

Morten Hjorth-Jensen, Maria Paola Lombardo, and  
Ubirajara van Kolck, Editors

# **An advanced course in computational nuclear physics**

Bridging the scales from quarks to neutron stars

May 31, 2016

## **No Title Given**

No Author Given



# Preface

This graduate-level text collects and synthesizes nine series of lectures on the nuclear quantum many-body problem - starting from our present understanding of the underlying forces with a presentation of recent advances within the field of lattice quantum chromodynamics, via effective field theories to central many-body methods like Monte Carlo methods, coupled cluster theories, similarity renormalization group and large-scale diagonalization approaches.

In particular algorithmic and computational advances show promise for breakthroughs in predictive power including proper error estimates, a better understanding of the underlying effective degrees of freedom and of the respective forces at play.

Enabled by recent advances in theoretical, experimental and numerical techniques, the modern and state-of-the art applications considered in this volume span the entire range from our smallest components, quarks and gluons as the mediators of the strong force to the computation of the equation of state for neutron star matter.

The present lectures provide a proper exposition of the underlying theoretical and algorithmic approaches as well as strong ties to the numerical implementation of the exposed methods. Each series of lectures provides a proper link to actual numerical software. The latter will enable the reader to build upon these and develop his/her own insights about these methods, as well as using the corresponding codes for developing own programs for tackling challenging nuclear many-body problems.



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# Chapter 1

## Motivation and overarching aims

Morten Hjorth-Jensen, Maria Paola Lombardo, and Ubirajara van Kolck

**Abstract** Our presentation

Nuclear physics has recently experienced several discoveries and technological advances that address the fundamental questions of the field, in particular how nuclei emerge from the strong dynamics of quantum chromodynamics (QCD). Many of these advances have been made possible by significant investments in frontier research facilities worldwide over the last two decades. Some of these discoveries are the detection of perhaps the most exotic state of matter, the quark-gluon plasma, which is believed to have existed in the very first moments of the Universe (refs). Recent experiments have validated the standard solar model and established that neutrinos have mass (refs). High-precision measurements of the quark structure of the nucleon are challenging existing theoretical understanding. Nuclear physicists have started to explore a completely unknown landscape of nuclei with extreme neutron-to-proton ratios using radioactive and short-lived ions, including rare and very neutron-rich isotopes. These experiments push us towards the extremes of nuclear stability. Moreover, these rare nuclei lie at the heart of nucleosynthesis processes in the universe and are therefore an important component in the puzzle of matter generation in the universe.

A firm experimental and theoretical understanding of nuclear stability in terms of the basic constituents is a huge intellectual endeavor. Experiments indicate that developing a comprehensive description of all nuclei and their reactions requires theoretical and experimental investigations of rare isotopes with unusual neutron-to-proton ratios that are very different from their stable counterparts. These rare nuclei are difficult to produce and study experimentally since they can have extremely short lifetimes. Theoretical approaches to these nuclei involve solving the nuclear many-body problem.

Accompanying these developments, a qualitative change has swept the nuclear theory landscape thanks to a combination of techniques that is allowing, for the first time, the direct connection between QCD and nuclear structure. This transformation has been brought by a dramatic improvement in the capability of numerical calculations both in QCD, via lattice simulations, and in the nuclear many-body problem, via "ab initio" methods for the diagonalization of non-relativistic Hamiltonians. Simultaneously, the framework of effective field

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theories builds a bridge between the two numerical approaches, allowing to convert the results of lattice QCD into input to ab initio methods.

Now, algorithmic and computational advances hold promise for breakthroughs in predictive power including proper error estimates, enhancing the already strong links between theory and experiment. These advances include better ab initio many-body methods as well as a better understanding of the underlying effective degrees of freedom and the respective forces at play. And obviously better numerical algorithms as well as developments in high-performance computing. This will provide us with important new insights about the stability of nuclear matter and allow us to relate these novel understandings to the underlying laws of motion, the corresponding forces and the pertinent fundamental building blocks.

Important issues such as whether we can explain from first-principle methods the existence of magic numbers and their vanishing as we add more and more nucleons, how the binding energy of neutron-rich nuclei behaves, or the radii, neutron skins, and many many other probes that extract information about many-body correlations as nuclei evolve towards their limits of stability — these are all fundamental questions which, combined with recent experimental and theoretical advances, will allow us to advance our basic knowledge about the limits of stability of matter, and, hopefully, help us in gaining a better understanding of visible matter.

It is within this framework the present texts finds its rationale. This text collects and synthesizes seven series of lectures on the nuclear many-body problem, starting from our present understanding of the underlying forces with a presentation of recent advances within the field of lattice QCD, via effective field theories to central many-body methods like Monte Carlo, coupled-cluster, and large-scale diagonalization methods. The applications span from our smallest components, quarks and gluons as the mediators of the strong force to the computation of the equation of state for infinite nuclear matter and neutron star matter. The lectures provide a proper exposition of the underlying theoretical and algorithmic approaches as well as strong ties to the numerical implementation of the exposed methods. The lectures propose exercises, often providing a proper link to actual numerical software. The latter will enable the reader to build upon these and develop his/her own insights about these methods, as well as using these codes for developing his/her own programs for tackling complicated many-body problems.

**Acknowledgements** If you want to include acknowledgments of assistance and the like at the end of an individual chapter please use the acknowledgement environment – it will automatically render Springer’s preferred layout.

## Appendix

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## Chapter 2

# Quantum chromodynamics, an introduction

Thomas Schaefer

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### 2.1 QCD and Symmetries

### 2.2 QCD at high Temperature

### 2.3 QCD at high Temperature: Experiment

### 2.4 QCD at Finite Density

### 2.5 Non-equilibrium QCD

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## Chapter 3

# Lattice quantum chromodynamics approach to nuclear physics

Tetsuo Hatsuda

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### 3.1 General Introduction

### 3.2 Continuum quantum chromodynamics: basics

### 3.3 Lattice quantum chromodynamics: basics

### 3.4 Lattice quantum chromodynamics: applications

### 3.5 Hadron interactions: basics

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## Chapter 4

# Theoretical aspects of few-body systems and effective field theories

Hans-Werner Hammer

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## 4.1 General Introduction

## 4.2 More stuff

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## Chapter 5

# Lattice methods and effective field theory

Amy Nicholson

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### 5.1 Introduction

### 5.2 Basics of lattice effective field theory

### 5.3 Calculating Observables

### 5.4 Systematic errors and improvement

### 5.5 Beyond simple leading order effective field theory

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## Chapter 6

# Lattice methods and the nuclear few- and many-body problem

Dean Lee

**Abstract** This chapter builds upon the review of lattice methods and effective field theory of the previous chapter. We begin with a brief overview of lattice calculations using chiral effective field theory. We then describe several methods for computing scattering on the lattice. After that we focus on the main goal, explaining the theory and algorithms relevant to lattice simulations of nuclear few- and many-body systems. We discuss the exact equivalence of four different lattice formalisms, the Grassmann path integral, transfer matrix operator, Grassmann path integral with auxiliary fields, and transfer matrix operator with auxiliary fields. Along with our analysis we include several coding examples and a number of exercises for the calculations of few- and many-body systems at leading order in chiral effective field theory.

### 6.1 Introduction

Effective field theory (EFT) provides a theoretical framework for organizing low-energy interactions in powers of particle momenta. Chiral effective field theory applies this framework to the low-energy interactions of protons and neutrons while explicitly including the interactions of pions [?, ?, ?, ?, ?, ?, ?, ?]. Pions are qualitatively different from other mesons since they become massless in the limit of massless quarks, thereby producing long-range exchange interactions. The low-energy expansion of chiral EFT is organized in powers of  $Q$ , where  $Q$  denotes the typical momentum of the nucleons as well as explicit factors of the pion mass. The most important interactions are called leading order (LO) or  $O(Q^0)$ . The next most important contributions are next-to-leading order (NLO) or  $O(Q^2)$ . The terms after this are next-to-next-to-leading order (NNLO) or  $O(Q^3)$ , and so on.

Lattice EFT refers generally to lattice simulations based upon the framework of effective field theory. There are a few reviews in the literature which discuss current methods used in lattice effective field theory [?, ?] as well as the discussion in the previous chapter of this volume. Many different phenomena can be studied in lattice EFT using the same lattice action. In principle all systematic errors are introduced up front when defining the low-energy effective theory, as opposed to the particular computational scheme used to calculate observables.

Lattice EFT has been aided by efficient lattice methods developed for lattice QCD and condensed matter applications. The methods include Markov Chain Monte Carlo techniques,

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auxiliary fields [?, ?], pseudofermion methods [?], and non-local updating schemes such as the hybrid Monte Carlo algorithm [?, ?, ?]. Lattice EFT was first used in studies of infinite nuclear matter [?] and infinite neutron matter with and without explicit pions [?, ?, ?, ?]. The method has also been used to study light nuclei in pionless EFT [?] and chiral EFT at leading order [?]. There have been further studies of neutron matter [?, ?, ?] and light nuclei [?, ?], and there have been several applications to nuclear structure and nuclear clustering [?, ?, ?, ?, ?, ?] as well as recent work on nuclear scattering and reactions [?, ?, ?].

## 6.2 Scattering on the lattice

At any given order in the chiral EFT expansion, there will be short-range interaction coefficients which depend on the chosen regularization of the large-momentum divergences. On the lattice this regularization is provided by the lattice spacing, unless some additional regularization is applied to the lattice interactions. In order to set the values of the short-range two-nucleon interaction coefficients, we make a comparison of nucleon-nucleon scattering on the lattice with experimental scattering data. The extension to three-nucleon interaction coefficients is also required at NNLO, and that procedure on the lattice has been discussed in Ref. [?]

As discussed in the previous chapter, Lüscher [?, ?, ?] has shown that the finite-volume energy levels for a two-body system in a periodic cubic box are related to the infinite-volume scattering matrix. While the method is very useful at low momenta, it can become less accurate at higher momenta and higher orbital angular momenta. Also spin-orbit coupling and partial-wave mixing are difficult to measure accurately using Lüscher's method due to scattering artifacts produced by the cubic periodic boundary. An alternative approach has been developed to measure phase shifts for particles on the lattice using a spherical wall boundary [?, ?].

In this approach, a hard spherical wall boundary is imposed on the relative separation between the two particles. This wall is placed at some chosen radius  $R_{\text{wall}}$ , and it removes copies of the interactions produced by the periodic lattice. Working in the center-of-mass frame, we solve the time-independent Schrödinger equation as a function of the relative separation between the particles and compute spherical standing waves which vanish at  $r = R_{\text{wall}}$ . At values of  $r$  beyond the range of the interaction, the spherical standing waves can be written as a superposition of products of spherical harmonics and spherical Bessel functions,

$$[\cos \delta_\ell \cdot j_\ell(kr) - \sin \delta_\ell \cdot y_\ell(kr)] Y_{\ell, \ell_z}(\theta, \phi). \quad (6.1)$$

Here  $k$  is the relative momentum between the scattering particles, and  $\delta_\ell$  is the phase shift for partial wave  $L$ . We can extract  $k$  from the energy of the standing wave, and the phase shift  $\delta_\ell$  is determined by setting the wave function in Eq. (6.1) to zero at the wall boundary.

When the total intrinsic spin of the two nucleons is nonzero, spin-orbit coupling generates mixing between partial waves. In this case the standing wave at the wall boundary is decomposed into spherical harmonics and coupled-channel equations are solved to extract the phase shifts and mixing angles. The spherical wall method was used to calculate phase shifts and mixing angle for low-energy nucleon-nucleon scattering [?]. Recently the spherical wall approach has been improved in accuracy and computational efficiency [?]. In the improved approach one projects onto spherical harmonics  $Y_{\ell, \ell_z}$  with angular momentum quantum numbers  $\ell, \ell_z$ . In this manner one constructs radial position states for a given partial wave,

$$|r\rangle^{\ell, \ell_z} = \sum_{\mathbf{r}'} Y_{\ell, \ell_z}(\hat{\mathbf{r}}') \delta_{r, |\mathbf{r}'|} |\mathbf{r}'\rangle. \quad (6.2)$$

We require that  $r$  is less than half the box length  $L/2$ . Using this technique we are essentially constructing a radial lattice Hamiltonian for each partial wave.

It is also useful to introduce auxiliary potentials in the region lying just in front of the spherical wall boundary [?]. We use the auxiliary potential to tune the energy of the scattering wave. This auxiliary potential is a spherical attractive well positioned in front of the spherical wall boundary. We can tune to any scattering energy by adjusting the depth of the well. For systems with partial wave mixing due to spin-orbit coupling, we also include a Hermitian but imaginary off-diagonal auxiliary potential for the two coupled channels. This breaks time reversal symmetry, and the resulting standing wave solutions now have both real and imaginary parts that are linearly independent. From the real and imaginary solutions one can determine the scattering phase shifts and mixing angle at any given value of the scattering energy.

This spherical wall approach has been used together with a technique called the adiabatic projection method to study nuclear scattering and reactions on the lattice. The adiabatic projection method [?, ?, ?, ?] is a general framework that produces a low-energy effective theory for clusters of particles which becomes exact in the limit of large projection time. For the case of two-cluster scattering, we consider a set of two cluster states  $|\mathbf{R}\rangle$  labeled by the spatial separation vector  $\mathbf{R}$ . The initial wave functions are wave packets which, for large  $|\mathbf{R}|$ , factorize into a product of two individual clusters,

$$|\mathbf{R}\rangle = \sum_{\mathbf{r}} |\mathbf{r} + \mathbf{R}\rangle_1 \otimes |\mathbf{r}\rangle_2. \quad (6.3)$$

The summation over  $\mathbf{r}$  is required to produce states with total momentum equal to zero. We bin the initial cluster states together according to radial distance and angular momentum. In this manner, we form radial position states with projected angular momentum quantum numbers, which we label  $|R\rangle^{J,J_z}$ .

The next step is to multiply by powers of the transfer matrix in order to form “dressed” cluster states. This produces states that approximately span the set of low-energy cluster-cluster scattering states in our periodic box. We discuss the transfer matrix formalism in detail later in this chapter. After  $n_t$  time steps, we have the dressed cluster states

$$|R\rangle_{n_t}^{J,J_z} = M^{n_t} |R\rangle^{J,J_z}. \quad (6.4)$$

These dressed cluster states are then used to compute matrix elements of the transfer matrix  $M$ ,

$$[M_{n_t}]_{R',R}^{J,J_z} = \langle R' | M | R \rangle_{n_t}^{J,J_z}. \quad (6.5)$$

Since such states are not orthogonal, we also compute a norm matrix

$$[N_{n_t}]_{R',R}^{J,J_z} = \langle R' | R \rangle_{n_t}^{J,J_z}. \quad (6.6)$$

The “radial adiabatic transfer matrix” is defined as the matrix product

$$[M_{n_t}^a]_{R',R}^{J,J_z} = \left[ N_{n_t}^{-\frac{1}{2}} M_{n_t} N_{n_t}^{-\frac{1}{2}} \right]_{R',R}^{J,J_z}, \quad (6.7)$$

and the scattering phase shifts can then be determined from the standing waves of the radial adiabatic transfer matrix.



### 6.3 Lattice formalisms

Throughout our discussion of the lattice formalism we use dimensionless parameters and operators corresponding with physical values times the appropriate power of the spatial lattice spacing  $a$ . In our notation the three-component integer vector  $\mathbf{n}$  labels the lattice sites of a three-dimensional periodic lattice with dimensions  $L^3$ . The spatial lattice unit vectors are denoted  $\hat{\mathbf{l}} = \hat{1}, \hat{2}, \hat{3}$ . We use  $n_t$  to label lattice steps in the temporal direction, and  $L_t$  denotes the total number of lattice time steps. The temporal lattice spacing is given by  $a_t$ , and  $\alpha_t = a_t/a$  is the ratio of the temporal to spatial lattice spacing. We also define  $h = \alpha_t/(2m)$ , where  $m$  is the nucleon mass in lattice units. In Fig. 6.1 we show a diagram of the four different but exactly equivalent lattice formulations that we discuss, the Grassmann path integral, transfer matrix operator, Grassmann path integral with auxiliary fields, and transfer matrix operator with auxiliary fields.

#### 6.3.1 Grassmann path integral

We define the lattice action starting from the lattice Grassmann path integral action without auxiliary fields. This is the simplest formulation in which to derive the lattice Feynman rules. We let  $c$  and  $c^*$  be anticommuting Grassmann fields for the nucleons. In our notation  $c$  is a column vector composed of the spin-isospin nucleon degrees of freedom  $c_i$ , while  $c^*$  is a row vector of the components  $c_i^*$ . The Grassmann fields are periodic with respect to the spatial extent of the  $L^3$  lattice,

$$c_i(\mathbf{n} + L\hat{1}, n_t) = c_i(\mathbf{n} + L\hat{2}, n_t) = c_i(\mathbf{n} + L\hat{3}, n_t) = c_i(\mathbf{n}, n_t), \quad (6.8)$$

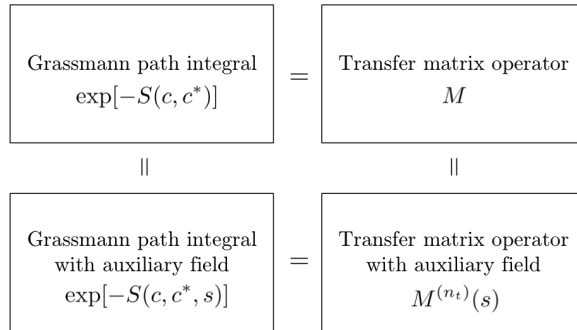
$$c_i^*(\mathbf{n} + L\hat{1}, n_t) = c_i^*(\mathbf{n} + L\hat{2}, n_t) = c_i^*(\mathbf{n} + L\hat{3}, n_t) = c_i^*(\mathbf{n}, n_t), \quad (6.9)$$

and antiperiodic along the temporal direction,

$$c_i(\mathbf{n}, n_t + L_t) = -c_i(\mathbf{n}, n_t), \quad (6.10)$$

$$c_i^*(\mathbf{n}, n_t + L_t) = -c_i^*(\mathbf{n}, n_t). \quad (6.11)$$

We write  $DcDc^*$  as shorthand for the integral measure,



**Fig. 6.1** A schematic diagram of the different lattice formulations, namely, the Grassmann path integral, transfer matrix operator, Grassmann path integral with auxiliary fields, and transfer matrix operator with auxiliary fields.

$$DcDc^* = \prod_{\mathbf{n}, n_t, i} dc_i(\mathbf{n}, n_t) dc_i^*(\mathbf{n}, n_t). \quad (6.12)$$

We use the usual convention for Grassmann integration,

$$\int dc_i(\mathbf{n}, n_t) = \int dc_i^*(\mathbf{n}, n_t) = 0, \quad (6.13)$$

$$\int dc_i(\mathbf{n}, n_t) c_i(\mathbf{n}, n_t) = \int dc_i^*(\mathbf{n}, n_t) c_i^*(\mathbf{n}, n_t) = 1 \quad (\text{no sum on } i). \quad (6.14)$$

We consider the Grassmann path integral

$$\mathcal{Z} = \int DcDc^* \exp[-S(c^*, c)], \quad (6.15)$$

where the lattice action can be broken into a free part and interacting part,

$$S(c^*, c) = S_{\text{free}}(c^*, c) + S_{\text{int}}(c^*, c). \quad (6.16)$$

The free part is the free non-relativistic nucleon action, which is

$$S_{\text{free}}(c^*, c) = \sum_{\mathbf{n}, n_t} c^*(\mathbf{n}, n_t) [c(\mathbf{n}, n_t + 1) - c(\mathbf{n}, n_t)] + \alpha_t \sum_{n_t} K^{(n_t)}(c^*, c), \quad (6.17)$$

where

$$K^{(n_t)}(c^*, c) = \sum_{k=0,1,2,\dots} (-1)^k \frac{w_k}{2m} \sum_{\mathbf{n}, \hat{\mathbf{l}}} c^*(\mathbf{n}, n_t) [c(\mathbf{n} + k\hat{\mathbf{l}}, n_t) + c(\mathbf{n} - k\hat{\mathbf{l}}, n_t)], \quad (6.18)$$

and the hopping coefficients  $w_k$  correspond to a hopping parameter expansion of the squared momentum,

$$P^2(\mathbf{p}) = 2 \sum_{k=0,1,2,\dots} \sum_{l=1,2,3} (-1)^k w_k \cos(kp_l). \quad (6.19)$$

The hopping coefficients can be chosen to match the continuum relation

$$P^2(\mathbf{p}) = \mathbf{p}^2, \quad (6.20)$$

up to some chosen level of lattice discretization error. The hopping coefficients  $w_k$  for a few different lattice actions are shown in Table 6.1.

**Table 6.1** Hopping coefficients  $w_k$  for several lattice actions

coefficient	standard	$O(a^2)$ -improved	$O(a^4)$ -improved
$w_0$	1	5/4	49/36
$w_1$	1	4/3	3/2
$w_2$	0	1/12	3/20
$w_3$	0	0	1/90

### 6.3.2 Transfer matrix operator

Let  $a_i(\mathbf{n})$  and  $a_i^\dagger(\mathbf{n})$  denote fermion annihilation and creation operators for the nucleon component  $i$  at lattice site  $\mathbf{n}$ . The shorthand  $a(\mathbf{n})$  represents a column vector of nucleon components  $a_i(\mathbf{n})$ , and  $a^\dagger(\mathbf{n})$  represents a row vector of components  $a_i^\dagger(\mathbf{n})$ . We can write any Grassmann path integral with instantaneous interactions as the trace of a product of operators using the identity [?, ?]

$$\begin{aligned} & \text{Tr} \left\{ : F_{L_t-1} [a^\dagger(\mathbf{n}'), a(\mathbf{n})] : \times \cdots \times : F_0 [a^\dagger(\mathbf{n}'), a(\mathbf{n})] : \right\} \\ &= \int Dc Dc^* \exp \left\{ \sum_{n_t=0}^{L_t-1} \sum_{\mathbf{n}, \mathbf{l}} c_i^*(\mathbf{n}, n_t) [c_i(\mathbf{n}, n_t) - c_i(\mathbf{n}, n_t + 1)] \right\} \\ & \quad \times \prod_{n_t=0}^{L_t-1} F_{n_t} [c^*(\mathbf{n}', n_t), c(\mathbf{n}, n_t)], \end{aligned} \quad (6.21)$$

where  $c_i(\mathbf{n}, L_t) = -c_i(\mathbf{n}, 0)$ .

Let us define the free non-relativistic lattice Hamiltonian

$$H_{\text{free}}(a^\dagger, a) = \sum_{k=0,1,2,\dots} (-1)^k \frac{W_k}{2m} \sum_{\mathbf{n}, \mathbf{l}} a^\dagger(\mathbf{n}) [a(\mathbf{n} + k\hat{\mathbf{l}}) + a(\mathbf{n} - k\hat{\mathbf{l}})]. \quad (6.22)$$

We write the interaction term as  $H_{\text{int}}(a^\dagger, a)$ , so that our total Hamiltonian is

$$H(a^\dagger, a) = H_{\text{free}}(a^\dagger, a) + H_{\text{int}}(a^\dagger, a). \quad (6.23)$$

Using the correspondence Eq. (6.21), we can rewrite the path integral  $\mathcal{Z}$  defined in Eq. (6.15) as a transfer-matrix partition function,

$$\mathcal{Z} = \text{Tr}(M^{L_t}), \quad (6.24)$$

where  $M$  is the normal-ordered transfer matrix operator

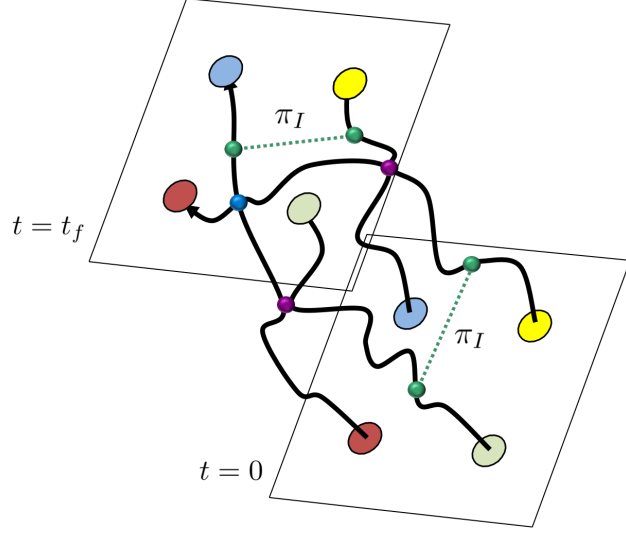
$$M = : \exp[-H(a^\dagger, a)\alpha_t] :. \quad (6.25)$$

Roughly speaking, the transfer matrix operator is the exponential of the Hamiltonian operator over one Euclidean lattice time step. In order to satisfy the identity Eq. (6.21), the exact definition of the transfer matrix is the normal-ordered exponential as defined in Eq. (6.25).

In this transfer matrix formalism, one can do simulations of nucleons using Monte Carlo, and this would essentially be a lattice version of diffusion or Green's function Monte Carlo [?]. Visually one can view the nucleons as interacting with each other while diffusing in space with each time step, as indicated in Fig. 6.2. At leading order in chiral effective field theory, the interactions include two independent S-wave contact interactions and the exchange of pions. We discuss these interactions in detail in the following.

### 6.3.3 Grassmann path integral with auxiliary field

We now assume that there exists an integral relation that allows us to write  $\exp[-S_{\text{int}}(c^*, c)]$  as an integral over auxiliary fields. The purpose of the auxiliary field transformation is to decouple the interactions among the nucleons. Instead the interactions will be between the nucleons and the auxiliary fields.



**Fig. 6.2** A sketch showing nucleons which evolve with each time step. At leading order in chiral effective field theory, the interactions include two contact interactions and the exchange of pions.

We now illustrate using the interactions that appear at leading order in chiral effective field theory. For pedagogical purposes we discuss the simplest possible implementation of the leading order action on the lattice. We first consider a zero-range contact interaction which is independent of nucleon spin and isospin. The action has the form

$$S_{\text{int}}^C(c^*, c) = \alpha_t \frac{C}{2} \sum_{\mathbf{n}, n_t} [c^*(\mathbf{n}, n_t) c(\mathbf{n}, n_t)]^2. \quad (6.26)$$

We can write this as

$$\exp[-S_{\text{int}}^C(c^*, c)] = \int Ds \exp[-S_{ss}(s) - S_s(c^*, c, s)] \quad (6.27)$$

for auxiliary field  $s(\mathbf{n}, n_t)$ , where

$$S_{ss}(s) = \frac{1}{2} \sum_{\mathbf{n}, n_t} s^2(\mathbf{n}, n_t), \quad (6.28)$$

$$S_s(c^*, c, s) = \sqrt{-C\alpha_t} \sum_{\mathbf{n}, n_t} s(\mathbf{n}, n_t) c^*(\mathbf{n}, n_t) c(\mathbf{n}, n_t). \quad (6.29)$$

In our definition of the integration measure  $Ds$ , we include a factor of  $1/\sqrt{2\pi}$  for each degree of freedom.

Next we consider an isospin-dependent contact interaction

$$S_{\text{int}}^{C'}(c^*, c) = \alpha_t \frac{C'}{2} \sum_{\mathbf{n}, n_t, I} [c^*(\mathbf{n}, n_t) \tau_I c(\mathbf{n}, n_t)]^2, \quad (6.30)$$

where  $\tau_I$  for  $I = 1, 2, 3$  are the Pauli matrices in isospin space. Then we can use

$$\exp[-S_{\text{int}}^{C'}(c^*, c)] = \int \prod_I Ds_I \exp[-S_{s_I s_I}(s_I) - S_{s_I}(c^*, c, s_I)] \quad (6.31)$$

for auxiliary fields  $s_I(\mathbf{n}, n_t)$  where

$$S_{s_I s_I}(s_I) = \frac{1}{2} \sum_{\mathbf{n}, n_t, I} s_I^2(\mathbf{n}, n_t), \quad (6.32)$$

$$S_{s_I}(c^*, c, s_I) = \sqrt{-C'} \alpha_t \sum_{\mathbf{n}, n_t, I} s_I(\mathbf{n}, n_t) c^*(\mathbf{n}, n_t) \tau_I c(\mathbf{n}, n_t). \quad (6.33)$$

Finally we work with the one-pion exchange potential (OPEP). In this case the pion acts much like the auxiliary fields. However there are also spatial correlations in the quadratic part of the pion action and a gradient coupling between the pions and nucleons. The one-pion exchange interaction on the lattice can be written as

$$\exp[-S_{\text{int}}^{\text{OPEP}}(c^*, c)] = \int \prod_I D\pi_I \exp[-S_{\pi_I \pi_I}(\pi_I) - S_{\pi_I}(c^*, c, \pi_I)]. \quad (6.34)$$

The free pion action is

$$S_{\pi_I \pi_I}(\pi_I) = \frac{1}{2} \alpha_t m_\pi^2 \sum_{\mathbf{n}, n_t, I} \pi_I^2(\mathbf{n}, n_t) \quad (6.35)$$

$$+ \frac{1}{2} \alpha_t \sum_{k=0,1,2,\dots} (-1)^k w_k \sum_{\mathbf{n}, n_t, I, \hat{\mathbf{l}}} \pi_I(\mathbf{n}, n_t) [\pi_I(\mathbf{n} + k\hat{\mathbf{l}}, n_t) + \pi_I(\mathbf{n} - k\hat{\mathbf{l}}, n_t)], \quad (6.36)$$

with the coefficient  $w_k$  as defined in Table 6.1 and  $m_\pi$  is the pion mass. At leading order we do not consider any isospin-breaking effects. The pion coupling to the nucleon is

$$S_{\pi_I}(c^*, c, \pi_I) = \frac{g_A \alpha_t}{2f_\pi} \sum_{\mathbf{n}, n_t, I, l} \Delta_k \pi_I(\mathbf{n}, n_t) c^*(\mathbf{n}, n_t) \sigma_k \tau_l c(\mathbf{n}, n_t), \quad (6.37)$$

where  $\sigma_l$  for  $l = 1, 2, 3$  are the Pauli matrices in spin space and

$$\Delta_l \pi_I(\mathbf{n}, n_t) = \frac{1}{2} \sum_{k=1,2,\dots} (-1)^{k-1} o_k [\pi_I(\mathbf{n} + k\hat{\mathbf{l}}, n_t) - \pi_I(\mathbf{n} - k\hat{\mathbf{l}}, n_t)], \quad (6.38)$$

with coefficients  $o_k$  corresponding to a hopping parameter expansion of the momentum,

$$P(p_l) = \sum_{k=1,2,\dots} (-1)^{k-1} o_k \sin(k p_l). \quad (6.39)$$

Here  $g_A$  is the axial-vector coupling constant, and  $f_\pi$  is the pion decay constant. The hopping coefficients can be chosen to match the continuum result

$$P(p_l) = p_l. \quad (6.40)$$

The hopping coefficients  $o_k$  for a few different lattice actions are shown in Table 6.2.

