Chapter 1

The renormalization of the NN potential

1.1 Introduction

First of all, it is worth to recall some of the basic features of the nucleon-nucleon (NN) potential V_{NN}, which can be inferred from the experimental data of the atomic nuclei:

- the V_{NN} is a short range potential. We can consider two major empirical observations.

  First, there is no need to consider the nuclear forces to describe atomic and molecular physics. Secondly, from the mass number $A = 4$ on the binding energy (BE) per nucleon of the atomic nuclei is nearly constant (about 8 MeV/nucleon), and the same feature holds for the nuclear density. A long-range force would originate a BE per nucleon that increase with A, as happens for nuclei with $A \leq 4$.

- The V_{NN} is attractive in its intermediate range. In fact, the data of the electron scattering on heavy nuclei are consistent with a nuclear density about 0.17 fm^{-3}, that is equivalent to a cube about 1.8 fm long.

- The V_{NN} presents a relevant tensor component, that it is needed to explain the quadrupole and magnetic moment of the deuteron, and providing the mixing of the S state with the D state.

- The NN potential owns a spin-orbit component, that has no relativistic origin. This spin-orbit force is responsible of the correct reproduction of the observed "magic numbers" in the many-nucleon systems.

- The V_{NN} exhibits a strong repulsive behavior in its short range, that in the momentum-space representation means that its matrix elements are strogly repulsive in the high-momentum regime. A clear sign of this

repulsive behavior is the experimental behavior of the ${}^1S_0$ phase-shifts of the NN scattering that turn to be negative around $E_{lab} = 250$ MeV.

It is worth to note that all these feature have been confirmed in some recent pioneering lattice QCD calculations, where the NN scattering is described in terms of quark and gluon degrees of freedom.

The main trouble is represented by the strong short-range repulsion, since it prevents to employ directly realistic NN potentials - able to reproduce the NN scattering data and describe the deuteron properties -within a many-body perturbative approach.

As a matter of fact, if we consider the eigenfunction Φ_0 of the unperturbed many-body hamiltonian $H_0 = T + U$, where U is a well-behaved auxiliary potential, then in the r space should be regular for $r \to 0$ and leading to a representation like the one in Fig. 1.1.

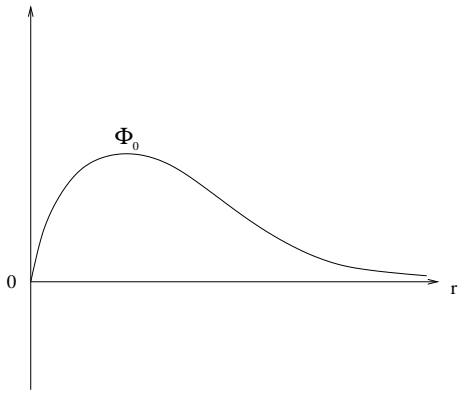


Figure 1.1: The unperturbed wave function Φ_0.

If we overlap the Φ_0 wave function with the behavior of an hard-core potential we have a picture like that in Fig. 1.2.

This would mean that the matrix element $\int \Phi_0^* V_{NN} \Phi_0 dr$ diverges, giving hard time when employing many-body perturbation theory to describe the physics of the atomic nuclei.

1.2 The Brueckner theory

The short-range repulsion of phenomenological V_{NN} makes highly desirable to built up an effective potential, whose action on an uncorrelated wave function Φ_0 is equal to the one of the original V_{NN} on the correlated wave function Ψ:

$$G\Phi_0 = V_{NN}\Psi \quad .$$

A well-known approach to this problem is the calculation of the Brueckner reaction matrix G starting from a realistic V_{NN}.

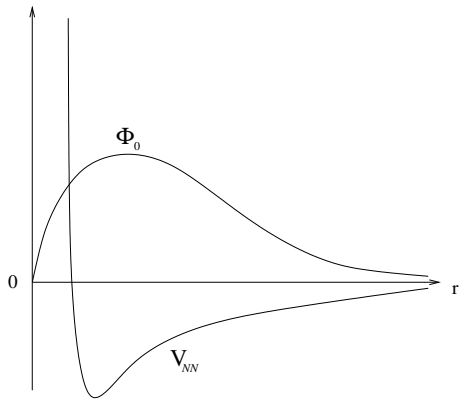


Figure 1.2: The overlap of the hard-core potential V_{NN} and the unperturbed wave function Φ_0.

Let's give a look how this idea comes out. We would like to calculate the ground-state energy E_{gs} of a nucleus using the perturbation theory. The hamiltonian H of the system may divided in an unperturbed term H_0 and an interaction term H_1 introducing an auxiliary potential U

$$H = H_0 + H_1 = (T + U) + (V - U) \quad .$$

The unperturbed eigenfunctions $|\Phi_0^i\rangle$ are solutions of the equation

$$H_0|\Phi_0^i\rangle = E_0^i|\Phi_0^i\rangle \quad .$$

The lowest unperturbed eigenvalue E_0^{gs} corresponds to a configuration, identified by the eigenfunction Φ_0^{gs}, where all the nucleons fill completely the orbitals below the Fermi surface. The orbitals are determined by the choice of U, for example the orbitals of a harmonic-oscillator well.

We want to calculate the ground state energy of the nucleus under consideration using the perturbation theory:

$$\begin{aligned} E_{\rm gs} &= E_0^{gs} + \langle\Phi_0^{gs}|H_1|\Phi_0^{gs}\rangle + \langle\Phi_0^{gs}|H_1\frac{Q}{E_0^{gs}-H_0}H_1|\Phi_0^{gs}\rangle + \\ &+ \langle\Phi_0^{gs}|H_1\frac{Q}{E_0^{gs}-H_0}H_1\frac{Q}{E_0^{gs}-H_0}H_1|\Phi_0^{gs}\rangle + \ ... \end{aligned}$$

The Pauli projection operator $Q = \sum_{i\neq gs}|\Phi_0^i\rangle\langle\Phi_0^i|$ prevents that $|\Phi_0^{gs}\rangle$ belongs to the possible intermediate states. The diagrammatic picture of $E_{gs}-E_0^{gs}$ Goldstone expansion is reported in Fig. 1.3, the dashed lines resembling the interaction vertices of V_{NN} and cross sign the insertion of the $-U$ potential.

