scattering it would be possible to build an accurate interaction, as it was done in the nucleon–nucleon case. However, because of the so short lifetime of hyperons, it is not possible to have accurate and sufficiently intense beams to do perform

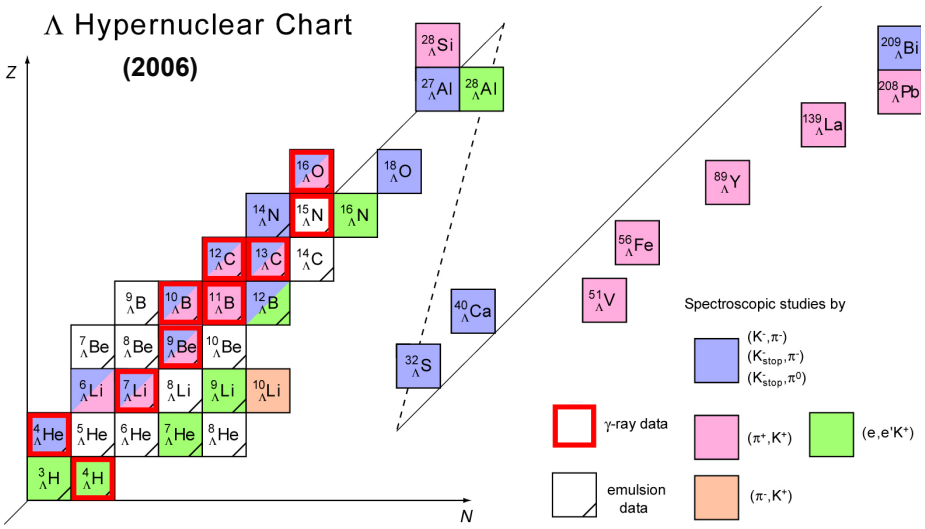

Figure 9.1: Hypernuclear chart as from [HT06]. In this table are shown the known single–Λ–hypernuclei and the available experiment measures. Moreover we know also 3 double–Λ–hypernuclei.

such experiments. The only data available so far are a few cross section data. Best experimental data about hyperons came from hypernuclei, i.e. from the study of nuclei including one or more hyperons. As we can see from the hypernuclear chart Fig. 9.1, about ~ 40 hypernuclei including a single Λ hyperon and only 3 double–Λ–hypernuclei been measured. Experimentally hypernuclei are produced exciting one nucleon to an hyperon. Hypernuclei have more or less the same lifetime of the single hyperon and therefore they are instable systems that decay in about 10^{-10}s. We substantially know only Λ–hypernuclei because the Λ hyperon is the lightest one.

9.2 History and experiments

Because of the previously explained properties of hyperons at present the only way to study the hyperon–hyperon and hyperon–nucleon interaction is related to the study of hypernuclei.

Hypernuclei were discovered in 1953. From that year Λ–hypernuclei were systematically studied with the available experimental technology. Until 1970's only experiments using emulsion plates were possible. So only the ground state of light Λ–hypernuclei ($A \leq 16$) were measured from their weak decays.

In the early 1970's with the availability of a K^- beam at CERN and later at Brookhaven National Laboratory (BNL), it became possible to do accurate spectroscopy experiments also for excited states. In that case reaction (K^-, π^-) was used. Also γ–ray hypernuclear spectroscopy started to be developed.

In the mid–1980's it was possible to have such an accurate and high energy

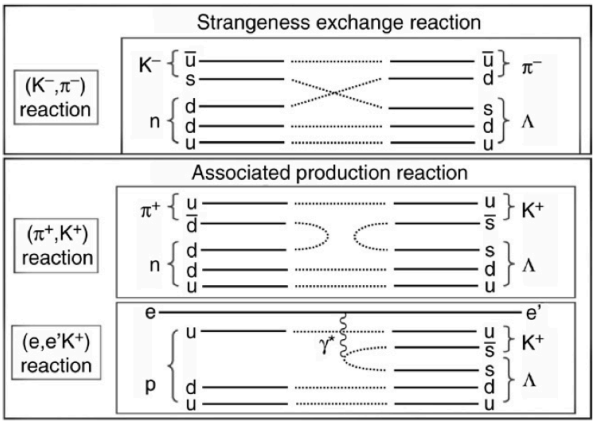

Figure 9.2: Schematic representation of three strangeness production reactions used to study hypernuclei. Figure from [HT06].

π^+ beam at the alternating gradient synchrotron (AGS) of BNL to make also possible to use the (π^+, K^+) reaction. Later on, the same process it was used also at the proton synchrotron (PS) of the High Energy Accelerator Organization (KEK) in Japan, where the superconducting kaon spectrometer (SKS) played a role in exploring Λ–hypernuclear spectroscopy. γ–ray spectroscopy developed reaching unprecedented resolution through the use of a germanium detector array called Hyperball and the high–quality and high–intensity electron beams available at the Thomas Jefferson National Accelerator Facility (JLab), USA. They permitted the first successful $(e, e'K^+)$ hypernuclear spectroscopy measurement. Today new experiments in these direction have been proposed, for example within the FINUDA project at DAΦNE facility, Frascati, Italy, and at the Japan Proton Accelerator Research Complex (J–PARC), where a new high–intensity proton synchrotron and a new better Hyperball are under construction.

Reaction spectroscopy is based on three typical strangeness reactions (K^-, π^-), (π^+, K^+) and $(e, e'K^+)$ which can excite a nucleon in the target to a Λ hyperon through the exchange of a couple s–d quark in the case of (K^-, π^-) or the creation of a s–$\bar{s}$ pair for the others, as shown in Fig. 9.2. The excellent resolution achieved using Hyperball detector is essential to resolving each member of the doublet in the hypernuclear fine structure: precise measures of the energies of various hypernuclear levels obtained by γ–ray spectroscopy allow the study of ΛN interaction in much grater detail. In particular, the spin–dependent interactions, the ΛN–ΣN coupling interaction in connection with the three–body ΛNN interaction, can be investigated.

Because of this extensive experimental activity, a parallel theoretical and computational work is needed to explain or predict experimental results. Moreover as we will explain in (§ 9.4), the hyperon interaction is not well known. Therefore any direct comparison with experiments is still not only interesting and useful, but fundamental to study better hyperon systems.

9.3 Astrophysical interest

Hyperons play a very important role in astrophysics because of their importance in neutron stars structure. We briefly summarize and show why hyperons are so relevant, and what is interesting to compute, in a way to discriminate between different neutron star models. Our intent is not a complete and detailed description of this argument; for a more accurate description we remand to [HHPY07].

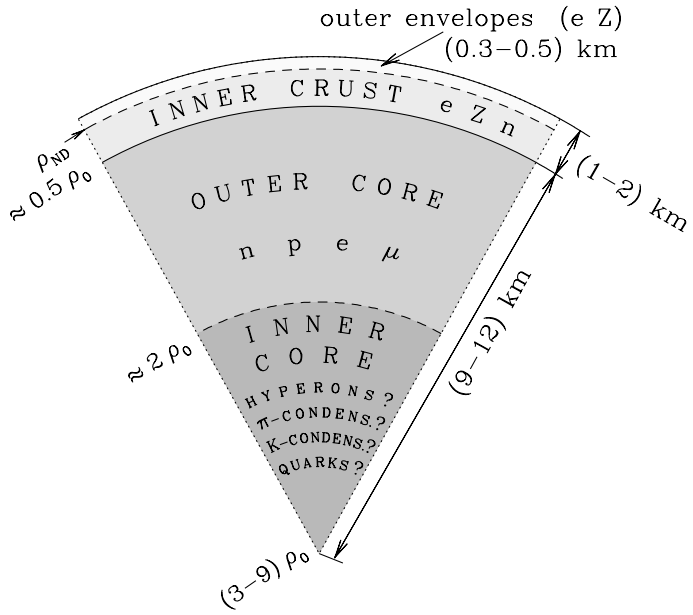

Figure 9.3: Schematic structure of a neutron star. Stellar parameter are model dependent. Figure from [HHPY07].