**Table 6.2** Hopping coefficients  $o_k$  for several lattice actions.

coefficient	standard	$O(a^2)$ -improved	$O(a^4)$ -improved
$o_1$	1	4/3	3/2
$o_2$	0	1/6	3/10
$o_3$	0	0	1/30

### 6.3.4 Transfer matrix operator with auxiliary field

Using the equivalence in Eq. (6.21), we can write  $\mathcal{Z}$  as the trace of a product of transfer matrix operators which depend on the auxiliary field,

$$\mathcal{Z} = \int Ds \prod_I (Ds_I D\pi_I) \exp[-S_{ss}(s) - S_{s_I s_I}(s_I) - S_{\pi_I \pi_I}(\pi_I)] \text{Tr} \left\{ M^{(L_t-1)} \dots M^{(0)} \right\}. \quad (6.41)$$

The transfer matrix at time step  $n_t$  is given by

$$M^{(n_t)} =: \exp \left[ -H^{(n_t)}(a^\dagger, a, s, s_I, \pi_I) \alpha_t \right] :, \quad (6.42)$$

where

$$H^{(n_t)}(a^\dagger, a, s, s_I, \pi_I) \alpha_t = H_{\text{free}}(a^\dagger, a) \alpha_t + S_s^{(n_t)}(a^\dagger, a, s) + S_{s_I}^{(n_t)}(a^\dagger, a, s_I) + S_{\pi_I}^{(n_t)}(a^\dagger, a, \pi_I), \quad (6.43)$$

and

$$S_s^{(n_t)}(a^\dagger, a, s) = \sqrt{-C\alpha_t} \sum_{\mathbf{n}} s(\mathbf{n}, n_t) a^\dagger(\mathbf{n}) a(\mathbf{n}), \quad (6.44)$$

$$S_{s_I}^{(n_t)}(a^\dagger, a, s_I) = \sqrt{-C'\alpha_t} \sum_{\mathbf{n}, I} s_I(\mathbf{n}, n_t) a^\dagger(\mathbf{n}) \tau_I a(\mathbf{n}), \quad (6.45)$$

$$S_{\pi_I}^{(n_t)}(a^\dagger, a, \pi_I) = \frac{g_A \alpha_t}{2f_\pi} \sum_{\mathbf{n}, k, I} \Delta_k \pi_I(\mathbf{n}, n_t) a^\dagger(\mathbf{n}) \sigma_k \tau_I a(\mathbf{n}). \quad (6.46)$$

## 6.4 Projection Monte Carlo

Let us consider a system with  $A$  nucleons. We can create a general single-nucleon state using creation operators acting on the vacuum with coefficient function  $f(\mathbf{n})$ . We write  $f(\mathbf{n})$  as a column vector in the space of nucleon spin and isospin components, and the single-nucleon state can be written as

$$|f\rangle = \sum_{\mathbf{n}} a^\dagger(\mathbf{n}) f(\mathbf{n}) |0\rangle. \quad (6.47)$$

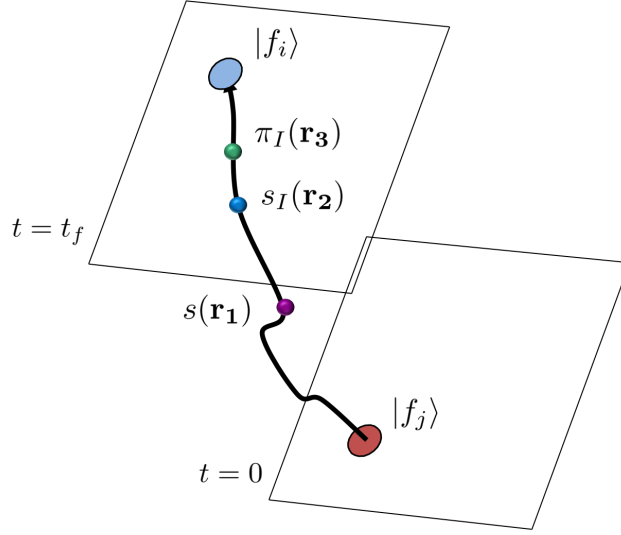
For our projection Monte Carlo calculation we take our  $A$ -body initial state to be a Slater determinant of single nucleon states,

$$|f_1, \dots, f_A\rangle = \left[ \sum_{\mathbf{n}} a^\dagger(\mathbf{n}) f_1(\mathbf{n}) \right] \cdots \left[ \sum_{\mathbf{n}} a^\dagger(\mathbf{n}) f_A(\mathbf{n}) \right] |0\rangle. \quad (6.48)$$

We use the same construction for the  $A$ -body final state.

For the purposes of coding the projection Monte Carlo calculation, it is convenient to view the identical nucleons as having a hidden index  $j = 1, \dots, A$  that makes all of the nucleons distinguishable. If we antisymmetrize all physical states over this extra index then all physical observables are exactly recovered. So our initial state  $|f_1, \dots, f_A\rangle$  becomes

$$\begin{aligned} & \frac{1}{\sqrt{A!}} \sum_P \left[ \sum_{\mathbf{n}} a_{[P(1)]}^\dagger(\mathbf{n}) f_1(\mathbf{n}) \right] \cdots \left[ \sum_{\mathbf{n}} a_{[P(A)]}^\dagger(\mathbf{n}) f_A(\mathbf{n}) \right] |0\rangle \\ &= \frac{1}{\sqrt{A!}} \sum_{P'} \text{sgn}(P') \left[ \sum_{\mathbf{n}} a_{[1]}^\dagger(\mathbf{n}) f_{P'(1)}(\mathbf{n}) \right] \cdots \left[ \sum_{\mathbf{n}} a_{[A]}^\dagger(\mathbf{n}) f_{P'(A)}(\mathbf{n}) \right] |0\rangle, \end{aligned} \quad (6.49)$$



**Fig. 6.3** A sketch showing the worldline for a single nucleon with a background of pion fields and auxiliary fields.

where the summations are over all permutations  $P$ , and  $\text{sgn}$  is the sign of the permutation. With these hidden indices our normal-ordered auxiliary-field transfer matrix  $M^{(n_t)}$  becomes

$$\left[1 - H^{(n_t)}(a_{[1]}^\dagger, a_{[1]}, s, s_I, \pi_I) \alpha_t\right] \cdots \left[1 - H^{(n_t)}(a_{[A]}^\dagger, a_{[A]}, s, s_I, \pi_I) \alpha_t\right] \quad (6.50)$$

We see that the higher-order powers of the exponential vanish due to normal ordering.

In the projection Monte Carlo calculation we compute the amplitude

$$Z(n_t) = \langle f_1, \dots, f_A | M^{(n_t-1)} \cdots M^{(0)} | f_1, \dots, f_A \rangle \quad (6.51)$$

for  $n_t = L_t$  and  $n_t = L_t - 1$ . In the limit of large  $L_t$  the amplitudes will be dominated by the state with the lowest energy  $E_0$  and nonzero overlap with  $|f_1, \dots, f_A\rangle$ . In this limit the ratio  $Z(n_t)/Z(n_t - 1)$  will converge to  $\exp(-E_0 \alpha_t)$  from above.

Each nucleon evolves as a particle in a fluctuating background of auxiliary fields and pion fields. The original interactions are reproduced after integrating over the fluctuating auxiliary and pion fields. For a simulation with  $A$  nucleons, the amplitude for a given configuration of pion and auxiliary fields is proportional to the determinant of an  $A \times A$  matrix  $\mathbf{M}$ . The entries of  $\mathbf{M}_{ij}$  are single nucleon worldline amplitudes for a nucleon starting at state  $|f_j\rangle$  at  $t = 0$  and ending at state  $|f_i\rangle$  at  $t = t_f = L_t \alpha_t$ . This is shown in Fig. 6.3.

In Fig. 6.4, we show a sample code which calculates the auxiliary-field transfer matrix multiplications on the left starting from the single-nucleon initial states. We only show the terms which arise from the free-nucleon transfer matrix and the auxiliary field  $s$ . Similarly, in Fig. 6.5, we show a sample code which calculates the auxiliary-field transfer matrix multiplications on the right starting from the single-nucleon final states. Again we present only the terms arising from the free-nucleon transfer matrix and the auxiliary field  $s$ . In Fig. 6.6 we show how these transfer matrix product multiplications are implemented as subroutines and used to compute the determinant and inverse of the matrix of single-nucleon amplitudes  $\mathbf{M}$ .

## 6.5 Importance sampling

We do importance sampling according to the positive measure

```

DO nt = nt1+1, nt2
  DO np = 0, num-1
    DO nz = 0, L-1; DO ny = 0, L-1; DO nx = 0, L-1
      DO ni = 0, 1; DO ns = 0, 1

        zvecs(nx,ny,nz,nt,ns,ni,np) = zvecs(nx,ny,nz,nt-1,ns,ni,np) &
          * (1.D0-6.D0*w0_N*h+CDSQRT(-c0*atovera*(1.D0,0.D0))*s(nx,ny,nz,nt-1))

        zvecs(nx,ny,nz,nt,ns,ni,np) = zvecs(nx,ny,nz,nt,ns,ni,np) &
          + w1_N*h*zvecs(MOD(nx+1,L),ny,nz,nt-1,ns,ni,np) &
          + w1_N*h*zvecs(MOD(nx-1+L,L),ny,nz,nt-1,ns,ni,np) &
          + w1_N*h*zvecs(nx,MOD(ny+1,L),nz,nt-1,ns,ni,np) &
          + w1_N*h*zvecs(nx,MOD(ny-1+L,L),nz,nt-1,ns,ni,np) &
          + w1_N*h*zvecs(nx,ny,MOD(nz+1,L),nt-1,ns,ni,np) &
          + w1_N*h*zvecs(nx,ny,MOD(nz-1+L,L),nt-1,ns,ni,np)

      IF (improveN >= 1) THEN
        zvecs(nx,ny,nz,nt,ns,ni,np) = zvecs(nx,ny,nz,nt,ns,ni,np) &
          - w2_N*h*zvecs(MOD(nx+2,L),ny,nz,nt-1,ns,ni,np) &
          - w2_N*h*zvecs(MOD(nx-2+L,L),ny,nz,nt-1,ns,ni,np) &
          - w2_N*h*zvecs(nx,MOD(ny+2,L),nz,nt-1,ns,ni,np) &
          - w2_N*h*zvecs(nx,MOD(ny-2+L,L),nz,nt-1,ns,ni,np) &
          - w2_N*h*zvecs(nx,ny,MOD(nz+2,L),nt-1,ns,ni,np) &
          - w2_N*h*zvecs(nx,ny,MOD(nz-2+L,L),nt-1,ns,ni,np)
      END IF

      IF (improveN == 2) THEN
        zvecs(nx,ny,nz,nt,ns,ni,np) = zvecs(nx,ny,nz,nt,ns,ni,np) &
          + w3_N*h*zvecs(MOD(nx+3,L),ny,nz,nt-1,ns,ni,np) &
          + w3_N*h*zvecs(MOD(nx-3+L,L),ny,nz,nt-1,ns,ni,np) &
          + w3_N*h*zvecs(nx,MOD(ny+3,L),nz,nt-1,ns,ni,np) &
          + w3_N*h*zvecs(nx,MOD(ny-3+L,L),nz,nt-1,ns,ni,np) &
          + w3_N*h*zvecs(nx,ny,MOD(nz+3,L),nt-1,ns,ni,np) &
          + w3_N*h*zvecs(nx,ny,MOD(nz-3+L,L),nt-1,ns,ni,np)
      END IF

    END DO; END DO
  END DO; END DO; END DO
END DO

```

**Fig. 6.4** Sample code which calculates the auxiliary-field transfer matrix multiplications on the left starting from the single-nucleon initial states. We only show the terms which arise from the free-nucleon transfer matrix and the auxiliary field  $s$ .

$$|Z(L_t)| \exp[-S_{ss}(s) - S_{s_I s_I}(s_I) - S_{\pi_I \pi_I}(\pi_I)], \quad (6.52)$$

and use hybrid Monte Carlo to do global updates of the auxiliary and pion fields. The hybrid Monte Carlo (HMC) algorithm [?, ?, ?] is efficient in quickly generating decorrelated configurations for each auxiliary and pion field. Here we describe the updating algorithm for the  $s$  field. The updating of the  $s_I$  and  $\pi_I$  fields proceed in a very similar fashion. In general terms, the HMC algorithm can be described by means of a probability weight  $P(s)$

$$P(s) \propto \exp[-V(s)], \quad (6.53)$$

where  $V(s)$  is in general a non-local function of the field  $s(\mathbf{n}, n_t)$ , and a molecular dynamics (MD) Hamiltonian,

$$H(s, p) \equiv \frac{1}{2} \sum_{\mathbf{n}, n_t} [p_s(\mathbf{n}, n_t)]^2 + V(s). \quad (6.54)$$

Classical Hamiltonian dynamics is introduced by defining the momentum  $p_s(\mathbf{n}, n_t)$  conjugate to  $s(\mathbf{n}, n_t)$ .



```

DO nt = nt2, nt1+1, -1
  DO np = 0, num-1
    DO nz = 0, L-1; DO ny = 0, L-1; DO nx = 0, L-1
      DO ni = 0, 1; DO ns = 0, 1

        zdualvecs(nx, ny, nz, nt-1, ns, ni, np) = zdualvecs(nx, ny, nz, nt, ns, ni, np) &
          * (1.D0-6.D0*w0_N*h+CDSQRT(-c0*atovera*(1.D0, 0.D0))*s(nx, ny, nz, nt-1))

        zdualvecs(nx, ny, nz, nt-1, ns, ni, np) = zdualvecs(nx, ny, nz, nt-1, ns, ni, np) &
          + w1_N*h*zdualvecs(MOD(nx+1, L), ny, nz, nt, ns, ni, np) &
          + w1_N*h*zdualvecs(MOD(nx-1+L, L), ny, nz, nt, ns, ni, np) &
          + w1_N*h*zdualvecs(nx, MOD(ny+1, L), nz, nt, ns, ni, np) &
          + w1_N*h*zdualvecs(nx, MOD(ny-1+L, L), nz, nt, ns, ni, np) &
          + w1_N*h*zdualvecs(nx, ny, MOD(nz+1, L), nt, ns, ni, np) &
          + w1_N*h*zdualvecs(nx, ny, MOD(nz-1+L, L), nt, ns, ni, np)

      IF (improveN >= 1) THEN
        zdualvecs(nx, ny, nz, nt-1, ns, ni, np) = zdualvecs(nx, ny, nz, nt-1, ns, ni, np) &
          - w2_N*h*zdualvecs(MOD(nx+2, L), ny, nz, nt, ns, ni, np) &
          - w2_N*h*zdualvecs(MOD(nx-2+L, L), ny, nz, nt, ns, ni, np) &
          - w2_N*h*zdualvecs(nx, MOD(ny+2, L), nz, nt, ns, ni, np) &
          - w2_N*h*zdualvecs(nx, MOD(ny-2+L, L), nz, nt, ns, ni, np) &
          - w2_N*h*zdualvecs(nx, ny, MOD(nz+2, L), nt, ns, ni, np) &
          - w2_N*h*zdualvecs(nx, ny, MOD(nz-2+L, L), nt, ns, ni, np)
      END IF

      IF (improveN == 2) THEN
        zdualvecs(nx, ny, nz, nt-1, ns, ni, np) = zdualvecs(nx, ny, nz, nt-1, ns, ni, np) &
          + w3_N*h*zdualvecs(MOD(nx+3, L), ny, nz, nt, ns, ni, np) &
          + w3_N*h*zdualvecs(MOD(nx-3+L, L), ny, nz, nt, ns, ni, np) &
          + w3_N*h*zdualvecs(nx, MOD(ny+3, L), nz, nt, ns, ni, np) &
          + w3_N*h*zdualvecs(nx, MOD(ny-3+L, L), nz, nt, ns, ni, np) &
          + w3_N*h*zdualvecs(nx, ny, MOD(nz+3, L), nt, ns, ni, np) &
          + w3_N*h*zdualvecs(nx, ny, MOD(nz-3+L, L), nt, ns, ni, np)
      END IF

    END DO; END DO
  END DO; END DO; END DO
END DO

```

**Fig. 6.5** Sample code which calculates auxiliary-field transfer matrix multiplications on the right starting from the single-nucleon final states. We only show terms involving the free-nucleon transfer matrix and the auxiliary field  $s$ .

**Fig. 6.6** Sample code showing how the transfer matrix product multiplications are called as subroutines and used to compute the determinant and inverse of the matrix of single-nucleon amplitudes.

```

CALL getzvecs(s, sI, zvecs, zwave, Lt, 0, &
  pion, ztau2x2, n_f)
CALL getzdualvecs(s, sI, zdualvecs, zdualwave, &
  Lt, 0, pion, ztau2x2, n_f)
CALL getinvcorr(zvecs, zdualvecs, zldeter, &
  zcorrmatrix, zcorrinv, Lt)
aldeterabs = DBLE(zldeter)
zdeterphase = CDEXP((0.D0, 1.D0)*DIMAG(zldeter))
act = bose - aldeterabs

```

Given an arbitrary initial configuration  $s^0(\mathbf{n}, n_t)$ , the conjugate momentum is chosen from a random Gaussian distribution according to

$$P[p_s^0(\mathbf{n}, n_t)] \propto \exp \left\{ -\frac{1}{2} [p_s^0(\mathbf{n}, n_t)]^2 \right\}, \quad (6.55)$$

after which the Hamiltonian equations of motion are integrated numerically with a small but nonzero step size  $\varepsilon_{\text{step}}$ . This method begins with a “half-step” forward in the conjugate momentum,

$$\tilde{p}_s^0(\mathbf{n}, n_t) = p_s^0(\mathbf{n}, n_t) - \frac{\epsilon_{\text{step}}}{2} \left[ \frac{\partial V(s)}{\partial s(\mathbf{n}, n_t)} \right]_{s=s^0}, \quad (6.56)$$

followed by repeated updates of  $s$  and  $\tilde{p}_s$  according to

$$s^{i+1}(\mathbf{n}, n_t) = s^i(\mathbf{n}, n_t) + \epsilon_{\text{step}} \tilde{p}_s^i(\mathbf{n}, n_t), \quad \tilde{p}_s^{i+1}(\mathbf{n}, n_t) = \tilde{p}_s^i(\mathbf{n}, n_t) - \epsilon_{\text{step}} \left[ \frac{\partial V(s)}{\partial s(\mathbf{n}, n_t)} \right]_{s=s^{i+1}}, \quad (6.57)$$

for a specified number of steps  $N_{\text{step}}$ . This is followed by an additional half-step backward in  $\tilde{p}_s$  given by

$$p_s^{N_{\text{step}}}(\mathbf{n}, n_t) = \tilde{p}_s^{N_{\text{step}}}(\mathbf{n}, n_t) + \frac{\epsilon_{\text{step}}}{2} \left[ \frac{\partial V(s)}{\partial s(\mathbf{n}, n_t)} \right]_{s=s^0}. \quad (6.58)$$

The length of such an MD “trajectory” should be taken large enough to ensure significant decorrelation between successive configurations of the auxiliary field. The evolved configuration is then subjected to a “Metropolis test” against a random number  $r \in [0, 1)$ . The new configuration is accepted if

$$r < \exp \left[ -H(s^{N_{\text{step}}}, p_s^{N_{\text{step}}}) + H(s^0, p_s^0) \right]. \quad (6.59)$$

It should be noted that although  $H$  is in principle conserved in the MD evolution, the truncation error of the leapfrog method introduces a systematic error. The Metropolis test eliminates the need for extrapolation in  $\epsilon_{\text{step}}$ .

In our case  $\exp[-V(s)]$  has the form

$$|Z(L_t)| \exp[-S_{ss}(s) - S_{s_I s_I}(s_I) - S_{\pi_I \pi_I}(\pi_I)], \quad (6.60)$$

where  $Z(L_t)$  is the determinant of an  $A \times A$  matrix of single-nucleon amplitudes  $\mathbf{M}$ . The derivative of  $V$  is then computed using

$$\begin{aligned} \frac{\partial V(s)}{\partial s(\mathbf{n}, n_t)} &= \frac{\partial S_{ss}(s)}{\partial s(\mathbf{n}, n_t)} - \frac{\partial \text{Re}[\ln(\det \mathbf{M})]}{\partial s(\mathbf{n}, n_t)} \\ &= \frac{\partial S_{ss}(s)}{\partial s(\mathbf{n}, n_t)} - \text{Re} \left[ \frac{1}{\det \mathbf{M}} \sum_{k,l} \frac{\partial \det \mathbf{M}}{\partial \mathbf{M}_{kl}} \frac{\partial \mathbf{M}_{kl}}{\partial s(\mathbf{n}, n_t)} \right] \\ &= \frac{\partial S_{ss}(s)}{\partial s(\mathbf{n}, n_t)} - \text{Re} \left[ \sum_{k,l} \mathbf{M}_{lk}^{-1} \frac{\partial \mathbf{M}_{kl}}{\partial s(\mathbf{n}, n_t)} \right]. \end{aligned} \quad (6.61)$$

In Fig. 6.7 we show a sample code calculating the quadratic part of the action due to the auxiliary fields and pion fields,

$$\frac{1}{2} \sum_{\mathbf{n}, n_t} [p_s(\mathbf{n}, n_t)]^2 + \frac{1}{2} \sum_{\mathbf{n}, n_t, I} [p_{s_I}(\mathbf{n}, n_t)]^2 + \frac{1}{2} \sum_{\mathbf{n}, n_t, I} [p_{\pi_I}(\mathbf{n}, n_t)]^2 + S_{ss}(s) + S_{s_I s_I}(s_I) + S_{\pi_I \pi_I}(\pi_I). \quad (6.62)$$

In the code we have found it convenient to rescale the pion field by a factor of  $\sqrt{q_\pi}$  where

$$q_\pi = \alpha_t (m_\pi^2 + 6w_0). \quad (6.63)$$

In Fig. 6.8 we show a sample code which calculates

$$\left[ \frac{\partial V(s)}{\partial s(\mathbf{n}, n_t)} \right]_{s=s^0} \quad (6.64)$$

and uses it to compute the half-step forward in the conjugate momentum,

```

bose = 0.D0
DO nt = 0, Lt-1
  DO nz = 0, L-1; DO ny = 0, L-1; DO nx = 0, L-1
    bose = bose &
      + s(nx,ny,nz,nt)**2.D0/2.D0 &
      + p_s(nx,ny,nz,nt)**2.D0/2.D0
  DO iso = 1,3
    bose = bose &
      + sI(nx,ny,nz,nt,iso)**2.D0/2.D0 &
      + p_sI(nx,ny,nz,nt,iso)**2.D0/2.D0 &
      + pion(nx,ny,nz,nt,iso)**2.D0/2.D0 &
      + atovera/qpi3*pion(nx,ny,nz,nt,iso)*( &
        - w1_P*pion(MOD(nx+1,L),ny,nz,nt,iso) &
        - w1_P*pion(nx,MOD(ny+1,L),nz,nt,iso) &
        - w1_P*pion(nx,ny,MOD(nz+1,L),nt,iso) &
        + w2_P*pion(MOD(nx+2,L),ny,nz,nt,iso) &
        + w2_P*pion(nx,MOD(ny+2,L),nz,nt,iso) &
        + w2_P*pion(nx,ny,MOD(nz+2,L),nt,iso) &
        - w3_P*pion(MOD(nx+3,L),ny,nz,nt,iso) &
        - w3_P*pion(nx,MOD(ny+3,L),nz,nt,iso) &
        - w3_P*pion(nx,ny,MOD(nz+3,L),nt,iso)) &
      + p_pion(nx,ny,nz,nt,iso)**2.D0/2.D0
  END DO
END DO; END DO; END DO
END DO

```

**Fig. 6.7** Sample code calculating the quadratic part of the action due to the auxiliary fields and pion fields.

```

DO npart1 = 0, n_f-1; DO npart2 = 0, n_f-1
  zdcorrmatrix(npart2,npart1) = 0.D0
  DO ni = 0,1; DO ns = 0,1
    zdcorrmatrix(npart2,npart1) = &
      zdcorrmatrix(npart2,npart1) + &
      zdualvecs(nx,ny,nz,nt+1,ns,ni,npart2) &
      *zvecs(nx,ny,nz,nt,ns,ni,npart1) &
      *CDSQRT(-c0*atovera*(1.D0,0.D0))/L**3
  END DO; END DO
END DO; END DO

dVds(nx,ny,nz,nt) = s(nx,ny,nz,nt)
DO npart1 = 0, n_f-1; DO npart2 = 0, n_f-1
  dVds(nx,ny,nz,nt) = dVds(nx,ny,nz,nt) &
    - DBLE(zdcorrmatrix(npart2,npart1) &
      *zcorrinv(npart1,npart2))
END DO; END DO

p_sHMC(nx,ny,nz,nt,0) = &
  p_s(nx,ny,nz,nt) - 0.5D0*eHMC*dVds(nx,ny,nz,nt)

```

**Fig. 6.8** Sample code which computes the derivative of the potential  $V(s)$  with respect to the auxiliary field  $s(\mathbf{n}, n_t)$  and uses it to compute the half-step forward in the conjugate momentum.

$$\tilde{p}_s^0(\mathbf{n}, n_t) = p_s^0(\mathbf{n}, n_t) - \frac{\epsilon_{\text{step}}}{2} \left[ \frac{\partial V(s)}{\partial s(\mathbf{n}, n_t)} \right]_{s=s^0}. \quad (6.65)$$

In Fig. 6.9 we show an example code which performs the Metropolis test against a random number  $r \in [0, 1)$ , with the new configuration being accepted if

$$r < \exp \left[ -H(s^{N_{\text{step}}}, p_s^{N_{\text{step}}}) + H(s^0, p_s^0) \right]. \quad (6.66)$$

Although importance sampling uses only the absolute volume, the complex phase of the determinant is treated as an observable and is collected with each configuration of the auxiliary and pion fields.

```

IF (ntrial .eq. 1 .or. grnd() .lt. DEXP(-actnew+act)) THEN
    accept = accept + 1.
DO nt = 0, Lt-1
    DO nz = 0, L-1; DO ny = 0, L-1; DO nx = 0, L-1
        s(nx,ny,nz,nt) = snew(nx,ny,nz,nt)
    END DO; END DO; END DO
END DO
DO nt = 0, Lt-1
    DO nz = 0, L-1; DO ny = 0, L-1; DO nx = 0, L-1
        DO iso = 1,3
            sI(nx,ny,nz,nt,iso) = sInew(nx,ny,nz,nt,iso)
            pion(nx,ny,nz,nt,iso) = pionnew(nx,ny,nz,nt,iso)
        END DO
    END DO; END DO; END DO
END DO
aldeterabs = aldeternewabs
zdeterphase = zdeternewphase
END IF

```

**Fig. 6.9** Sample code showing the Metropolis condition used to determine whether the new configuration is accepted or rejected.

## 6.6 Exercises

**6.1.** Write a lattice hybrid Monte Carlo code involving only the quadratic part of the action due to the auxiliary fields and pions,

$$\frac{1}{2} \sum_{\mathbf{n}, n_t} [p_s(\mathbf{n}, n_t)]^2 + \frac{1}{2} \sum_{\mathbf{n}, n_t, I} [p_{s_I}(\mathbf{n}, n_t)]^2 + \frac{1}{2} \sum_{\mathbf{n}, n_t, I} [p_{\pi_I}(\mathbf{n}, n_t)]^2 + S_{ss}(s) + S_{s_I s_I}(s_I) + S_{\pi_I \pi_I}(\pi_I). \quad (6.67)$$

Verify that the change in the action produced by the hybrid Monte Carlo update is scaling quadratically in the step size,  $\epsilon_{\text{step}}$ , in the limit  $\epsilon_{\text{step}} \rightarrow 0$  with  $N_{\text{step}} \epsilon_{\text{step}}$  held fixed.

**6.2.** Write a subroutine that generates the single-nucleon states on the lattice corresponding to the Slater-determinant state of four nucleons — proton spin-up, proton spin-down, neutron spin-up, and neutron spin-down — each with zero momentum.