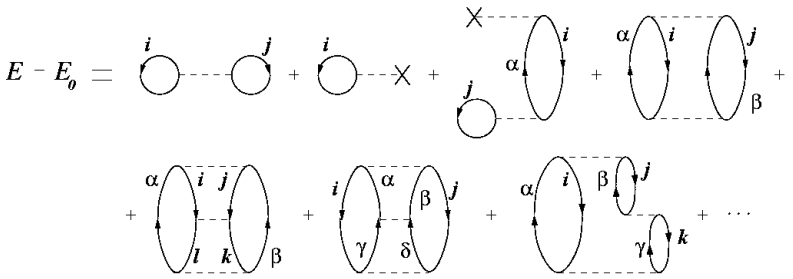


Figure 1.3: Goldstone expansion of the ground-state energy of a nucleus, latin letters indicate hole state below the Fermi surface, the greek ones particle states above the Fermi surface (see text for details).

From the sum of diagrams in Fig. 1.3 we consider the collection of the so-called ladder diagrams, as reported in Fig. 1.4.

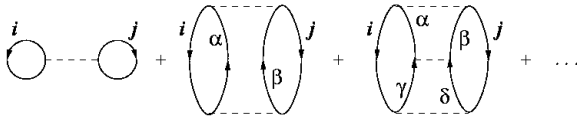


Figure 1.4: Sum of the Goldstone ladder diagrams.

The sum of the diagrams in Fig. 1.4 is equal to:

$$\frac{1}{2}\sum_{ij} V_{NN}(ij,ij) + \frac{1}{4}\sum_{ij,\alpha\beta}\frac{|V_{NN}(ij,\alpha\beta)|^2}{\epsilon_i+\epsilon_j-\epsilon_\alpha-\epsilon_\beta} + \tag{1.1}$$
$$+\frac{1}{8}\sum_{ij,\alpha\beta\gamma\delta} V_{NN}(ij,\gamma\delta)\frac{1}{\epsilon_i+\epsilon_j-\epsilon_\gamma-\epsilon_\delta}V_{NN}(\gamma\delta,\alpha\beta)\frac{1}{\epsilon_i+\epsilon_j-\epsilon_\alpha-\epsilon_\beta}V_{NN}(\alpha\beta,ij)+... \quad ,$$

where we have denoted with latin letters the hole states belonging to the set of those orbitals below the Fermi surface, the greek letters indicate the particle ones above the Fermi surface.

The expression 1.2 suggests to introduce the so-called reaction matrix G via the following integral equation

$$G(ab,cd) = V_{NN}(ab,cd) + \frac{1}{2}\sum_{\alpha\beta}\frac{V_{NN}(ab,\alpha\beta)G(\alpha\beta,cd)}{\epsilon_c+\epsilon_d-\epsilon_\alpha-\epsilon_\beta} \quad ,$$

that can be also written in an operatorial form as

$$G(\omega) = V_{NN} + V_{NN}\frac{Q_{2p}}{\omega - H_0}G(\omega) \quad .$$

Finally we can re-write the diagrammatic expression of the Goldstone expansion in Fig. 1.3 in terms of the G-matrix vertices, as reported in Fig. 1.5

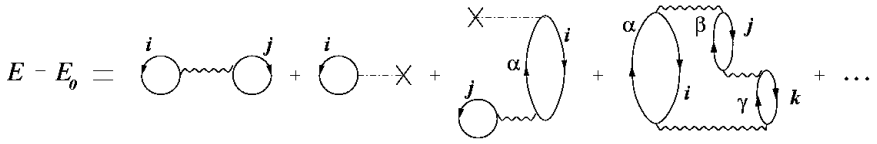


Figure 1.5: Goldstone expansion of the ground-state energy of a nucleus in terms of G-matrix vertices, reported now as wavy lines.

Now, some considerations are in order. We define the correlated wave function $\Psi(\omega)$ as

$$|\Psi(\omega)\rangle = |\Phi_0\rangle + \frac{Q_{2p}}{\omega - H_0} V_{NN} |\Psi(\omega)\rangle \quad ,$$

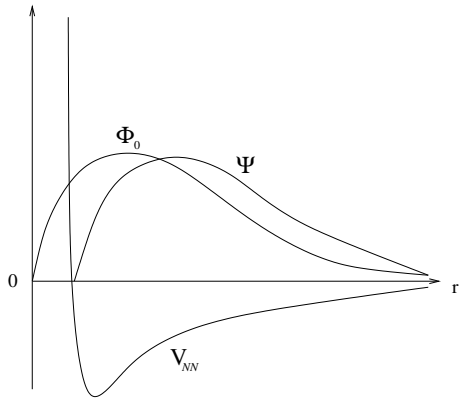
where the uncorrelated wave function Φ_0 is the solution of the Schrödinger equation for the unperturbed hamiltonian H_0. If we iterate the expression defining the correlated wave function $\Psi(\omega)$, we can re-write the latter in terms of the reaction matrix G:

$$|\Psi(\omega)\rangle = |\Phi_0\rangle + \frac{Q_{2p}}{\omega - H_0} G(\omega) |\Phi_0\rangle \quad .$$

So it holds the following identity

$$G(\omega)|\Phi_0\rangle = V_{NN}|\Psi(\omega)\rangle \quad ,$$

which evidences that the G-matrix is an effective interaction whose action on the uncorrelated wave function - that is the one used in the perturbative expansion - is equal to the action of V_{NN} on the correlated one.



It is worth now to consider an example to show how the G-matrix is able to "heal' ' the divergencies of the NN potential. Let's consider a separable realistic potential

$$V_{NN}(ij,kl) = \lambda u(ij)v(kl) \quad .$$

We construct its reaction matrix G by assuming that it can be written in a separable form too:

$$G(ij,kl) = \eta_{kl} u(ij)v(kl) \quad ,$$

the matrix elements of G will be then univocously determined by the η_{kl} coefficient. The integral equation of the G matrix of our V_{NN} is:

$$\begin{aligned} \eta_{kl} u(ij)v(kl) &= \lambda u(ij)v(kl) + \frac{1}{2}\sum_{\alpha\beta} \lambda u(ij)v(\alpha\beta) \\ &\times \frac{1}{\epsilon_i + \epsilon_j - \epsilon_\alpha - \epsilon_\beta} \eta_{kl} u(\alpha\beta)v(kl) \quad , \end{aligned}$$

$$\eta_{kl}\left[u(ij)v(kl) - \frac{\lambda}{2}\sum_{\alpha\beta} \frac{u(ij)v(\alpha\beta)u(\alpha\beta)v(kl)}{\epsilon_i + \epsilon_j - \epsilon_\alpha - \epsilon_\beta} \right] = \lambda u(ij)v(kl) \quad .$$

Finally, we have

$$\begin{aligned} \eta_{kl} &= \frac{\lambda u(ij)v(kl)}{\left[u(ij)v(kl) - \frac{\lambda}{2}\sum_{\alpha\beta} \frac{u(ij)v(\alpha\beta)u(\alpha\beta)v(kl)}{\epsilon_i+\epsilon_j-\epsilon_\alpha-\epsilon_\beta}\right]} = \\ &= \frac{u(ij)v(kl)}{\left[\frac{u(ij)v(kl)}{\lambda} - \frac{1}{2}\sum_{\alpha\beta} \frac{u(ij)v(\alpha\beta)u(\alpha\beta)v(kl)}{\epsilon_i+\epsilon_j-\epsilon_\alpha-\epsilon_\beta}\right]} \quad . \end{aligned}$$

The above expression of η_{kl} is finite when $\lambda \to \infty$ and the V_{NN} diverges, showing that G is regular in the poles of its original potential.