We can roughly describe a neutron star as a sequence of layers of matter of different densities, as shown in Fig. 9.3. While the knowledge of the atmosphere and of the crust is quite well established, we do not know anything certainly about the inner core. There are several models and hypothesis, but for densities bigger than $2\rho_0$, where $\rho_0 = 0.16\text{fm}^{-3}$ is the nuclear saturation density, we have very different possible scenarios: Fermion/Boson condensates such hyperons, a pion condensate, a kaon condensate or even an uniform quark matter. All these possible pictures strictly depend on the details of the hadron–hadron interaction scheme assumed. It is therefore difficult to discriminate among them because of the lack in experimental data. The hypothesis that we want to test by means of AFDMC methods is that at densities $2\rho_0 < \rho < 3\rho_0$, Σ_- hyperons become stable in the uniform matter, contributing to the moderate softening in the equation of state that seems necessary to fit the constraints determined by astrophysical observations. Bruckner Hartree Fock (BHF) calculations, like that in Fig. 9.4 [HHPY07], suggest that hyperons are indeed important to determine the equation of state. At smaller densities we have the presence of only Σ_- hyperons, at

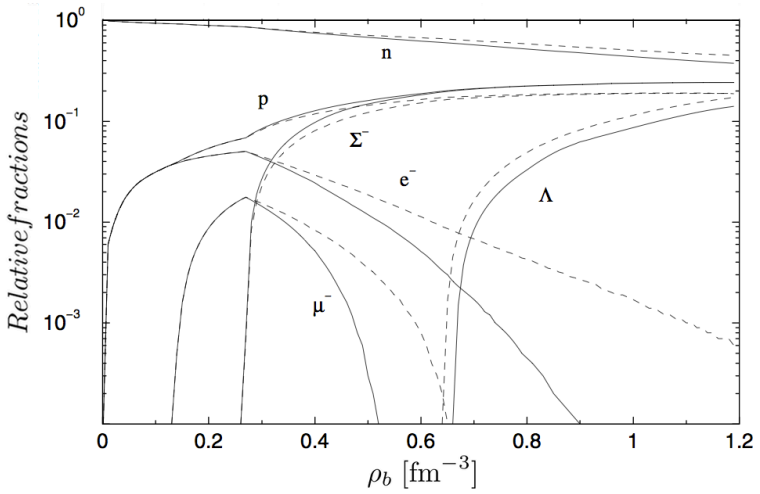

Figure 9.4: Relative fraction of different particles in a neutron star, as a function of the core density. From [HHPY07], obtained from a BHF calculation with the NSC97e potential.

higher ones also Λ hyperons become present. As clear from Fig. 9.5 an accurate knowledge of the EOS including hyperons could be very important to compare different models and astrophysical observations. From the figure we can also see how poor is our knowledge of nucleon and nucleon–hyperon interaction. In fact, using different potentials (with or without hyperons) very different results are obtained, for instance in the estimate of radii or masses of neutron stars. The problem is not just related to the potential or to the model of the neutron star. It is also very important to verify the accuracy of the calculations that we use to derive the EOS. In the case of the cited BHF ones, for example, all the three body correlations are neglected. As we can see in a while, for the Nijmegen nucleon–hyperon potential used, it is crucial to include also these correlations. We could conclude asserting that we are able to improve the previous calculations only when we can stronger constraint the interaction and use an accurate computational method.

9.4 Hyperon potentials

From experiments we only know a few hyperon–nucleon cross sections and the ground state energy or some excited states of single Λ hypernuclei. Because of that the knowledge relative to the hyperon potential is mainly related to the interaction between the Λ hyperon and nucleons. Moreover, it is not so easy to extract accurate microscopic information about the hyperon–nucleon potential from hypernuclei because of the presence of many–body effects. Because of that, at present only three interaction types are present:

Phenomenological interaction. It is mainly used with shell model calcula-

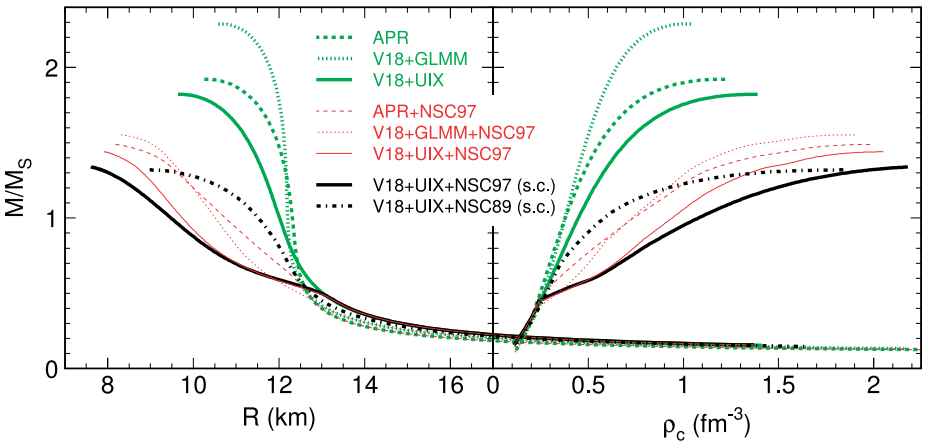

Figure 9.5: Mass of neutron star as function of it is radius (left) and central density (right) for different potentials, with and without hyperons. From BHF calculations [SVn06].

tion. It is written in a form like

$$V_{\Lambda N}(r) = V_0(r) + V_\sigma(r)\sigma_\Lambda\sigma_N + V_\Lambda(r)l_{\Lambda N}\sigma_\Lambda + V_N(r)l_{\Lambda N}\sigma_N + V_T(r)S_{12} \tag{9.1}$$

with

$$S_{12} = 3(\sigma_\Lambda\hat{r})(\sigma_N\hat{r}) - \sigma_\Lambda\sigma_N \tag{9.2}$$

The interaction is described by a two body effective force containing a central term, a spin dependent term, other two terms depending on the relative angular momentum and a last one tensor term. This is the interaction used in shell model calculations[Hiy09, Hiy08, HKM$^+$98, HKM$^+$96, HKYM10, HY09, HYRM06] giving results in excellent agreement with experimental data, with a very high accuracy. However, we cannot conclude that the interaction is known. In fact because of the shell model used in calculations, all the many body effects are hidden in appropriate effective potentials that describe the interaction between different clusters.

Usmani potential. It is a phenomenological potential[Bod84, UBS08] derived in the same way as the Argonne nuclear potential. It is built taking into account different diagrammatic contributions, mainly due to pion exchange. Like explained in the next section, it contains two–body ΛN terms and also three–body ΛNN terms. These three body terms are very important because describe effectively the excitation of the Λ hyperon to a Σ hyperon, in the same way as three body NNN Urbana potential terms describe the possibility of exciting one nucleon to a Δ. However because of the smaller mass difference between Λ and Σ respect to the difference between the nucleon and Δ masses, we have that the inclusion of the ΛNN term is fundamental and not simply a small correction to the two–body ΛN term.

Nijmegen potential. It is based on a theoretical $SU(3)$ model[NRdS77, Tak80, Hal99, Hal00]. Because of that it describes the interaction between all the

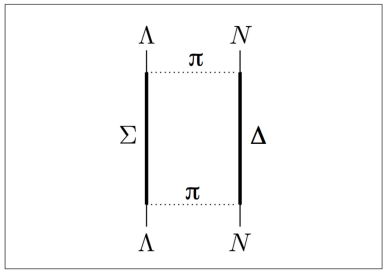

Figure 9.6: Two pion exchange term

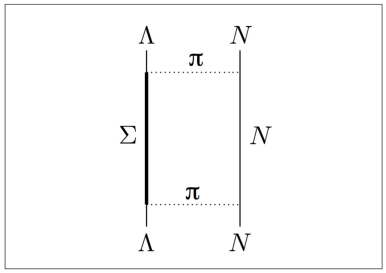

Figure 9.7: Two pion exchange term

hyperons themselves, and not only those between nucleons and hyperons or one hyperon species. Hence, it is the most widespread used interaction. However, several different parametrizations of this potential exist and all of them are far to reach the accuracy of the previous potential results. Without describing the potential in detail, we want to underline that because of the inclusion of all the hyperon types the potential contains only two–body terms. The exciting of a Λ hyperon to a Σ, which description requires the use of a three body term in the previous approach, can be described directly taking into account a two body force but including also the Σ hyperon in the calculation.