**6.3.** Write a subroutine that extends the sample code in Fig. 6.4 to repeatedly multiply the auxiliary-field transfer matrix on the left starting from some initial single-nucleon wave functions. Include the contributions from the auxiliary fields  $s$  and  $s_I$  as well as the pion field  $\pi_I$ .

**6.4.** Write a subroutine that extends the sample code in Fig. 6.5 to repeatedly multiply the auxiliary-field transfer matrix on the right starting from some final single-nucleon wave functions. Include the contributions from the auxiliary fields  $s$  and  $s_I$  as well as the pion field  $\pi_I$ .

**6.5.** Use the Slater-determinant state constructed in Prob. 6.2 as the initial and final states. Apply the subroutines written in Prob. 6.3 and Prob. 6.4 with all coupling constants set to zero. Verify that this state is the ground state of the non-interacting system with energy equal to zero.

**6.6.** Use the Slater-determinant state constructed in Prob. 6.2 as the initial and final states. Then implement the subroutines written in Prob. 6.3 and Prob. 6.4 and extend the sample code in Fig. 6.8 to compute the derivatives of  $V(s)$  with respect to  $s(\mathbf{n}, n_t)$ ,  $s_I(\mathbf{n}, n_t)$ , and  $\pi_I(\mathbf{n}, n_t)$ .

**6.7.** Take the code you have written for Prob. 6.6 and complete the remaining steps needed to do hybrid Monte Carlo updates for  $s$ ,  $s_I$ , and  $\pi_I$ . Verify that the change in the action produced by the hybrid Monte Carlo update is scaling quadratically in  $\epsilon_{\text{step}}$  in the limit  $\epsilon_{\text{step}} \rightarrow 0$  with  $N_{\text{step}} \epsilon_{\text{step}}$  held fixed.

**6.8.** Take the code you have written for Prob. 6.7 and complete the remaining steps needed to calculate the energy of the four-nucleon ground state by computing the ratio of the amplitudes  $Z(L_t)/Z(L_t - 1)$ .

## Acknowledgements

The author is grateful for discussions with Amy Nicholson and Morten Hjorth-Jensen. He is also greatly indebted to his collaborators Jose Alarcón, Dechuan Du, Serdar Elhatisari, Evgeny Epelbaum, Nico Klein, Hermann Krebs, Timo Lähde, Ning Li, Bing-nan Lu, Thomas Luu, Ulf-G. Meißner, Alexander Rokash, and Gautam Rupak. Partial financial support provided by the U.S. Department of Energy (DE-FG02-03ER41260). Computational resources were provided by the Jülich Supercomputing Centre.

## Chapter 7

# From few to many nucleons and methods for nuclear reactions

Giuseppina Orlandini

**Abstract** Each chapter should be preceded by an abstract (10–15 lines long) that summarizes the content. The abstract will appear *online* at [www.SpringerLink.com](http://www.SpringerLink.com) and be available with unrestricted access. This allows unregistered users to read the abstract as a teaser for the complete chapter. As a general rule the abstracts will not appear in the printed version of your book unless it is the style of your particular book or that of the series to which your book belongs.

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### 7.1 The Nuclear few- and many-body problem

### 7.2 Methods for bound states based on the variational principle I: The No Core Shell Model (NCSM)

### 7.3 Methods for bound states based on the variational principle II: The Hyperspherical Harmonics (HH) method

### 7.4 Methods for reactions involving continuum states I: Perturbation induced reactions and integral transforms

### 7.5 Methods for reactions involving continuum states II: The continuum state problem reduced to a bound state problem

**Acknowledgements** If you want to include acknowledgments of assistance and the like at the end of an individual chapter please use the acknowledgement environment – it will automatically render Springer’s preferred layout.

## Appendix

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- The *two* recommended styles for references in books on *mathematical, physical, statistical and computer sciences* are depicted in [?, ?, ?, ?, ?] and [?, ?, ?, ?, ?].
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## Chapter 8

# High-performance computing Many-body methods and infinite nuclear matter

Justin G. Lietz, Samuel Novario, Gustav R. Jansen, Gaute Hagen, and Morten Hjorth-Jensen,

**Abstract** We present a computational approach to infinite nuclear matter employing Hartree-Fock theory, many-body perturbation theory and coupled cluster theory. These lectures are closely linked with those in chapters ?? and ?? and serve as input for the correlation functions employed in Monte Carlo calculations and in-medium similarity renormalization group theory of dense fermionic systems. We provide extensive code examples and benchmark calculations, allowing thereby an eventual reader to start writing her/his own codes. We start with an object-oriented serial code and end with in-depth discussions on strategies for porting the code to present and planned high-performance computing facilities.

### 8.1 Introduction

Studies of infinite nuclear matter play an important role in nuclear physics. The aim of this part of the lectures is to provide the necessary ingredients for performing studies of neutron star matter (or matter in  $\beta$ -equilibrium) and symmetric nuclear matter. The framework and formalism can easily be extended to other dense and homogeneous fermionic systems such as the electron gas in two and three dimensions.

Studies of dense baryonic matter are of central importance to our basic understanding of the stability of nuclear matter, spanning from matter at high densities and temperatures to matter as found within dense astronomical objects like neutron stars.

---

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Neutron star matter at densities of  $0.1 \text{ fm}^{-3}$  and greater, is often assumed to be made of mainly neutrons, protons, electrons and muons in beta equilibrium. However, other baryons like various hyperons may exist, as well as possible mesonic condensates and transitions to quark degrees of freedom at higher densities. In these notes we limit ourselves to matter composed of neutrons and protons only in chemical and electrical equilibrium. Furthermore, we will also consider matter at temperatures much lower than the typical Fermi energies. The equilibrium conditions are governed by the weak processes (normally referred to as the processes for  $\beta$ -equilibrium)

$$b_1 \rightarrow b_2 + l + \bar{\nu}_l \quad b_2 + l \rightarrow b_1 + \nu_l, \quad (8.1)$$

where  $b_1$  and  $b_2$  refer to e.g. the baryons being a neutron and a proton, respectively,  $l$  is either an electron or a muon and  $\bar{\nu}_l$  and  $\nu_l$  their respective anti-neutrinos and neutrinos. Muons typically appear at a density close to nuclear matter saturation density, the latter being

$$n_0 \approx 0.16 \pm 0.02 \quad \text{fm}^{-3},$$

with a corresponding binding energy  $\mathcal{E}_0$  for symmetric nuclear matter at saturation density of

$$\mathcal{E}_0 = B/A = -15.6 \pm 0.2 \quad \text{MeV}.$$

The pressure  $P$  is defined through the relation

$$P = n^2 \frac{\partial \mathcal{E}}{\partial n} = n \frac{\partial \mathcal{E}}{\partial n} - \mathcal{E}. \quad (8.2)$$

Similarly, the chemical potential for particle species  $i$  is given by

$$\mu_i = \left( \frac{\partial \mathcal{E}}{\partial n_i} \right). \quad (8.3)$$

In calculations of properties of neutron star matter in  $\beta$ -equilibrium, we will need to calculate the energy per baryon  $\mathcal{E}$  for e.g. several proton fractions  $x_p$ , which corresponds to the ratio of protons as compared to the total nucleon number ( $Z/A$ ), defined as

$$x_p = \frac{n_p}{n}, \quad (8.4)$$

where  $n = n_p + n_n$ , the total baryonic density if neutrons and protons are the only baryons present. In that case, the total Fermi momentum  $k_F$  and the Fermi momenta  $k_{Fp}$ ,  $k_{Fn}$  for protons and neutrons are related to the total nucleon density  $n$  by

$$\begin{aligned} n &= \frac{2}{3\pi^2} k_F^3 \\ &= x_p n + (1 - x_p) n \\ &= \frac{1}{3\pi^2} k_{Fp}^3 + \frac{1}{3\pi^2} k_{Fn}^3. \end{aligned} \quad (8.5)$$

The energy per baryon will thus be labelled as  $\mathcal{E}(n, x_p)$ .  $\mathcal{E}(n, 0)$  will then refer to the energy per baryon for pure neutron matter (PNM) while  $\mathcal{E}(n, \frac{1}{2})$  is the corresponding value for SNM. Furthermore, in this work, subscripts  $n, p, e, \mu$  will always refer to neutrons, protons, electrons and muons, respectively.

Since the mean free path of a neutrino in a neutron star is bigger than the typical radius of such a star ( $\sim 10 \text{ km}$ ), we will throughout assume that neutrinos escape freely from the neutron star, see for example the work of Prakash et al. for a discussion on trapped neutrinos.

Eq. (8.1) yields then the following conditions for matter in  $\beta$  equilibrium with for example nucleonic degrees freedom only

$$\mu_n = \mu_p + \mu_e, \quad (8.6)$$

and

$$n_p = n_e, \quad (8.7)$$

where  $\mu_i$  and  $n_i$  refer to the chemical potential and number density in  $\text{fm}^{-3}$  of particle species  $i$ . If muons are present as well, we need to modify the equation for charge conservation, Eq. (8.7), to read

$$n_p = n_e + n_\mu,$$

and require that  $\mu_e = \mu_\mu$ .

An important ingredient in the discussion of the EoS and the criteria for matter in  $\beta$ -equilibrium is the so-called symmetry energy  $\mathcal{S}(n)$ , defined as the difference in energy for symmetric nuclear matter and pure neutron matter

$$\mathcal{S}(n) = \mathcal{E}(n, x_p = 0) - \mathcal{E}(n, x_p = 1/2). \quad (8.8)$$

If we expand the energy per baryon in the case of nucleonic degrees of freedom only in the proton concentration  $x_p$  about the value of the energy for SNM ( $x_p = \frac{1}{2}$ ), we obtain,

$$\mathcal{E}(n, x_p) = \mathcal{E}(n, x_p = \frac{1}{2}) + \frac{1}{2} \frac{d^2 \mathcal{E}}{dx_p^2}(n) (x_p - 1/2)^2 + \dots, \quad (8.9)$$

where the term  $d^2 \mathcal{E} / dx_p^2$  is to be associated with the symmetry energy  $\mathcal{S}(n)$  in the empirical mass formula. If we assume that higher order derivatives in the above expansion are small (we will see examples of this in the next subsection), then through the conditions for  $\beta$ -equilibrium of Eqs. (8.6) and (8.7) and Eq. (8.3) we can define the proton fraction by the symmetry energy as

$$\hbar c (3\pi^2 n x_p)^{1/3} = 4\mathcal{S}(n) (1 - 2x_p), \quad (8.10)$$

where the electron chemical potential is given by  $\mu_e = \hbar c k_F$ , i.e. ultrarelativistic electrons are assumed. Thus, the symmetry energy is of paramount importance for studies of neutron star matter in  $\beta$ -equilibrium. One can extract information about the value of the symmetry energy at saturation density  $n_0$  from systematic studies of the masses of atomic nuclei. However, these results are limited to densities around  $n_0$  and for proton fractions close to  $\frac{1}{2}$ . Typical values for  $\mathcal{S}(n)$  at  $n_0$  are in the range 27 – 38 MeV. For densities greater than  $n_0$  it is more difficult to get a reliable information on the symmetry energy, and thereby the related proton fraction. We will shed more light on this topic in the next subsection.

## 8.2 Single-particle basis, Hamiltonians and models for the nuclear force

We begin our discussion

$$\Phi_{AS}(\alpha_1, \dots, \alpha_A; x_1, \dots, x_A) = \frac{1}{\sqrt{A}} \sum_{\vec{p}} (-1)^P \hat{P} \prod_{i=1}^A \psi_{\alpha_i}(x_i),$$

which is equivalent with  $|\alpha_1 \dots \alpha_A\rangle = a_{\alpha_1}^\dagger \dots a_{\alpha_A}^\dagger |0\rangle$ . We have also

$$a_p^\dagger |0\rangle = |p\rangle, \quad a_p |q\rangle = \delta_{pq} |0\rangle$$

$$\delta_{pq} = \{a_p, a_q^\dagger\},$$

and

$$\begin{aligned} 0 &= \{a_p^\dagger, a_q\} = \{a_p, a_q\} = \{a_p^\dagger, a_q^\dagger\} \\ |\Phi_0\rangle &= |\alpha_1 \dots \alpha_A\rangle, \quad \alpha_1, \dots, \alpha_A \leq \alpha_F \\ \{a_p^\dagger, a_q\} &= \delta_{pq}, p, q \leq \alpha_F \\ \{a_p, a_q^\dagger\} &= \delta_{pq}, p, q > \alpha_F \end{aligned}$$

with  $i, j, \dots \leq \alpha_F$ ,  $a, b, \dots > \alpha_F$ ,  $p, q, \dots$  – any

$$a_i |\Phi_0\rangle = |\Phi_i\rangle, \quad a_a^\dagger |\Phi_0\rangle = |\Phi^a\rangle$$

and

$$a_i^\dagger |\Phi_0\rangle = 0 \quad a_a |\Phi_0\rangle = 0$$

The one-body operator is defined as

$$\hat{F} = \sum_{pq} \langle p | \hat{f} | q \rangle a_p^\dagger a_q$$

while the two-body operator is defined as

$$\hat{V} = \frac{1}{4} \sum_{pqrs} \langle pq | \hat{v} | rs \rangle_{AS} a_p^\dagger a_q^\dagger a_s a_r$$

where we have defined the antisymmetric matrix elements

$$\langle pq | \hat{v} | rs \rangle_{AS} = \langle pq | \hat{v} | rs \rangle - \langle pq | \hat{v} | sr \rangle.$$

We can also define a three-body operator

$$\hat{V}_3 = \frac{1}{36} \sum_{pqrst} \langle pqr | \hat{v}_3 | stu \rangle_{AS} a_p^\dagger a_q^\dagger a_r^\dagger a_u a_t a_s$$

with the antisymmetrized matrix element

$$\langle pqr | \hat{v}_3 | stu \rangle_{AS} = \langle pqr | \hat{v}_3 | stu \rangle + \langle pqr | \hat{v}_3 | tus \rangle + \langle pqr | \hat{v}_3 | ust \rangle - \langle pqr | \hat{v}_3 | sut \rangle - \langle pqr | \hat{v}_3 | tsu \rangle - \langle pqr | \hat{v}_3 | uts \rangle. \quad (8.11)$$

$$\hat{H}_0 = \sum_{pq} \langle p | \hat{h}_0 | q \rangle a_p^\dagger a_q,$$

$$\hat{H}_0 = \sum_{pq} \langle p | \hat{h}_0 | q \rangle \{a_p^\dagger a_q\} + \sum_i \langle i | \hat{h}_0 | i \rangle.$$

$$\hat{H}_I = \frac{1}{4} \sum_{pqrs} \langle pq | \hat{v} | rs \rangle a_p^\dagger a_q^\dagger a_s a_r,$$

$$\hat{H}_I = \frac{1}{4} \sum_{pqrs} \langle pq | \hat{v} | rs \rangle \{a_p^\dagger a_q^\dagger a_s a_r\} + \sum_{pqi} \langle pi | \hat{v} | qi \rangle \{a_p^\dagger a_q\} + \frac{1}{2} \sum_{ij} \langle ij | \hat{v} | ij \rangle.$$

Explain again the meaning of the various symbols.

$$\hat{H}_3 = \frac{1}{36} \sum_{pqr \atop stu} \langle pqr | \hat{v}_3 | stu \rangle a_p^\dagger a_q^\dagger a_r^\dagger a_u a_t a_s,$$

and specify the contributions to the twobody, onebody and the scalar part.

This is a homogeneous system and the one-particle wave functions are given by plane wave functions normalized to a volume  $\Omega$  for a box with length  $L$  (the limit  $L \rightarrow \infty$  is to be taken after we have computed various expectation values)

$$\psi_{\mathbf{k}\sigma}(\mathbf{r}) = \frac{1}{\sqrt{\Omega}} \exp(i\mathbf{k}\mathbf{r}) \xi_{\sigma}$$

where  $\mathbf{k}$  is the wave number and  $\xi_{\sigma}$  is a spin function for either spin up or down

$$\xi_{\sigma=+1/2} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \xi_{\sigma=-1/2} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

We assume that we have periodic boundary conditions which limit the allowed wave numbers to

$$k_i = \frac{2\pi n_i}{L} \quad i = x, y, z \quad n_i = 0, \pm 1, \pm 2, \dots$$

We assume first that the electrons interact via a central, symmetric and translationally invariant interaction  $V(r_{12})$  with  $r_{12} = |\mathbf{r}_1 - \mathbf{r}_2|$ . The interaction is spin independent.

The total Hamiltonian consists then of kinetic and potential energy

$$\hat{H} = \hat{T} + \hat{V}.$$

The operator for the kinetic energy can be written as

$$\hat{T} = \sum_{\mathbf{k}\sigma} \frac{\hbar^2 k^2}{2m} a_{\mathbf{k}\sigma}^{\dagger} a_{\mathbf{k}\sigma}.$$

The Hamiltonian operator is given by

$$\hat{H} = \hat{H}_{el} + \hat{H}_b + \hat{H}_{el-b},$$

When using periodic boundary conditions, the discrete-momentum single-particle basis functions

$$\phi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} / L^{d/2}$$

are associated with the single-particle energy

$$\epsilon_{n_x, n_y} = \frac{\hbar^2}{2m} \left( \frac{2\pi}{L} \right)^2 (n_x^2 + n_y^2) \quad (8.12)$$

for two-dimensional systems and

$$\epsilon_{n_x, n_y, n_z} = \frac{\hbar^2}{2m} \left( \frac{2\pi}{L} \right)^2 (n_x^2 + n_y^2 + n_z^2) \quad (8.13)$$

for three-dimensional systems.

We choose the single-particle basis such that both the occupied and unoccupied single-particle spaces have a closed-shell structure. This means that all single-particle states corresponding to energies below a chosen cutoff are included in the basis. We study only the unpolarized spin phase, in which all orbitals are occupied with one spin-up and one spin-down electron.

The single-particle kinetic energy defined as

$$\frac{\hbar^2}{2m} (k_{n_x}^2 + k_{n_y}^2 + k_{n_z}^2),$$

and

$$k_{n_i} = \frac{2\pi n_i}{L} \quad n_i = 0, \pm 1, \pm 2, \dots,$$

we can set up a similar table and obtain (assuming identical particles one and including spin up and spin down solutions) for energies less than or equal to  $n_x^2 + n_y^2 + n_z^2 \leq 3$

$n_x^2 + n_y^2 + n_z^2$	$n_x$	$n_y$	$n_z$	$N_{\uparrow\downarrow}$
0	0	0	0	2
1	-1	0	0	
1	1	0	0	
1	0	-1	0	
1	0	1	0	
1	0	0	-1	
1	0	0	1	14
2	-1	-1	0	
2	-1	1	0	
2	1	-1	0	
2	1	1	0	
2	-1	0	-1	
2	-1	0	1	
2	1	0	-1	
2	1	0	1	
2	0	-1	-1	
2	0	-1	1	
2	0	1	-1	
2	0	1	1	38
3	-1	-1	-1	
3	-1	-1	1	
3	-1	1	-1	
3	-1	1	1	
3	1	-1	-1	
3	1	-1	1	
3	1	1	-1	
3	1	1	1	54

Continuing in this way we get for  $n_x^2 + n_y^2 + n_z^2 = 4$  a total of 22 additional states, resulting in 76 as a new magic number. For the lowest six energy values the degeneracy in energy gives us 2, 14, 38, 54, 76 and 114 as magic numbers. These numbers will then define our Fermi level when we compute the energy in a Cartesian basis. When performing calculations based on many-body perturbation theory, Coupled cluster theory or other many-body methods, we need then to add states above the Fermi level in order to sum over single-particle states which are not occupied.

If we wish to study infinite nuclear matter with both protons and neutrons, the above magic numbers become 4, 28, 76, 108, 132, 228, ...

Every number of particles for filled shells defines also the number of particles to be used in a given calculation. Use the number of particles to define the density of the system

$$\rho = g \frac{k_F^3}{6\pi^2},$$

where you need to define  $k_F$  and the degeneracy  $g$ , which is two for one type of spin-1/2 particles and four for symmetric nuclear matter.

Use the density to find the length  $L$  of the box used with periodic boundary contributions, that is use the relation

$$V = L^3 = \frac{A}{\rho}.$$

You can use  $L$  to define the spacing to set up the spacing between various  $k$ -values, that is

$$\Delta k = \frac{2\pi}{L}.$$

Here,  $A$  can be the number of nucleons. If we deal with the electron gas only, this needs to be replaced by the number of electrons  $N$ .

The total Hamiltonian consists then of kinetic and potential energy

$$\hat{H} = \hat{T} + \hat{V}.$$

The operator for the kinetic energy can be written as

$$\hat{T} = \sum_{\mathbf{k}\sigma} \frac{\hbar^2 k^2}{2m} a_{\mathbf{k}\sigma}^\dagger a_{\mathbf{k}\sigma}.$$

As mentioned above, we will employ a plane wave basis for our calculations of infinite matter properties. With a cartesian basis it means that we can calculate directly the various matrix elements, as discussed in the previous subsection. However, a cartesian basis represents an approximation to the thermodynamical limit. In order to compare the stability of our basis with results from the thermodynamical limit, it is convenient to rewrite the nucleon-nucleon interaction in terms of a partial wave expansion. This will allow us to compute the Hartree-Fock energy of the ground state in the thermodynamical limit (with the caveat that we need to limit the number of partial waves). In order to find the expressions for the Hartree-Fock energy in a partial wave basis, we will find it convenient to rewrite our two-body force in terms of the relative and center-of-mass motion momenta.

The direct matrix element, with single-particle three-dimensional momenta  $\mathbf{k}_i$ , spin  $\sigma_i$  and isospin  $\tau_i$ , is defined as

$$\langle \mathbf{k}_a \sigma_a \tau_a \mathbf{k}_b \sigma_b \tau_b | \hat{v} | \mathbf{k}_c \sigma_c \tau_c \mathbf{k}_d \sigma_d \tau_d \rangle,$$

or in a more compact form as  $\langle \mathbf{a} \mathbf{b} | \hat{v} | \mathbf{c} \mathbf{d} \rangle$  where the boldfaced letters  $\mathbf{a}$  etc represent the relevant quantum numbers, here momentum, spin and isospin. Introducing the relative momentum

$$\mathbf{k} = \frac{1}{2} (\mathbf{k}_a - \mathbf{k}_b),$$

and the center-of-mass momentum

$$\mathbf{K} = \mathbf{k}_a + \mathbf{k}_b,$$

we have

$$\langle \mathbf{k}_a \sigma_a \tau_a \mathbf{k}_b \sigma_b \tau_b | \hat{v} | \mathbf{k}_c \sigma_c \tau_c \mathbf{k}_d \sigma_d \tau_d \rangle = \langle \mathbf{K} \mathbf{K} \sigma_a \tau_a \sigma_b \tau_b | \hat{v} | \mathbf{K}' \mathbf{K}' \sigma_c \tau_c \sigma_d \tau_d \rangle.$$

The nucleon-nucleon interaction conserves the total momentum and is charge invariant, implying that the above uncoupled matrix element reads

$$\langle \mathbf{K} \mathbf{K} \sigma_a \tau_a \sigma_b \tau_b | \hat{v} | \mathbf{K}' \mathbf{K}' \sigma_c \tau_c \sigma_d \tau_d \rangle = \delta_{T_z, T'_z} \delta(\mathbf{K} - \mathbf{K}') \langle \mathbf{k} T_z S_z = (\sigma_a + \sigma_b) | \hat{v} | \mathbf{k}' T'_z S'_z = (\sigma_c + \sigma_d) \rangle,$$

where we have defined the isospin projections  $T_z = \tau_a + \tau_b$  and  $T'_z = \tau_c + \tau_d$ . Defining  $\hat{v} = \hat{v}(\mathbf{k}, \mathbf{k}')$ , we can rewrite the previous equation in a more compact form as

$$\delta_{T_z, T'_z} \delta(\mathbf{K} - \mathbf{K}') \langle \mathbf{k} T_z S_z = (\sigma_a + \sigma_b) | \hat{v} | \mathbf{k}' T'_z S'_z = (\sigma_c + \sigma_d) \rangle = \delta_{T_z, T'_z} \delta(\mathbf{K} - \mathbf{K}') \langle T_z S_z | \hat{v}(\mathbf{k}, \mathbf{k}') | T'_z S'_z \rangle.$$

These matrix elements can in turn be rewritten in terms of the total two-body quantum numbers for the spin  $S$  of two spin-1/2 fermions as

$$\langle \mathbf{k} T_z S_z | \hat{v}(\mathbf{k}, \mathbf{k}') | \mathbf{k}' T'_z S'_z \rangle = \sum_{SS'} \langle \frac{1}{2} \sigma_a \frac{1}{2} \sigma_b | SS_z \rangle \langle \frac{1}{2} \sigma_c \frac{1}{2} \sigma_d | S' S'_z \rangle \langle \mathbf{k} T_z SS_z | \hat{v}(\mathbf{k}, \mathbf{k}') | \mathbf{k}' T'_z S' S'_z \rangle$$

The coefficients  $\langle \frac{1}{2}\sigma_a \frac{1}{2}\sigma_b | SS_z \rangle$  are so-called Clebsch-Gordan recoupling coefficients. We will assume that our interactions break charge and isospin symmetry. We will refer to  $T_z = 0$  as the  $pn$  (proton-neutron) channel,  $T_z = -1$  as the  $pp$  (proton-proton) channel and  $T_z = 1$  as the  $nn$  (neutron-neutron) channel.

The nucleon-nucleon force is often derived and analyzed theoretically in terms of a partial wave expansion. A state with linear momentum  $\mathbf{k}$  can be written as

$$|\mathbf{k}\rangle = \sum_{l=0}^{\infty} \sum_{l_l=-l}^l t^l Y_l^{m_l}(\hat{\mathbf{k}}) |klm_l\rangle.$$

In terms of the relative and center-of-mass momenta  $\mathbf{k}$  and  $\mathbf{K}$ , the potential in momentum space is related to the nonlocal operator  $V(\mathbf{r}, \mathbf{r}')$  by

$$\langle \mathbf{k}' \mathbf{K}' | \hat{v} | \mathbf{k} \mathbf{K} \rangle = \int d\mathbf{r} d\mathbf{r}' e^{-i\mathbf{k}'\mathbf{r}'} V(\mathbf{r}', \mathbf{r}) e^{i\mathbf{k}\mathbf{r}} \delta(\mathbf{K}, \mathbf{K}'). \quad (8.14)$$

We will assume that the interaction is spherically symmetric and use the partial wave expansion of the plane waves in terms of spherical harmonics. This means that we can separate the radial part of the wave function from its angular dependence. The wave function of the relative motion is described in terms of plane waves as

$$e^{i\mathbf{k}\mathbf{r}} = \langle \mathbf{r} | \mathbf{k} \rangle = 4\pi \sum_{lm} t^l j_l(kr) Y_{lm}^*(\hat{\mathbf{k}}) Y_{lm}(\hat{\mathbf{r}}), \quad (8.15)$$

where  $j_l$  is a spherical Bessel function and  $Y_{lm}$  the spherical harmonic. This partial wave basis is useful for defining the operator for the nucleon-nucleon interaction, which is symmetric with respect to rotations, parity and isospin transformations. These symmetries imply that the interaction is diagonal with respect to the quantum numbers of total angular momentum  $J$ , spin  $S$  and isospin  $T$ . Using the above plane wave expansion, and coupling to final  $J$ ,  $S$  and  $T$  we get

$$\langle \mathbf{k}' | V | \mathbf{k} \rangle = (4\pi)^2 \sum_{JM} \sum_{lm} \sum_{l'm'} t^{l+l'} Y_{lm}^*(\hat{\mathbf{k}}) Y_{l'm'}(\hat{\mathbf{k}}') \mathcal{C}_{m'M_S M}^{l'SJ} \mathcal{C}_{m'M_S M}^{l'SJ} \langle k'l'STJM | V | k'l'STJM \rangle, \quad (8.16)$$

where we have defined

$$\langle k'l'STJM | V | k'l'STJM \rangle = \int j_{l'}(k'r') \langle l'STJM | V(r', r) | l'STJM \rangle j_l(kr) r'^2 dr' r^2 dr. \quad (8.17)$$

We have omitted the momentum of the center-of-mass motion  $\mathbf{K}$  and the corresponding orbital momentum  $L$ , since the interaction is diagonal in these variables. The potentials we will employ in this work, like those of the Bonn group, are all non-local potentials defined in momentum space, and we will therefore not need the last equation.

### 8.3 Hartree-Fock theory

Hartree-Fock (HF) theory is an algorithm for finding an approximative expression for the ground state of a given Hamiltonian. The basic ingredients are Define a single-particle basis  $\{\psi_\alpha\}$  so that

$$\hat{h}^{\text{HF}} \psi_\alpha = \varepsilon_\alpha \psi_\alpha$$

with the Hartree-Fock Hamiltonian defined as

$$\hat{h}^{\text{HF}} = \hat{t} + \hat{u}_{\text{ext}} + \hat{u}^{\text{HF}}$$

The term  $\hat{u}^{\text{HF}}$  is a single-particle potential to be determined by the HF algorithm. The HF algorithm means to choose  $\hat{u}^{\text{HF}}$  in order to have

$$\langle \hat{H} \rangle = E^{\text{HF}} = \langle \Phi_0 | \hat{H} | \Phi_0 \rangle$$

that is to find a local minimum with a Slater determinant  $\Phi_0$  being the ansatz for the ground state. The variational principle ensures that  $E^{\text{HF}} \geq E_0$ , with  $E_0$  the exact ground state energy.