However, nothwistanding this feature, there is a major shortcoming when employing a G matrix as vertex of the perturbation expansion. The G matrix is energy-dependent, more precisely it depends by definition on the unperturbed energy of the system of the two incoming nucleons, and consequentely it depends on the choice of the auxiliary potential U

1.3 The V_{low-k} approach

Nowadays, there are alternative approaches to the renormalization of the NN potential, which have been inspired by the effective field theory (EFT) and the renormalization group (RG) techniques.

From the EFT perspective, that is the one inspiring the construction of chiral potentials as have been introduced in his lectures by Michele Viviani, the NN potential is not an observable to be determined on experimental data, but there is an infinite class of NN potentials capable to reproduce accurately the low-energy physics.

It is worth to note that chiral potentials have a sort of free parameter, that is the momentum cutoff appearing in.

Two different cutoffs correspond to different chiral potentials, but the opportune renormalization of the LECs belonging to the two-body, three-body, four-body ... N-body terms will provide the preservation of the same observables by the two different chiral potentials.

Now, starting from these basic concepts, one may think to derive an infinite class of phase-equivalent potentials, that, via a RG process, decouple the low-momentum subspace from the high-momentum one.

The RG approach to a two-nucleon system requires that the solutions of the half-on-shell Lippmann-Schwinger equation has to be preserved

$$T(k,k',k'^2) = V(k,k') + \frac{2}{\pi}\mathcal{P}\int_0^\infty q^2 dq \frac{V(k,q)T(q,k',k'^2)}{k^2-q^2} \quad .$$

The solution of this equation, the so-called T-matrix, provides all the physical observables of the two-nucleon system. Diagonal matrix elements are equal, apart from a factor, to the phase-shifts of the NN scattering, and it can be shown that they provide also the bound eigenvalue of the deuteron hamiltonian.

Preserving the T-matrix means that for our decoupled potential

$$T_{low-k}(k,k',k'^2) = V_{low-k}(k,k') + \frac{2}{\pi}\mathcal{P}\int_0^\Lambda q^2 dq \frac{V_{low-k}(k,q)T_{low-k}(q,k',k'^2)}{k^2-q^2}$$

for any $k,k' \leq \Lambda$,

$$T_{high-k}(k,k',k'^2) = V_{high-k}(k,k') + \frac{2}{\pi}\mathcal{P}\int_\Lambda^\infty q^2 dq \frac{V_{high-k}(k,q)T_{high-k}(q,k',k'^2)}{k^2-q^2}$$

for any $k,k' > \Lambda$.

To solve this problem we can follow three ways, that give the same solutions:

1. to solve the integral equation by matrix inversion (it is complicated by solving numerically the principal value integration very accurately);
2. to integrate the RG equation

$$\frac{d}{d\Lambda}V_{low-k}(k',k) = \frac{2}{\pi}\frac{V_{low-k}(k',\Lambda)T_{low-k}(\Lambda,k,\Lambda^2)}{1-\left(\frac{k}{\Lambda}\right)^2} \quad ;$$

3. employing the Lee-Suzuki similarity transformation.

Let's now consider the latter approach.

1.3.1 The Lee-Suzuki transformation

The starting point is the two-nucleon hamiltonian and its eigenvalue problem in the momentum space

$$\int_0^\infty [H_0(k,k') + V_{NN}(k,k')]\langle k|\Psi_\nu\rangle k^2 dk = E_\nu \langle k'|\Psi_\nu\rangle \quad .$$

Our goal is to construct an effective hamiltonian that is defined in a subspace P of the Hilbert space spanned by all relative momenta smaller than a chosen cutoff Λ

$$P = \int_0^\Lambda |k\rangle\langle k| k^2 dk$$

This effective hamiltonian has to be obtained with a similarity transformation Ω

$$\mathcal{H} = \Omega^{-1} H \Omega$$

The decoupling condition between the P-space and its complementary space $Q = 1 - P = \int_\Lambda^\infty |k\rangle\langle k| k^2 dk$ is

$$Q\mathcal{H}P = 0 \quad .$$

Obviously, this decoupling equation is not able itself to identify the operator Ω, the so-called wave operator, and Lee and Suzuki have suggested that a convenient form could be like this

$$\begin{aligned} P\Omega P &= 1 \qquad & P\Omega Q &= 0 \\ Q\Omega P &= \omega \qquad & Q\Omega Q &= 0 \quad . \end{aligned}$$

This form of Ω will make $\mathcal{H}$ to satisfy the following identities in the P and Q subspaces

$$P\mathcal{H}P = PHP + PHQ\omega \quad ,$$

$$P\mathcal{H}Q = PHQ \quad ,$$

$$Q\mathcal{H}Q = QHQ - \omega PHQ \quad ,$$

and finally

$$Q\mathcal{H}P = QHP + QHQ\omega - \omega PHP - \omega PHQ\omega \quad .$$

Since it holds the decoupling condition between P and Q spaces, we obtain the following matrix equation for ω

$$Q\mathcal{H}P = QHP + QHQ\omega - \omega PHP - \omega PHQ\omega = 0 \quad .$$

This non-linear matrix equation for ω is amenable of numerical solution via iterative procedures, and one of them will be presented in the following.

Let us consider,

$$p(\omega) = PHP + PHQ\omega \quad ,$$

$$q(\omega) = QHQ - \omega PHQ \quad .$$

Now if we construct

$$\begin{aligned} x_0 &= -(QHQ)^{-1}QHP \quad , \\ x_1 &= q^{-1}(x_0)x_0 p(x_0) \quad , \\ &... \\ x_n &= q^{-1}(x_0 + x_1 + ... + x_{n-1})x_{n-1}p(x_0 + x_1 + ... + x_{n-1}) \quad . \end{aligned}$$

Then when $x_n \to 0$

$$\omega = \omega_n = \sum_{i=0}^{n} x_i \quad ,$$

the following condition has to be verified

$$p(\omega_n) = p(\omega_{n-1}) \quad .$$

Finally, it is worth to evaluate the action of the V_{low-k} approach on a realistic potential. In Fig. 1.6 they are reported the diagonal matrix elements of many different high-precision NN potentials, that fit equally well the two-nucleon data up to the inhelastic treshold at $E_{lab} = 350$ MeV.