In our work, we chose to use the Usmani potential.

9.5 Usmani potential

The Usmani interaction includes a short range Wood–Saxon potential that describes effectively all the short–range, high energy behaviors. The long range part is described by meson exchange terms. So we can take into account the diagrams in figure Fig. 9.8, Fig. 9.6 and Fig. 9.7, i.e. a one–kaon exchange and two–pions exchange graphs. Clearly a one–pion exchanged is denied. The kaon exchange term is substantially canceled by the correspondent anti-kaon exchange term. So the main part of the two body interaction will be described by the two–pion exchange process. Now we can write the two body term of the

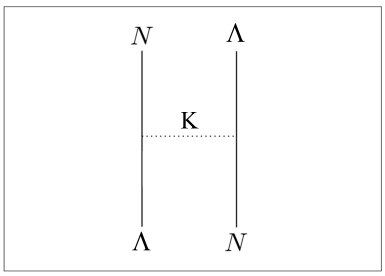

Figure 9.8: One kaon exchange

ΛN potential as

$$V_{\Lambda N}(r) = v_0(r) + v_0(r)\varepsilon(P_x - 1) + (v_\sigma/4)T_\pi^2(m_\pi r)\boldsymbol{\sigma}_\Lambda \cdot \boldsymbol{\sigma}_N, \tag{9.3}$$

where the term v_0 is the direct ΛN term, i.e. the repulsive Woods–Saxon potential v_c plus the two–pions attractive one

$$v_0(r) = v_c(r) + v_{2\pi}(r), \tag{9.4}$$

plus the spin dependent two–pions exchange term. We use these definitions

$$v_c(r) = W_c/[1 + \exp\{(r - R)/a\}] \tag{9.5}$$

$$v_{2\pi} = \overline{v}T_\pi^2(m_\pi r), \tag{9.6}$$

$$\overline{v} = (v_s + 3v_t)/4, \tag{9.7}$$

$$v_\sigma = v_s - v_t, \tag{9.8}$$

$$T_\pi(x) = \left(1 + \frac{3}{x} + \frac{3}{x^2}\right)\frac{e^{-x}}{x}\xi_T(r), \tag{9.9}$$

and this regularization cut–off:

$$\xi_Y(r) = \xi_T^{1/2}(r) = \left(1 - e^{-cr^2}\right). \tag{9.10}$$

The second term of the interaction is a space–exchange term potential, where P_x is the exchange operator, defined as $P_x = (-1)^l$ with l is the momentum eigenvalue of the nucleon–hyperon pair. This term is added to explicitly include parity violation. Althogh there is a clear experimental evidence for this effect, it has not well quantitatively fixed yet. The source of this term is simply the kaon exchange term of figure Fig. 9.8. I guess that it might be a reasonable improvement in the accuracy of the potential, directly including the one kaon exchange term in Fig. 9.8, even if quite small. With the previous description of the parity violation term we are instead using for the potential a shape characteristic of the two–pion exchange rather than that of the kaon exchange. Explicitly including the one kaon exchange we would also be to introduce tensor terms just in the two body sector of the interaction. This could be an interesting and useful study.
Now we have to take into account also the possibility to excite a Λ hyperon

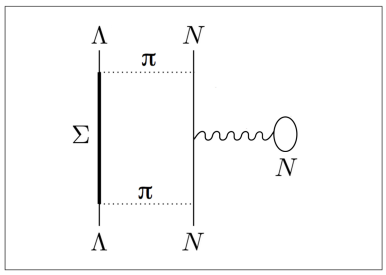

Figure 9.9: Two pion exchange, dispersive term.

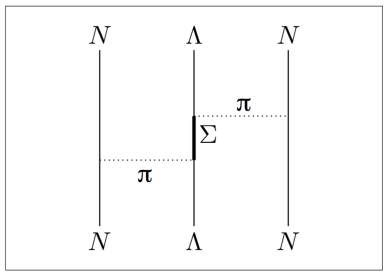

Figure 9.10: Two pion exchange, P wave term.

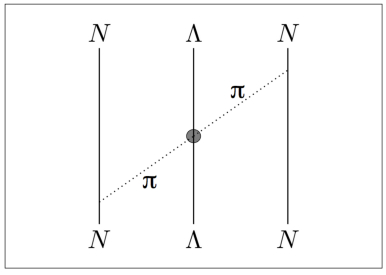

Figure 9.11: Two pion exchange, S wave term.

Constant	Value	
W_c	2137	MeV
R	0.5	fm
a	0.2	fm
ε	$0.1 \div 0.38$	
$\overline{v}$	6.15(5)	MeV
v_σ	0.24(5)	MeV
c	2.0	fm^-1
W^D	$0.01 \div 0.1$	MeV
C^P	$0.4 \div 2.0$	MeV
C^S	$1 \div 2$	MeV

Table 9.2: Parameters of the $N\Lambda$ potential used in AFDMC calculations.

to a Σ one. Like explained previously it is very important to include also this term into the potential because of the small mass differences between the two hyperons.

So considering the diagrams in figure we can write a three body force like

$$V_{\Lambda ij} = V^D_{\Lambda ij} + V^{2\pi}_{\Lambda ij}, \tag{9.11}$$

where $V^D_{\Lambda ij}$ is relative to the two pion dispersive term of graph Fig. 9.9:

$$V^D_{\Lambda ij} = W^D T^2_\pi(m_\pi r_{\Lambda i}) T^2_\pi(m_\pi r_{\Lambda j})[1 + \boldsymbol{\sigma}_\Lambda \cdot (\boldsymbol{\sigma}_i + \boldsymbol{\sigma}_j)/6], \tag{9.12}$$

while $V^{2\pi}_{\Lambda ij}$

$$V^{2\pi}_{\Lambda ij} = V^P_{\Lambda ij} + V^S_{\Lambda ij}, \tag{9.13}$$

is the sum of the S–wave (Fig. 9.11) and P–wave (Fig. 9.10) two pion exchange terms

$$V^P_{\Lambda ij} = -\left(C^P/6\right)(\boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j)\{X_{i\Lambda}, X_{\Lambda j}\}, \tag{9.14}$$

$$V^S_{\Lambda ij} = C^S Z(m_\pi r_{i\Lambda}) Z(m_\pi r_{j\Lambda}) \boldsymbol{\sigma}_i \cdot \hat{\mathbf{r}}_{i\Lambda} \boldsymbol{\sigma}_j \cdot \hat{\mathbf{r}}_{j\Lambda} \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j, \tag{9.15}$$

with:

$$X_{\Lambda i} = (\boldsymbol{\sigma}_\Lambda \cdot \boldsymbol{\sigma}_i) Y_\pi(m_\pi r_{\Lambda i}) + S_{\Lambda i} T_\pi(m_\pi r_{\Lambda i}), \tag{9.16}$$

$$Z(x) = \frac{x}{3}[Y_\pi(x) - T_\pi(x)], \tag{9.17}$$

$$Y_\pi(x) = \frac{e^{-x}}{x}\xi_Y(r), \tag{9.18}$$

$$S_{\Lambda i} = 3(\boldsymbol{\sigma}_\Lambda \cdot \hat{\boldsymbol{r}}_{\Lambda i})(\boldsymbol{\sigma}_i \cdot \hat{\boldsymbol{r}}_{\Lambda i}) - \boldsymbol{\sigma}_\Lambda \boldsymbol{\sigma}_i. \tag{9.19}$$

Summarizing, the full nucleon-hyperon interaction, assuming $A_\Lambda = 1$, has the following form:

$$H_{\Lambda N} = \sum_i^{A_N} V_{\Lambda i} + \sum_{i<j}^{A_N} V_{\Lambda ij}. \tag{9.20}$$

Now we need to determine the parameters of the potential like in table Tab. 9.2. As we can see from the values in the table, cross section data fix reasonably well the two body terms except for the exchange term coefficient ε. But for coefficients relative to the three body potential we can fix only their range with theoretical considerations related to the $SU(3)$ approximate symmetry. Then they could be well fixed reproducing the binding energies of some hypernuclei. This work was performed several times from Usmani et al., but because of the use of different nucleon–nucleon potentials or because of the perturbative inclusion of the exchange term, they never use the same parameters. So before using this potential we have to fit the three body parameters.