We will show that the Hartree-Fock Hamiltonian  $\hat{h}^{\text{HF}}$  equals our definition of the operator  $\hat{f}$  discussed in connection with the new definition of the normal-ordered Hamiltonian (see later lectures), that is we have, for a specific matrix element

$$\langle p | \hat{h}^{\text{HF}} | q \rangle = \langle p | \hat{f} | q \rangle = \langle p | \hat{t} + \hat{u}_{\text{ext}} | q \rangle + \sum_{i \leq F} \langle p i | \hat{V} | q i \rangle_{AS},$$

meaning that

$$\langle p | \hat{u}^{\text{HF}} | q \rangle = \sum_{i \leq F} \langle p i | \hat{V} | q i \rangle_{AS}.$$

The so-called Hartree-Fock potential  $\hat{u}^{\text{HF}}$  brings an explicit medium dependence due to the summation over all single-particle states below the Fermi level  $F$ . It brings also in an explicit dependence on the two-body interaction (in nuclear physics we can also have complicated three- or higher-body forces). The two-body interaction, with its contribution from the other bystander fermions, creates an effective mean field in which a given fermion moves, in addition to the external potential  $\hat{u}_{\text{ext}}$  which confines the motion of the fermion. For systems like nuclei, there is no external confining potential. Nuclei are examples of self-bound systems, where the binding arises due to the intrinsic nature of the strong force. For nuclear systems thus, there would be no external one-body potential in the Hartree-Fock Hamiltonian.

Another possibility is to expand the single-particle functions in a known basis and vary the coefficients, that is, the new single-particle wave function is written as a linear expansion in terms of a fixed chosen orthogonal basis (for example the well-known harmonic oscillator functions or the hydrogen-like functions etc). We define our new Hartree-Fock single-particle basis by performing a unitary transformation on our previous basis (labelled with greek indices) as

$$\psi_p^{\text{HF}} = \sum_{\lambda} C_{p\lambda} \phi_{\lambda}. \quad (8.18)$$

In this case we vary the coefficients  $C_{p\lambda}$ . If the basis has infinitely many solutions, we need to truncate the above sum. We assume that the basis  $\phi_{\lambda}$  is orthogonal. A unitary transformation keeps the orthogonality, as discussed in exercise 1 below.

It is normal to choose a single-particle basis defined as the eigenfunctions of parts of the full Hamiltonian. The typical situation consists of the solutions of the one-body part of the Hamiltonian, that is we have

$$\hat{h}_0 \phi_{\lambda} = \epsilon_{\lambda} \phi_{\lambda}.$$

The single-particle wave functions  $\phi_{\lambda}(\mathbf{r})$ , defined by the quantum numbers  $\lambda$  and  $\mathbf{r}$  are defined as the overlap

$$\phi_{\lambda}(\mathbf{r}) = \langle \mathbf{r} | \lambda \rangle.$$

In our discussions hereafter we will use our definitions of single-particle states above and below the Fermi ( $F$ ) level given by the labels  $ijkl \dots \leq F$  for so-called single-hole states and  $abcd \dots > F$  for so-called particle states. For general single-particle states we employ the labels  $pqrs \dots$ .

$$E[\Phi] = \sum_{\mu=1}^A \langle \mu | h | \mu \rangle + \frac{1}{2} \sum_{\mu=1}^A \sum_{\nu=1}^A \langle \mu \nu | \hat{v} | \mu \nu \rangle_{AS},$$



we found the expression for the energy functional in terms of the basis function  $\phi_\lambda(\mathbf{r})$ . We then varied the above energy functional with respect to the basis functions  $|\mu\rangle$ . Now we are interested in defining a new basis defined in terms of a chosen basis as defined in Eq. (refeq:newbasis). We can then rewrite the energy functional as

$$E[\Phi^{HF}] = \sum_{i=1}^A \langle i|h|i\rangle + \frac{1}{2} \sum_{ij=1}^A \langle ij|\hat{v}|ij\rangle_{AS}, \quad (8.19)$$

where  $\Phi^{HF}$  is the new Slater determinant defined by the new basis of Eq. (refeq:newbasis).

Using Eq. (8.18) we can rewrite Eq. (8.19) as

$$E[\Psi] = \sum_{i=1}^A \sum_{\alpha\beta} C_{i\alpha}^* C_{i\beta} \langle \alpha|h|\beta\rangle + \frac{1}{2} \sum_{ij=1}^A \sum_{\alpha\beta\gamma\delta} C_{i\alpha}^* C_{j\beta}^* C_{i\gamma} C_{j\delta} \langle \alpha\beta|\hat{v}|\gamma\delta\rangle_{AS}. \quad (8.20)$$

We wish now to minimize the above functional. We introduce again a set of Lagrange multipliers, noting that since  $\langle i|j\rangle = \delta_{i,j}$  and  $\langle \alpha|\beta\rangle = \delta_{\alpha,\beta}$ , the coefficients  $C_{i\gamma}$  obey the relation

$$\langle i|j\rangle = \delta_{i,j} = \sum_{\alpha\beta} C_{i\alpha}^* C_{i\beta} \langle \alpha|\beta\rangle = \sum_{\alpha} C_{i\alpha}^* C_{i\alpha},$$

which allows us to define a functional to be minimized that reads

$$F[\Phi^{HF}] = E[\Phi^{HF}] - \sum_{i=1}^A \varepsilon_i \sum_{\alpha} C_{i\alpha}^* C_{i\alpha}. \quad (8.21)$$

Minimizing with respect to  $C_{i\alpha}^*$ , remembering that the equations for  $C_{i\alpha}^*$  and  $C_{i\alpha}$  can be written as two independent equations, we obtain

$$\frac{d}{dC_{i\alpha}^*} \left[ E[\Phi^{HF}] - \sum_j \varepsilon_j \sum_{\alpha} C_{j\alpha}^* C_{j\alpha} \right] = 0,$$

which yields for every single-particle state  $i$  and index  $\alpha$  (recalling that the coefficients  $C_{i\alpha}$  are matrix elements of a unitary (or orthogonal for a real symmetric matrix) matrix) the following Hartree-Fock equations

$$\sum_{\beta} C_{i\beta} \langle \alpha|h|\beta\rangle + \sum_{j=1}^A \sum_{\beta\gamma\delta} C_{j\beta}^* C_{j\delta} C_{i\gamma} \langle \alpha\beta|\hat{v}|\gamma\delta\rangle_{AS} = \varepsilon_i^{HF} C_{i\alpha}.$$

We can rewrite this equation as (changing dummy variables)

$$\sum_{\beta} \left\{ \langle \alpha|h|\beta\rangle + \sum_j \sum_{\gamma\delta} C_{j\gamma}^* C_{j\delta} \langle \alpha\gamma|\hat{v}|\beta\delta\rangle_{AS} \right\} C_{i\beta} = \varepsilon_i^{HF} C_{i\alpha}.$$

Note that the sums over greek indices run over the number of basis set functions (in principle an infinite number).

Defining

$$h_{\alpha\beta}^{HF} = \langle \alpha|h|\beta\rangle + \sum_{j=1}^A \sum_{\gamma\delta} C_{j\gamma}^* C_{j\delta} \langle \alpha\gamma|\hat{v}|\beta\delta\rangle_{AS},$$

we can rewrite the new equations as

$$\sum_{\gamma} h_{\alpha\beta}^{HF} C_{i\beta} = \varepsilon_i^{HF} C_{i\alpha}. \quad (8.22)$$

The latter is nothing but a standard eigenvalue problem. Compared with Eq. (refeq:hartreefockcoordinatespace), we see that we do not need to compute any integrals in an iterative procedure for solving the equations. It suffices to tabulate the matrix elements  $\langle \alpha | h | \beta \rangle$  and  $\langle \alpha \gamma | \hat{v} | \beta \delta \rangle_{AS}$  once and for all. Successive iterations require thus only a look-up in tables over one-body and two-body matrix elements. These details will be discussed below when we solve the Hartree-Fock equations numerical.

Our Hartree-Fock matrix is thus

$$\hat{h}_{\alpha\beta}^{HF} = \langle \alpha | \hat{h}_0 | \beta \rangle + \sum_{j=1}^A \sum_{\gamma\delta} C_{j\gamma}^* C_{j\delta} \langle \alpha \gamma | \hat{v} | \beta \delta \rangle_{AS}.$$

The Hartree-Fock equations are solved in an iterative waym starting with a guess for the coefficients  $C_{j\gamma} = \delta_{j,\gamma}$  and solving the equations by diagonalization till the new single-particle energies  $\epsilon_i^{HF}$  do not change anymore by a prefixed quantity.

Normally we assume that the single-particle basis  $|\beta\rangle$  forms an eigenbasis for the operator  $\hat{h}_0$ , meaning that the Hartree-Fock matrix becomes

$$\hat{h}_{\alpha\beta}^{HF} = \epsilon_\alpha \delta_{\alpha,\beta} + \sum_{j=1}^A \sum_{\gamma\delta} C_{j\gamma}^* C_{j\delta} \langle \alpha \gamma | \hat{v} | \beta \delta \rangle_{AS}.$$

The Hartree-Fock eigenvalue problem

$$\sum_{\beta} \hat{h}_{\alpha\beta}^{HF} C_{i\beta} = \epsilon_i^{HF} C_{i\alpha},$$

can be written out in a more compact form as

$$\hat{h}^{HF} \hat{C} = \epsilon^{HF} \hat{C}.$$

The Hartree-Fock equations are, in their simplest form, solved in an iterative way, starting with a guess for the coefficients  $C_{i\alpha}$ . We label the coefficients as  $C_{i\alpha}^{(n)}$ , where the subscript  $n$  stands for iteration  $n$ . To set up the algorithm we can proceed as follows:

We start with a guess  $C_{i\alpha}^{(0)} = \delta_{i,\alpha}$ . Alternatively, we could have used random starting values as long as the vectors are normalized. Another possibility is to give states below the Fermi level a larger weight. The Hartree-Fock matrix simplifies then to (assuming that the coefficients  $C_{i\alpha}$  are real)

$$\hat{h}_{\alpha\beta}^{HF} = \epsilon_\alpha \delta_{\alpha,\beta} + \sum_{j=1}^A \sum_{\gamma\delta} C_{j\gamma}^{(0)} C_{j\delta}^{(0)} \langle \alpha \gamma | \hat{v} | \beta \delta \rangle_{AS}.$$

Solving the Hartree-Fock eigenvalue problem yields then new eigenvectors  $C_{i\alpha}^{(1)}$  and eigenvalues  $\epsilon_i^{HF(1)}$ . With the new eigenvalues we can set up a new Hartree-Fock potential

$$\sum_{j=1}^A \sum_{\gamma\delta} C_{j\gamma}^{(1)} C_{j\delta}^{(1)} \langle \alpha \gamma | \hat{v} | \beta \delta \rangle_{AS}.$$

The diagonalization with the new Hartree-Fock potential yields new eigenvectors and eigenvalues. This process is continued till for example

$$\frac{\sum_p |\epsilon_i^{(n)} - \epsilon_i^{(n-1)}|}{m} \leq \lambda,$$

where  $\lambda$  is a user prefixed quantity ( $\lambda \sim 10^{-8}$  or smaller) and  $p$  runs over all calculated single-particle energies and  $m$  is the number of single-particle states.

We can rewrite the ground state energy by adding and subtracting  $\hat{u}^{HF}(x_i)$

$$E_0^{HF} = \langle \Phi_0 | \hat{H} | \Phi_0 \rangle = \sum_{i \leq F}^A \langle i | \hat{h}_0 + \hat{u}^{HF} | j \rangle + \frac{1}{2} \sum_{i \leq F}^A \sum_{j \leq F}^A [\langle ij | \hat{v} | ij \rangle - \langle ij | \hat{v} | ji \rangle] - \sum_{i \leq F}^A \langle i | \hat{u}^{HF} | i \rangle,$$

which results in

$$E_0^{HF} = \sum_{i \leq F}^A \epsilon_i^{HF} + \frac{1}{2} \sum_{i \leq F}^A \sum_{j \leq F}^A [\langle ij | \hat{v} | ij \rangle - \langle ij | \hat{v} | ji \rangle] - \sum_{i \leq F}^A \langle i | \hat{u}^{HF} | i \rangle.$$

Our single-particle states  $ijk \dots$  are now single-particle states obtained from the solution of the Hartree-Fock equations.

Using our definition of the Hartree-Fock single-particle energies we obtain then the following expression for the total ground-state energy

$$E_0^{HF} = \sum_{i \leq F}^A \epsilon_i - \frac{1}{2} \sum_{i \leq F}^A \sum_{j \leq F}^A [\langle ij | \hat{v} | ij \rangle - \langle ij | \hat{v} | ji \rangle].$$

### 8.3.1 Introducing our first ansatz for the ground state

### 8.3.2 Slater determinants as basis states

The simplest possible choice for many-body wavefunctions are **product** wavefunctions. That is

$$\Psi(x_1, x_2, x_3, \dots, x_A) \approx \phi_1(x_1) \phi_2(x_2) \phi_3(x_3) \dots$$

because we are really only good at thinking about one particle at a time. Such product wavefunctions, without correlations, are easy to work with; for example, if the single-particle states  $\phi_i(x)$  are orthonormal, then the product wavefunctions are easy to orthonormalize.

Similarly, computing matrix elements of operators are relatively easy, because the integrals factorize.

The price we pay is the lack of correlations, which we must build up by using many, many product wavefunctions.

Because we have fermions, we are required to have antisymmetric wavefunctions, that is

$$\Psi(x_1, x_2, x_3, \dots, x_A) = -\Psi(x_2, x_1, x_3, \dots, x_A)$$

etc. This is accomplished formally by using the determinantal formalism

$$\Psi(x_1, x_2, \dots, x_A) = \frac{1}{\sqrt{A!}} \det \begin{vmatrix} \phi_1(x_1) & \phi_1(x_2) & \dots & \phi_1(x_A) \\ \phi_2(x_1) & \phi_2(x_2) & \dots & \phi_2(x_A) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_A(x_1) & \phi_A(x_2) & \dots & \phi_A(x_A) \end{vmatrix}$$

Product wavefunction + antisymmetry (Pauli principle) = Slater determinant.

Properties of the determinant (interchange of any two rows or any two columns yields a change in sign; thus no two rows and no two columns can be the same) lead to the following consequence of the Pauli principle:

- No two particles can be at the same place (two columns the same); and
- No two particles can be in the same state (two rows the same).

As a practical matter, however, Slater determinants beyond  $N = 4$  quickly become unwieldy. Thus we turn to the **occupation representation** or **second quantization** to simplify calculations.

The occupation representation, using fermion **creation** and **annihilation** operators, is compact and efficient. It is also abstract and, at first encounter, not easy to internalize. It is inspired by other operator formalism, such as the ladder operators for the harmonic oscillator or for angular momentum, but unlike those cases, the operators **do not have coordinate space representations**.

Instead, one can think of fermion creation/annihilation operators as a game of symbols that compactly reproduces what one would do, albeit clumsily, with full coordinate-space Slater determinants.

We start with a set of orthonormal single-particle states  $\{\phi_i(x)\}$ . (Note: this requirement, and others, can be relaxed, but leads to a more involved formalism.) **Any** orthonormal set will do.

To each single-particle state  $\phi_i(x)$  we associate a creation operator  $\hat{a}_i^\dagger$  and an annihilation operator  $\hat{a}_i$ .

When acting on the vacuum state  $|0\rangle$ , the creation operator  $\hat{a}_i^\dagger$  causes a particle to occupy the single-particle state  $\phi_i(x)$ :

$$\phi_i(x) \rightarrow \hat{a}_i^\dagger |0\rangle$$

But with multiple creation operators we can occupy multiple states:

$$\phi_i(x)\phi_j(x')\phi_k(x'') \rightarrow \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_k^\dagger |0\rangle.$$

Now we impose antisymmetry, by having the fermion operators satisfy **anticommutation relations**:

$$\hat{a}_i^\dagger \hat{a}_j^\dagger + \hat{a}_j^\dagger \hat{a}_i^\dagger = [\hat{a}_i^\dagger, \hat{a}_j^\dagger]_+ = \{\hat{a}_i^\dagger, \hat{a}_j^\dagger\} = 0$$

so that

$$\hat{a}_i^\dagger \hat{a}_j^\dagger = -\hat{a}_j^\dagger \hat{a}_i^\dagger$$

Because of this property, automatically  $\hat{a}_i^\dagger \hat{a}_i^\dagger = 0$ , enforcing the Pauli exclusion principle. Thus when writing a Slater determinant using creation operators,

$$\hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_k^\dagger \dots |0\rangle$$

each index  $i, j, k, \dots$  must be unique.

### 8.3.3 The Brueckner $G$ -matrix

The Brueckner  $G$ -matrix has historically been an important ingredient in many-body calculations of nuclear systems. In this section, we will briefly survey the philosophy behind the  $G$ -matrix.

Historically, the  $G$ -matrix was developed in microscopic nuclear matter calculations using realistic nucleon-nucleon (NN) interactions. It is an ingenious as well as an interesting method to overcome the difficulties caused by the strong, short-range repulsive core contained in all modern models for the NN interaction. The  $G$ -matrix method was originally developed by Brueckner, and further developed by Goldstone and Bethe, Brandow and Petschek. In the literature it is generally referred to as the Brueckner theory or the Brueckner-Bethe-Goldstone theory.

Suppose we want to calculate the nuclear matter ground-state energy  $E_0$  using the non-relativistic Schrödinger equation

$$H\Psi_0(A) = E_0(A)\Psi_0(A), \quad (8.23)$$

with  $H = T + V$  where  $A$  denotes the number of particles,  $T$  is the kinetic energy and  $V$  is the nucleon-nucleon (NN) potential. Models for the NN interaction are discussed in the chapter on nuclear forces. The corresponding unperturbed problem is

$$H_0\psi_0(A) = W_0(A)\psi_0(A). \quad (8.24)$$

Here  $H_0$  is just kinetic energy  $T$  and  $\psi_0$  is a Slater determinant representing the Fermi sea, where all orbits through the Fermi momentum  $k_F$  are filled. We write

$$E_0 = W_0 + \Delta E_0, \quad (8.25)$$

where  $\Delta E_0$  is the ground-state energy shift or correlation energy as it was defined in many-body perturbation theory. If we know how to calculate  $\Delta E_0$ , then we know  $E_0$ , since  $W_0$  is easily obtained. In the limit  $A \rightarrow \infty$ , the quantities  $E_0$  and  $\Delta E_0$  themselves are not well defined, but the ratios  $E_0/A$  and  $\Delta E_0/A$  are. The nuclear-matter binding energy per nucleon is commonly denoted by  $BE/A$ , which is just  $-E_0/A$ . In passing, we note that the empirical value for symmetric nuclear matter (proton number  $Z$ =neutron number  $N$ ) is  $\approx 16$  MeV. There exists a formal theory for the calculation of  $\Delta E_0$ . According to the well-known Goldstone linked-diagram theory, the energy shift  $\Delta E_0$  is given exactly by the diagrammatic expansion shown in Fig. ???. This theory, is a linked-cluster perturbation expansion for the ground state energy of a many-body system, and applies equally well to both nuclear matter and closed-shell nuclei such as the doubly magic nucleus  $^{40}\text{Ca}$ . We will not discuss the Goldstone expansion, but rather discuss briefly how it is used in calculations.

Using the standard diagram rules (see the discussion on coupled-cluster theory and many-body perturbation theory), the various diagrams contained in the above figure can be readily calculated (in an uncoupled scheme)

$$(i) = \frac{(-)^{n_h+n_l}}{2^{n_{ep}}} \sum_{ij \leq k_F} \langle ij | \hat{v} | ij \rangle_{AS}, \quad (8.26)$$

with  $n_h = n_l = 2$  and  $n_{ep} = 1$ . As discussed in connection with the diagram rules in the many-body perturbation theory chapter,  $n_h$  denotes the number of hole lines,  $n_l$  the number of closed fermion loops and  $n_{ep}$  is the number of so-called equivalent pairs. The factor  $1/2^{n_{ep}}$  is needed since we want to count a pair of particles only once. We will carry this factor  $1/2$  with us in the equations below. The subscript  $AS$  denotes the antisymmetrized and normalized matrix element

$$\langle ij | \hat{v} | ij \rangle_{AS} = \langle ij | \hat{v} | ij \rangle - \langle ji | \hat{v} | ij \rangle. \quad (8.27)$$

Similarly, diagrams (ii) and (iii) read

$$(ii) = \frac{(-)^{2+2}}{2^2} \sum_{ij \leq k_F} \sum_{ab > k_F} \frac{\langle ij | \hat{v} | ab \rangle_{AS} \langle ab | \hat{v} | ij \rangle_{AS}}{\epsilon_i + \epsilon_j - \epsilon_a - \epsilon_b}, \quad (8.28)$$

and

$$(iii) = \frac{(-)^{2+2}}{2^3} \sum_{k_i, k_j \leq k_F} \sum_{abcd > k_F} \frac{\langle ij | \hat{v} | ab \rangle_{AS} \langle ab | \hat{v} | cd \rangle_{AS} \langle cd | \hat{v} | ij \rangle_{AS}}{(\epsilon_i + \epsilon_j - \epsilon_a - \epsilon_b)(\epsilon_i + \epsilon_j - \epsilon_c - \epsilon_d)}. \quad (8.29)$$

In the above,  $\epsilon$  denotes the sp energies defined by  $H_0$ . The steps leading to the above expressions for the various diagrams are rather straightforward. Though, if we wish to compute

the matrix elements for the interaction  $v$ , a serious problem arises. Typically, the matrix elements will contain a term (see the next section for the formal details)  $V(|\mathbf{r}|)$ , which represents the interaction potential  $V$  between two nucleons, where  $\mathbf{r}$  is the internucleon distance. All modern models for  $V$  have a strong short-range repulsive core. Hence, matrix elements involving  $V(|\mathbf{r}|)$ , will result in large (or infinitely large for a potential with a hard core) and repulsive contributions to the ground-state energy. Thus, the diagrammatic expansion for the ground-state energy in terms of the potential  $V(|\mathbf{r}|)$  becomes meaningless.

One possible solution to this problem is provided by the well-known Brueckner theory or the Brueckner  $G$ -matrix, or just the  $G$ -matrix. In fact, the  $G$ -matrix is an almost indispensable tool in almost every microscopic nuclear structure calculation. Its main idea may be paraphrased as follows. Suppose we want to calculate the function  $f(x) = x/(1+x)$ . If  $x$  is small, we may expand the function  $f(x)$  as a power series  $x + x^2 + x^3 + \dots$  and it may be adequate to just calculate the first few terms. In other words,  $f(x)$  may be calculated using a low-order perturbation method. But if  $x$  is large (or infinitely large), the above power series is obviously meaningless. However, the exact function  $x/(1+x)$  is still well defined in the limit of  $x$  becoming very large.

These arguments suggest that one should sum up the diagrams (i), (ii), (iii) in fig. ?? and the similar ones to all orders, instead of computing them one by one. Denoting this all-order sum as  $1/2\tilde{G}_{ijij}$ , where we have introduced the shorthand notation  $\tilde{G}_{ijij} = \langle k_i k_j | \tilde{G} | k_i k_j \rangle_{AS}$  (and similarly for  $\tilde{v}$ ), we have that

$$\begin{aligned} \frac{1}{2}\tilde{G}_{ijij} = & \frac{1}{2}\hat{v}_{ijij} + \sum_{ab > k_F} \frac{1}{2}\hat{v}_{ijab} \frac{1}{\epsilon_i + \epsilon_j - \epsilon_a - \epsilon_b} \\ & \times \left[ \frac{1}{2}\hat{v}_{abij} + \sum_{cd > k_F} \frac{1}{2}\hat{v}_{abcd} \frac{1}{\epsilon_i + \epsilon_j - \epsilon_c - \epsilon_d} \frac{1}{2}V_{cdij} + \dots \right]. \end{aligned} \quad (8.30)$$

The factor  $1/2$  is the same as that discussed above, namely we want to count a pair of particles only once. The quantity inside the brackets is just  $1/2\tilde{G}_{mni j}$  and the above equation can be rewritten as an integral equation

$$\tilde{G}_{ijij} = \tilde{V}_{ijij} + \sum_{ab > F} \frac{1}{2}\hat{v}_{ijab} \frac{1}{\epsilon_i + \epsilon_j - \epsilon_a - \epsilon_b} \tilde{G}_{abij}. \quad (8.31)$$

Note that  $\tilde{G}$  is the antisymmetrized  $G$ -matrix since the potential  $\tilde{v}$  is also antisymmetrized. This means that  $\tilde{G}$  obeys

$$\tilde{G}_{ijij} = -\tilde{G}_{jiij} = -\tilde{G}_{ijji}. \quad (8.32)$$

The  $\tilde{G}$ -matrix is defined as

$$\tilde{G}_{ijij} = G_{ijij} - G_{jiij}, \quad (8.33)$$

and the equation for  $G$  is

$$G_{ijij} = V_{ijij} + \sum_{ab > k_F} V_{ijab} \frac{1}{\epsilon_i + \epsilon_j - \epsilon_a - \epsilon_b} G_{abij}, \quad (8.34)$$

which is the familiar  $G$ -matrix equation. The above matrix is specifically designed to treat a class of diagrams contained in  $\Delta E_0$ , of which typical contributions were shown in fig. ?. In fact the sum of the diagrams in fig. ?? is equal to  $1/2(G_{ijij} - G_{jiij})$ .

Let us now define a more general  $G$ -matrix as

$$G_{ijij} = V_{ijij} + \sum_{mn > 0} V_{ijmn} \frac{Q(mn)}{\omega - \epsilon_m - \epsilon_n} G_{mni j}, \quad (8.35)$$

which is an extension of Eq. (8.34). Note that Eq. (8.34) has  $\varepsilon_i + \varepsilon_j$  in the energy denominator, whereas in the latter equation we have a general energy variable  $\omega$  in the denominator. Furthermore, in Eq. (8.34) we have a restricted sum over  $mn$ , while in Eq. (8.35) we sum over all  $ab$  and we have introduced a weighting factor  $Q(ab)$ . In Eq. (8.35)  $Q(ab)$  corresponds to the choice

$$Q(a, b) = \begin{cases} 1, & \min(a, b) > k_F \\ 0, & \text{else.} \end{cases}, \quad (8.36)$$

where  $Q(ab)$  is usually referred to as the  $G$ -matrix Pauli exclusion operator. The role of  $Q$  is to enforce a selection of the intermediate states allowed in the  $G$ -matrix equation. The above  $Q$  requires that the intermediate particles  $a$  and  $b$  must be both above the Fermi surface defined by  $F$ . We may enforce a different requirement by using a summation over intermediate states different from that in Eq. (8.35). An example is the Pauli operator for the model-space Brueckner-Hartree-Fock method discussed below.

Before ending this section, let us rewrite the  $G$ -matrix equation in a more compact form. The sp energies  $\varepsilon$  and wave functions are defined by the unperturbed hamiltonian  $H_0$  as

$$H_0|\psi_a\psi_b\rangle = (\varepsilon_a + \varepsilon_b)|\psi_a\psi_b\rangle. \quad (8.37)$$

The  $G$ -matrix equation can then be rewritten in the following compact form

$$G(\omega) = V + V \frac{\hat{Q}}{\omega - H_0} G(\omega), \quad (8.38)$$

with  $\hat{Q} = \sum_{ab} |\psi_a\psi_b\rangle\langle\psi_a\psi_b|$ . In terms of diagrams,  $G$  corresponds to an all-order sum of the "ladder-type" interactions between two particles with the intermediate states restricted by  $Q$ .

The  $G$ -matrix equation has a very simple form. But its calculation is rather complicated, particularly for finite nuclear systems such as the nucleus  $^{18}\text{O}$ . There are a number of complexities. To mention a few, the Pauli operator  $Q$  may not commute with the unperturbed hamiltonian  $H_0$  and we have to make the replacement

$$\frac{Q}{\omega - H_0} \rightarrow Q \frac{1}{\omega - QH_0Q} Q.$$

The determination of the starting energy  $\omega$  is also another problem.