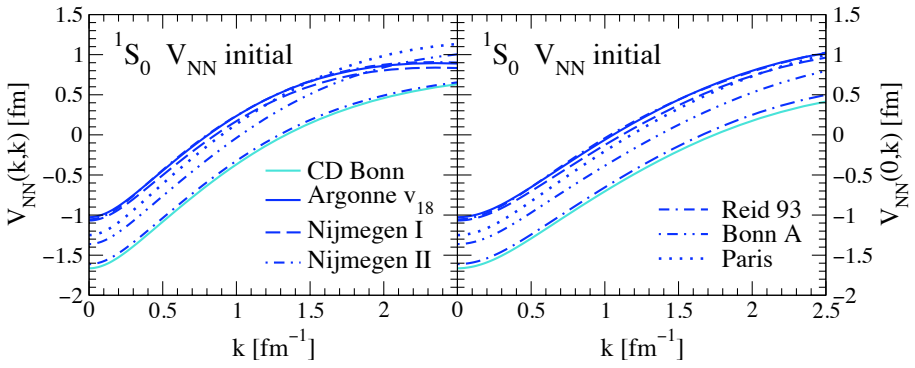


Figure 1.6: Diagonal matrix elements of the $^1S_0$ partial wave for many different modern realistic potentials.

As can be seen, the different V_{NN}s exhibit a repulsive behavior when increasing the k, k' momenta, and their matrix elements are very different each other.

The V_{low-k} diagonal matrix elements calculated from the potentials considered in Fig. 1.6 with a cutoff momentum $\Lambda = 2.1$ fm^{-1} are reported in Fig. 1.7.

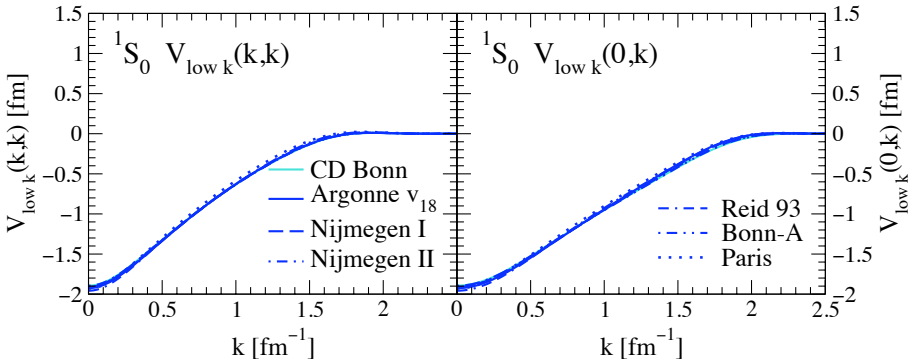


Figure 1.7: Diagonal matrix elements of the $^1S_0$ partial wave of V_{low-k}s calculated from the same potentials reported in Fig. 1.6 for a cutoff $\Lambda = 2.1$ fm^{-1}.

From the inspection of Fig. 1.7, it can be seen that the V_{low-k} matrix elements are always attractive and goes to zero at $k, k' = \Lambda$. Moreover, now all V_{low-k} have substantially identical matrix elements.

1.4 The SRG approach

An evolution of the V_{low-k} renormalization procedure is the so-called similarity renormalization-group (SRG) approach. The SRG renormalization procedure provides a more flexible choice of the decoupling between the low- and high-momentum regime. As a matter of fact, using this approach one decouples the two subspaces via a continuous sequence of unitary transformations that suppresses gradually the off-diagonal matrix elements of the effective two-nucleon hamiltonian. What we will get at the end of this flow of unitary transformations is a band-diagonal potential that preserves the physics of the original potential, but a weak coupling between low- and high-momentum regimes.

Let's now sketch briefly the procedures to reach this.

The full hamiltonian H is, as usual,

$$H = T_{rel} + V \quad .$$

We will transform the hamiltonian H into another one H_s, where s is the so-called flow parameter, by way of a unitary transformation:

$$H_s = U_s H U_s^\dagger = T_{rel} + V_s \quad ,$$

this means that the kinetic energy operator T_{rel} is independent of s, $U_s T_{rel} U_s^\dagger = T_{rel}$.

This evolution happens according to the flow equation

$$\frac{dH_s}{ds} = [\eta_s, H_s] \quad ,$$

where

$$\eta_s = \frac{dU_s}{ds} U_s^\dagger = -\eta_s^\dagger \quad .$$

The choice of η_s will specify the characteristics of our unitary transformation. This can be stressed writing η_s as a commutator of a generator operator G_s:

$$\eta_s = [G_s, H_s] \quad ,$$

so we obtain

$$\frac{dH_s}{ds} = [[G_s, H_s], H_s] \quad .$$

A possible choice of the generator G_s that drives H_s towards a band-diagonal form is:

$$G_s \equiv T_{rel} \quad ,$$

so

$$\frac{dH_s}{ds} = [[T_{rel}, H_s], H_s] \quad .$$

Since it holds that

$$\frac{dH_s}{ds} = \frac{d}{ds}(T_{rel} + V_s) = \frac{dV_s}{ds} \quad ,$$

we can derive a differential equation for V_s

$$\begin{aligned} \frac{dV_s(k,k')}{ds} &= -(k^2 - k'^2)^2 V_s(k,k') + \\ &+ \frac{2}{\pi} \int_0^\infty q^2 dq (k^2 + k'^2 - 2q^2) V_s(k,q) V_s(q,k') \quad . \end{aligned} \tag{1.2}$$

Exercise: Please, write all expressions needed to derive Eq. 1.2
Hint: remember that explicitly

$$\begin{aligned} \eta_s(k,k') &= k^2 H_s(k,k') - H_s(k,k')k'^2 \quad , \\ [\eta_s, H_s] &= \frac{2}{\pi}\int_0^\infty q^2 dq \, [\eta_s(k,q)H_s(q,k') - H_s(k,q)\eta_s(q,k')] \quad . \end{aligned}$$

Observe that for off-diagonal matrix elements ($|k-k'|$) very large, the first term on the right side of Eq. 1.2 prevails, and we can approximate the differential equation for V_s with

$$\frac{dV_s(k,k')}{ds} \approx -(k^2 - k'^2)^2 V_s(k,k') \quad ,$$

and its solution would be

$$V_s(k,k') = V_{s=0}(k,k')e^{-s(k^2-k'^2)^2} = V(k,k')e^{-s(k^2-k'^2)^2} \quad .$$

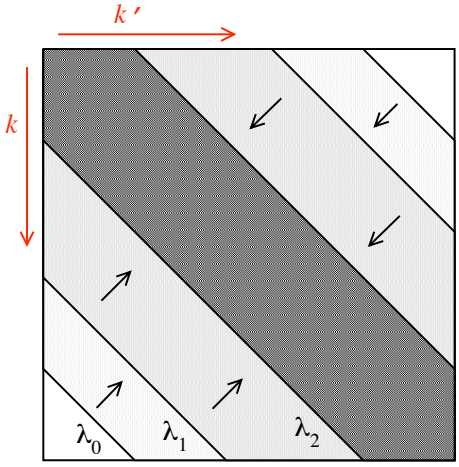


Figure 1.8: Evolution of the matrix elements of V_s as a function of the parameter $\lambda = s^{-1/4}$.