Chapter 10

AFDMC for Hypernuclei

In the previous chapter we summarized the physics and the present status of the knowledge relative to hypernuclei. It would be of high interest to compute an accurate EOS with hyperons to be used for neutron star models. However we have seen that at present there is no definite knowledge of the nucleon–hyperon interaction, nor an accurate theoretical framework is available to determine it only from experimental data. Before trying to solve this problem we want to verify the accuracy of the potential used and of the proposed AFDMC method that we want to use. So we focus on the study of hypernuclear systems, to be able to compare directly our calculations with the available experimental results.
We choose the AFDMC method and so we take into account only the ground states of hypernuclei. Now we proceed with clarifying some details needed to implement the AFDMC algorithm before to report the results.

10.1 Conventions and assumptions

We use the following conventions:

- A_Λ is the number of hyperons (we assume $A_\Lambda = 1$);
- A_N is the number of nucleons;
- $A = A_\Lambda + A_N$ is the number of nucleons plus hyperons;
- indexes with Greek letters are referred to hyperons;
- indexes with Latin letters are referred to nucleons.

The Hamiltonian used is

$$H = H_N + H_{\Lambda N} + H_\Lambda, \tag{10.1}$$

where H_N is the nucleon Hamiltonian term, i.e. nucleon kinetic term plus a standard Argonne Av_6' nucleon–nucleon potential. For more details about this interaction we refer to [WSS95, WP02]. The H_Λ is the pure hyperon Hamiltonian term. In the case of $A_\Lambda = 1$ it is simply the Λ kinetic term. The other $H_{\Lambda N}$ term is the ΛN potential term like defined in Eq(9.20).

10.2 Trial wavefunction

We assume the following ansatz for the wavefunction:

$$\psi = J_{\Lambda n} J_{nn} \mathrm{Det}_\Lambda \mathrm{Det}_n, \tag{10.2}$$

where $J_{\Lambda n}$ is a nucleon–hyperon central Jastrow factor, J_{nn} the nucleon–nucleon one, Det_Λ a Slater determinant of single Λ wavefunctions, and Det_n Slater determinant of single nucleon wavefunctions. For the single nucleon wavefunctions we use spherical harmonics and radial orbitals obtained by an Hartree Fock calculation with Skyrme interaction. We use the same form for the hyperon orbitals. The central Jastrow correlations are determined solving the two body problem with the central part of the nucleon–nucleon and nucleon–hyperon potential. The single nucleon spin/isospin state is simply a four–dimensional spinor; the hyperon Λ has the only spin 1/2 degrees of freedom and so the spin state is represented only by a two–dimensional spinor. With these assumptions we consider the hyperon and nucleons as distinct particles. It is very important to notice that in this way we are not able to include the exchange term in the AFDMC propagator, because it mixes nucleon and hyperon states. We will dedicate a section to discuss this problem in details.

10.3 Center of mass correction terms

In order to have a simple form for of the wavefunction that is an eigenstate of J, we define single particle orbitals with respect to the center of mass of the hypernucleus. To study finite size systems we also have to remove from the Hamiltonian the kinetic term relative to the center of mass. Hence, we see the details for a system with different mass particles like an hypernucleus. Calling ρ_i the relative coordinates and r_i the absolute ones, we have:

$$\rho_i = r_i - \sum_j \frac{r_j m_j}{M}, \qquad \rho_{cm} = \sum_j \frac{r_j m_j}{M}, \qquad M = \sum_i m_i, \tag{10.3}$$

$$\frac{\partial \rho_i}{\partial r_i} = \delta_{ij} - \frac{m_j}{M}, \tag{10.4}$$

$$\frac{\partial}{\partial r_i} \quad f(\rho_1 ... \rho_N) = \left[\frac{\partial}{\partial \rho_i} - \frac{m_i}{M} \sum_j \frac{\partial}{\partial \rho_j} \right] \quad f(\rho_1 ... \rho_N). \tag{10.5}$$

If $f(\rho_1 ... \rho_N)$ is a Slater determinant, the previous can be efficiently computed using Eq(10.17).

$$\frac{\partial^2}{\partial r_i^2} f(\rho_1 ... \rho_N) = \left[\frac{\partial^2}{\partial \rho_i^2} - 2\frac{m_i}{M} \sum_j \frac{\partial^2}{\partial \rho_i \partial \rho_j} + \frac{m_i^2}{M^2} \sum_{jk} \frac{\partial^2}{\partial \rho_k \partial \rho_j} \right] f(\rho_1 ... \rho_N). \tag{10.6}$$

Clearly because of the independence of $f(\rho_1 ... \rho_N)$ from ρ_{cm} we have that the center of mass kinetic contribution is vanishing:

$$\left(\sum_i \frac{\partial}{\partial r_i} \right)^2 \quad f(\rho_1 ... \rho_N) = 0 \tag{10.7}$$

From Eq(10.6) we derive the following expression that can be efficiently computed using Eq(10.17), Eq(10.25) and (10.26):

$$\begin{aligned}\frac{\partial^2}{\partial r_i^2}f(\rho_1...\rho_N) &= \left[\frac{\partial^2}{\partial\rho_i^2} - 2\frac{m_i}{M}\sum_j\frac{\partial^2}{\partial\rho_i\partial\rho_j} + \frac{m_i^2}{M^2}\sum_{jk}\frac{\partial^2}{\partial\rho_k\partial\rho_j}\right]f(\rho_1...\rho_N)\\ &= \left[\left(1-2\frac{m_i}{M}\right)\frac{\partial^2}{\partial\rho_i^2} - 2\frac{m_i}{M}\sum_{j,j\neq i}\frac{\partial^2}{\partial\rho_i\partial\rho_j} + \right.\\ &\quad \left. +2\frac{m_i^2}{M^2}\sum_{j<k}\frac{\partial^2}{\partial\rho_k\partial\rho_j} + \frac{m_i^2}{M^2}\sum_j\frac{\partial^2}{\partial\rho_j^2}\right]f(\rho_1...\rho_N);\end{aligned} \tag{10.8}$$

$$\begin{aligned}\sum_i\frac{\partial^2}{\partial r_i^2}f(\rho_1...\rho_N) &= \left[\sum_i\frac{\partial^2}{\partial\rho_i^2} - 2\sum_{ij}\frac{m_i}{M}\frac{\partial^2}{\partial\rho_i\partial\rho_j} + \right.\\ &\quad \left. +\sum_i\frac{m_i^2}{M^2}\sum_{jk}\frac{\partial^2}{\partial\rho_k\partial\rho_j}\right]f(\rho_1...\rho_N) =\\ &= \left[\sum_i\frac{\partial^2}{\partial\rho_i^2} + \sum_{ij}\frac{\partial^2}{\partial\rho_i\partial\rho_j}\left(-2\frac{m_i}{M} + \sum_k\frac{m_k^2}{M^2}\right)\right]f(\rho_1...\rho_N)\\ &= \left[\sum_i\left(1-2\frac{m_i}{M} + \sum_k\frac{m_k^2}{M^2}\right)\frac{\partial^2}{\partial\rho_i^2} + \right.\\ &\quad \left. +2\sum_{i<j}\left(-2\frac{m_i}{M} + \sum_k\frac{m_k^2}{M^2}\right)\frac{\partial^2}{\partial\rho_i\partial\rho_j}\right]f(\rho_1...\rho_N).\end{aligned} \tag{10.9}$$