In a medium such as nuclear matter we must account for the fact that certain states are not available as intermediate states in the calculation of the  $G$ -matrix. Following the discussion above this is achieved by introducing the medium dependent Pauli operator  $Q$ . Further, the energy  $\omega$  of the incoming particles, given by a pure kinetic term in a scattering problem between two unbound particles (for example two colliding protons), must be modified so as to allow for medium corrections. How to evaluate the Pauli operator for nuclear matter is, however, not straightforward. Before discussing how to evaluate the Pauli operator for nuclear matter, we note that the  $G$ -matrix is conventionally given in terms of partial waves and the coordinates of the relative and center-of-mass motion. If we assume that the  $G$ -matrix is diagonal in  $\alpha$  ( $\alpha$  is a shorthand notation for  $J, S, L$  and  $T$ ), we write the equation for the  $G$ -matrix as a coupled-channels equation in the relative and center-of-mass system

$$G_{ll'}^\alpha(kk'K\omega) = V_{ll'}^\alpha(kk') + \sum_{l''} \int \frac{d^3q}{(2\pi)^3} V_{ll''}^\alpha(kq) \frac{Q(q, K)}{\omega - H_0} G_{l''l'}^\alpha(qk'K\omega). \quad (8.39)$$

This equation is similar in structure to the scattering equations discussed in connection with nuclear forces (see the chapter on models for nuclear forces), except that we now have introduced the Pauli operator  $Q$  and a medium dependent two-particle energy  $\omega$ . The notations in

this equation follow those of the chapter on nuclear forces where we discuss the solution of the scattering matrix  $T$ . The numerical details on how to solve the above  $G$ -matrix equation through matrix inversion techniques are discussed below. Note however that the  $G$ -matrix may not be diagonal in  $\alpha$ . This is due to the fact that the Pauli operator  $Q$  is not diagonal in the above representation in the relative and center-of-mass system. The Pauli operator depends on the angle between the relative momentum and the center of mass momentum. This angle dependence causes  $Q$  to couple states with different relative angular momenta  $\mathcal{J}$ , rendering a partial wave decomposition of the  $G$ -matrix equation rather difficult. The angle dependence of the Pauli operator can be eliminated by introducing the angle-average Pauli operator, where one replaces the exact Pauli operator  $Q$  by its average  $\bar{Q}$  over all angles for fixed relative and center-of-mass momenta. The choice of Pauli operator is decisive to the determination of the sp spectrum. Basically, to first order in the reaction matrix  $G$ , there are three commonly used sp spectra, all defined by the solution of the following equations

$$\varepsilon_m = \varepsilon(k_m) = t_m + u_m = \frac{k_m^2}{2M_N} + u_m, \quad (8.40)$$

and

$$u_m = \sum_{h \leq k_F} \langle mh | G(\omega = \varepsilon_m + \varepsilon_h) | mh \rangle_{AS} \quad k_m \leq k_M, \quad (8.41)$$

$$(8.42)$$

$$u_m = 0, k_m > k_M. \quad (8.43)$$

For notational economy, we set  $|\mathbf{k}_m| = k_m$ . Here we employ antisymmetrized matrix elements (AS), and  $k_M$  is a cutoff on the momentum. Further,  $t_m$  is the sp kinetic energy and similarly  $u_m$  is the sp potential. The choice of cutoff  $k_M$  is actually what determines the three commonly used sp spectra. In the conventional BHF approach one employs  $k_M = k_F$ , which leads to a Pauli operator  $Q_{\text{BHF}}$  (in the laboratory system) given by

$$Q_{\text{BHF}}(k, k_n) = \begin{cases} 1, & \min(k, k_n) > k_F \\ 0, & \text{else.} \end{cases}, \quad (8.44)$$

or, since we will define an angle-average Pauli operator in the relative and center-of-mass system, we have

$$\bar{Q}_{\text{BHF}}(k, K) = \begin{cases} 0, & k \leq \sqrt{k_F^2 - K^2/4} \\ 1, & k \geq k_F + K/2 \\ \frac{K^2/4 + k^2 - k_F^2}{kK}, & \text{else,} \end{cases} \quad (8.45)$$

with  $k_F$  the momentum at the Fermi surface.

The BHF choice sets  $u_k = 0$  for  $k > k_F$ , which leads to an unphysical, large gap at the Fermi surface, typically of the order of 50 – 60 MeV. To overcome the gap problem, Mahaux and collaborators introduced a continuous sp spectrum for all values of  $k$ . The divergencies which then may occur in Eq. (8.39) are taken care of by introducing a principal value integration in Eq. (8.39), to retain only the real part contribution to the  $G$ -matrix.

To define the energy denominators we will also make use of the angle-average approximation. The angle dependence is handled by the so-called effective mass approximation. The single-particle energies in nuclear matter are assumed to have the simple quadratic form



$$\begin{aligned}\varepsilon(k_m) &= \frac{\hbar^2 k_m^2}{2M_N^*} + \Delta, \quad k_m \leq k_F \\ &= \frac{\hbar^2 k_m^2}{2M_N}, \quad k_m > k_F,\end{aligned}\tag{8.46}$$

where  $M_N^*$  is the effective mass of the nucleon and  $M_N$  is the bare nucleon mass. For particle states above the Fermi sea we choose a pure kinetic energy term, whereas for hole states, the terms  $M_N^*$  and  $\Delta$ , the latter being an effective single-particle potential related to the  $G$ -matrix, are obtained through the self-consistent Brueckner-Hartree-Fock procedure. The sp potential is obtained through the same angle-average approximation

$$\begin{aligned}U(k_m) &= \sum_{l\alpha} (2T+1)(2J+1) \left\{ \frac{8}{\pi} \int_0^{(k_F-k_m)/2} k^2 dk G_{ll}^\alpha(k, \bar{K}_1) \right. \\ &\quad \left. + \frac{1}{\pi k_m} \int_{(k_F-k_m)/2}^{(k_F+k_m)/2} k dk (k_F^2 - (k_m - 2k)^2) G_{ll}^\alpha(k, \bar{K}_2) \right\},\end{aligned}\tag{8.47}$$

where we have defined

$$\bar{K}_1^2 = 4(k_m^2 + k^2),\tag{8.48}$$

and

$$\bar{K}_2^2 = 4(k_m^2 + k^2) - (2k + k_m - k_F)(2k + k_1 + k_F).\tag{8.49}$$

This self-consistency scheme consists in choosing adequate initial values of the effective mass and  $\Delta$ . The obtained  $G$ -matrix is in turn used to obtain new values for  $M_N^*$  and  $\Delta$ . This procedure continues until these parameters vary little.

## 8.4 Full Configuration Interaction Theory

We have defined the ansatz for the ground state as

$$|\Phi_0\rangle = \left( \prod_{i \leq F} \hat{a}_i^\dagger \right) |0\rangle,$$

where the index  $i$  defines different single-particle states up to the Fermi level. We have assumed that we have  $N$  fermions. A given one-particle-one-hole ( $1p1h$ ) state can be written as

$$|\Phi_i^a\rangle = \hat{a}_a^\dagger \hat{a}_i |\Phi_0\rangle,$$

while a  $2p2h$  state can be written as

$$|\Phi_{ij}^{ab}\rangle = \hat{a}_a^\dagger \hat{a}_b^\dagger \hat{a}_j \hat{a}_i |\Phi_0\rangle,$$

and a general  $ApAh$  state as

$$|\Phi_{ijk\dots}^{abc\dots}\rangle = \hat{a}_a^\dagger \hat{a}_b^\dagger \hat{a}_c^\dagger \dots \hat{a}_k \hat{a}_j \hat{a}_i |\Phi_0\rangle.$$

We use letters  $ijkl\dots$  for states below the Fermi level and  $abcd\dots$  for states above the Fermi level. A general single-particle state is given by letters  $pqrs\dots$ .

We can then expand our exact state function for the ground state as

$$|\Psi_0\rangle = C_0 |\Phi_0\rangle + \sum_{ai} C_i^a |\Phi_i^a\rangle + \sum_{abij} C_{ij}^{ab} |\Phi_{ij}^{ab}\rangle + \dots = (C_0 + \hat{C}) |\Phi_0\rangle,$$

where we have introduced the so-called correlation operator

$$\hat{C} = \sum_{ai} C_i^a \hat{a}_a^\dagger \hat{a}_i + \sum_{abij} C_{ij}^{ab} \hat{a}_a^\dagger \hat{a}_b^\dagger \hat{a}_j \hat{a}_i + \dots$$

Since the normalization of  $\Psi_0$  is at our disposal and since  $C_0$  is by hypothesis non-zero, we may arbitrarily set  $C_0 = 1$  with corresponding proportional changes in all other coefficients. Using this so-called intermediate normalization we have

$$\langle \Psi_0 | \Phi_0 \rangle = \langle \Phi_0 | \Phi_0 \rangle = 1,$$

resulting in

$$|\Psi_0\rangle = (1 + \hat{C})|\Phi_0\rangle.$$

We rewrite

$$|\Psi_0\rangle = C_0|\Phi_0\rangle + \sum_{ai} C_i^a |\Phi_i^a\rangle + \sum_{abij} C_{ij}^{ab} |\Phi_{ij}^{ab}\rangle + \dots,$$

in a more compact form as

$$|\Psi_0\rangle = \sum_{PH} C_H^P \Phi_H^P = \left( \sum_{PH} C_H^P \hat{A}_H^P \right) |\Phi_0\rangle,$$

where  $H$  stands for  $0, 1, \dots, n$  hole states and  $P$  for  $0, 1, \dots, n$  particle states. Our requirement of unit normalization gives

$$\langle \Psi_0 | \Psi_0 \rangle = \sum_{PH} |C_H^P|^2 = 1,$$

and the energy can be written as

$$E = \langle \Psi_0 | \hat{H} | \Psi_0 \rangle = \sum_{PP'HH'} C_H^{*P} \langle \Phi_H^P | \hat{H} | \Phi_{H'}^{P'} \rangle C_{H'}^{P'}.$$

Normally

$$E = \langle \Psi_0 | \hat{H} | \Psi_0 \rangle = \sum_{PP'HH'} C_H^{*P} \langle \Phi_H^P | \hat{H} | \Phi_{H'}^{P'} \rangle C_{H'}^{P'},$$

is solved by diagonalization setting up the Hamiltonian matrix defined by the basis of all possible Slater determinants. A diagonalization is equivalent to finding the variational minimum of

$$\langle \Psi_0 | \hat{H} | \Psi_0 \rangle - \lambda \langle \Psi_0 | \Psi_0 \rangle,$$

where  $\lambda$  is a variational multiplier to be identified with the energy of the system.

The minimization process results in

$$\delta \left[ \langle \Psi_0 | \hat{H} | \Psi_0 \rangle - \lambda \langle \Psi_0 | \Psi_0 \rangle \right] = \sum_{P'H'} \left\{ \delta[C_H^{*P}] \langle \Phi_H^P | \hat{H} | \Phi_{H'}^{P'} \rangle C_{H'}^{P'} + C_H^{*P} \langle \Phi_H^P | \hat{H} | \Phi_{H'}^{P'} \rangle \delta[C_{H'}^{P'}] - \lambda (\delta[C_H^{*P}] C_{H'}^{P'} + C_H^{*P} \delta[C_{H'}^{P'}]) \right\} = 0.$$

Since the coefficients  $\delta[C_H^{*P}]$  and  $\delta[C_{H'}^{P'}]$  are complex conjugates it is necessary and sufficient to require the quantities that multiply with  $\delta[C_H^{*P}]$  to vanish.

This leads to

$$\sum_{P'H'} \langle \Phi_H^P | \hat{H} | \Phi_{H'}^{P'} \rangle C_{H'}^{P'} - \lambda C_H^P = 0,$$

for all sets of  $P$  and  $H$ .

If we then multiply by the corresponding  $C_H^{*P}$  and sum over  $PH$  we obtain

$$\sum_{PP'HH'} C_H^{*P} \langle \Phi_H^P | \hat{H} | \Phi_{H'}^{P'} \rangle C_{H'}^{P'} - \lambda \sum_{PH} |C_H^P|^2 = 0,$$

leading to the identification  $\lambda = E$ . This means that we have for all  $PH$  sets

$$\sum_{P'H'} \langle \Phi_H^P | \hat{H} - E | \Phi_{H'}^{P'} \rangle = 0. \quad (8.50)$$

An alternative way to derive the last equation is to start from

$$(\hat{H} - E) |\Psi_0\rangle = (\hat{H} - E) \sum_{P'H'} C_{H'}^{P'} |\Phi_{H'}^{P'}\rangle = 0,$$

and if this equation is successively projected against all  $\Phi_H^P$  in the expansion of  $\Psi$ , we end up with Eq. (8.50).

One solves this equation normally by diagonalization. If we are able to solve this equation exactly (that is numerically exactly) in a large Hilbert space (it will be truncated in terms of the number of single-particle states included in the definition of Slater determinants), it can then serve as a benchmark for other many-body methods which approximate the correlation operator  $\hat{C}$ .

### 8.4.1 Example of a Hamiltonian matrix

Suppose, as an example, that we have six fermions below the Fermi level. This means that we can make at most  $6p - 6h$  excitations. If we have an infinity of single particle states above the Fermi level, we will obviously have an infinity of say  $2p - 2h$  excitations. Each such way to configure the particles is called a **configuration**. We will always have to truncate in the basis of single-particle states. This gives us a finite number of possible Slater determinants. Our Hamiltonian matrix would then look like (where each block can have a large dimensionalities):

	$0p-0h$	$1p-1h$	$2p-2h$	$3p-3h$	$4p-4h$	$5p-5h$	$6p-6h$
$0p-0h$	x	x	x	0	0	0	0
$1p-1h$	x	x	x	x	0	0	0
$2p-2h$	x	x	x	x	x	0	0
$3p-3h$	0	x	x	x	x	x	0
$4p-4h$	0	0	x	x	x	x	x
$5p-5h$	0	0	0	x	x	x	x
$6p-6h$	0	0	0	0	x	x	x

with a two-body force. Why are there non-zero blocks of elements? If we use a Hartree-Fock basis, this corresponds to a particular unitary transformation where matrix elements of the type  $\langle 0p-0h | \hat{H} | 1p-1h \rangle = \langle \Phi_0 | \hat{H} | \Phi_i^a \rangle = 0$  and our Hamiltonian matrix becomes

	$0p-0h$	$1p-1h$	$2p-2h$	$3p-3h$	$4p-4h$	$5p-5h$	$6p-6h$
$0p-0h$	$\tilde{x}$	0	$\tilde{x}$	0	0	0	0
$1p-1h$	0	$\tilde{x}$	$\tilde{x}$	$\tilde{x}$	0	0	0
$2p-2h$	$\tilde{x}$	$\tilde{x}$	$\tilde{x}$	$\tilde{x}$	$\tilde{x}$	0	0
$3p-3h$	0	$\tilde{x}$	$\tilde{x}$	$\tilde{x}$	$\tilde{x}$	$\tilde{x}$	0
$4p-4h$	0	0	$\tilde{x}$	$\tilde{x}$	$\tilde{x}$	$\tilde{x}$	$\tilde{x}$
$5p-5h$	0	0	0	$\tilde{x}$	$\tilde{x}$	$\tilde{x}$	$\tilde{x}$
$6p-6h$	0	0	0	0	$\tilde{x}$	$\tilde{x}$	$\tilde{x}$

If we do not make any truncations in the possible sets of Slater determinants (many-body states) we can make by distributing  $A$  nucleons among  $n$  single-particle states, we call such a calculation for

- Full configuration interaction theory

If we make truncations, we have different possibilities

- The standard nuclear shell-model. Here we define an effective Hilbert space with respect to a given core. The calculations are normally then performed for all many-body states that can be constructed from the effective Hilbert spaces. This approach requires a properly defined effective Hamiltonian
- We can truncate in the number of excitations. For example, we can limit the possible Slater determinants to only  $1p-1h$  and  $2p-2h$  excitations. This is called a configuration interaction calculation at the level of singles and doubles excitations, or just CISD.
- We can limit the number of excitations in terms of the excitation energies. If we do not define a core, this defines normally what is called the no-core shell-model approach.

What happens if we have a three-body interaction and a Hartree-Fock basis?

Full configuration interaction theory calculations provide in principle, if we can diagonalize numerically, all states of interest. The dimensionality of the problem explodes however quickly.

The total number of Slater determinants which can be built with say  $N$  neutrons distributed among  $n$  single particle states is

$$\binom{n}{N} = \frac{n!}{(n-N)!N!}.$$

For a model space which comprises the first four major shells only  $0s$ ,  $0p$ ,  $1s0d$  and  $1p0f$  we have 40 single particle states for neutrons and protons. For the eight neutrons of oxygen-16 we would then have

$$\binom{40}{8} = \frac{40!}{(32)!8!} \sim 10^9,$$

and multiplying this with the number of proton Slater determinants we end up with approximately with a dimensionality  $d$  of  $d \sim 10^{18}$ .

This number can be reduced if we look at specific symmetries only. However, the dimensionality explodes quickly!

- For Hamiltonian matrices of dimensionalities which are smaller than  $d \sim 10^5$ , we would use so-called direct methods for diagonalizing the Hamiltonian matrix
- For larger dimensionalities iterative eigenvalue solvers like Lanczos' method are used. The most efficient codes at present can handle matrices of  $d \sim 10^{10}$ .

### 8.4.2 A non-practical way of solving the eigenvalue problem

For reasons to come (links with Coupled-Cluster theory and Many-Body perturbation theory), we will rewrite Eq. (8.50) as a set of coupled non-linear equations in terms of the unknown coefficients  $C_H^P$ . To obtain the eigenstates and eigenvalues in terms of non-linear equations is not a very practical approach. However, it serves the scope of linking FCI theory with approximative solutions to the many-body problem.

To see this, we look at the contributions arising from

$$\langle \Phi_H^P | = \langle \Phi_0 |$$

in Eq. (8.50), that is we multiply with  $\langle \Phi_0 |$  from the left in

$$(\hat{H} - E) \sum_{P'H'} C_{H'}^{P'} |\Phi_{H'}^{P'}\rangle = 0.$$

If we assume that we have a two-body operator at most, Slater's rule gives then an equation for the correlation energy in terms of  $C_i^a$  and  $C_{ij}^{ab}$  only. We get then

$$\langle \Phi_0 | \hat{H} - E | \Phi_0 \rangle + \sum_{ai} \langle \Phi_0 | \hat{H} - E | \Phi_i^a \rangle C_i^a + \sum_{abij} \langle \Phi_0 | \hat{H} - E | \Phi_{ij}^{ab} \rangle C_{ij}^{ab} = 0,$$

or

$$E - E_0 = \Delta E = \sum_{ai} \langle \Phi_0 | \hat{H} | \Phi_i^a \rangle C_i^a + \sum_{abij} \langle \Phi_0 | \hat{H} | \Phi_{ij}^{ab} \rangle C_{ij}^{ab},$$

where the energy  $E_0$  is the reference energy and  $\Delta E$  defines the so-called correlation energy. The single-particle basis functions could be the results of a Hartree-Fock calculation or just the eigenstates of the non-interacting part of the Hamiltonian.

In our notes on Hartree-Fock calculations, we have already computed the matrix  $\langle \Phi_0 | \hat{H} | \Phi_i^a \rangle$  and  $\langle \Phi_0 | \hat{H} | \Phi_{ij}^{ab} \rangle$ . If we are using a Hartree-Fock basis, then the matrix elements  $\langle \Phi_0 | \hat{H} | \Phi_i^a \rangle = 0$  and we are left with a *correlation energy* given by

$$E - E_0 = \Delta E^{HF} = \sum_{abij} \langle \Phi_0 | \hat{H} | \Phi_{ij}^{ab} \rangle C_{ij}^{ab}.$$

Inserting the various matrix elements we can rewrite the previous equation as

$$\Delta E = \sum_{ai} \langle i | \hat{f} | a \rangle C_i^a + \sum_{abij} \langle ij | \hat{v} | ab \rangle C_{ij}^{ab}.$$

This equation determines the correlation energy but not the coefficients  $C$ . We need more equations. Our next step is to set up

$$\langle \Phi_i^a | \hat{H} - E | \Phi_0 \rangle + \sum_{bj} \langle \Phi_i^a | \hat{H} - E | \Phi_j^b \rangle C_j^b + \sum_{bcjk} \langle \Phi_i^a | \hat{H} - E | \Phi_{jk}^{bc} \rangle C_{jk}^{bc} + \sum_{bcdjkl} \langle \Phi_i^a | \hat{H} - E | \Phi_{jkl}^{bcd} \rangle C_{jkl}^{bcd} = 0,$$

as this equation will allow us to find an expression for the coefficients  $C_i^a$  since we can rewrite this equation as

$$\langle i | \hat{f} | a \rangle + \langle \Phi_i^a | \hat{H} | \Phi_i^a \rangle C_i^a + \sum_{bj \neq ai} \langle \Phi_i^a | \hat{H} | \Phi_j^b \rangle C_j^b + \sum_{bcjk} \langle \Phi_i^a | \hat{H} | \Phi_{jk}^{bc} \rangle C_{jk}^{bc} + \sum_{bcdjkl} \langle \Phi_i^a | \hat{H} | \Phi_{jkl}^{bcd} \rangle C_{jkl}^{bcd} = E C_i^a.$$

We see that on the right-hand side we have the energy  $E$ . This leads to a non-linear equation in the unknown coefficients. These equations are normally solved iteratively ( that is we can start with a guess for the coefficients  $C_i^a$ ). A common choice is to use perturbation theory for the first guess, setting thereby

$$C_i^a = \frac{\langle i | \hat{f} | a \rangle}{\epsilon_i - \epsilon_a}.$$

The observant reader will however see that we need an equation for  $C_{jk}^{bc}$  and  $C_{jkl}^{bcd}$  as well. To find equations for these coefficients we need then to continue our multiplications from the left with the various  $\Phi_H^P$  terms.

For  $C_{jk}^{bc}$  we need then

$$\begin{aligned} & \langle \Phi_{ij}^{ab} | \hat{H} - E | \Phi_0 \rangle + \sum_{kc} \langle \Phi_{ij}^{ab} | \hat{H} - E | \Phi_k^c \rangle C_k^c + \\ & \sum_{cdkl} \langle \Phi_{ij}^{ab} | \hat{H} - E | \Phi_{kl}^{cd} \rangle C_{kl}^{cd} + \sum_{cdeklm} \langle \Phi_{ij}^{ab} | \hat{H} - E | \Phi_{klm}^{cde} \rangle C_{klm}^{cde} + \sum_{cdefklmn} \langle \Phi_{ij}^{ab} | \hat{H} - E | \Phi_{klmn}^{cdef} \rangle C_{klmn}^{cdef} = 0, \end{aligned}$$

and we can isolate the coefficients  $C_{kl}^{cd}$  in a similar way as we did for the coefficients  $C_i^a$ . A standard choice for the first iteration is to set

$$C_{ij}^{ab} = \frac{\langle ij|\hat{v}|ab\rangle}{\epsilon_i + \epsilon_j - \epsilon_a - \epsilon_b}.$$

At the end we can rewrite our solution of the Schroedinger equation in terms of  $n$  coupled equations for the coefficients  $C_H^p$ . This is a very cumbersome way of solving the equation. However, by using this iterative scheme we can illustrate how we can compute the various terms in the wave operator or correlation operator  $\hat{C}$ . We will later identify the calculation of the various terms  $C_H^p$  as parts of different many-body approximations to full CI. In particular, we can relate this non-linear scheme with Coupled Cluster theory and many-body perturbation theory.

### 8.4.3 Summarizing FCI and bringing in approximative methods

If we can diagonalize large matrices, FCI is the method of choice since:

- It gives all eigenvalues, ground state and excited states
- The eigenvectors are obtained directly from the coefficients  $C_H^p$  which result from the diagonalization
- We can compute easily expectation values of other operators, as well as transition probabilities
- Correlations are easy to understand in terms of contributions to a given operator beyond the Hartree-Fock contribution. This is the standard approach in many-body theory.

The correlation energy is defined as, with a two-body Hamiltonian,

$$\Delta E = \sum_{ai} \langle i|\hat{f}|a\rangle C_i^a + \sum_{abij} \langle ij|\hat{v}|ab\rangle C_{ij}^{ab}.$$

The coefficients  $C$  result from the solution of the eigenvalue problem. The energy of say the ground state is then

$$E = E_{ref} + \Delta E,$$

where the so-called reference energy is the energy we obtain from a Hartree-Fock calculation, that is

$$E_{ref} = \langle \Phi_0 | \hat{H} | \Phi_0 \rangle.$$

However, as we have seen, even for a small case like the four first major shells and a nucleus like oxygen-16, the dimensionality becomes quickly intractable. If we wish to include single-particle states that reflect weakly bound systems, we need a much larger single-particle basis. We need thus approximative methods that sum specific correlations to infinite order.

Popular methods are

- Many-body perturbation theory (in essence a Taylor expansion)
- Coupled cluster theory (coupled non-linear equations)
- Green's function approaches (matrix inversion)
- Similarity group transformation methods (coupled ordinary differential equations)

All these methods start normally with a Hartree-Fock basis as the calculational basis.

### 8.4.4 Building a many-body basis

Here we will discuss how we can set up a single-particle basis which we can use in the various parts of our projects, from the simple pairing model to infinite nuclear matter. We will use here the simple pairing model to illustrate in particular how to set up a single-particle basis. We will also use this to discuss standard FCI approaches like:

1. Standard shell-model basis in one or two major shells
2. Full CI in a given basis and no truncations
3. CISD and CISDT approximations
4. No-core shell model and truncation in excitation energy

An important step in an FCI code is to construct the many-body basis.

While the formalism is independent of the choice of basis, the **effectiveness** of a calculation will certainly be basis dependent.

Furthermore there are common conventions useful to know.

First, the single-particle basis has angular momentum as a good quantum number. You can imagine the single-particle wavefunctions being generated by a one-body Hamiltonian, for example a harmonic oscillator. Modifications include harmonic oscillator plus spin-orbit splitting, or self-consistent mean-field potentials, or the Woods-Saxon potential which mocks up the self-consistent mean-field. For nuclei, the harmonic oscillator, modified by spin-orbit splitting, provides a useful language for describing single-particle states.

Each single-particle state is labeled by the following quantum numbers:

- Orbital angular momentum  $l$
- Intrinsic spin  $s = 1/2$  for protons and neutrons
- Angular momentum  $j = l \pm 1/2$
- $z$ -component  $j_z$  (or  $m$ )
- Some labeling of the radial wavefunction, typically  $n$  the number of nodes in the radial wavefunction, but in the case of harmonic oscillator one can also use the principal quantum number  $N$ , where the harmonic oscillator energy is  $(N + 3/2)\hbar\omega$ . For our nuclear matter projects, you will need to change the quantum numbers to those relevant for calculations

in three-dimensional cartesian basis, see the relevante lectures.

In this format one labels states by  $n(l)_j$ , with  $(l)$  replaced by a letter:  $s$  for  $l = 0$ ,  $p$  for  $l = 1$ ,  $d$  for  $l = 2$ ,  $f$  for  $l = 3$ , and thenceforth alphabetical.

In practice the single-particle space has to be severely truncated. This truncation is typically based upon the single-particle energies, which is the effective energy from a mean-field potential.

Sometimes we freeze the core and only consider a valence space. For example, one may assume a frozen  $^4\text{He}$  core, with two protons and two neutrons in the  $0s_{1/2}$  shell, and then only allow active particles in the  $0p_{1/2}$  and  $0p_{3/2}$  orbits.

Another example is a frozen  $^{16}\text{O}$  core, with eight protons and eight neutrons filling the  $0s_{1/2}$ ,  $0p_{1/2}$  and  $0p_{3/2}$  orbits, with valence particles in the  $0d_{5/2}$ ,  $1s_{1/2}$  and  $0d_{3/2}$  orbits.

Sometimes we refer to nuclei by the valence space where their last nucleons go. So, for example, we call  $^{12}\text{C}$  a  $p$ -shell nucleus, while  $^{26}\text{Al}$  is an  $sd$ -shell nucleus and  $^{56}\text{Fe}$  is a  $pf$ -shell nucleus.

There are different kinds of truncations.

- For example, one can start with ‘filled’ orbits (almost always the lowest), and then allow one, two, three... particles excited out of those filled orbits. These are called 1p-1h, 2p-2h, 3p-3h excitations.

- Alternately, one can state a maximal orbit and allow all possible configurations with particles occupying states up to that maximum. This is called *full configuration*.
- Finally, for particular use in nuclear physics, there is the *energy* truncation, also called the  $N\hbar\Omega$  or  $N_{max}$  truncation.

Here one works in a harmonic oscillator basis, with each major oscillator shell assigned a principal quantum number  $N = 0, 1, 2, 3, \dots$ . The  $N\hbar\Omega$  or  $N_{max}$  truncation: Any configuration is given an noninteracting energy, which is the sum of the single-particle harmonic oscillator energies. (Thus this ignores spin-orbit splitting.)

Excited state are labeled relative to the lowest configuration by the number of harmonic oscillator quanta.

This truncation is useful because if one includes *all* configuration up to some  $N_{max}$ , and has a translationally invariant interaction, then the intrinsic motion and the center-of-mass motion factor. In other words, we can know exactly the center-of-mass wavefunction.

In almost all cases, the many-body Hamiltonian is rotationally invariant. This means it commutes with the operators  $\hat{J}^2, \hat{J}_z$  and so eigenstates will have good  $J, M$ . Furthermore, the eigenenergies do not depend upon the orientation  $M$ .

Therefore we can choose to construct a many-body basis which has fixed  $M$ ; this is called an  $M$ -scheme basis.

Alternately, one can construct a many-body basis which has fixed  $J$ , or a  $J$ -scheme basis.

The Hamiltonian matrix will have smaller dimensions (a factor of 10 or more) in the  $J$ -scheme than in the  $M$ -scheme. On the other hand, as we'll show in the next slide, the  $M$ -scheme is very easy to construct with Slater determinants, while the  $J$ -scheme basis states, and thus the matrix elements, are more complicated, almost always being linear combinations of  $M$ -scheme states.  $J$ -scheme bases are important and useful, but we'll focus on the simpler  $M$ -scheme.

The quantum number  $m$  is additive (because the underlying group is Abelian): if a Slater determinant  $\hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_k^\dagger \dots |0\rangle$  is built from single-particle states all with good  $m$ , then the total

$$M = m_i + m_j + m_k + \dots$$

This is *not* true of  $J$ , because the angular momentum group  $SU(2)$  is not Abelian.

The upshot is that

- It is easy to construct a Slater determinant with good total  $M$ ;
- It is trivial to calculate  $M$  for each Slater determinant;
- So it is easy to construct an  $M$ -scheme basis with fixed total  $M$ .

Note that the individual  $M$ -scheme basis states will *not*, in general, have good total  $J$ . Because the Hamiltonian is rotationally invariant, however, the eigenstates will have good  $J$ . (The situation is muddled when one has states of different  $J$  that are nonetheless degenerate.)