This leads to solutions whose matrix elements evolves as in Fig. 1.8.

It is worth pointing out that the sharp cutoff V_{low-k} can be obtained by choosing as the generator function G_s a block-diagonal operator such as:

$$G_s = \begin{pmatrix} PH_sP & 0 \\ 0 & QH_sQ \end{pmatrix}$$

In such a case the V_s matrix elements will evolve as in Fig. 1.9.

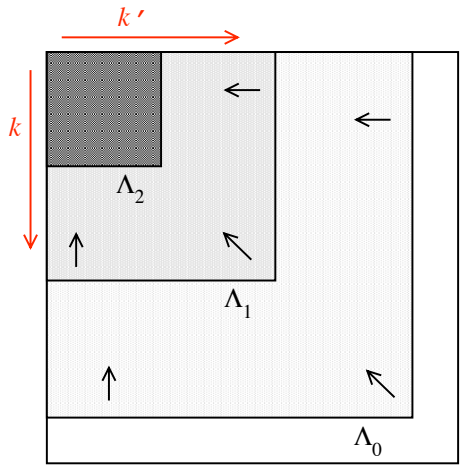


Figure 1.9: Evolution of the matrix elements of the $V_s = V_{low-k}$ as a function of the sharp cutoff Λ.

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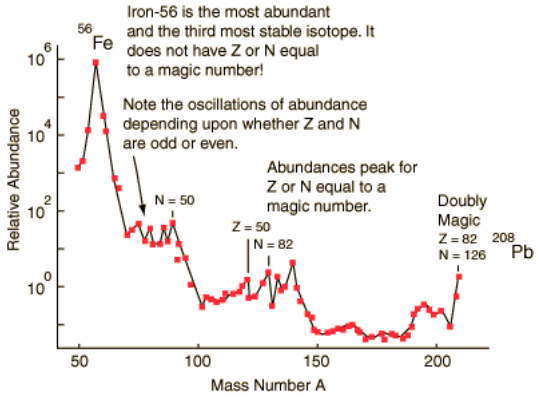
Chapter 2

The nuclear shell model

2.1 Introduction

The nuclear shell model is still one of the most powerful tools to study an extensive number of nuclear properties along the whole nuclide chart. The concept is analogous to the atomic shell model and is rooted in the observation of regularities in the nuclei when evolving the number of protons and neutrons. In particular, the observation that are peak of abundance of tightly bound nuclei with a number of protons and neutrons equal to 2, 8, 20, 28, 50, 82, ... with respect to nuclei with higher or lower N, Z, induces that an independent-particle model, with a single-particle hamiltonian $h_0(r) = p^2/2M + u(r)$, may describe reasonably well the properties of atomic nuclei.



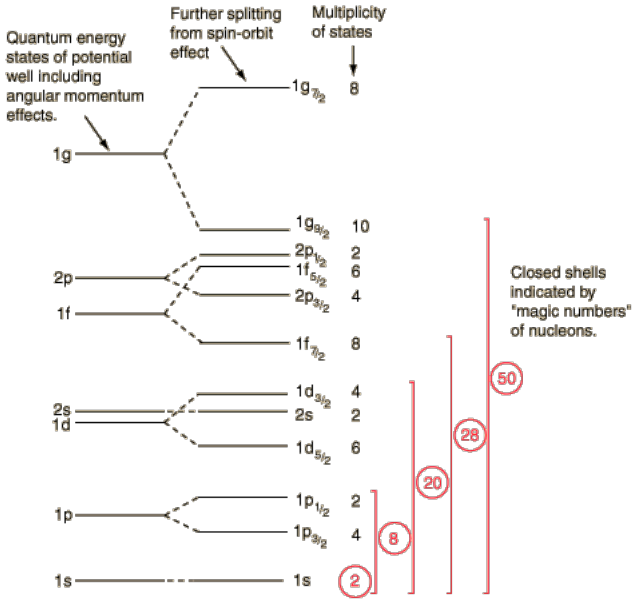
So the correlated many-body wave function of an A-nucleon system is well approximated by a Slater determinant of single-particle eigenfunctions of h_0:

$$\Phi(A) = \begin{vmatrix} \phi_1(r_1) & \phi_1(r_2) & ... & \phi_1(r_A) \\ \phi_2(r_1) & \phi_2(r_2) & ... & \phi_2(r_A) \\ ... & ... & ... & ... \\ \phi_A(r_1) & \phi_A(r_2) & ... & \phi_A(r_A) \end{vmatrix}$$

With the opportune auxiliary potential $u(r)$ the above wave function may be able to predict the correct ground-state total angular momenta of most existing even-even and odd-even mass nuclei.

The role of the choice of the potential $u(r)$ is crucial. For example, if we deal with a simple harmonic-oscillator potentials it can be observed that the sequence of its eigenvalues would lead to shell closures in correspondance of a number of protons or netutrons equal to 2, 8, 20, 40, 70, ..., that resembles the observed "magic numbers", but after $Z, N = 20$ is completely wrong.

The sole $u(r) = 1/2M\omega^2 r^2$ is not satisfacory , unless a spin-orbit is taken into account in order to remove the degeneracy of the harmonic-oscillator potential.



It is worth to note that in atomic physics is a relativistic correction to the atomic hamiltonian. Actually, the spin-orbit force in nuclear physics is more consistent, about a few MeV contribution, and originates from the basic components of the free nucleon-nucleon potential.

However, the independent-particle hamiltonian $H_0 = \sum_{i=1}^{A} h_0^i$ is not able to describe alone satisfactorily the large amount of experimental data. We need to provide a mixing of the single-particle configurations, that is brovided by the inclusion in the shell-model hamiltonian of the residual two-body interaction

V^{res}, which will break the degeneracy of states with different total angular momenta but the same single-particle configuration.