We apply the previous formula to compute the derivative of the trial wavefunction defined in Eq(10.2)

$$\partial_\Lambda\psi = \psi\left(\frac{\partial_\Lambda J_{\Lambda n}}{J_{\Lambda n}} + \frac{\partial_\Lambda \mathrm{Det}_\Lambda}{\mathrm{Det}_\Lambda}\right); \tag{10.10}$$

$$\partial_n\psi = \psi\left(\frac{\partial_n J_{\Lambda n}}{J_{\Lambda n}} + \frac{\partial_n J_{nn}}{J_{nn}} + \frac{\partial_n \mathrm{Det}_n}{\mathrm{Det}_n}\right); \tag{10.11}$$

$$\begin{aligned}\partial_\Lambda\partial_n\psi = \psi \quad &\left[\left(\frac{\partial_\Lambda J_{\Lambda n}}{J_{\Lambda n}} + \frac{\partial_\Lambda \mathrm{Det}_\Lambda}{\mathrm{Det}_\Lambda}\right)\left(\frac{\partial_n J_{\Lambda n}}{J_{\Lambda n}} + \frac{\partial_n J_{nn}}{J_{nn}} + \frac{\partial_n \mathrm{Det}_n}{\mathrm{Det}_n}\right)\right.\\ &\left. + \left(\frac{\partial_\Lambda\partial_n J_{\Lambda n}}{J_{\Lambda n}} - \frac{\partial_n J_{\Lambda n}}{J_{\Lambda n}}\frac{\partial_\Lambda J_{\Lambda n}}{J_{\Lambda n}}\right)\right];\end{aligned} \tag{10.12}$$

$$\begin{aligned}\partial_n^2\psi = \psi\left[\frac{\partial_n^2 J_{nn}}{J_{nn}} + \frac{\partial_n^2 J_{\Lambda n}}{J_{\Lambda n}}\frac{\partial_n^2 \mathrm{Det}_n}{\mathrm{Det}_n} + 2\frac{\partial_n J_{nn}}{J_{nn}}\frac{\partial_n J_{\Lambda n}}{J_{\Lambda n}} + \right.\\ \left. +2\frac{\partial_n J_{nn}}{J_{nn}}\frac{\partial_n \mathrm{Det}_n}{\mathrm{Det}_n} + 2\frac{\partial_n J_{\Lambda n}}{J_{\Lambda n}}\frac{\partial_n \mathrm{Det}_n}{\mathrm{Det}_n}\right];\end{aligned} \tag{10.13}$$

$$\partial_\Lambda^2\psi = \psi\left[\frac{\partial_\Lambda^2 J_{n\Lambda}}{J_{n\Lambda}} + \frac{\partial_\Lambda^2 \mathrm{Det}_\Lambda}{\mathrm{Det}_\Lambda} + 2\frac{\partial_\Lambda J_{\Lambda n}}{J_{\Lambda n}}\frac{\partial_\Lambda \mathrm{Det}_\Lambda}{\mathrm{Det}_\Lambda}\right]. \tag{10.14}$$

10.4 Derivative of Slater Determinant

In this section we describe how to compute in an efficient way the derivative of a Slater determinant. This is very important to have a good efficiency for the AFDMC algorithm. Moreover we want to stress that this technique can be generalized to compute any one–body operator or product of two one–body operators applied to a Slater determinant; so we use this trick in our AFDMC to compute efficiently any two–body expectation value.
Define the Slater determinant $A_{ij} = f_i(j)$ so that $\partial_j A_{ij} = f_i'(j)$. ${}^iB$ is a matrix equal to A but with column i replaced by derivative of f: ${}^iB_{ki} = f_k'(i)$, and ${}^iB_{kj} = f_k(j)$ for $j \neq i$. Considering the trivial identity

$$|Q| = |Q| \sum_i Q_{ij} Q^{-1}_{ji} = \sum_i Q_{ij} (Q^{-1}_{ji} |Q|), \tag{10.15}$$

and at the following relation

$$(Q^{-1}_{ji}|Q|) = (-1)^{i+j} |\mathrm{Minor}_{(ij)}|, \tag{10.16}$$

the cofactor $|\mathrm{Minor}_{(ij)}|$ is, by definition, j–independent. So for a derivative of Slater determinant follows that

$$\partial_j |A| = |A| \sum_i A^{-1}_{ji} (\partial_j A_{ij}) = |A| \sum_i A^{-1}_{ji} f_i'(j), \tag{10.17}$$

but we have also that $|{}^jB| = \partial_j |A|$ from which:

$$|{}^jB| = |A| \sum_i A^{-1}_{ji} f_i'(j). \tag{10.18}$$

Using Eq(10.17) for $|{}^iB|$, now we try to compute

$$\partial_j \partial_i |A| = \partial_j |{}^iB| = |{}^iB| \sum_k ({}^iB)^{-1}_{jk} (\partial_j {}^iB_{kj}). \tag{10.19}$$

Choosing $i \neq j$ we have that $(\partial_j {}^iB_{kj}) = (\partial_j A_{kj}) = f_k'(j)$. Using Eq(10.18) we rewrite the previous equation

$$\partial_j \partial_i |A| = \left(\sum_k f_k'(j) \quad ({}^iB)^{-1}_{jk} \right) \left(\sum_k f_k'(i) A^{-1}_{ik} \right) |A| \tag{10.20}$$

Now we use the Sherman–Morrison Formula to compute $({}^iB)^{-1}$:

$$(A + u \otimes v)^{-1} = A^{-1} - \frac{(A^{-1} \cdot u) \otimes (v \cdot A^{-1})}{1 + v \cdot A^{-1} \cdot u}, \tag{10.21}$$

with u, v vectors. To have that $(A + u \otimes v) = {}^iB$, we choose for u:

$$u_k = f_k'(i) - f_k(i), \tag{10.22}$$

and for v: $v_k = 0$ except for $k = i$, with $v_i = 1$. So using Eq(10.21) we obtain

$$({}^iB)^{-1}_{kj} = A^{-1}_{jk} - A^{-1}_{ik} \frac{\left(\sum_k A^{-1}_{jk} f_k'(i)\right) - \left(\sum_k A^{-1}_{jk} f_k(i)\right)}{1 + \left(\sum_k A^{-1}_{ik} f_k'(i)\right) - \left(\sum_k A^{-1}_{ik} f_k(i)\right)}. \tag{10.23}$$

Remembering that $A_{ki} = f_k(i)$ and assuming $i \neq j$ we have

$$({}^iB)^{-1}_{kj} = A^{-1}_{jk} - A^{-1}_{ik} \frac{\left(\sum_k A^{-1}_{jk} f'_k(i)\right) - \cancelto{0}{\left(\sum_k A^{-1}_{jk} A_{ki}\right)}}{\cancel{1} + \left(\sum_k A^{-1}_{ik} f'_k(i)\right) - \cancel{\left(\sum_k A^{-1}_{ik} A_{ki}\right)}}. \tag{10.24}$$

So finally we obtain for $i \neq j$.

$$\begin{aligned} \partial_j \partial_i |A| = |A| \left(\sum_k f'_k(j) \quad A^{-1}_{jk} \right) \left(\sum_k f'_k(i) A^{-1}_{ik} \right) \\ -|A| \left(\sum_k f'_k(j) \quad A^{-1}_{ik} \right) \left(\sum_k f'_k(i) A^{-1}_{jk} \right). \end{aligned} \tag{10.25}$$

For $i = j$ we can use Eq(10.17), obtaining:

$$\partial^2_i |A| = |A| \sum_k A^{-1}_{ik} (\partial^2_j A_{ki}) = |A| \sum_k A^{-1}_{ik} f''_k(i). \tag{10.26}$$

10.5 Propagator for two–body hyperon–nucleon terms

We have to carefully apply the AFDMC propagator term relative to the $N\Lambda$ potential term, because we have to well understand how it operates on different nucleon and hyperon spaces. So considering the following propagator $\mathcal{P}$ (remember conventions of (§ 3.3) and that Greek letters are referred to hyperons and Latin ones to nucleons) we have:

$$\mathcal{P} = e^{-dt \sum_{i\alpha} V_{i\alpha} \hat{O}_i \otimes \hat{\theta}_\alpha} = \prod_{i\alpha} e^{-dt V_{i\alpha} \hat{O}_i \otimes \hat{\theta}_\alpha} + \mathcal{O}(dt^2). \tag{10.27}$$

But we want to rewrite the exponent as

$$\hat{O}_i \otimes \hat{\theta}_\alpha = \frac{1}{2} \left((\hat{O}_i \oplus \hat{\theta}_\alpha)^2 - (\hat{O}_i \otimes \hat{\mathbb{I}})^2 - (\hat{\mathbb{I}} \otimes \hat{\theta}_\alpha)^2 \right); \tag{10.28}$$

and, neglecting commutators of order $\mathcal{O}(dt^2)$, we have that:

$$\mathcal{P} \simeq \prod_{i\alpha} \left(e^{-dt V_{i\alpha} \frac{(\hat{O}_i \oplus \hat{\theta}_\alpha)^2}{2}} \cdot e^{dt V_{i\alpha} \frac{(\hat{O}_i \otimes \hat{\mathbb{I}})^2}{2}} \cdot e^{dt V_{i\alpha} \frac{(\hat{\mathbb{I}} \otimes \hat{\theta}_\alpha)^2}{2}} \right). \tag{10.29}$$