Example: two  $j = 1/2$  orbits

Index	$n$	$l$	$j$	$m_j$
1	0	0	1/2	-1/2
2	0	0	1/2	1/2
3	1	0	1/2	-1/2
4	1	0	1/2	1/2

Note that the order is arbitrary. There are  $\binom{4}{2} = 6$  two-particle states, which we list with the total  $M$ :



Occupied $M$	
1,2	0
1,3	-1
1,4	0
2,3	0
2,4	1
3,4	0

and 1 each with  $M = \pm 1$ .

As another example, consider using only single particle states from the  $0d_{5/2}$  space. They have the following quantum numbers

Index	$n$	$l$	$j$	$m_j$
1	0	2	5/2	-5/2
2	0	2	5/2	-3/2
3	0	2	5/2	-1/2
4	0	2	5/2	1/2
5	0	2	5/2	3/2
6	0	2	5/2	5/2

There are  $\binom{6}{2} = 15$  two-particle states, which we list with the total  $M$ :

Occupied $M$		Occupied $M$		Occupied $M$	
1,2	-4	2,3	-2	3,5	1
1,3	-3	2,4	-1	3,6	2
1,4	-2	2,5	0	4,5	2
1,5	-1	2,6	1	4,6	3
1,6	0	3,4	0	5,6	4

## 8.5 Many-body perturbation theory

### 8.5.1 Many-body perturbation theory

We assume here that we are only interested in the ground state of the system and expand the exact wave function in term of a series of Slater determinants

$$|\Psi_0\rangle = |\Phi_0\rangle + \sum_{m=1}^{\infty} C_m |\Phi_m\rangle,$$

where we have assumed that the true ground state is dominated by the solution of the unperturbed problem, that is

$$\hat{H}_0 |\Phi_0\rangle = W_0 |\Phi_0\rangle.$$

The state  $|\Psi_0\rangle$  is not normalized, rather we have used an intermediate normalization  $\langle \Phi_0 | \Psi_0 \rangle = 1$  since we have  $\langle \Phi_0 | \Phi_0 \rangle = 1$ .

The Schroedinger equation is

$$\hat{H} |\Psi_0\rangle = E |\Psi_0\rangle,$$

and multiplying the latter from the left with  $\langle \Phi_0 |$  gives

$$\langle \Phi_0 | \hat{H} | \Psi_0 \rangle = E \langle \Phi_0 | \Psi_0 \rangle = E,$$

and subtracting from this equation

$$\langle \Psi_0 | \hat{H}_0 | \Phi_0 \rangle = W_0 \langle \Psi_0 | \Phi_0 \rangle = W_0,$$

and using the fact that the both operators  $\hat{H}$  and  $\hat{H}_0$  are hermitian results in

$$\Delta E = E - W_0 = \langle \Phi_0 | \hat{H}_I | \Psi_0 \rangle,$$

which is an exact result. We call this quantity the correlation energy.

This equation forms the starting point for all perturbative derivations. However, as it stands it represents nothing but a mere formal rewriting of Schroedinger's equation and is not of much practical use. The exact wave function  $|\Psi_0\rangle$  is unknown. In order to obtain a perturbative expansion, we need to expand the exact wave function in terms of the interaction  $\hat{H}_I$ .

Here we have assumed that our model space defined by the operator  $\hat{P}$  is one-dimensional, meaning that

$$\hat{P} = |\Phi_0\rangle\langle\Phi_0|,$$

and

$$\hat{Q} = \sum_{m=1}^{\infty} |\Phi_m\rangle\langle\Phi_m|.$$

We can thus rewrite the exact wave function as

$$|\Psi_0\rangle = (\hat{P} + \hat{Q})|\Psi_0\rangle = |\Phi_0\rangle + \hat{Q}|\Psi_0\rangle.$$

Going back to the Schrödinger equation, we can rewrite it as, adding and a subtracting a term  $\omega|\Psi_0\rangle$  as

$$(\omega - \hat{H}_0)|\Psi_0\rangle = (\omega - E + \hat{H}_I)|\Psi_0\rangle,$$

where  $\omega$  is an energy variable to be specified later.

We assume also that the resolvent of  $(\omega - \hat{H}_0)$  exists, that is it has an inverse which defined the unperturbed Green's function as

$$(\omega - \hat{H}_0)^{-1} = \frac{1}{(\omega - \hat{H}_0)}.$$

We can rewrite Schroedinger's equation as

$$|\Psi_0\rangle = \frac{1}{\omega - \hat{H}_0} (\omega - E + \hat{H}_I) |\Psi_0\rangle,$$

and multiplying from the left with  $\hat{Q}$  results in

$$\hat{Q}|\Psi_0\rangle = \frac{\hat{Q}}{\omega - \hat{H}_0} (\omega - E + \hat{H}_I) |\Psi_0\rangle,$$

which is possible since we have defined the operator  $\hat{Q}$  in terms of the eigenfunctions of  $\hat{H}$ .

These operators commute meaning that

$$\hat{Q} \frac{1}{(\omega - \hat{H}_0)} \hat{Q} = \hat{Q} \frac{1}{(\omega - \hat{H}_0)} = \frac{\hat{Q}}{(\omega - \hat{H}_0)}.$$

With these definitions we can in turn define the wave function as

$$|\Psi_0\rangle = |\Phi_0\rangle + \frac{\hat{Q}}{\omega - \hat{H}_0} (\omega - E + \hat{H}_I) |\Psi_0\rangle.$$

This equation is again nothing but a formal rewrite of Schrödinger's equation and does not represent a practical calculational scheme. It is a non-linear equation in two unknown quan-

ties, the energy  $E$  and the exact wave function  $|\Psi_0\rangle$ . We can however start with a guess for  $|\Psi_0\rangle$  on the right hand side of the last equation.

The most common choice is to start with the function which is expected to exhibit the largest overlap with the wave function we are searching after, namely  $|\Phi_0\rangle$ . This can again be inserted in the solution for  $|\Psi_0\rangle$  in an iterative fashion and if we continue along these lines we end up with

$$|\Psi_0\rangle = \sum_{i=0}^{\infty} \left\{ \frac{\hat{Q}}{\omega - \hat{H}_0} (\omega - E + \hat{H}_I) \right\}^i |\Phi_0\rangle,$$

for the wave function and

$$\Delta E = \sum_{i=0}^{\infty} \langle \Phi_0 | \hat{H}_I \left\{ \frac{\hat{Q}}{\omega - \hat{H}_0} (\omega - E + \hat{H}_I) \right\}^i | \Phi_0 \rangle,$$

which is now a perturbative expansion of the exact energy in terms of the interaction  $\hat{H}_I$  and the unperturbed wave function  $|\Psi_0\rangle$ .

In our equations for  $|\Psi_0\rangle$  and  $\Delta E$  in terms of the unperturbed solutions  $|\Phi_i\rangle$  we have still an undetermined parameter  $\omega$  and a dependency on the exact energy  $E$ . Not much has been gained thus from a practical computational point of view.

In Brilluoin-Wigner perturbation theory it is customary to set  $\omega = E$ . This results in the following perturbative expansion for the energy  $\Delta E$

$$\begin{aligned} \Delta E &= \sum_{i=0}^{\infty} \langle \Phi_0 | \hat{H}_I \left\{ \frac{\hat{Q}}{\omega - \hat{H}_0} (\omega - E + \hat{H}_I) \right\}^i | \Phi_0 \rangle = \\ &\langle \Phi_0 | \left( \hat{H}_I + \hat{H}_I \frac{\hat{Q}}{E - \hat{H}_0} \hat{H}_I + \hat{H}_I \frac{\hat{Q}}{E - \hat{H}_0} \hat{H}_I \frac{\hat{Q}}{E - \hat{H}_0} \hat{H}_I + \dots \right) | \Phi_0 \rangle. \\ \Delta E &= \sum_{i=0}^{\infty} \langle \Phi_0 | \hat{H}_I \left\{ \frac{\hat{Q}}{\omega - \hat{H}_0} (\omega - E + \hat{H}_I) \right\}^i | \Phi_0 \rangle = \\ &\langle \Phi_0 | \left( \hat{H}_I + \hat{H}_I \frac{\hat{Q}}{E - \hat{H}_0} \hat{H}_I + \hat{H}_I \frac{\hat{Q}}{E - \hat{H}_0} \hat{H}_I \frac{\hat{Q}}{E - \hat{H}_0} \hat{H}_I + \dots \right) | \Phi_0 \rangle. \end{aligned}$$

This expression depends however on the exact energy  $E$  and is again not very convenient from a practical point of view. It can obviously be solved iteratively, by starting with a guess for  $E$  and then solve till some kind of self-consistency criterion has been reached.

Actually, the above expression is nothing but a rewrite again of the full Schrödinger equation.

Defining  $e = E - \hat{H}_0$  and recalling that  $\hat{H}_0$  commutes with  $\hat{Q}$  by construction and that  $\hat{Q}$  is an idempotent operator  $\hat{Q}^2 = \hat{Q}$ . Using this equation in the above expansion for  $\Delta E$  we can write the denominator

$$\begin{aligned} \hat{Q} \frac{1}{e - \hat{Q} \hat{H}_I \hat{Q}} &= \\ \hat{Q} \left[ \frac{1}{e} + \frac{1}{e} \hat{Q} \hat{H}_I \hat{Q} \frac{1}{e} + \frac{1}{e} \hat{Q} \hat{H}_I \hat{Q} \frac{1}{e} \hat{Q} \hat{H}_I \hat{Q} \frac{1}{e} + \dots \right] \hat{Q}. \end{aligned}$$

Inserted in the expression for  $\Delta E$  leads to

$$\Delta E = \langle \Phi_0 | \hat{H}_I + \hat{H}_I \hat{Q} \frac{1}{E - \hat{H}_0 - \hat{Q} \hat{H}_I \hat{Q}} \hat{Q} \hat{H}_I | \Phi_0 \rangle.$$

In RS perturbation theory we set  $\omega = W_0$  and obtain the following expression for the energy difference

$$\Delta E = \sum_{i=0}^{\infty} \langle \Phi_0 | \hat{H}_I \left\{ \frac{\hat{Q}}{W_0 - \hat{H}_0} (\hat{H}_I - \Delta E) \right\}^i | \Phi_0 \rangle =$$

$$\langle \Phi_0 | \left( \hat{H}_I + \hat{H}_I \frac{\hat{Q}}{W_0 - \hat{H}_0} (\hat{H}_I - \Delta E) + \hat{H}_I \frac{\hat{Q}}{W_0 - \hat{H}_0} (\hat{H}_I - \Delta E) \frac{\hat{Q}}{W_0 - \hat{H}_0} (\hat{H}_I - \Delta E) + \dots \right) | \Phi_0 \rangle.$$

Recalling that  $\hat{Q}$  commutes with  $\hat{H}_0$  and since  $\Delta E$  is a constant we obtain that

$$\hat{Q} \Delta E | \Phi_0 \rangle = \hat{Q} \Delta E | \hat{Q} \Phi_0 \rangle = 0.$$

Inserting this results in the expression for the energy results in

$$\Delta E = \langle \Phi_0 | \left( \hat{H}_I + \hat{H}_I \frac{\hat{Q}}{W_0 - \hat{H}_0} \hat{H}_I + \hat{H}_I \frac{\hat{Q}}{W_0 - \hat{H}_0} (\hat{H}_I - \Delta E) \frac{\hat{Q}}{W_0 - \hat{H}_0} \hat{H}_I + \dots \right) | \Phi_0 \rangle.$$

We can now this expression in terms of a perturbative expression in terms of  $\hat{H}_I$  where we iterate the last expression in terms of  $\Delta E$

$$\Delta E = \sum_{i=1}^{\infty} \Delta E^{(i)}.$$

We get the following expression for  $\Delta E^{(i)}$

$$\Delta E^{(1)} = \langle \Phi_0 | \hat{H}_I | \Phi_0 \rangle,$$

which is just the contribution to first order in perturbation theory,

$$\Delta E^{(2)} = \langle \Phi_0 | \hat{H}_I \frac{\hat{Q}}{W_0 - \hat{H}_0} \hat{H}_I | \Phi_0 \rangle,$$

which is the contribution to second order.

$$\Delta E^{(3)} = \langle \Phi_0 | \hat{H}_I \frac{\hat{Q}}{W_0 - \hat{H}_0} \hat{H}_I \frac{\hat{Q}}{W_0 - \hat{H}_0} \hat{H}_I | \Phi_0 \rangle - \langle \Phi_0 | \hat{H}_I \frac{\hat{Q}}{W_0 - \hat{H}_0} \langle \Phi_0 | \hat{H}_I | \Phi_0 \rangle \frac{\hat{Q}}{W_0 - \hat{H}_0} \hat{H}_I | \Phi_0 \rangle,$$

being the third-order contribution.

### 8.5.2 Interpreting the correlation energy and the wave operator

In the shell-model lectures we showed that we could rewrite the exact state function for say the ground state, as a linear expansion in terms of all possible Slater determinants. That is, we define the ansatz for the ground state as

$$| \Phi_0 \rangle = \left( \prod_{i \leq F} \hat{a}_i^\dagger \right) | 0 \rangle,$$

where the index  $i$  defines different single-particle states up to the Fermi level. We have assumed that we have  $N$  fermions. A given one-particle-one-hole (1p1h) state can be written as

$$| \Phi_i^a \rangle = \hat{a}_a^\dagger \hat{a}_i | \Phi_0 \rangle,$$

while a 2p2h state can be written as

$$| \Phi_{ij}^{ab} \rangle = \hat{a}_a^\dagger \hat{a}_b^\dagger \hat{a}_j \hat{a}_i | \Phi_0 \rangle,$$

and a general  $ApAh$  state as

$$|\Phi_{ijkl\dots}^{abc\dots}\rangle = \hat{a}_a^\dagger \hat{a}_b^\dagger \hat{a}_c^\dagger \dots \hat{a}_k \hat{a}_j \hat{a}_i |\Phi_0\rangle.$$

We use letters  $ijkl\dots$  for states below the Fermi level and  $abcd\dots$  for states above the Fermi level. A general single-particle state is given by letters  $pqrs\dots$ .

We can then expand our exact state function for the ground state as

$$|\Psi_0\rangle = C_0 |\Phi_0\rangle + \sum_{ai} C_i^a |\Phi_i^a\rangle + \sum_{abij} C_{ij}^{ab} |\Phi_{ij}^{ab}\rangle + \dots = (C_0 + \hat{C}) |\Phi_0\rangle,$$

where we have introduced the so-called correlation operator

$$\hat{C} = \sum_{ai} C_i^a \hat{a}_a^\dagger \hat{a}_i + \sum_{abij} C_{ij}^{ab} \hat{a}_a^\dagger \hat{a}_b^\dagger \hat{a}_j \hat{a}_i + \dots$$

Since the normalization of  $\Psi_0$  is at our disposal and since  $C_0$  is by hypothesis non-zero, we may arbitrarily set  $C_0 = 1$  with corresponding proportional changes in all other coefficients. Using this so-called intermediate normalization we have

$$\langle \Psi_0 | \Phi_0 \rangle = \langle \Phi_0 | \Phi_0 \rangle = 1,$$

resulting in

$$|\Psi_0\rangle = (1 + \hat{C}) |\Phi_0\rangle.$$

In a shell-model calculation, the unknown coefficients in  $\hat{C}$  are the eigenvectors which result from the diagonalization of the Hamiltonian matrix.

How can we use perturbation theory to determine the same coefficients? Let us study the contributions to second order in the interaction, namely

$$\Delta E^{(2)} = \langle \Phi_0 | \hat{H}_I \frac{\hat{Q}}{W_0 - \hat{H}_0} \hat{H}_I | \Phi_0 \rangle.$$

The intermediate states given by  $\hat{Q}$  can at most be of a  $2p - 2h$  nature if we have a two-body Hamiltonian. This means that second order in the perturbation theory can have  $1p - 1h$  and  $2p - 2h$  at most as intermediate states. When we diagonalize, these contributions are included to infinite order. This means that higher-orders in perturbation theory bring in more complicated correlations.

If we limit the attention to a Hartree-Fock basis, then we have that  $\langle \Phi_0 | \hat{H}_I | 2p - 2h \rangle$  is the only contribution and the contribution to the energy reduces to

$$\Delta E^{(2)} = \frac{1}{4} \sum_{abij} \langle ij | \hat{v} | ab \rangle \frac{\langle ab | \hat{v} | ij \rangle}{\epsilon_i + \epsilon_j - \epsilon_a - \epsilon_b}.$$

If we compare this to the correlation energy obtained from full configuration interaction theory with a Hartree-Fock basis, we found that

$$E - E_0 = \Delta E = \sum_{abij} \langle ij | \hat{v} | ab \rangle C_{ij}^{ab},$$

where the energy  $E_0$  is the reference energy and  $\Delta E$  defines the so-called correlation energy.

We see that if we set

$$C_{ij}^{ab} = \frac{1}{4} \frac{\langle ab | \hat{v} | ij \rangle}{\epsilon_i + \epsilon_j - \epsilon_a - \epsilon_b},$$

we have a perfect agreement between FCI and MBPT. However, FCI includes such  $2p - 2h$  correlations to infinite order. In order to make a meaningful comparison we would at least need to sum such correlations to infinite order in perturbation theory.

Summing up, we can see that

- MBPT introduces order-by-order specific correlations and we make comparisons with exact calculations like FCI
- At every order, we can calculate all contributions since they are well-known and either tabulated or calculated on the fly.
- MBPT is a non-variational theory and there is no guarantee that higher orders will improve the convergence.
- However, since FCI calculations are limited by the size of the Hamiltonian matrices to diagonalize (today's most efficient codes can attach dimensionalities of ten billion basis states, MBPT can function as an approximative method which gives a straightforward (but tedious) calculation recipe.
- MBPT has been widely used to compute effective interactions for the nuclear shell-model.
- But there are better methods which sum to infinite order important correlations. Coupled cluster theory is one of these methods.

## 8.6 Coupled cluster theory

### 8.7 Introduction

Coester and Kummel first developed the ideas that led to coupled-cluster theory in the late 1950s. The basic idea is that the correlated wave function of a many-body system  $|\Psi\rangle$  can be formulated as an exponential of correlation operators  $T$  acting on a reference state  $|\Phi\rangle$

$$|\Psi\rangle = \exp(-\hat{T}) |\Phi\rangle.$$

We will discuss how to define the operators later in this work. This simple ansatz carries enormous power. It leads to a non-perturbative many-body theory that includes summation of ladder diagrams, ring diagrams, and an infinite-order generalization of many-body perturbation theory.

Developments and applications of coupled-cluster theory took different routes in chemistry and nuclear physics. In quantum chemistry, coupled-cluster developments and applications have proven to be extremely useful, see for example the review by Barrett and Musial as well as the recent textbook by Shavitt and Barrett. Many previous applications to nuclear physics struggled with the repulsive character of the nuclear forces and limited basis sets used in the computations. Most of these problems have been overcome during the last decade and coupled-cluster theory is one of the computational methods of preference for doing nuclear physics, with applications ranging from light nuclei to medium-heavy nuclei, see for example the recent review by Hagen, Papenbrock, Hjorth-Jensen and Dean.

#### 8.7.1 A non-practical way of solving the eigenvalue problem

Before we proceed with the derivation of the Coupled cluster equations, let us repeat some of the arguments we presented during our FCI lectures. In our FCI discussions, we rewrote the solution of the Schrodinger equation as a set of coupled equations in the unknown coeffi-

cients  $C$ . Let us repeat some of these arguments. To obtain the eigenstates and eigenvalues in terms of non-linear equations is not a very practical approach. However, it serves the scope of linking FCI theory with approximative solutions to the many-body problem like Coupled cluster (CC) theory

If we assume that we have a two-body operator at most, the Slater-Condon rule gives then an equation for the correlation energy in terms of  $C_i^a$  and  $C_{ij}^{ab}$  only. We get then

$$\langle \Phi_0 | \hat{H} - E | \Phi_0 \rangle + \sum_{ai} \langle \Phi_0 | \hat{H} - E | \Phi_i^a \rangle C_i^a + \sum_{abij} \langle \Phi_0 | \hat{H} - E | \Phi_{ij}^{ab} \rangle C_{ij}^{ab} = 0,$$

or

$$E - E_0 = \Delta E = \sum_{ai} \langle \Phi_0 | \hat{H} | \Phi_i^a \rangle C_i^a + \sum_{abij} \langle \Phi_0 | \hat{H} | \Phi_{ij}^{ab} \rangle C_{ij}^{ab},$$

where the energy  $E_0$  is the reference energy and  $\Delta E$  defines the so-called correlation energy. The single-particle basis functions could be the results of a Hartree-Fock calculation or just the eigenstates of the non-interacting part of the Hamiltonian.

In our notes on Hartree-Fock calculations, we have already computed the matrix  $\langle \Phi_0 | \hat{H} | \Phi_i^a \rangle$  and  $\langle \Phi_0 | \hat{H} | \Phi_{ij}^{ab} \rangle$ . If we are using a Hartree-Fock basis, then the matrix elements  $\langle \Phi_0 | \hat{H} | \Phi_i^a \rangle = 0$  and we are left with a *correlation energy* given by

$$E - E_0 = \Delta E^{HF} = \sum_{abij} \langle \Phi_0 | \hat{H} | \Phi_{ij}^{ab} \rangle C_{ij}^{ab}.$$

Inserting the various matrix elements we can rewrite the previous equation as

$$\Delta E = \sum_{ai} \langle i | \hat{f} | a \rangle C_i^a + \sum_{abij} \langle ij | \hat{v} | ab \rangle C_{ij}^{ab}.$$

This equation determines the correlation energy but not the coefficients  $C$ . We need more equations. Our next step is to set up

$$\langle \Phi_i^a | \hat{H} - E | \Phi_0 \rangle + \sum_{bj} \langle \Phi_i^a | \hat{H} - E | \Phi_j^b \rangle C_j^b + \sum_{bcjk} \langle \Phi_i^a | \hat{H} - E | \Phi_{jk}^{bc} \rangle C_{jk}^{bc} + \sum_{bcdjkl} \langle \Phi_i^a | \hat{H} - E | \Phi_{jkl}^{bcd} \rangle C_{jkl}^{bcd} = 0,$$

as this equation will allow us to find an expression for the coefficients  $C_i^a$  since we can rewrite this equation as

$$\langle i | \hat{f} | a \rangle + \langle \Phi_i^a | \hat{H} | \Phi_i^a \rangle C_i^a + \sum_{bj \neq ai} \langle \Phi_i^a | \hat{H} | \Phi_j^b \rangle C_j^b + \sum_{bcjk} \langle \Phi_i^a | \hat{H} | \Phi_{jk}^{bc} \rangle C_{jk}^{bc} + \sum_{bcdjkl} \langle \Phi_i^a | \hat{H} | \Phi_{jkl}^{bcd} \rangle C_{jkl}^{bcd} = E C_i^a.$$

We see that on the right-hand side we have the energy  $E$ . This leads to a non-linear equation in the unknown coefficients. These equations are normally solved iteratively ( that is we can start with a guess for the coefficients  $C_i^a$ ). A common choice is to use perturbation theory for the first guess, setting thereby

$$C_i^a = \frac{\langle i | \hat{f} | a \rangle}{\epsilon_i - \epsilon_a}.$$

The observant reader will however see that we need an equation for  $C_{jk}^{bc}$  and  $C_{jkl}^{bcd}$  as well. To find equations for these coefficients we need then to continue our multiplications from the left with the various  $\Phi_H^P$  terms.

For  $C_{jk}^{bc}$  we need then

$$\langle \Phi_{ij}^{ab} | \hat{H} - E | \Phi_0 \rangle + \sum_{kc} \langle \Phi_{ij}^{ab} | \hat{H} - E | \Phi_k^c \rangle C_k^c +$$

$$\sum_{cdkl} \langle \Phi_{ij}^{ab} | \hat{H} - E | \Phi_{kl}^{cd} \rangle C_{kl}^{cd} + \sum_{cdeklm} \langle \Phi_{ij}^{ab} | \hat{H} - E | \Phi_{klm}^{cde} \rangle C_{klm}^{cde} + \sum_{cdefklmn} \langle \Phi_{ij}^{ab} | \hat{H} - E | \Phi_{klmn}^{cdef} \rangle C_{klmn}^{cdef} = 0,$$

and we can isolate the coefficients  $C_{kl}^{cd}$  in a similar way as we did for the coefficients  $C_i^a$ . A standard choice for the first iteration is to set

$$C_{ij}^{ab} = \frac{\langle ij | \hat{v} | ab \rangle}{\epsilon_i + \epsilon_j - \epsilon_a - \epsilon_b}.$$

At the end we can rewrite our solution of the Schroedinger equation in terms of  $n$  coupled equations for the coefficients  $C_H^P$ . This is a very cumbersome way of solving the equation. However, by using this iterative scheme we can illustrate how we can compute the various terms in the wave operator or correlation operator  $\hat{C}$ . We will later identify the calculation of the various terms  $C_H^P$  as parts of different many-body approximations to full CI. In particular, we can relate this non-linear scheme with Coupled Cluster theory and many-body perturbation theory.

### 8.7.2 Summarizing FCI and bringing in approximative methods

If we can diagonalize large matrices, FCI is the method of choice since:

- It gives all eigenvalues, ground state and excited states
- The eigenvectors are obtained directly from the coefficients  $C_H^P$  which result from the diagonalization
- We can compute easily expectation values of other operators, as well as transition probabilities
- Correlations are easy to understand in terms of contributions to a given operator beyond the Hartree-Fock contribution. This is the standard approach in many-body theory.

The correlation energy is defined as, with a two-body Hamiltonian,

$$\Delta E = \sum_{ai} \langle i | \hat{f} | a \rangle C_i^a + \sum_{abij} \langle ij | \hat{v} | ab \rangle C_{ij}^{ab}.$$

The coefficients  $C$  result from the solution of the eigenvalue problem. The energy of say the ground state is then

$$E = E_{ref} + \Delta E,$$

where the so-called reference energy is the energy we obtain from a Hartree-Fock calculation, that is

$$E_{ref} = \langle \Phi_0 | \hat{H} | \Phi_0 \rangle.$$

However, as we have seen, even for a small case like the four first major shells and a nucleus like oxygen-16, the dimensionality becomes quickly intractable. If we wish to include single-particle states that reflect weakly bound systems, we need a much larger single-particle basis. We need thus approximative methods that sum specific correlations to infinite order.

Popular methods are

- Many-body perturbation theory (in essence a Taylor expansion)
- Coupled cluster theory (coupled non-linear equations)
- Green's function approaches (matrix inversion)
- Similarity group transformation methods (coupled ordinary differential equations)

All these methods start normally with a Hartree-Fock basis as the calculational basis.



### 8.7.3 A quick tour of Coupled Cluster theory

The ansatz for the wavefunction (ground state) is given by

$$|\Psi\rangle = |\Psi_{CC}\rangle = e^{\hat{T}}|\Phi_0\rangle = \left(\sum_{n=1}^A \frac{1}{n!} \hat{T}^n\right) |\Phi_0\rangle,$$

where  $A$  represents the maximum number of particle-hole excitations and  $\hat{T}$  is the cluster operator defined as

$$\begin{aligned} \hat{T} &= \hat{T}_1 + \hat{T}_2 + \dots + \hat{T}_A \\ \hat{T}_n &= \left(\frac{1}{n!}\right)^2 \sum_{\substack{i_1, i_2, \dots, i_n \\ a_1, a_2, \dots, a_n}} t_{i_1 i_2 \dots i_n}^{a_1 a_2 \dots a_n} a_{a_1}^\dagger a_{a_2}^\dagger \dots a_{a_n}^\dagger a_{i_n} \dots a_{i_2} a_{i_1}. \end{aligned}$$

The energy is given by

$$E_{CC} = \langle \Phi_0 | \bar{H} | \Phi_0 \rangle,$$

where  $\bar{H}$  is a similarity transformed Hamiltonian

$$\begin{aligned} \bar{H} &= e^{-\hat{T}} \hat{H}_N e^{\hat{T}} \\ \hat{H}_N &= \hat{H} - \langle \Phi_0 | \hat{H} | \Phi_0 \rangle. \end{aligned}$$

The coupled cluster energy is a function of the unknown cluster amplitudes  $t_{i_1 i_2 \dots i_n}^{a_1 a_2 \dots a_n}$ , given by the solutions to the amplitude equations

$$0 = \langle \Phi_{i_1 \dots i_n}^{a_1 \dots a_n} | \bar{H} | \Phi_0 \rangle.$$

The similarity transformed Hamiltonian  $\bar{H}$  is expanded using the Baker-Campbell-Hausdorff expression,

$$\begin{aligned} \bar{H} &= \hat{H}_N + [\hat{H}_N, \hat{T}] + \frac{1}{2} [[\hat{H}_N, \hat{T}], \hat{T}] + \dots \\ &\quad \frac{1}{n!} [\dots [\hat{H}_N, \hat{T}], \dots \hat{T}] + \dots \end{aligned}$$

and simplified using the connected cluster theorem

$$\bar{H} = \hat{H}_N + (\hat{H}_N \hat{T})_c + \frac{1}{2} (\hat{H}_N \hat{T}^2)_c + \dots + \frac{1}{n!} (\hat{H}_N \hat{T}^n)_c + \dots$$

A much used approximation is to truncate the cluster operator  $\hat{T}$  at the  $n = 2$  level. This defines the so-called singles and doubles approximation to the Coupled Cluster wavefunction, normally shortened to CCSD..