The shell-model hamiltonian is then

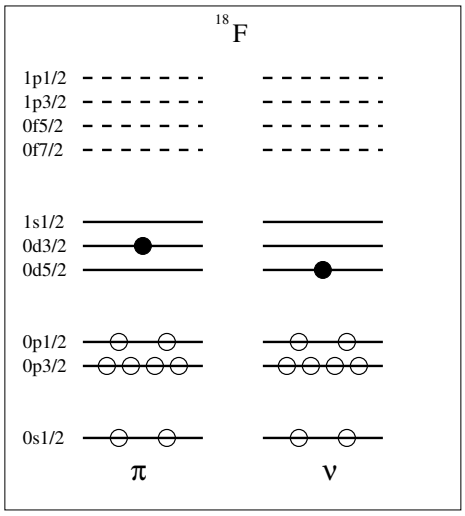
$$H = H_0 + H_1 = \sum_{i=1}^{A} \left(\frac{p_i^2}{2M} + u_i \right) + \sum_{i<j} V_{ij}^{res} \quad . \tag{2.1}$$

2.1.1 The configuration mixing

As a matter of fact the hamiltonian in Eq. 2.1 is impossible to be diagonalized, except for light systems. We need then to reduce the degrees of freedom of the eigenvalue problem.

First of all, a reasonable truncation could be to freeze all the degrees of freedom of a number of nucleons that is equal to a magic number.

For example, ^{18}F is built up by 9 protons and 9 neutrons, and 9 is very close to the magic number 8. This would correspond to the filling of the $0s_{1/2}$, $0p_{3/2}$, and $0p_{1/2}$ orbitals of the doubly magic ^{16}O



Freezing the 16 nucleons below the Fermi surface of ^{16}O reduces the problem to 1 proton and 1 neutron interacting in all the major shells that are placed in energy above the ones blonging to the core. This is, however, still a problem that, when the interacting particles start to increase, is very difficult to be solved computationally.

It should be noted that, since the unperturbed hamiltonian provides that the major shells are well-separated in energy, we may reduce the active orbitals to those belonging to one major shell just above the Fermi surface. So, the eigenvalue problem becomes much simpler and feasible. For the ^{18}F system this means 1 proton and 1 neutron interacting in the $1s0d$ proton-neutron shells,

J^π	dimension
0^+	3×3
1^+	7×7
2^+	8×8
3^+	6×6
4^+	3×3
5^+	1×1

and, for example, the eigenvalue problem of the $J^\pi = 0^+$ states is to diagonalize a 3×3 matrix.

Let's write down the shell-model hamiltonian in the second-quantization form

$$H = \sum_{i=1}^{n} \epsilon_i a_i^\dagger a_i + \sum_{ijkl} V_{ijkl}^{res} a_i^\dagger a_j^\dagger a_l a_k \quad .$$

Its eigenfunctions $|\Psi_\alpha\rangle$ will be linear combinations of antisymmetrized products of single-particle wave functions.

$$|\Psi_\alpha\rangle = \sum_\beta c_\alpha^\beta |\Phi_\alpha^\beta\rangle \quad ,$$

where

$$|\Phi_\alpha^\beta\rangle = \left[(a_1^\dagger)^{k_1} (a_2^\dagger)^{k_2} ... (a_n^\dagger)^{k_n} \right]_{\alpha\beta} |\Psi_c\rangle \quad ,$$

and

$$\sum_i k_i = A_{val} = \text{total number of valence nucleons} \; .$$

2.2 The parameters of the shell-model hamiltonian

Now, to solve the shell-model eigenvalue problem we need to know the parameters of the shell-model hamiltonian, the single-particle energies ϵ_j and the two-body matrix elements (TBME) of the residual potential V^{res}.

The ϵ_j may be taken from the experiment: in terms of the Koopmans' theorem the shell-model ϵ_js correspond to the experimental energy spectrum of the single-particle states of the nuclei with only one-valence nucleon with respect to the closed core.

The TBME can be determined following three major approaches:

- empirical V^{res} with a simple analytical expression;
- empirical TBME fitted on experimental data;
- realistic effective V^{res} derived microscopically from the free NN potential.

2.2.1 Schematic shell-model interactions

A way to derive the TBME of the residual potential is to resort to the so-called schematic interactions.

They are interactions with a simple analytical expression, and very few parameters to be fitted to the experimental data. They ususally contain only some relevant component of the NN potential, and can be expressed as gaussian or yukawian radial functions coupled to exchange operators consistent with the free NN potential:

$$V^{res} = V_0(r) + V_\sigma \sigma_1 \cdot \sigma_2 + V_\tau \tau_1 \cdot \tau_2 + V_{\sigma\tau} (\sigma_1 \cdot \sigma_2)(\tau_1 \cdot \tau_2) + V_T \frac{(\sigma_1 \cdot \mathbf{r})(\sigma_2 \cdot \mathbf{r}) - (\sigma_1 \cdot \sigma_2)}{r^2}$$

Other schematic interactions may have an even simpler form, containg only one or two relevant components of V_{NN} and a very small number of free parameters:

- the pairing or pairing plus quadrupole interactions;
- the surface delta interaction (SDI);
- the spin and isospin dependent Migdal interaction.

The schematic interactions may be very useful in order to understand what is the relevant physics underlying the spectroscopic structure of the nuclei. However, they provide a low resolution in the reproduction of the experimental data, and nowadays they are considered out-of-date.

2.2.2 Empirical effective interactions

The most successful approach to the derivation of the shell-model TBME may be considered the one that provides the residual interactions fitting the TBME so to reproduce a set of experimental data of the nuclei with a few valence particles.

Let us consider a very simple case: nuclei with valence particle outside ^{40}Ca. As the model space, we can use a very small one spanned by the sole $0f_{7/2}$ orbital for both protons and neutrons.

The single-particle energies ϵ_j can be obtained from the experimental ground-state energies of ^{41}Sc and ^{41}Ca with respect to ^{40}Ca (experimental data may be found at the web page http://amdc.impcas.ac.cn/evaluation/data2012/data/mass.mas12):

$$\begin{aligned} \epsilon^{\pi}_{0f_{7/2}} &= -1.09 \text{ MeV} \\ \epsilon^{\nu}_{0f_{7/2}} &= -8.36 \text{ MeV} \quad . \end{aligned}$$

The TBME can be derived from the experimental spectra and ground-state energies of ^{42}Ti, ^{42}Ca, and ^{42}Sc.