For the last relation we can use the Hubbard–Stratonovich transform (3.14):

$$\begin{aligned} \mathcal{P} \simeq & \prod_{i\alpha} \frac{1}{(2\pi)^{3/2}} \iiint dx\, dy\, dz\; e^{-\frac{x^2+y^2+z^2}{2}}\; e^{-x\sqrt{-dtV_{i\alpha}}(\hat{O}_i \oplus \hat{\theta}_\alpha)} \cdot \\ & \cdot\; e^{-y\sqrt{dtV_{i\alpha}}(\hat{O}_i \otimes \hat{\mathbb{I}})} \cdot e^{-z\sqrt{dtV_{i\alpha}}(\hat{\mathbb{I}} \otimes \hat{\theta}_\alpha)} \\ \simeq & \frac{1}{(2\pi)^{\frac{3(i\,\cdot\,\alpha)}{2}}} \iiint dx^{i\alpha}\, dy^{i\alpha}\, dz^{i\alpha}\; e^{-\frac{\sum_{i\alpha} x^2_{i\alpha} + y^2_{i\alpha} + z^2_{i\alpha}}{2}} \cdot \\ & \cdot \prod_{i\alpha} \left(e^{-x_{i\alpha}\sqrt{-dtV_{i\alpha}}(\hat{O}_i \oplus \hat{\theta}_\alpha)} \cdot\; e^{-y_{i\alpha}\sqrt{dtV_{i\alpha}}(\hat{O}_i \otimes \hat{\mathbb{I}})} \cdot e^{-z_{i\alpha}\sqrt{dtV_{i\alpha}}(\hat{\mathbb{I}} \otimes \hat{\theta}_\alpha)} \right) \end{aligned} \tag{10.30}$$

Now using the equation (3.24) we can rewrite the previous, up to terms $\mathcal{O}(dt^2)$, as

$$\begin{aligned}\mathcal{P} \simeq & \frac{1}{(2\pi)^{\frac{3(i\cdot\alpha)}{2}}} \iiint dx^{i\alpha}\, dy^{i\alpha}\, dz^{i\alpha}\; e^{-\frac{\sum_{i\alpha} x_{i\alpha}^2+y_{i\alpha}^2+z_{i\alpha}^2}{2}} \cdot \\ & \cdot e^{-\sum_{i\alpha} x_{i\alpha}\sqrt{-dtV_{i\alpha}}(\hat{O}_i\oplus\hat{\theta}_\alpha)+y_{i\alpha}\sqrt{dtV_{i\alpha}}(\hat{O}_i\otimes\hat{\mathbb{I}})+z_{i\alpha}\sqrt{dtV_{i\alpha}}(\hat{\mathbb{I}}\otimes\hat{\theta}_\alpha)}.\end{aligned} \tag{10.31}$$

But

$$(\hat{O}_i \oplus \hat{\theta}_\alpha) = (\hat{O}_i \otimes \hat{\mathbb{I}}) + (\hat{\mathbb{I}} \otimes \hat{\theta}_\alpha), \tag{10.32}$$

so we have that:

$$\begin{aligned}&\sum_{i\alpha} x_{i\alpha}\sqrt{-dtV_{i\alpha}}(\hat{O}_i \oplus \hat{\theta}_\alpha) + y_{i\alpha}\sqrt{dtV_{i\alpha}}(\hat{O}_i \otimes \hat{\mathbb{I}}) + z_{i\alpha}\sqrt{dtV_{i\alpha}}(\hat{\mathbb{I}} \otimes \hat{\theta}_\alpha) = \\ &= \sum_{i\alpha}(x_{i\alpha}\sqrt{-dtV_{i\alpha}} + y_{i\alpha}\sqrt{dtV_{i\alpha}})(\hat{O}_i \otimes \hat{\mathbb{I}}) + \\ &\quad + (x_{i\alpha}\sqrt{-dtV_{i\alpha}} + z_{i\alpha}\sqrt{dtV_{i\alpha}})(\hat{\mathbb{I}} \otimes \hat{\theta}_\alpha) = \\ &= \sum_i \left(\sum_\alpha x_{i\alpha}\sqrt{-dtV_{i\alpha}} + y_{i\alpha}\sqrt{dtV_{i\alpha}}\right)(\hat{O}_i \otimes \hat{\mathbb{I}}) + \\ &+ \sum_\alpha \left(\sum_i x_{i\alpha}\sqrt{-dtV_{i\alpha}} + z_{i\alpha}\sqrt{dtV_{i\alpha}}\right)(\hat{\mathbb{I}} \otimes \hat{\theta}_\alpha) \\ &= \left(\bigoplus_i \left(\sum_\alpha x_{i\alpha}\sqrt{-dtV_{i\alpha}} + y_{i\alpha}\sqrt{dtV_{i\alpha}}\right) O_i\right) \oplus \\ &\quad \oplus \left(\bigoplus_\alpha \left(\sum_i x_{i\alpha}\sqrt{-dtV_{i\alpha}} + z_{i\alpha}\sqrt{dtV_{i\alpha}}\right)\theta_\alpha\right).\end{aligned} \tag{10.33}$$

Replacing the last result in the previous equation and recalling Eq(3.10) we have that:

$$\begin{aligned}\mathcal{P} &= e^{-dt\sum_{i\alpha} V_{i\alpha}\hat{O}_i\otimes\hat{\theta}_\alpha} \\ &\simeq \frac{1}{(2\pi)^{\frac{3(i\cdot\alpha)}{2}}} \iiint dx^{i\alpha}\, dy^{i\alpha}\, dz^{i\alpha}\; e^{-\frac{\sum_{i\alpha} x_{i\alpha}^2+y_{i\alpha}^2+z_{i\alpha}^2}{2}} \cdot \\ &\quad \cdot \left(\bigotimes_i e^{-\left(\sum_\alpha x_{i\alpha}\sqrt{-dtV_{i\alpha}}+y_{i\alpha}\sqrt{dtV_{i\alpha}}\right)O_i}\right) \otimes \\ &\quad \otimes \left(\bigotimes_\alpha e^{-\left(\sum_i x_{i\alpha}\sqrt{-dtV_{i\alpha}}+z_{i\alpha}\sqrt{dtV_{i\alpha}}\right)\theta_\alpha}\right).\end{aligned} \tag{10.34}$$

Now we are able to apply the previous propagator. Clearly we can improve the previous expansion of the propagator using the importance sampling as described in the AFDMC chapter.

10.6 Details on 3–body ΛNN term

We know that in AFDMC code we are not able to include three body operatorial terms. However in our potential Eq(9.20) we also have a three body

component. Now we have shown that it is possible to rewrite these terms simply like two operators terms, and so it is possible to use them in the AFDMC propagator. Assume for this paragraph the following notations:

$$T_{\Lambda i} = T_\pi(m_\pi r_{\Lambda i}) \tag{10.35}$$
$$Y_{\Lambda i} = Y_\pi(m_\pi r_{\Lambda i}) \tag{10.36}$$
$$C_{\Lambda i} = Y_{\Lambda i} - T_{\Lambda i} \tag{10.37}$$
$$\Xi_{i,j}^{\alpha,\beta} = \textstyle\sum_\Lambda \frac{m_\pi^2}{9} C^S C_{\Lambda i} C_{\Lambda j} |r_{i\Lambda}||r_{j\Lambda}| \hat{r}_{i\Lambda}^\alpha \hat{r}_{j\Lambda}^\beta \tag{10.38}$$
$$\Theta_{\Lambda,i}^{\alpha,\beta} = C_{\Lambda i}\delta^{\alpha,\beta} + 3T_{\Lambda i}\hat{r}_{\Lambda i}^\alpha \hat{r}_{\Lambda i}^\beta. \tag{10.39}$$