The coupled cluster wavefunction is now given by

$$|\Psi_{CC}\rangle = e^{\hat{T}_1 + \hat{T}_2} |\Phi_0\rangle$$

where

$$\begin{aligned} \hat{T}_1 &= \sum_{ia} t_i^a a_a^\dagger a_i \\ \hat{T}_2 &= \frac{1}{4} \sum_{ijab} t_{ij}^{ab} a_a^\dagger a_b^\dagger a_j a_i. \end{aligned}$$

The amplitudes  $t$  play a role similar to the coefficients  $C$  in the shell-model calculations. They are obtained by solving a set of non-linear equations similar to those discussed above in connection with the FCI discussion.

If we truncate our equations at the CCSD level, it corresponds to performing a transformation of the Hamiltonian matrix of the following type for a six particle problem (with a two-body Hamiltonian):

	$0p-0h$	$1p-1h$	$2p-2h$	$3p-3h$	$4p-4h$	$5p-5h$	$6p-6h$
$0p-0h$	$\tilde{x}$	$\tilde{x}$	$\tilde{x}$	0	0	0	0
$1p-1h$	0	$\tilde{x}$	$\tilde{x}$	$\tilde{x}$	0	0	0
$2p-2h$	0	$\tilde{x}$	$\tilde{x}$	$\tilde{x}$	$\tilde{x}$	0	0
$3p-3h$	0	$\tilde{x}$	$\tilde{x}$	$\tilde{x}$	$\tilde{x}$	$\tilde{x}$	0
$4p-4h$	0	0	$\tilde{x}$	$\tilde{x}$	$\tilde{x}$	$\tilde{x}$	$\tilde{x}$
$5p-5h$	0	0	0	$\tilde{x}$	$\tilde{x}$	$\tilde{x}$	$\tilde{x}$
$6p-6h$	0	0	0	0	$\tilde{x}$	$\tilde{x}$	$\tilde{x}$

In our FCI discussion the correlation energy is defined as, with a two-body Hamiltonian,

$$\Delta E = \sum_{ai} \langle i | \hat{f} | a \rangle C_i^a + \sum_{abij} \langle ij | \hat{v} | ab \rangle C_{ij}^{ab}.$$

In Coupled cluster theory it becomes (irrespective of level of truncation of  $T$ )

$$\Delta E = \sum_{ai} \langle i | \hat{f} | a \rangle t_i^a + \sum_{abij} \langle ij | \hat{v} | ab \rangle t_{ij}^{ab}.$$

Coupled cluster theory has several interesting computational features and is the method of choice in quantum chemistry. The method was originally proposed by Coester and Kummel, two nuclear physicists (way back in the fifties). It came back in full strength in nuclear physics during the last decade.

There are several interesting features:

- With a truncation like CCSD or CCSDT, we can include to infinite order correlations like  $2p-2h$ .
- We can include a large basis of single-particle states, not possible in standard FCI calculations

However, Coupled Cluster theory is

- non-variational
- if we want to find properties of excited states, additional calculations via for example equation of motion methods are needed
- if correlations are strong, a single-reference ansatz may not be the best starting point
- we cannot quantify properly the error we make when truncations are made in the cluster operator

### 8.7.4 The CCD approximation

We will now approximate the cluster operator  $\hat{T}$  to include only  $2p-2h$  correlations. This leads to the so-called CCD approximation, that is

$$\hat{T} \approx \hat{T}_2 = \frac{1}{4} \sum_{abij} t_{ij}^{ab} a_a^\dagger a_b^\dagger a_j a_i,$$

meaning that we have

$$|\Psi_0\rangle \approx |\Psi_{CCD}\rangle = \exp(\hat{T}_2)|\Phi_0\rangle.$$

Inserting these equations in the expression for the computation of the energy we have, with a Hamiltonian defined with respect to a general vacuum (see the exercises in the second quantization part)

$$\hat{H} = \hat{H}_N + E_{\text{ref}},$$

with

$$\hat{H}_N = \sum_{pq} \langle p|\hat{f}|q\rangle a_p^\dagger a_q + \frac{1}{4} \sum_{pqrs} \langle pq|\hat{v}|rs\rangle a_p^\dagger a_q^\dagger a_s a_r,$$

we obtain that the energy can be written as

$$\langle \Phi_0 | \exp(-\hat{T}_2) \hat{H}_N \exp(\hat{T}_2) | \Phi_0 \rangle = \langle \Phi_0 | \hat{H}_N (1 + \hat{T}_2) | \Phi_0 \rangle = E_{CCD}.$$

This quantity becomes

$$E_{CCD} = E_{\text{ref}} + \frac{1}{4} \sum_{abij} \langle ij|\hat{v}|ab\rangle t_{ij}^{ab},$$

where the latter is the correlation energy from this level of approximation of CC theory. Similarly, the expression for the amplitudes reads

$$\langle \Phi_{ij}^{ab} | \exp(-\hat{T}_2) \hat{H}_N \exp(\hat{T}_2) | \Phi_0 \rangle = 0.$$

These equations can be reduced to (after several applications of Wick's theorem) to, for all  $i > j$  and all  $a > b$ ,

$$\begin{aligned} 0 = & \langle ab|\hat{v}|ij\rangle + (\varepsilon_a + \varepsilon_b - \varepsilon_i - \varepsilon_j) t_{ij}^{ab} \\ & + \frac{1}{2} \sum_{cd} \langle ab|\hat{v}|cd\rangle t_{ij}^{cd} + \frac{1}{2} \sum_{kl} \langle kl|\hat{v}|ij\rangle t_{kl}^{ab} + \hat{P}(ij|ab) \sum_{kc} \langle kb|\hat{v}|cj\rangle t_{ik}^{ac} \\ & + \frac{1}{4} \sum_{klcd} \langle kl|\hat{v}|cd\rangle t_{ij}^{cd} t_{kl}^{ab} + \hat{P}(ij) \sum_{klcd} \langle kl|\hat{v}|cd\rangle t_{ik}^{ac} t_{jl}^{bd} \\ & - \frac{1}{2} \hat{P}(ij) \sum_{klcd} \langle kl|\hat{v}|cd\rangle t_{ik}^{dc} t_{lj}^{ab} - \frac{1}{2} \hat{P}(ab) \sum_{klcd} \langle kl|\hat{v}|cd\rangle t_{lk}^{ac} t_{ij}^{db}, \end{aligned} \quad (8.51)$$

where we have defined

$$\hat{P}(ab) = 1 - \hat{P}_{ab},$$

where  $\hat{P}_{ab}$  interchanges two particles occupying the quantum numbers  $a$  and  $b$ . The operator  $\hat{P}(ij|ab)$  is defined as

$$\hat{P}(ij|ab) = (1 - \hat{P}_{ij})(1 - \hat{P}_{ab}).$$

Recall also that the unknown amplitudes  $t_{ij}^{ab}$  represent anti-symmetrized matrix elements, meaning that they obey the same symmetry relations as the two-body interaction, that is

$$t_{ij}^{ab} = -t_{ji}^{ab} = -t_{ij}^{ba} = t_{ji}^{ba}.$$

The two-body matrix elements are also anti-symmetrized, meaning that

$$\langle ab|\hat{v}|ij\rangle = -\langle ab|\hat{v}|ji\rangle = -\langle ba|\hat{v}|ij\rangle = \langle ba|\hat{v}|ji\rangle.$$

The non-linear equations for the unknown amplitudes  $t_{ij}^{ab}$  are solved iteratively. We discuss the implementation of these equations below.

Approximations to the full CCD equations.

It is useful to make approximations to the equations for the amplitudes. The standard method for solving these equations is to set up an iterative scheme where method's like Newton's method or similar root searching methods are used to find the amplitudes. Iterative solvers need a guess for the amplitudes. A good starting point is to use the correlated wave operator from perturbation theory to first order in the interaction. This means that we define the zeroth approximation to the amplitudes as

$$t^{(0)} = \frac{\langle ab|\hat{v}|ij\rangle}{(\epsilon_i + \epsilon_j - \epsilon_a - \epsilon_b)},$$

leading to our first approximation for the correlation energy at the CCD level to be equal to second-order perturbation theory without  $1p-1h$  excitations, namely

$$\Delta E_{\text{CCD}}^{(0)} = \frac{1}{4} \sum_{abij} \frac{\langle ij|\hat{v}|ab\rangle \langle ab|\hat{v}|ij\rangle}{(\epsilon_i + \epsilon_j - \epsilon_a - \epsilon_b)}.$$

With this starting point, we are now ready to solve Eq. (8.51) iteratively. Before we attack the full equations, it is however instructive to study a truncated version of the equations. We will first study the following approximation where we take away all terms except the linear terms that involve the single-particle energies and the the two-particle intermediate excitations, that is

$$0 = \langle ab|\hat{v}|ij\rangle + (\epsilon_a + \epsilon_b - \epsilon_i - \epsilon_j) t_{ij}^{ab} + \frac{1}{2} \sum_{cd} \langle ab|\hat{v}|cd\rangle t_{ij}^{cd}. \quad (8.52)$$

Setting the single-particle energies for the hole states equal to an energy variable  $\omega = \epsilon_i + \epsilon_j$ , Eq. (8.52) reduces to the well-known equations for the so-called  $G$ -matrix, widely used in infinite matter and finite nuclei studies. The equation can then be reordered and solved by matrix inversion. To see this let us define the following quantity

$$\tau_{ij}^{ab} = (\omega - \epsilon_a - \epsilon_b) t_{ij}^{ab},$$

and inserting

$$1 = \frac{(\omega - \epsilon_c - \epsilon_d)}{(\omega - \epsilon_c - \epsilon_d)},$$

in the intermediate sums over  $cd$  in Eq. (8.52), we can rewrite the latter equation as

$$\tau_{ij}^{ab}(\omega) = \langle ab|\hat{v}|ij\rangle + \frac{1}{2} \sum_{cd} \langle ab|\hat{v}|cd\rangle \frac{1}{\omega - \epsilon_c - \epsilon_d} \tau_{ij}^{cd}(\omega),$$

where we have indicated an explicit energy dependence. This equation, transforming a two-particle configuration into a single index, can be transformed into a matrix inversion problem. Solving the equations for a fixed energy  $\omega$  allows us to compare directly with results from Green's function theory when only two-particle intermediate states are included.

To solve Eq. (8.52), we would thus start with a guess for the unknown amplitudes, typically using the wave operator defined by first order in perturbation theory, leading to a zeroth approximation to the energy given by second-order perturbation theory for the correlation energy. A simple approach to the solution of Eq. (8.52), is to thus to

1. Start with a guess for the amplitudes and compute the zeroth approximation to the correlation energy

2. Use the ansatz for the amplitudes to solve Eq. (8.52) via for example your root-finding method of choice (Newton's method or modifications thereof can be used) and continue these iterations till the correlation energy does not change more than a prefixed quantity  $\lambda$ ;  $\Delta E_{\text{CCD}}^{(i)} - \Delta E_{\text{CCD}}^{(i-1)} \leq \lambda$ .
3. It is common during the iterations to scale the amplitudes with a parameter  $\alpha$ , with  $\alpha \in (0, 1]$  as  $t^{(i)} = \alpha t^{(i)} + (1 - \alpha)t^{(i-1)}$ .

The next approximation is to include the two-hole term in Eq. (8.51), a term which allow us to make a link with Green's function theory with two-particle and two-hole correlations. This means that we solve

$$0 = \langle ab|\hat{v}|ij\rangle + (\epsilon_a + \epsilon_b - \epsilon_i - \epsilon_j)t_{ij}^{ab} + \frac{1}{2} \sum_{cd} \langle ab|\hat{v}|cd\rangle t_{ij}^{cd} + \frac{1}{2} \sum_{kl} \langle kl|\hat{v}|ij\rangle t_{kl}^{ab}. \quad (8.53)$$

This equation is solved the same way as we would do for Eq. (8.52). The final step is then to include all terms in Eq. (8.51).

## 8.8 Developing a numerical project

This section will focus on writing a working CCD code from scratch. If you are familiar with writing quantum many-body physics codes, feel free to skip ahead as we are going to go into some detail about implementing CCD as a computer code now. As we saw earlier, the CCD equations can be written as

$$\begin{aligned} (\epsilon_i + \epsilon_j - \epsilon_a - \epsilon_b)t_{ij}^{ab} = & \langle ab|\hat{v}|ij\rangle \\ & + \frac{1}{2} \sum_{cd} \langle ab|\hat{v}|cd\rangle t_{ij}^{cd} + \frac{1}{2} \sum_{kl} \langle kl|\hat{v}|ij\rangle t_{kl}^{ab} + \hat{P}(ij|ab) \sum_{kc} \langle kb|\hat{v}|cj\rangle t_{ik}^{ac} \\ & + \frac{1}{4} \sum_{klcd} \langle kl|\hat{v}|cd\rangle t_{ij}^{cd} t_{kl}^{ab} + \hat{P}(ij) \sum_{klcd} \langle kl|\hat{v}|cd\rangle t_{ik}^{ac} t_{jl}^{bd} \\ & - \frac{1}{2} \hat{P}(ij) \sum_{klcd} \langle kl|\hat{v}|cd\rangle t_{ik}^{dc} t_{lj}^{ab} - \frac{1}{2} \hat{P}(ab) \sum_{klcd} \langle kl|\hat{v}|cd\rangle t_{lk}^{ac} t_{ij}^{db}, \end{aligned} \quad (8.54)$$

for all  $i < j$  and all  $a < b$ , using the standard notation that  $a, b, \dots$  are particle states and  $i, j, \dots$  are hole states. With the CCD correlation energy given by

$$\Delta E_{\text{CCD}} = \frac{1}{4} \sum_{ijab} \langle ij|\hat{v}|ab\rangle t_{ij}^{ab}. \quad (8.55)$$

One way to solve these equations, is to write equation (8.54) as a series of iterative nonlinear algebraic equations.

$$\begin{aligned} t_{ij}^{ab(n+1)} = & \frac{1}{\epsilon_{ij}^{ab}} \left( \langle ab|\hat{v}|ij\rangle \right. \\ & + \frac{1}{2} \sum_{cd} \langle ab|\hat{v}|cd\rangle t_{ij}^{cd(n)} + \frac{1}{2} \sum_{kl} \langle kl|\hat{v}|ij\rangle t_{kl}^{ab(n)} + \hat{P}(ij|ab) \sum_{kc} \langle kb|\hat{v}|cj\rangle t_{ik}^{ac(n)} \\ & + \frac{1}{4} \sum_{klcd} \langle kl|\hat{v}|cd\rangle t_{ij}^{cd(n)} t_{kl}^{ab(n)} + \hat{P}(ij) \sum_{klcd} \langle kl|\hat{v}|cd\rangle t_{ik}^{ac(n)} t_{jl}^{bd(n)} \\ & \left. - \frac{1}{2} \hat{P}(ij) \sum_{klcd} \langle kl|\hat{v}|cd\rangle t_{ik}^{dc(n)} t_{lj}^{ab(n)} - \frac{1}{2} \hat{P}(ab) \sum_{klcd} \langle kl|\hat{v}|cd\rangle t_{lk}^{ac(n)} t_{ij}^{db(n)} \right), \end{aligned} \quad (8.56)$$

for all  $i < j$  and all  $a < b$ , where  $\varepsilon_{ij}^{ab} = (\varepsilon_i + \varepsilon_j - \varepsilon_a - \varepsilon_b)$ , and  $t_{ij}^{ab(n)}$  is the  $t$  amplitude for the  $n$ th iteration of the series. This way, given some starting guess  $t_{ij}^{ab(0)}$ , we can generate subsequent  $t$  amplitudes that converges to some value. Discussion of the mathematical details regarding convergence will be tabled for later; for now we will talk about implementing these equations into a computer program and assume convergence. In pseudocode, the function that updates the  $t$  amplitudes looks like

```

CCD_Update()
for  $i \in \{0, N_{fermi} - 1\}$  do
  for  $j \in \{0, N_{fermi} - 1\}$  do
    for  $a \in \{N_{fermi}, N_{sp} - 1\}$  do
      for  $b \in \{N_{fermi}, N_{sp} - 1\}$  do
        sum  $\leftarrow$  TBME[index( $a, b, i, j$ )]
        for  $c \in \{N_{fermi}, N_{sp} - 1\}$  do
          for  $d \in \{N_{fermi}, N_{sp} - 1\}$  do
            sum  $\leftarrow$  sum + 0.5 * ME[index( $a, b, c, d$ )] *  $t\_amplitudes\_old$ [index( $c, d, i, j$ )]
          end for
        end for
      end for
    end for
    ...
    sum  $\leftarrow$  sum + (all other terms)
    ...
    energy_denom = SP_energy[ $i$ ] + SP_energy[ $j$ ] - SP_energy[ $a$ ] - SP_energy[ $b$ ]
     $t\_amplitudes$ [index( $a, b, i, j$ )] = sum/energy_denom
  end for
end for
end for

```

Where  $N_{fermi}$  is the fermi level and  $N_{sp}$  is the total number of single particle (s.p.) states, indexed from 0 to  $N_{sp} - 1$ . At the most basic level, the CCD equations are just the addition of many products containing  $t_{ij}^{ab}$  amplitudes and two-body matrix elements (TBMEs)  $\langle ij|\hat{v}|ab\rangle$ , so a lot of care should be placed into how we store these objects. These are both objects with four indices, so a sensible first implementation of the CCD equations would be to create two 4-D arrays to store the objects. However, it is often more convenient to work with simple 1-D arrays instead. `index()` is a function that maps the four indices onto one index so that a 1-D array can be used. An example of such a function is:

```

function index( $p, q, r, s$ )
  return  $p * N_{sp}^3 + q * N_{sp}^2 + r * N_{sp} + s$ 
end function

```

Because elements with repeated indices vanish,  $t_{ii}^{ab} = t_{ij}^{aa} = 0$  and  $\langle pp|\hat{v}|rs\rangle = \langle pq|\hat{v}|rr\rangle = 0$ , data structures using this index function will contain many elements that are automatically zero, so we will discuss more efficient storage strategies later. Notice also that we are looping over all  $i, j, a, b$ , rather than the restricted indices. This means that we are doing redundant work, but it is simpler to code up, and we will want to unrestrict these indices later anyways.

The goal of this code is to calculate the correlation energy,  $\Delta E_{CCD}$ , so after each iteration of our equation, we use our newest  $t$  amplitudes to update this value,

$$\Delta E_{CCD}^{(n)} = \frac{1}{4} \sum_{ijab} \langle ij|\hat{v}|ab\rangle t_{ij}^{ab(n)}. \quad (8.57)$$

We check that our result is converged by checking that to see if the most recent iteration has changed the correlation energy by less than some tolerance threshold  $\eta$ ,

$$\eta > |\Delta E_{CCD}^{(n+1)} - \Delta E_{CCD}^{(n)}|. \quad (8.58)$$

The basic structure of the iterative process will look like:

```
while (abs(energy_Diff) > tolerance) do
  CCD_Update()
  correlation_Energy ← CCD_Corr_Energy()
  energy_Diff ← correlation_Energy - correlation_Energy_old
  correlation_Energy_old ← correlation_Energy
  t_amplitudes_old ← t_amplitudes
end while
```

Prior to this algorithm, the  $t$  amplitudes should be initialized,  $t_{ij}^{ab(0)}$ . A particularly convenient choice is to set  $t_{ij}^{ab(0)} = 0$ . Notice that if this starting point is used, then

$$t_{ij}^{ab(1)} = \frac{\langle ab|\hat{v}|ij\rangle}{\epsilon_{ij}^{ab}} \quad (8.59)$$

$$\Delta E_{CCD}^{(1)} = \frac{1}{4} \sum_{ijab} \frac{\langle ab|\hat{v}|ij\rangle}{\epsilon_{ij}^{ab}}, \quad (8.60)$$

which is the result from MBPT2. This is a useful, as one iteration of the CCD equations can be ran, and checked against MBPT2 to give some confidence that everything is working so far. To check that everything is working, it is useful to run the code using a minimal example. A simple pairing model Hamiltonian is a nice place to start.

$$\hat{H}_0 = \xi \sum_{p\sigma} (p-1) a_{p\sigma}^\dagger a_{p\sigma} \quad (8.61)$$

$$\hat{V} = -\frac{1}{2} g \sum_{pq} a_{p+}^\dagger a_{p-}^\dagger a_{q-} a_{q+} \quad (8.62)$$

which represents a basic pairing model with  $p$  levels each with a spin degeneracy of 2. The form of the coupled cluster equations in (Eq) uses single-particle states that are eigenstates of the Hartree-Fock operator,  $(\hat{u} + \hat{u}_{\text{HF}}|p\rangle = \epsilon_p|p\rangle$ . In the pairing model, this condition is already fulfilled. All we have to do is define the lowest  $N_{\text{fermi}}$  states as holes then redefine the single-particle energies,

$$\epsilon_q = h_{qq} + \sum_i \langle qi||qi\rangle. \quad (8.63)$$

To be more specific, let's look at this pairing model with 4 particles and 8 single-particle states. These states (with  $\xi = 1.0$ ) could be labeled as such with

State Label	p	2s <sub>z</sub>	E	type
0	1	1	-g/2	hole
1	1	-1	-g/2	hole
2	2	1	1-g/2	hole
3	2	-1	1-g/2	hole
4	3	1	2	particle
5	3	-1	2	particle
6	4	1	3	particle
7	4	-1	3	particle

Here are some more results for specific values of  $g$  that can be used for benchmarking.

g	E <sub>ref</sub>	$\Delta E_{MBPT2}$	$\Delta E_{CCD}$
-1.0	3	-0.46667	-0.21895*
-0.5	2.5	-0.08874	-0.06306
0.0	2	0	0
0.5	1.5	-0.06239	-0.08336
1.0	1	-0.21905	-0.36956

The  $g = -1.0$  case diverges without implementing iterative mixing. Sometimes iterative solvers run into oscillating solutions, and mixing can help the iterations break this cycle.

$$t^{(i)} = \alpha t_{no\_mixing}^{(i)} + (1 - \alpha)t^{(i-1)} \quad (8.64)$$

In the case of this simple pairing model, it is easy to calculate  $\Delta E_{MBPT2}$  by hand, which is useful to check the code's calculation of this value, as well as the first CCD iteration.

$$\Delta E_{MBPT2} = \frac{1}{4} \sum_{abij} \frac{\langle ij||ab \rangle \langle ab||ij \rangle}{\epsilon_{ij}^{ab}} = \sum_{a < b, i < j} \frac{\langle ij||ab \rangle \langle ab||ij \rangle}{\epsilon_{ij}^{ab}} \quad (8.65)$$

For our pairing example:

$$\Delta E_{MBPT2} = \frac{\langle 01||45 \rangle^2}{\epsilon_{01}^{45}} + \frac{\langle 01||67 \rangle^2}{\epsilon_{01}^{67}} + \frac{\langle 23||45 \rangle^2}{\epsilon_{23}^{45}} + \frac{\langle 23||67 \rangle^2}{\epsilon_{23}^{67}}$$

$$\Delta E_{MBPT2} = -\frac{g^2}{4} \left( \frac{1}{4+g} + \frac{1}{6+g} + \frac{1}{2+g} + \frac{1}{4+g} \right),$$

which is a nice expression which can be used to check the results for any value of  $g$ .

Once a working pairing model has been implemented, improvements can start to be made, all the while using the pairing model to make sure that the code is still working and giving correct answers. Realistic systems will be much larger than this small pairing example.

One limitation that will be ran into while trying to do realistic CCD calculations is that of memory. The 4-indexed TBMEs and  $t$ -amplitudes have to store a lot of elements, and the size of these arrays can quite become larger than that of the available memory on the machine. If calculation wants to use 500 s.p. basis states, then a structure like  $\langle pq|v|rs \rangle$  will have length 500 for each of its four indices, which means it will have  $500^4 = 625 * 10^8$  elements. To get a handle on how much memory is used, consider the elements as double-precision floating point type. One double takes up 8 bytes of memory. So this array would take up  $8 * 625 * 10^8$  bytes =  $5000 * 10^8$  bytes = 500 Gbytes of memory. Most personal computers in 2016 have 4-8 Gbytes of RAM, so this calculation would be way out of reach. There are supercomputers that can handle applications using 500 Gbytes of memory, but we can quickly reduce the total memory required by applying some physical arguments. In addition to vanishing elements with repeated indices, mentioned above, elements that do not obey certain symmetries are also zero. Almost all realistic two-body forces preserve some quantities due to symmetries in the interaction. For example, an interaction with rotational symmetry will conserve angular momentum. This means that a two-body ket state  $|rs \rangle$ , which has some set of quantum numbers, will retain quantum numbers corresponding to the interaction symmetries after being acted on by  $\hat{v}$ . This state is then projected onto  $|pq \rangle$  with its own set of quantum numbers. Thus  $\langle pq|v|rs \rangle$  is only non-zero if  $|pq \rangle$  and  $|rs \rangle$  share the same quantum numbers that are preserved by  $\hat{v}$ . In addition, because the cluster operators represent excitations due to the interaction,  $t_{ij}^{ab}$  is only non-zero if  $|ij \rangle$  has the same relevant quantum numbers as  $|ab \rangle$ .

To take advantage of this, these two-body ket states can be organized into “channels” of shared quantum numbers. In the case of the pairing model, the interaction preserves the total spin projection of a two-body state,  $S_z = s_{z1} + s_{z2}$ . The single particle states can have spin of



+1/2 or -1/2, so there can be three two-body channels with  $S_z = -1, 0, +1$ . These channels can then be indexed with a unique label in a similar way to the single particle index scheme. In more complicated systems, there will be many more channels involving multiple symmetries, so it is useful to create a data structure that stores the relevant two-body quantum numbers to keep track of the labeling scheme.

Now it is more efficient to use two-dimensional array data structures, where the first index refers to the channel number and the second refers to the element within that channel. So to access matrix elements or  $t$  amplitudes, you can loop over the channels first, then the indices within that channel. To get an idea of the savings using this block diagonal structure, let's look at a case with a plane wave basis, with three momentum and one spin quantum numbers, with an interaction that conserves linear momentum in all three dimensions, as well as the total spin projection. Using 502 basis states, the TBME's require about 0.23 Gb of memory in block diagonal form, which is an enormous saving from the 500 Gb mentions earlier in the naïve storage scheme.

Since the calculation of all of these zeros can now be avoided, improvements in speed as memory will now follow. To get a handle on how example these CCD calculations are we need only to look at the most expensive sum in equation 8.54. This corresponds to the sum over  $klcd$ . Since this sum is repeated for all  $i < j$  and  $a < b$ , that means these equations will scale as  $\mathcal{O}(n_p^4 n_h^4)$ . However, (as we saw earlier?), they can be rewritten using intermediates as

$$\begin{aligned} 0 = \langle ab|\hat{v}|ij\rangle + \hat{P}(ab) \sum_c \langle b|\chi|c\rangle \langle ac|t|ij\rangle - \hat{P}(ij) \sum_k \langle k|\chi|j\rangle \langle ab|t|ik\rangle \\ + \frac{1}{2} \sum_{cd} \langle ab|\chi|cd\rangle \langle cd|t|ij\rangle + \frac{1}{2} \sum_{kl} \langle ab|t|kl\rangle \langle kl|\chi|ij\rangle \\ + \hat{P}(ij) \hat{P}(ab) \sum_{kc} \langle ac|t|ik\rangle \langle kb|\chi|cj\rangle \end{aligned} \quad (8.66)$$

for all  $i, j, a, b$ , the reason why these indices are now unrestricted will be explained later. Where the intermediates  $\chi$  are

$$\langle b|\chi|c\rangle = \langle b|f|c\rangle - \frac{1}{2} \sum_{kl} \langle bd|t|kl\rangle \langle kl|v|cd\rangle \quad (8.67)$$

$$\langle k|\chi|j\rangle = \langle k|f|j\rangle + \frac{1}{2} \sum_{cd} \langle kl|v|cd\rangle \langle cd|t|jl\rangle \quad (8.68)$$

$$\langle kl|\chi|ij\rangle = \langle kl|v|ij\rangle + \frac{1}{2} \sum_{cd} \langle kl|v|cd\rangle \langle cd|t|ij\rangle \quad (8.69)$$

$$\langle kb|\chi|cj\rangle = \langle kb|v|cj\rangle + \frac{1}{2} \sum_{dl} \langle kl|v|cd\rangle \langle db|t|lj\rangle \quad (8.70)$$

$$\langle ab|\chi|cd\rangle = \langle ab|v|cd\rangle \quad (8.71)$$

Maybe demonstrate how these equations are equal here?

Now the CCD equations will scale as  $\mathcal{O}(n_h^2 n_p^4)$  which is quite a bit better than before. This is of course at the cost of computing the intermediates at the beginning of each iteration, which the most expensive one,  $\langle kb|\chi|cj\rangle$ , will scale as  $\mathcal{O}(n_h^3 n_p^3)$ . To further speed these computations up, we see that these sums can be written as matrix-matrix multiplication. It is not obvious how to write all of these sums in such a way, but it is useful to first remember that to write out the multiplication of matrices  $\hat{C} = \hat{A} * \hat{B}$  is

$$C_{ij} = \sum_k A_{ik} * B_{kj}. \quad (8.72)$$

Notice that equation (8.69) can be written as

$$\langle K|\chi|I\rangle = \langle K|v|I\rangle + \frac{1}{2} \sum_C \langle K|v|C\rangle \langle C|t|I\rangle$$

by mapping the two index pairs  $kl \rightarrow K, ij \rightarrow I, cd \rightarrow C$ . So now the sum looks like a matrix-matrix multiplication. This is useful because there are packages like BLAS (Basic Linear Algebra Subprograms) which have extremely fast implementations of matrix-matrix multiplication.