For example, for ^{42}Ca we have that

$$\begin{aligned} E_{gs} &= E(J^\pi = 0^+; T_z = -1) = \epsilon^\nu_{7/2} \langle (0f_{7/2})^2 | a^\dagger_{0f_{7/2}} a_{0f_{7/2}} | (0f_{7/2})^2 \rangle + \\ &+ \langle (0f_{7/2})^2; J = 0^+; T_z = -1 | V^{res} | (0f_{7/2})^2; J = 0^+; T_z = -1 \rangle = \\ &= 2\epsilon^\nu_{7/2} + \langle (0f_{7/2})^2; J = 0^+; T_z = -1 | V^{res} | (0f_{7/2})^2; J = 0^+; T_z = -1 \rangle \quad . \end{aligned}$$

Since, experimentally, the ground-state energy of ^{42}Ca with respect to ^{40}Ca is $E^{expt}_{gs} = -19.84$ MeV, we have that

$$\langle (0f_{7/2})^2; J = 0^+; T_z = -1 | V^{res} | (0f_{7/2})^2; J = 0^+; T_z = -1 \rangle = E^{expt}_{gs} - 2\epsilon^\nu_{7/2} = -3.12 \text{ MeV} \quad .$$

Experimentally, in the ^{42}Ca the energy relative to the ground state of the first excited $J^\pi = 2^+$ is $E^{expt}_{2^+} = 1.53$ MeV (visit the website http://www.nndc.bnl.gov/ensdf/), then

$$\begin{aligned} E(J^\pi = 0^+; Tz = -1) &= E^{expt}_{2^+} + E^{expt}_{gs} = \epsilon^\nu_{7/2} \langle (0f_{7/2})^2 | a^\dagger_{0f_{7/2}} a_{0f_{7/2}} | (0f_{7/2})^2 \rangle + \\ &+ \langle (0f_{7/2})^2; J = 2^+; T_z = -1 | V^{res} | (0f_{7/2})^2; J = 2^+; T_z = -1 \rangle \quad . \end{aligned}$$

Finally

$$\langle (0f_{7/2})^2; J = 2^+; T_z = -1 | V^{res} | (0f_{7/2})^2; J = 2^+; T_z = -1 \rangle = E^{expt}_{2^+} + E^{expt}_{gs} - 2\epsilon^\nu_{7/2} = -1.59 \text{ MeV} \quad .$$

Exercise: Please, following the above procedure for ^{42}Ca, ^{42}Ti, and ^{42}Sc, derive all TBME needed for the shell-model hamiltonian:

configuration	J^π	T_z	TBME (in MeV)
$(0f_{7/2})^2$	0^+	-1	-3.12
$(0f_{7/2})^2$	2^+	-1	-1.59
$(0f_{7/2})^2$	4^+	-1	?
$(0f_{7/2})^2$	6^+	-1	?
$(0f_{7/2})^2$	0^+	+1	?
$(0f_{7/2})^2$	2^+	+1	?
$(0f_{7/2})^2$	4^+	+1	?
$(0f_{7/2})^2$	6^+	+1	?
$(0f_{7/2})^2$	0^+	0	?
$(0f_{7/2})^2$	1^+	0	?
$(0f_{7/2})^2$	2^+	0	?
$(0f_{7/2})^2$	3^+	0	?
$(0f_{7/2})^2$	4^+	0	?
$(0f_{7/2})^2$	5^+	0	?
$(0f_{7/2})^2$	6^+	0	?
$(0f_{7/2})^2$	7^+	0	?

2.2.3 Realistic effective shell-model interaction

There is a third possibility: to derive the residual two-body shell-model interaction V^{res} from a realistic free NN potential. This would mean that no parameters are involved, except for those fixed to reproduce the NN scattering data and deuteron binding energy, but the theory is a bit complicated and now let's outline it briefly.

The Schrödinger equation for a A-nucleon system is:

$$H|\Psi_\nu\rangle = E_\nu|\Psi_\nu\rangle \quad .$$

Let us consider a unitary transformation Ω that defines an effective hamiltonian H_{eff} that is defined only for a few valence nucleons in a reduced model space

$$H_{eff} = \Omega^{-1} H \Omega \quad ,$$

and,

$$H_{eff}|\phi_\nu\rangle = E_\nu|\phi_\nu\rangle \quad ,$$
$$|\phi_\nu\rangle\Omega^{-1}|\Psi_\nu\rangle \quad .$$

We use the Lee-Suzuki approach to derive Ω in terms of ω operator, as introduced in section 1.3.1. First of all, we rewrite H in terms of an unperturbed degenerate hamiltonian H_0

$$H = H_0 + H_1 \quad ,$$

where

$$PH_0P = \epsilon_0 P \quad .$$

Using the decoupling condition as in Eq. 1.3.1, we can write H_1^{eff} in terms of ω:

$$H_1^{eff} = H^{eff} - PH_0P = PH_1P + PH_1Q\omega \quad .$$

Let us calculate ω as a function of H_1^{eff}

$$\omega = Q\frac{1}{\epsilon_0 - QHQ}QH_1P - Q\frac{1}{\epsilon_0 - QHQ}\omega H_1^{eff} \quad .$$

The latter is used to obtain a recursive equation for H_1^{eff}

$$H_1^{eff}(\omega) = PH_1P + PH_1Q\frac{1}{\epsilon_0 - QHQ}QH_1P - PH_1Q\frac{1}{\epsilon_0 - QHQ}\omega H_1^{eff}(\omega) \quad .$$

We call $\hat{Q}$-box the operator

$$\hat{Q}(\epsilon) = PH_1P + PH_1Q\frac{1}{\epsilon_0 - QHQ}QH_1P \quad ,$$

and rewrite H_1^{eff} in terms of the $\hat{Q}$-box

$$H_1^{eff}(\omega) = \hat{Q}(\epsilon_0) - PH_1Q\frac{1}{\epsilon_0 - QHQ}\omega H_1^{eff}(\omega) \quad .$$

The above recursive equation may be solved using iterative solutions. Lee and Suzuki provided also a solution for the equation in terms of the derivatives with respect to ϵ of the $\hat{Q}$-box

$$H_1^{eff}(\omega_n) = [1 - \hat{Q}_1 - \sum_{m=2}^{n-1} \prod_{k=n-m+1}^{n-1} H_1^{eff}(\omega_k)]^{-1} \hat{Q} \quad ,$$

where the iteration starts with

$$H_1^{eff}(\omega_1) = \hat{Q}(\epsilon_0) \quad ,$$

and

$$\hat{Q}_m = \frac{1}{m!} \left[\frac{d^m \hat{Q}(\epsilon)}{d\epsilon^m} \right]_{\epsilon=\epsilon_0} \quad .$$

The knot to be solved is the calculation of the $\hat{Q}$-box.