Now we can write

$$V_{\Lambda NN}^S = \frac{1}{2}\sum_{i\neq j}\sum_{\alpha,\beta,\gamma} \Xi_{i,j}^{\alpha,\beta} \left(\tau_i^\gamma \sigma_i^\alpha\right) \left(\tau_j^\gamma \sigma_j^\beta\right), \tag{10.40}$$

$$V_{\Lambda NN}^P = \frac{1}{2}\sum_{i\neq j}\sum_{\alpha,\beta,\gamma} \left(-\frac{C^P}{3}\sum_\delta \sum_\Lambda \Theta_{\Lambda,i}^{\alpha,\delta}\Theta_{\Lambda,j}^{\beta,\delta}\right) \left(\tau_i^\gamma \sigma_i^\alpha\right) \left(\tau_j^\gamma \sigma_j^\beta\right), \tag{10.41}$$

and considering this definition

$$\begin{aligned}\omega_{i,j,\Lambda}^{\alpha,\beta} = \Bigg[&-\frac{1}{3}C^P C_{\Lambda i} C_{\Lambda j}\delta^{\alpha,\beta} - C^P C_{\Lambda j} T_{\Lambda i}\hat{r}_i^\alpha \hat{r}_i^\beta - C^P C_{\Lambda i} T_{\Lambda j}\hat{r}_j^\alpha \hat{r}_j^\beta + \\ &\left(\frac{m_\pi^2}{9} C^S C_{\Lambda i} C_{\Lambda j}|r_{i\Lambda}||r_{j\Lambda}| - 3T_{\Lambda i}T_{\Lambda j}C^P\left(\sum_\delta \hat{r}_i^\delta \hat{r}_j^\delta\right)\right)\hat{r}_i^\alpha \hat{r}_j^\beta\Bigg],\end{aligned} \tag{10.42}$$

we have that:

$$V_{\Lambda NN}^D = \frac{1}{2}\sum_{\Lambda, i\neq j} W^D T_{\Lambda i}^2 T_{\Lambda j}^2 + \sum_{\Lambda, i\neq j}\sum_\alpha \left(\frac{W^D}{6} T_{\Lambda i}^2 T_{\Lambda j}^2\right)\left(\sigma_\Lambda^\alpha \sigma_i^\alpha\right), \tag{10.43}$$

and

$$V_{\Lambda NN}^{2\pi} = V_{\Lambda NN}^S + V_{\Lambda NN}^P = \frac{1}{2}\sum_{\Lambda, i\neq j}\sum_{\alpha,\beta,\gamma} \omega_{i,j,\Lambda}^{\alpha,\beta}\left(\tau_i^\gamma \sigma_i^\alpha\right) \left(\tau_j^\gamma \sigma_j^\beta\right). \tag{10.44}$$

Remembering that

$$V_{\Lambda NN} = V_{\Lambda NN}^D + V_{\Lambda NN}^{2\pi}, \tag{10.45}$$

it is possible to see that this 3–body potential contains only 2–body operators and can be included into the AFDMC propagator.

10.7 Nucleon–hyperon Exchange term

Consider the nucleon–hyperon potential of Eq(9.3). As seen in previous paragraphs, we are now able to include all the terms of this potential in our AFDMC calculations with the exception of the exchange term P_x. At first we can try to include it perturbatively. Doing that is fairly simple. The operator P_x between one nucleon and one hyperon simply exchanges their position respect to their center of mass. That is, for each configuration that we sample, to

compute this potential contribution, we have to sum over all nucleon–hyperon pairs. Because of the mass differences between nucleon and hyperon, when we exchange the pair coordinates with respect to their center of mass, remembering that in this way we are changing also the total center of mass coordinate. Although not very efficient, we can compute perturbatively the exchange term. Anyway, we want to underline that including this term only perturbatively is not a good approximation. As shown in [SUB98, Usm06, UK08] the exchange operator induces strong correlations and a perturbative treatment is not appropriate. On the other hand all other calculations with this potential, except the cited ones, include this term only perturbatively.
Therefor we outline a proposal for directly implementing the exchange propagator. At first, rewrite the exchange term in a simpler form. The exchange term mixes the hyperon and nucleon states. So, instead of describing the nucleons and hyperons as distinct particles, we can describe them with a sort of "isospin" with three states:

$$\begin{pmatrix} n \\ p \\ \Lambda \end{pmatrix}. \tag{10.46}$$

So, if we start from a wavefunction that is antisymmetric, i.e. that is an eigenstate of the permutation operator, we have that

$$-1 = P_{TOT} = P_x P_\sigma P_\lambda, \tag{10.47}$$

where P_{TOT} is a pair exchange operator, P_x as previously defined, the operator that exchanges only the coordinates, P_σ the one exchanges spins only and P_λ that exchanging the extended isospins only:

$$P_\sigma(i \leftrightarrow j) = \frac{1}{2}\left(\mathbb{I} + \sum_{\alpha\in\{xyz\}} \sigma_i^\alpha \sigma_j^\alpha\right), \tag{10.48}$$

$$P_\lambda(i \leftrightarrow j) = \frac{1}{2}\left(\frac{2}{3}\mathbb{I} + \sum_{\alpha=1}^{8} \lambda_i^\alpha \lambda_j^\alpha\right), \tag{10.49}$$

where λ_i are the eight Gell-Mann matrices. So from Eq(10.47) we can use instead of P_x

$$-P_\sigma P_\lambda = P_x, \tag{10.50}$$

that is in a form suitable to use into the propagator. Clearly this approach requires a deep change in the structure of the code for a hypernuclear system. Instead of having a trial wavefunction that is simply a product of a Slater determinant of nucleons times another Slater determinant of hyperon single particle wavefunction, we require the construction of a determinant including the states of all the particles. The isospin matrices τ become the first three Gell-Mann matrices. All the potential operators acting on nucleons must be preceded by a projector on the nucleon state, i.e.

$$Q_N = \frac{2\mathbb{I} + \sqrt{3}\lambda^8}{3} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \tag{10.51}$$

and similarly for operators that act on hyperons we have to add the projector:

$$Q_\Lambda = \frac{\mathbb{I} - \sqrt{3}\lambda^8}{3} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{10.52}$$

We have to notice that because of the non–negligible differences between the hyperon and nucleon masses, we have to use the trick explained into (§ 3.11) to be able to implement a diffusive term of the propagator as:

$$e^{-dt\sum_i \frac{P_i^2 O_i}{2}}, \tag{10.53}$$

with:

$$O_i = \begin{pmatrix} 1/m_N & 0 & 0 \\ 0 & 1/m_N & 0 \\ 0 & 0 & 1/m_\Lambda \end{pmatrix}. \tag{10.54}$$

that is we have to split the P_i operator from the O_i one. We also have to notice that within this approach, the 3–body $NN\Lambda$ terms, containing at most two operators in the old approach, in this way, because of the presence of the projector operators Q_N and Q_Λ, become 3–body terms with 3 explicits operators. So we can suppose that it is not possible to easily include three body terms, like for 3–body NNN Urbana potential. Fortunately that is not the case. In fact, in the Usmani 3–body potential we only have $NN\Lambda$ terms, i.e two operators that act on nucleons and another acting on hyperons. We can note that all nucleon operators commute with hyperon operators, and so we can apply twice the Hubbard Stratonovich transform like we have done to include spin–orbit, L^2 or different mass terms, i.e. we can satisfy a relation similar to equations Eq(3.89), Eq(3.116), Eq(3.124).

10.8 Results

With the previously described elements, we are now able to compute the binding energy of a hypernucleus. Anyway we cannot compare our results directly with experiments, because of the use of a too poor nuclear potential, the Argonne $Av6'$. We point out that this calculation has serious shortcoming because of the limited form of the nucleon–nucleon potential used (Argonne $Av6'$). However, the underlying assumption is that the Λ–hyperon binding energy:

$$BE_\Lambda = BE(\text{hypernucleus}) - BE(\text{hypernucleus without hyperon}) \tag{10.55}$$

being the difference of two quantities computes using the same NN potential, has a systematic error smaller than that on the absolute energy of the nucleons of the hypernucleus. Clearly this is still an approximation, but reasonable, universally used. For the nuclei energies we use that one reported in table Tab. 3.1.