Now that we have a working CCD program, we can move on to more realistic cases. One such case is infinite nuclear matter using a plane-wave basis. These states are solutions to the free-particle Hamiltonian,

$$\frac{-\hbar^2}{2m} \nabla^2 \phi(\mathbf{x}) = \varepsilon \phi(\mathbf{x}). \quad (8.73)$$

For a finite basis, we approximate the problem by constructing a box with sides of length  $L$ , which quantizes the momentum, and impose periodic boundary conditions in each direction.

$$\phi(x_i) = \phi(x_i + L) \quad (8.74)$$

$$\phi_{\mathbf{k}}(\mathbf{x}) = \frac{1}{\sqrt{L^3}} e^{i\mathbf{k}\cdot\mathbf{x}}, \quad \mathbf{k} = \frac{2\pi\mathbf{n}}{L}, \quad n_i \quad (8.75)$$

The first step in calculating infinite matter is to construct a model space by finding every single-particle state relevant to a given problem. In our case, this amounts to looping over the quantum numbers for spin, isospin, and the three momentum directions. To control the model space size, the momentum can be truncated to give a cubic space, where  $n_i \leq n_{\max}$ , or a spherical space, where  $n_x^2 + n_y^2 + n_z^2 \leq N_{\max}$ . The number of single-particle states in a cubic space increases rapidly with  $n_{\max}$  compared to the spherical case with  $N_{\max}$ . For example, in pure neutron matter a cubic space with  $n_{\max} = 3$  has 668 states while the spherical space with  $N_{\max} = 17$  has 610 states. Therefore, the spherical case will be used for the rest of the calculations here. The loop increases in energy by counting the number of shells, so states can be ‘filled’ by labeling the first  $P$  proton and  $N$  neutron states as holes. The following loop is for pure neutron matter and requires the number of neutrons,  $N$  and density,  $\rho = N/L^3$ , as input. Symmetric nuclear matter requires an extra loop over isospin.

```

n = 0
for shell  $\in \{0, \dots, N_{\max}\}$  do
  for  $-\sqrt{N_{\max}} \leq n_x \leq \sqrt{N_{\max}}$  do
    for  $-\sqrt{N_{\max}} \leq n_y \leq \sqrt{N_{\max}}$  do
      for  $-\sqrt{N_{\max}} \leq n_z \leq \sqrt{N_{\max}}$  do
        for  $s_z \in \{-\frac{1}{2}, \frac{1}{2}\}$  do
          if  $n_x^2 + n_y^2 + n_z^2 = \text{shell}$  then
            Energy =  $\frac{4\pi^2\hbar^2}{2m} \times \text{shell}$ 
            if  $n < N$  then
              type = “hole”
            else
              type = “particle”
            end if
            STATES  $\leftarrow (n, n_x, n_y, n_z, s_z, \text{Energy}, \text{type})$ 
             $n \leftarrow n + 1$ 
          end if
        end for
      end for
    end for
  end for
end for

```

**end for**  
**end for**  
**end for**

The next step is to build every two-body state in the model space and separate them by their particle/hole character and combined quantum numbers. While each single-particle state was unique, two-body states can share quantum numbers with members of a particular two-body channel. These channels allow us to remove matrix elements and cluster amplitudes that violate the symmetries of the interaction and greatly reduces the size and speed of the calculation. Our structures will depend on direct two-body channels,  $T$ , where the quantum numbers are added and cross two-body channels,  $X$ , where the quantum numbers are subtracted. Before filling the channels, it's helpful to order them with an index function which returns a unique index for a given set of two-body quantum numbers. Without an index function, one has to loop over all the channels for each two-body state which adds a substantial amount of time to this algorithm. An example of an index function for the direct channels in symmetric nuclear matter is, for  $N_x = n_{x,1} + n_{x,2}$ ,  $N_y = n_{y,1} + n_{y,2}$ ,  $N_z = n_{z,1} + n_{z,2}$ ,  $S_z = s_{z,1} + s_{z,2}$ ,  $T_z = t_{z,1} + t_{z,2}$ ,  $m = 2\lfloor\sqrt{N_{\max}}\rfloor$ , and  $M = 2m + 1$ ,

$$\text{Ind}(N_x, N_y, N_z, S_z, T_z) = 2(N_x + m)M^3 + 2(N_y + m)M^2 + 2(N_z + m)M + 2(S_z + 1) + (T_z + 1). \quad (8.76)$$

This function, which can also be used for the cross-channel index function, is well suited for a cubic model space but can be applied in either case. An additional restriction for two-body states is that they must be composed of two different states to satisfy the Pauli-exclusion principle.

```
for sp1  $\in$  STATES do
  for sp2  $\in$  STATES do
    if sp1  $\neq$  sp2 then
       $N_i \leftarrow n_{i,1} + n_{i,2}$ 
       $S_z \leftarrow s_{z,1} + s_{z,2}$ 
       $T_z \leftarrow t_{z,1} + t_{z,2}$ 
       $i\_dir \leftarrow \text{Ind}(N_x, N_y, N_z, S_z, T_z)$ 
       $T \leftarrow (\text{sp1}, \text{sp2}, i\_dir)$ 
       $N'_i \leftarrow n_{i,1} - n_{i,2}$ 
       $S'_z \leftarrow s_{z,1} - s_{z,2}$ 
       $T'_z \leftarrow t_{z,1} - t_{z,2}$ 
       $i\_cross \leftarrow \text{Ind}(N'_x, N'_y, N'_z, S'_z, T'_z)$ 
       $X \leftarrow (\text{sp1}, \text{sp2}, i\_cross)$ 
    end if
  end for
end for
```

From the cross channels, one can construct the cross channel compliments,  $X'$ , where  $X(pq) \equiv X'(qp)$ . Also from the direct channels, one can construct one-body, and correspondent three-body, channels for each single-particle state,  $K$  by finding every combination of two two-body states within a direct channel that contains that single particle state,  $T(pq) = T(rs) \Rightarrow K_p \leftarrow (qrs)$ .

```
for Chan  $\in$  T do
  for tb1  $\in$  Chan do
    for tb2  $\in$  Chan do
       $K \leftarrow \text{tb1}_1$ 
       $K_{\text{tb1}_1} \leftarrow \text{tb1}_2, \text{tb2}_1, \text{tb2}_2$ 
    end for
  end for
```

**end for**

These different sctructures can be further categorized by a two-body state's particle-hole character,  $\langle pp|t|hh\rangle$ ,  $\langle hh|v|hh\rangle$ ,  $\langle pp|v|pp\rangle$ ,  $\langle hh|v|pp\rangle$ , and  $\langle hp|v|hp\rangle$ , which greatly simplifies the matrix-matrix multiplications of the CCD iterations by indexing the summed variables in a systematic way. Summations are constructed by placing two structures next to each other in such a way that the inner, summed indices are of the same channel. The resulting structure is indexed by the outer channels.

$$\langle b|\chi|c\rangle = \langle b|f|c\rangle - \frac{1}{2} \sum_{kl} \langle bd|t|kl\rangle \langle kl|v|cd\rangle \rightarrow f_c^b(K(b), K(c)) - \frac{1}{2} t_{kl}^{bd}(K(b), K_b(kld)) \cdot v_{cd}^{kl}(K_c(kld), K(c)) \quad (8.77)$$

$$\langle k|\chi|j\rangle = \langle k|f|j\rangle + \frac{1}{2} \sum_{cd} \langle kl|v|cd\rangle \langle cd|t|jl\rangle \rightarrow f_j^k(K(k), K(j)) + \frac{1}{2} v_{cd}^{kl}(K(k), K_k(cdl)) \cdot t_{jl}^{cd}(K_j(cdl), K(j)) \quad (8.78)$$

$$\langle kl|\chi|ij\rangle = \langle kl|v|ij\rangle + \frac{1}{2} \sum_{cd} \langle kl|v|cd\rangle \langle cd|t|ij\rangle \rightarrow v_{ij}^{kl}(T(kl), T(ij)) + \frac{1}{2} v_{cd}^{kl}(T(kl), T(cd)) \cdot t_{ij}^{cd}(T(cd), T(ij)) \quad (8.79)$$

$$\langle kb|\chi|cj\rangle = \langle kb|v|cj\rangle + \frac{1}{2} \sum_{dl} \langle kl|v|cd\rangle \langle db|t|lj\rangle \rightarrow v_{cj}^{kb}(X(kc), X(jb)) + \frac{1}{2} v_{cd}^{kl}(X(kc), X(dl)) \cdot t_{lj}^{db}(X(dl), X(jb)) \quad (8.80)$$

$$\langle ab|\chi|cd\rangle = \langle ab|v|cd\rangle \rightarrow v_{cd}^{ab}(T(ab), T(cd)) \quad (8.81)$$

$$\sum_c \langle b|\chi|c\rangle \langle ac|t|ij\rangle \rightarrow \chi_c^b(K(b), K(c)) \cdot t_{ij}^{ac}(K(c), K_c(ija)) \quad (8.82)$$

$$\sum_k \langle k|\chi|j\rangle \langle ab|t|ik\rangle \rightarrow \chi_j^k(K(j), K(k)) \cdot t_{ik}^{ab}(K(c), K_c(ija)) \quad (8.83)$$

$$\sum_{cd} \langle ab|\chi|cd\rangle \langle cd|t|ij\rangle \rightarrow \chi_{cd}^{ab}(T(ab), T(cd)) \cdot t_{ij}^{cd}(T(cd), T(ij)) \quad (8.84)$$

$$\sum_{kl} \langle ab|t|kl\rangle \langle kl|\chi|ij\rangle \rightarrow t_{kl}^{ab}(T(ab), T(kl)) \cdot \chi_{ij}^{kl}(T(kl), T(ij)) \quad (8.85)$$

$$\sum_{kc} \langle ac|t|ik\rangle \langle kb|\chi|cj\rangle = \sum_{kc} \langle ai^{-1}|t|kc^{-1}\rangle \langle kc^{-1}|\chi|jb^{-1}\rangle \rightarrow t_{ik}^{ac}(X(ia), X(kc)) \cdot \chi_{cj}^{kb}(X(kc), X(jb)) \quad (8.86)$$

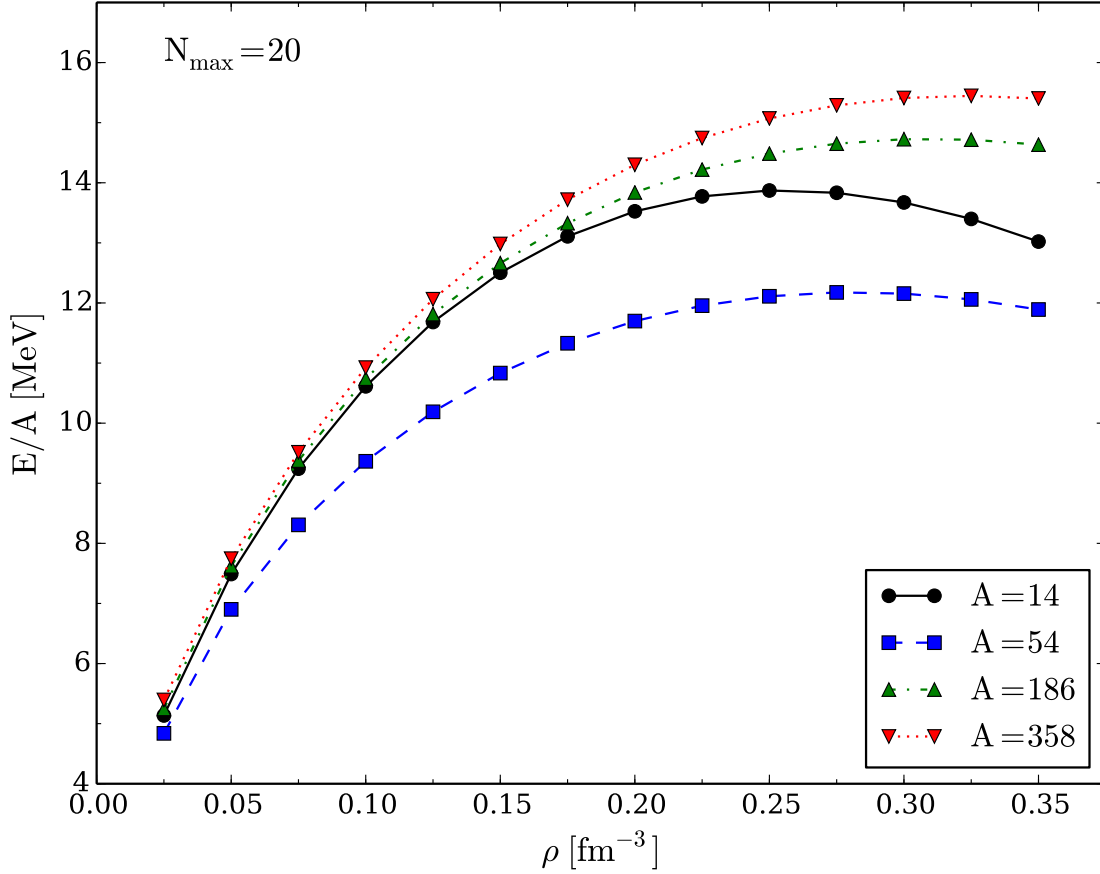
The interaction we will use for these calculations is a semirealistic nucleon-nucleon potential known as the Minnesota potential which has the form,  $V_\alpha(r) = V_\alpha e^{-\alpha r^2}$ . The spin and isospin dependence of the Minnesota potential is given by,

$$V(r) = \frac{1}{2} \left( V_R + \frac{1}{2} (1 + P_{12}^\sigma) V_T + \frac{1}{2} (1 - P_{12}^\sigma) V_S \right) (1 - P_{12}^\sigma P_{12}^\tau), \quad (8.87)$$

where  $P_{12}^\sigma = \frac{1}{2} (1 + \sigma_1 \cdot \sigma_2)$  and  $P_{12}^\tau = \frac{1}{2} (1 + \tau_1 \cdot \tau_2)$  are the spin and isospin exchange operators, respectively. When this potential is integrated over space, the result depends only on the magnitude of the momentum transfer,  $\mathbf{q} = \frac{1}{2} (\mathbf{k}_p - \mathbf{k}_q - \mathbf{k}_r + \mathbf{k}_s)$ , as well as the spin and isospin dependencies,

$$\langle pq|V_\alpha|rs\rangle = \frac{V_\alpha}{L^3} \left( \frac{\pi}{\alpha} \right)^{3/2} e^{-\frac{q^2}{4\alpha}} \delta_{\mathbf{k}_p+\mathbf{k}_q, \mathbf{k}_r+\mathbf{k}_s} \quad (8.88)$$

$\alpha$	$V_\alpha$	$\kappa_\alpha$
$R$	200 MeV	$1.487 \text{ fm}^{-2}$
$T$	178 MeV	$0.639 \text{ fm}^{-2}$
$S$	91.85 MeV	$0.465 \text{ fm}^{-2}$



**Fig. 8.1** Energy per particle of pure neutron matter computed in the CCD approximation with the Minnesota potential for different numbers of particles with  $N_{\max} = 20$ .

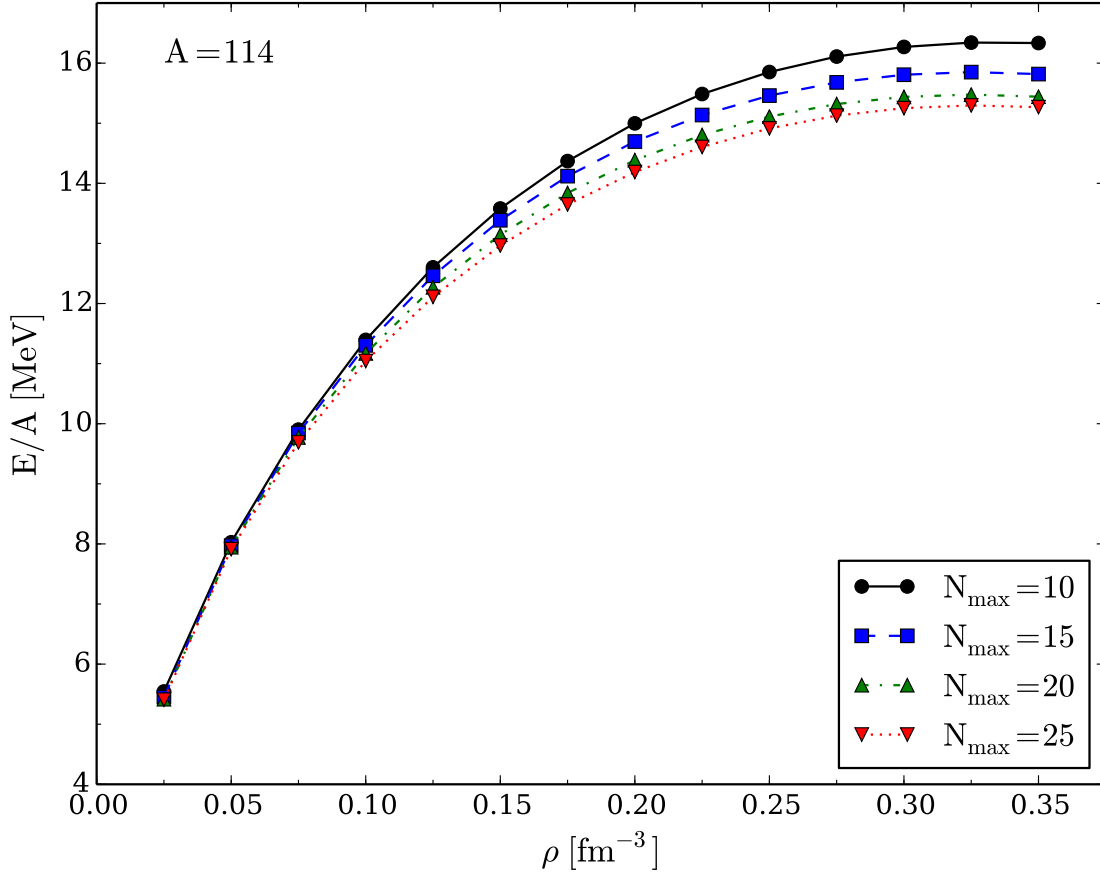
We approximated our problem with periodic boundary conditions,  $\phi(x_i) = \phi(x_i + L)$ , but we could have chosen anti-periodic boundary conditions,  $\phi(x_i) = -\phi(x_i + L)$ . The difference between these two shows how the correlation energy contains finite-size effects. One solution to this problem is by integrating over solutions between periodic and anti-periodic conditions, known as twist-averaging. First, we multiply the single-particle states by a phase for each direction, characterized by a twist-angle,  $\theta_i$ .

$$\phi_{\mathbf{k}}(\mathbf{x} + \mathbf{L}) \rightarrow e^{i\theta} \phi_{\mathbf{k}}(\mathbf{x}) \quad (8.89)$$

$\theta_i = 0$  for PBC and  $\theta_i = \pi$  for APBC

$$\mathbf{k} \rightarrow \mathbf{k} + \frac{\theta}{L} \quad (8.90)$$

$$\varepsilon_{\mathbf{k}} \rightarrow \varepsilon_{\mathbf{k}} + \frac{\pi}{L} \mathbf{k} \cdot \theta + \frac{\pi^2}{L^2} \quad (8.91)$$



**Fig. 8.2** Energy per particle of pure neutron matter computed in the CCD approximation with the Minnesota potential for different model space sizes with  $A = 20$ .

Adding these phases changes the single-particle energies, the correction of which disappear as  $L \rightarrow \infty$ , depending on  $\theta$  and thus changes the shell structure so that hole states can jump up to particle states and vis a versa. So it's necessary to fill hole states separately for each  $\theta$ . Integration over some quantity is approximated by a weighted sum, such as Gauss-Legendre quadrature, over the quantity for each set of twist angles.

Build mesh points and weights for each direction  $i$ :  $\{\theta_i, w_i\}$

$E_{\text{twist}} = 0$

**for**  $(\theta_x, w_x) \in \{\theta_x, w_x\}$  **do**

**for**  $(\theta_y, w_y) \in \{\theta_y, w_y\}$  **do**

**for**  $(\theta_z, w_z) \in \{\theta_z, w_z\}$  **do**

      Build Basis States with  $k_i \rightarrow k_i + \frac{\theta_i}{L}$

      Order States by Energy and Fill Holes

      Get Result  $E$  (T,HF,CCD)

$E_{\text{twist}} = E_{\text{twist}} + \frac{1}{\pi^3} w_x w_y w_z E$

**end for**

**end for**

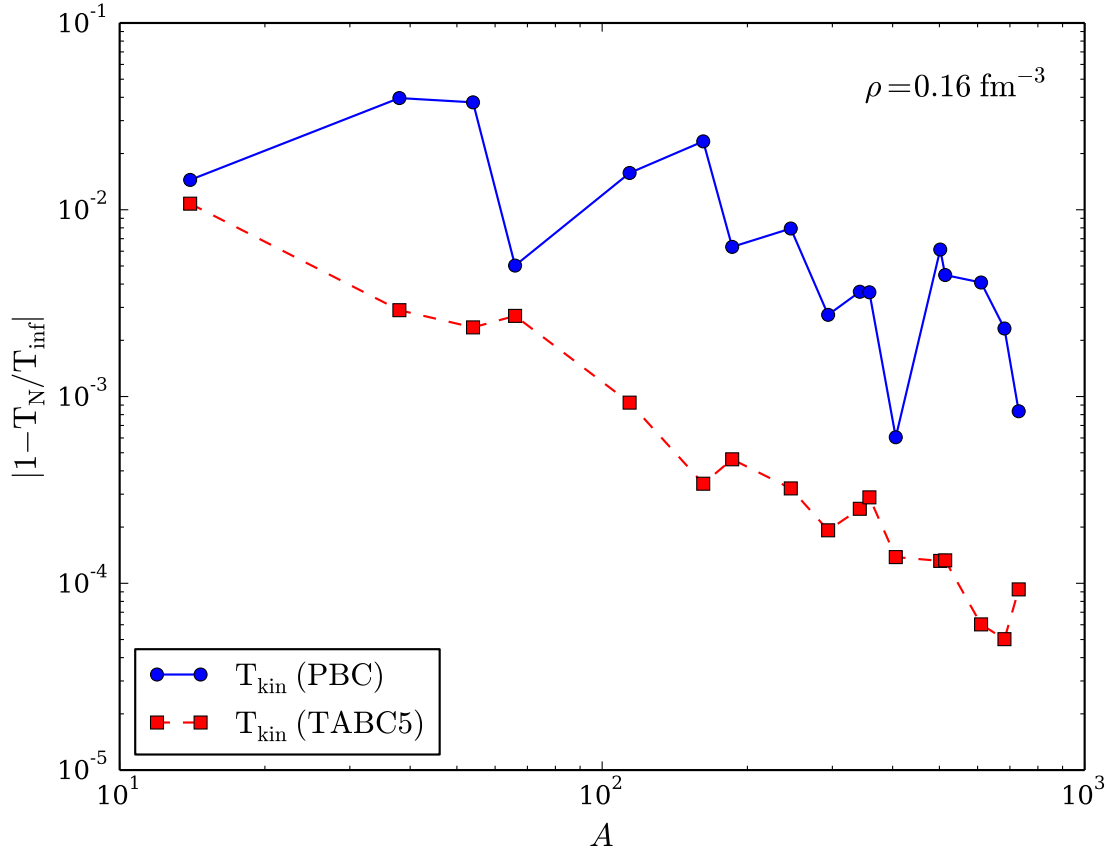
**end for**

This technique gives results which depend much less on the particle number, but requires a full calculation for each set of twist angles, which can grow very quickly. For example, using 10 twist angles in each direction requires 1000 calculations. To see the effects of twist

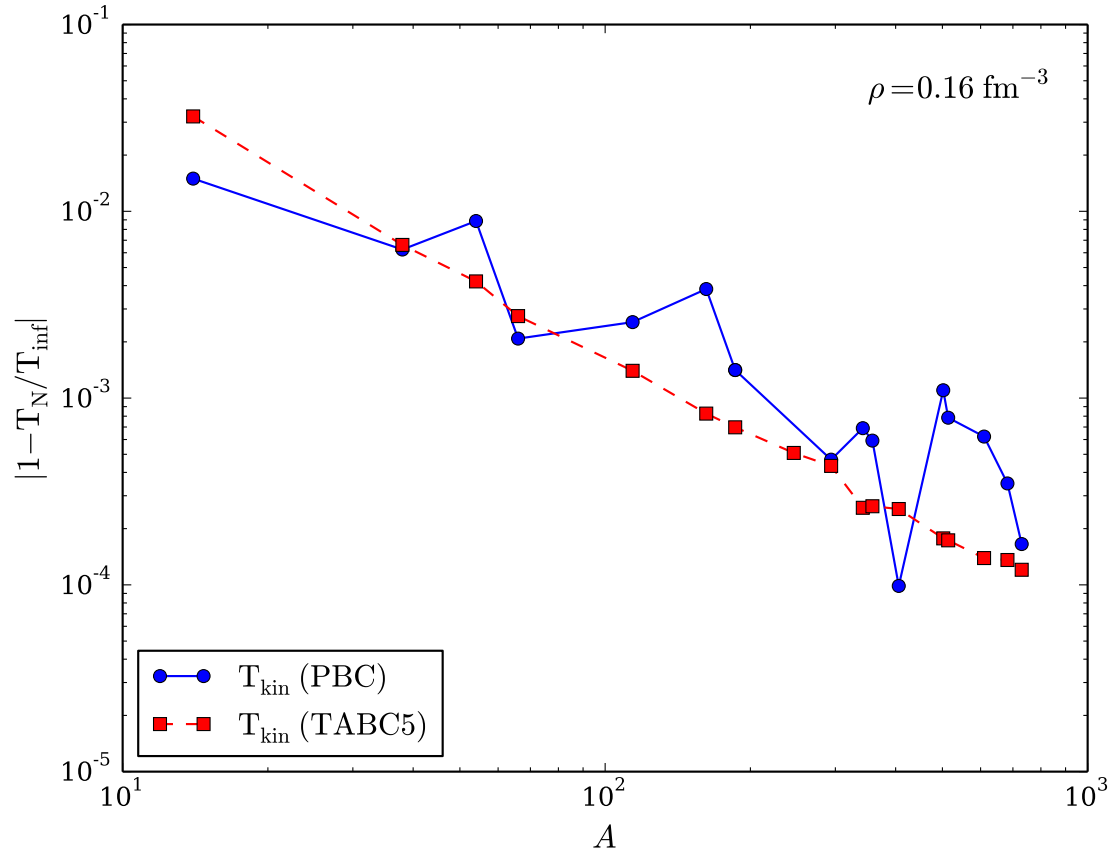
averaging, it's easy to calculate the kinetic energy per particle and the Hartree-Fock energy per particle, which avoids the full CCD calculation. These calculations can be compared to the exact values for infinite matter, which are calculated by integrating the the relevent values up to the fermi surface.

$$T_{\text{inf}} = \frac{3\hbar^2 k_f^2}{10m} \quad (8.92)$$

$$\text{HF}_{\text{inf}} = \frac{1}{(2\pi)^6} \frac{L^3}{2\rho} \int_0^{k_f} d\mathbf{k}_1 \int_0^{k_f} d\mathbf{k}_2 \langle \mathbf{k}_1 \mathbf{k}_2 | \hat{v} | \mathbf{k}_1 \mathbf{k}_2 \rangle \quad (8.93)$$



**Fig. 8.3** Finite-size effects in the kinetic energy of pure neutron matter computed with the Minnesota potential as a function of the number of particles for both periodic boundary conditions and twist-averaged boundary conditions.



**Fig. 8.4** Finite-size effects in the Hartree-Fock energy of pure neutron matter computed with the Minnesota potential as a function of the number of particles for both periodic boundary conditions and twist-averaged boundary conditions.





## Chapter 9

# Variational and diffusion Monte Carlo approaches to the nuclear few- and many-body problem

Francesco Pederiva

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### 9.1 The Nuclear few- and many-body problem

### 9.2 Methods for bound states based on the variational principle I: The No Core Shell Model (NCSM)

### 9.3 Methods for bound states based on the variational principle II: The Hyperspherical Harmonics (HH) method

### 9.4 Methods for reactions involving continuum states I: Perturbation induced reactions and integral transforms

### 9.5 Methods for reactions involving continuum states II: The continuum state problem reduced to a bound state problem

**Acknowledgements** If you want to include acknowledgments of assistance and the like at the end of an individual chapter please use the acknowledgement environment – it will automatically render Springer’s preferred layout.

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## Chapter 10

# In-medium SRG approaches to infinite nuclear matter

Scott K. Bogner, Heiko Hergert, Titus Morris, Nathan Parzuchowski, and Fei Yuan

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### 10.1 Introduction

### 10.2 The similarity renormalization group approach

### 10.3 In-medium SRG studies of infinite matter

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## Chapter 11

# Concluding remarks and perspectives

Morten Hjorth-Jensen, Maria Paola Lombardo, and Ubirajara van Kolck

**Abstract** Here Morten the Roman-Viking (who has never admitted his Norse roots) goes finally berserk in a classical Norse way and and Bira, clad in his befitting apologetic suit, presents himself as the true messiah of EFT and shouts stand up all ye infidels and hail the master. Halleluja and amen. Maria Paola is left speechless and runs for shelter somewhere in lovely Frascati (we envy her).

### 11.1 Concluding remarks

### 11.2 Perspectives

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