An exact one is impossible to be calculated, it is better to resort to a perturbative expansion. The analytic form of the $\hat{Q}$-box induces that the diagrammatic expansion of the $\hat{Q}$-box includes only valence linked (the incoming and outcoming lines should belong to the model space P) and irreducible diagrams.

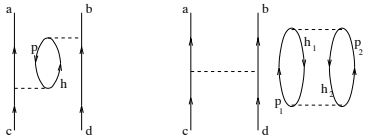


Figure 2.1: An example of a linked second-order Goldstone diagram (left) and non-linked one (right)

Without including phenomenological parameters, if:

- the realistic potential is reliable;
- the model space is large enough to contain the needed degrees of freedom;
- the perturbative properties of the expansion of H_{eff} are satisfactory;

then the predictive power of the shell-model calculation is enhanced.

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Chapter 3

The coupled-cluster approach

There are some considerations that make the coupled-cluster (CC) approach a profitable way to microscopic nuclear structure calculations.

CC is fully microscopic and capable of systematic and hyerarchical improvements of the unavoidable truncations needed to make the calculations feasible.

In fact, when expanding the cluster operator to all A nucleons belonging to a nucleus, one obtains the exact correlated wave function of the nucleus.

The CC method is size extensive, which means that only linked diagrams appear in the calculation of the energy, and this implies that the nuclear separation energy tends to a constant in the infinite system size, and the total energy is proportional to the number of the nucleons.

The CC method is size consistent, this means that if the system presents two well-separated non-interacting subsystems, the total energy of the system is equal to the sum of the energy of the two subsystems.

If we deal with a two-body potential only, then the CC equations need only two-body formalism to be written down.

Let's consider first the A-body product state $|\Phi\rangle$

$$|\Phi\rangle = \prod_{\alpha=1}^{A} a_\alpha^\dagger |0\rangle \quad ,$$

that will be our reference state.

This reference state could be either the result of a Hartree-Fock calculation or simply obtained filling the harmonic-oscillator orbitals. From now on greek letters will refer to occupied states below the Fermi surface, latin ones to any orbital.

In order to easily derive the CC equations, it is useful to normal order the

two-body hamiltonian in second quantization

$$H = \sum_{ij} \epsilon_{ij} a_i^\dagger a_j + \frac{1}{4} \sum_{ijkl} \langle ij|V|jk\rangle a_i^\dagger a_j^\dagger a_l a_k \quad ,$$

with respect to the reference state $|\Phi\rangle$.

The normal ordered hamiltonian H_N is then definied as

$$H = H_N + E_0 = H_N + \sum_{\alpha} \epsilon_\alpha + \frac{1}{2} \sum_{\alpha\beta} \langle \alpha\beta|V|\alpha\beta\rangle \quad .$$

It can be easily seen that H_N can be written as

$$\begin{aligned} H_N &= \sum_{ij} \left(\epsilon_{ij} + \frac{1}{2} \sum_{\alpha} \langle \alpha i|V|\alpha j\rangle \right) : a_i^\dagger a_j : + \frac{1}{2} \sum_{ijkl} \langle ij|V|jk\rangle : a_i^\dagger a_j^\dagger a_l a_k : \\ &= \sum_{ij} f_{ij} : a_i^\dagger a_j : + \frac{1}{2} \sum_{ijkl} \langle ij|V|jk\rangle : a_i^\dagger a_j^\dagger a_l a_k : \quad . \end{aligned}$$

Please note that this formalism can be easily extended to the case of an hamiltonian including also a three-body potential.

Note that, by construction

$$\langle \Phi|H_N|\Phi\rangle = 0 \quad .$$

The core of the CC method is to build up a similarity transformed hamiltonian H_{CC}

$$H_{CC} = e^{-T} H e^{T} \quad ,$$

where T will be the cluster operator that is definied with respect to the refernce state in the following way

$$T = T_1 + T_2 + ... + T_A \quad ,$$

and

$$\begin{aligned} T_1 &= \sum_{a\alpha} t_a^\alpha a_a^\dagger a_\alpha \\ T_2 &= \frac{1}{4} \sum_{a\alpha b\beta} t_{\alpha\beta}^{ab} a_a^\dagger a_b^\dagger a_\beta a_\alpha \\ &... \end{aligned}$$

It is evident that the generic T_n operator generates n-particle n-hole excitations with respect to the reference state $|\Phi\rangle$. The truncation of the number of the T_n operators to 1 defines the CC approximation with singles

$$\begin{aligned} \text{CCS} &\rightarrow T_1 \\ \text{CCSD} &\rightarrow T_1 + T_2 \\ \text{CCSDT} &\rightarrow T_1 + T_2 + T_3 \end{aligned}$$

and so on.

The Baker-Hausdorff relation allows to write H_{CC} as

$$H_{CC} = e^{-T} H_N e^T = H_N + [H_N, T] + \frac{1}{2}[[H_N, T], T] + \\ + \frac{1}{3!}[[[H_N, T], T], T] + + \frac{1}{4!}[[[[H_N, T], T], T], T] + ...$$

If we deal only with a two-body potential we have only four-fold nested commutators, if we include a three-body potential, up to six-fold nested commutators are needed.

The eigenvalue problem of the gorund-state energy would be

$$E = \langle \Phi | H_{CC} | \Phi \rangle \quad ,$$

and to calculate E we need to derive the n-particle n-hole amplitudes t. This can be done observing that

$$\begin{aligned} \langle \Phi | a_a a_\alpha^\dagger H_{CC} | \Phi \rangle &= 0 \\ \langle \Phi | a_a a_b a_\beta^\dagger a_\alpha^\dagger H_{CC} | \Phi \rangle &= 0 \\ &... \end{aligned}$$

Using the above set of equations and the Wick's theorem to contract all a and $a^\dagger$ operators, one obtains the equations for the amplitudes t. For simplicity we consider only CCS approximation (coupled-cluster with singles)

$$f_{\alpha\alpha} + \sum_b f_{ab} t_\alpha^b - \sum_{beta} f_{\beta\alpha} t_\beta^a + \sum_{\beta b} \langle \beta a | V | b\alpha \rangle t_\beta^b + \\ - \frac{1}{2} \sum_{\beta b} f_{\beta b} t_\alpha^b t_\beta^a - \sum_{\beta\gamma b} \langle \beta\gamma | V | b\alpha \rangle t_\beta^b t_\gamma^a + \\ + \sum_{\beta bc} \langle \beta a | V | bc \rangle t_\beta^a t_\alpha^c - \sum_{\beta\gamma bc} \langle \beta\gamma | V | bc \rangle t_\beta^b t_\alpha^c t_\gamma^a = 0$$

This system of equations can be easily solved with iterative techniques.

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