10.8.1 2–body interaction only

As a first step we try to do calculations using only the 2–body terms of the hyperon—nucleon interaction. We do calculations for the ${}^{5}_{\Lambda}$He hypernucleus, i.e.

	BE [MeV]	error [MeV]	BE_Λ [MeV]	exp [MeV]
${}^{5}_{\Lambda}$He	-33.4	0.1	6.6	3.12
${}^{17}_{\Lambda}$O	-138.0	0.3	32.6	(13.5)
${}^{41}_{\Lambda}$Ca	-326.	2.	47.	($\sim$ 19)

Table 10.1: BE_Λ computed with AFDMC and compared with expected BE_Λ values (experimentally for ${}^{4}_{\Lambda}$He,theoretically estimated for ${}^{17}_{\Lambda}$O). We use $Av6'$ potential for the nuclear interaction and the Usmany tipe of Eq(9.3) but without the exchange and the three body terms, i.e. with $\varepsilon = 0$, $W^D = 0$, $C^P = 0$ and $C^S = 0$.

the ^{4}He nucleus plus the Λ hyperon, for ${}^{17}_{\Lambda}$O and for ${}^{41}_{\Lambda}$Ca. Results are reported in Tab. 10.1. As we can see from the table we are quite far from the expected values of BE_Λ. Anyway, how explained and shown in [BUC84], this overbinding effect is due to the neglected three body terms. With this observation we want to underline the importance of the three body terms in hyperon interaction. To do a realistic calculation it is necessary to include it, both for hypernuclei and for nuclear matter with hyperons. Clearly an equivalent approach is to use only two–body potentials like Nijmegen, but being sure to take into account 3–body correlations that allows the possibility to excite a Λ to a Σ hyperon.

10.8.2 With 3–body terms

Now we try to compute BE_Λ including also the three body terms of the nucleon–hyperon interaction. As said before we have to fix the parameters relative to these three body terms, i.e. W^D, C^P and C^S coefficients. To do that we try to reproduce the BE_Λ of some hypernuclei. We focus on ${}^{5}_{\Lambda}He$ and ${}^{17}_{\Lambda}$O; these are closed shell systems, therefore simpler and faster to compute. As we saw from our calculations and as observed in [UK08], the S–wave term contribution is negligible. So we assume $C^S = 0$. The result for different values of C^P and W^D are reported in the plot Fig. 10.1. With parameters $W^D = 0.06$ MeV, $C^P = 0.7$ MeV and $C^S = 0$ we also performed calculations also for other hypernuclei, as reported in table Tab. 10.2. As we can see, we have to better the three body coefficients. However, because of the uncertainties in the AFDMC fixed–phase approximation used, we have first to solve these algorithm problems.

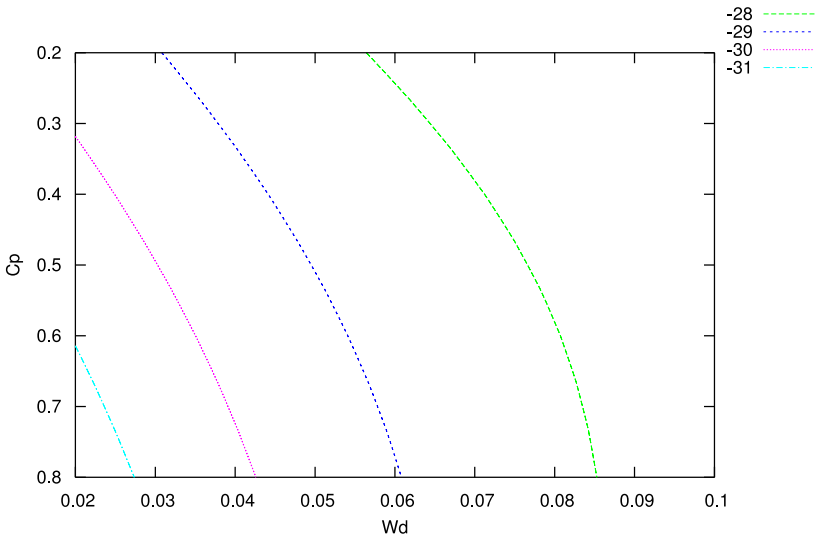

Figure 10.1: Total BE of ${}^{5}_{\Lambda}$He as functions of C^P and W^D. Unit measure is MeV. We use $Av6'$ potential for the nuclear interaction and the Usmani type of Eq(9.3) without the exchange term, assuming $\varepsilon = 0$, $\bar{v} = 6.15$ MeV, $v_\sigma = 0.24$ MeV, and $C^S = 0$.

	BE [MeV]	error [MeV]	BE_Λ [MeV]	exp [MeV]
${}^{5}_{\Lambda}$He	-30.4	0.2	3.59	3.12
${}^{7}_{\Lambda}$He	-29.5	0.3	4.46	5.23
${}^{9}_{\Lambda}$He	-28.3	0.3	4.29	?
${}^{16}_{\Lambda}$O	-102.9	0.6	13.02	12.5
${}^{17}_{\Lambda}$O	-117.3	0.7	11.94	(13.5)
${}^{18}_{\Lambda}$O	-118.	1	13.40	?
${}^{40}_{\Lambda}$Ca	-275.	5	13.50	18.7
${}^{41}_{\Lambda}$Ca	-293.	2	13.65	?

Table 10.2: BE_Λ computed with AFDMC and compared with experimental BE_Λ values where available(theoretically estimated and computed[UPU95] for ${}^{17}_{\Lambda}$O). We use $Av6'$ potential for the nuclear interaction and the Usmani type of Eq(9.3) without the exchange term. We use $\varepsilon = 0$, $\bar{v} = 6.15$ MeV, $v_\sigma = 0.24$ MeV, $W^D = 0.06$ MeV, $C^P = 0.7$ MeV and $C^S = 0$.

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Conclusions

This thesis work consisted of three distinct set of results. First, we studied some improvements relative to the the Monte Carlo methods:

- The fixed–hypernode extension is a possible improvement scheme on the fixed–node approximation used in DMC algorithm. It is necessary to proceed with more systematic study to understand when we can obtain reasonable benefits using this method.
- We show how is possible to include nonlocal terms (spin–orbit, L^2) and exchange terms in the propagator of the AFDMC algorithm. This theoretical work is interesting and open the possibilities to generally improve the AFDMC and maybe also the GFMC calculations. But they are not usable until we do not solve or reduce the problems related to the fixed phase approximation.

The second part concerns the development of an algorithm of Diffusion Monte Carlo class to solve EFT Hamiltonians, explicitly including pion degrees of freedom. These are the main findings.

- The study of the pion dynamic effects in the interaction is very interesting to be investigate; but maybe it is necessary a more theoretical and analytic work to have a better trial wave function.
- The inclusion of next order terms in chiral expansion requires an accurate study to check the feasibility of such calculation. A more extensive and accurate theoretical and analytic study is required.
- We need a better method than the current version of AFDMC that we use.
- As shown in the section relative to instantaneous pion fields, maybe it might be convenient to represent pion fields in momentum space instead of in coordinate space.
- The idea of representing nucleons in the continuum is not a such a good idea: we have problems computing derivative terms and an infinite dimensional wavefunction space. Representing nucleons on lattice we can work with a finite basis set for nucleons and we do not introduce any more

approximation; pions are represented on a lattice anyway, and our physics is anyway well described only for distances larger than the lattice cell size.

- It is interesting to consider instantaneous pion fields, but only to find corrective terms to the existent potential. If we want to do that, I think that a better regularization should be chosen (a continuous one, not on lattice), and moreover more terms of the EFT theory must be include, at least to N^2LO. A study of nucleonic systems using an instantaneous pion field on lattice limited to the leading order EFT is useless.

The last part concerned the development of an AFDMC algorithm for studying mixed nucleon–hyperon systems.

- Accurate microscopic calculations on hypernuclei are very useful to fit accurate hyperon potential on available experimental data, i.e. on the hypernuclei binding energies. To this end we need an accurate method to compute binding energies. From the tests performed, we saw that the current AFDMC algorithm is insufficient for this purpose. We look at AFQMC algorithm on which we are working.

- It might be very interesting an accurate evaluation of Hypernuclei using different existent potentials, to stress different properties and behaviors.

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