EFFECTIVE NUCLEAR OPERATORS WITH THE COUPLED-CLUSTER METHOD

By

Samuel John Novario

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KEY TO SYMBOLS AND ABBREVIATIONS

Ap-Bh	A-particle, B-hole excitation or de-excitation from the reference state
$\|0\rangle$	vacuum state
$\|\Phi_0\rangle$	reference state
$\|\Psi\rangle$	correlated ground state
$\|\Phi^{a_1\cdots a_A}_{i_1\cdots i_B}\rangle$	specific Ap-Bh state
$\{\cdots\}$	normal-ordered with respect to the reference state
$\hbar\omega$	harmonic oscillator energy scale
$\hat{H}$	Hamiltonian
$\overline{H}$	similarity-transformed Hamiltonian
$\hat{H}_{\mathrm{N}}$	normal-ordered Hamiltonian
$\overline{H}_{\mathrm{N}}$	normal-ordered similarity-transformed Hamiltonian
$\hat{T}$	cluster operator
$\varepsilon^{a_1\cdots a_A}_{i_1\cdots i_B}$	energy denominator, $f^{i_1}_{i_1} + \cdots + f^{i_B}_{i_B} - f^{a_1}_{a_1} - \cdots - f^{a_A}_{a_A}$
CC	coupled cluster
CCD	coupled cluster with doubles
CCSD	coupled cluster with singles and doubles
CCSDT	coupled cluster with singles, doubles, and triples
CCSD(T)	coupled cluster with singles, doubles, and triples approximation
Λ-CCSD(T)	coupled cluster with singles, doubles, and Λ-triples approximation
CI	configuration interaction
FCI	full configuration interaction
COM	center of mass
EOM	equations-of-motion
PA	particle-attached

PR	particle-removed
EOM	equations-of-motion
EOM-CC	equations-of-motion coupled cluster
EOM-CCSD	equations-of-motion coupled cluster with singles and doubles
HF	Hartree-Fock
IM-SRG	in-medium similarity renormalization group
HO	harmonic oscillator
LECs	low-energy constants
MBPT	many-body perturbation theory
WS	Woods-Saxon
DIIS	direct-inversion of the iterative subspace
QCD	quantum chromodynamics
EFT	effective field theory
NN	nucleon-nucleon
3N	three-nucleon
NLO	next-to leading order
N^2LO	next-to-next-to leading order
N^3LO	next-to-next-to-next-to leading order

Chapter 1

Introduction

Steady progress in any modern scientific endeavor requires a strong, dynamic relationship between experimental data to paint an accurate picture of some natural phenomena and theoretical models to interpret those phenomena with respect to the growing network of other scientific models. Conversely, the predictive capability of theoretical models can highlight blurry or unfinished areas of that picture which can be clarified or completed by new or improved experimental techniques. In the pursuit to understand and describe the atomic nucleus and the corresponding implications from quarks to neutron stars, this push-and-pull coordination between theory and experiment makes progress in modern nuclear physics robust and persistent.

An integral component of modern nuclear physics is describing the structure and emergent properties of self-bound systems of protons and neutrons. The systems in questions can be stable nuclei, rare isotopes far from stability, and even infinite nuclear matter which can be used to model neutron stars. Relevant properties to nuclear structure include ground-state energies–for determining nuclear masses, excited-state energies–for identification in gamma or neutron spectroscopy, and transition or decay amplitudes–for calculating the respective rates for those processes. This wide array of emergent properties inserts both nuclear structure theory and experiment into a prominent role within every other subfield of modern nuclear physics, from lattice quantum chromodynamics (QCD) to nuclear astrophysics, and beyond, to questions about fundamental symmetries and dark matter. However, two inextricable characteristics of a comprehensive model of nuclear structure–the increasingly large

size of many-body nuclear systems and the complexity and strength of the nucleon-nucleon interactions–have been imposing hurdles for theorists to overcome.

1.1 A Brief History of Nuclear Structure Theory

The project to solve the correlation problem in many-fermion systems began with the work of Brueckner, Bethe, and Goldstone [17, 7, 1] with the reformulation of the nuclear interaction by accounting for two-body correlations from the nuclear medium. This work continued with the work of Coester and Kummel [25, 26, 57] with a further resummation of nuclear correlations in the form of an exponential ansatz into what would become coupled-cluster (CC) theory. However, there were two major obstacles that hindered the progress in this area for decades. First, while these methods were systematically improvable by including progressively higher-level correlations, the highly-nonperturbatuve nature of the nuclear force required computationally infeasible summations. Second, there wasn't a reliable and consistent theory to model nucleon-nucleon interactions.

However, the well-known and highly-perturbative Coulomb force, which underlies the many-electron systems in atoms and molecules, made consistent advances in ab-initio quantum chemistry possible since the 1950s. Along with the quasi-exact method of configuration interaction (CI) [77, 27, 3, 94] which physicists have utilized since the formulation of quantum mechanics, chemists successfully employed approximate methods like many-body perturbation theory (MBPT) [49, 50, 73, 75] and coupled-cluster theory [23, 21, 22, 66, 75].

Fortunately, within the past decade, two breakthroughs have allowed ab-initio nuclear structure to resurface and thrive the way that quantum chemistry had done in the previous decades. First was the invention of chiral effective field theory (EFT) [32, 60] which gave theorists the ability to construct nucleon-nucleon interactions consistent with the underlying

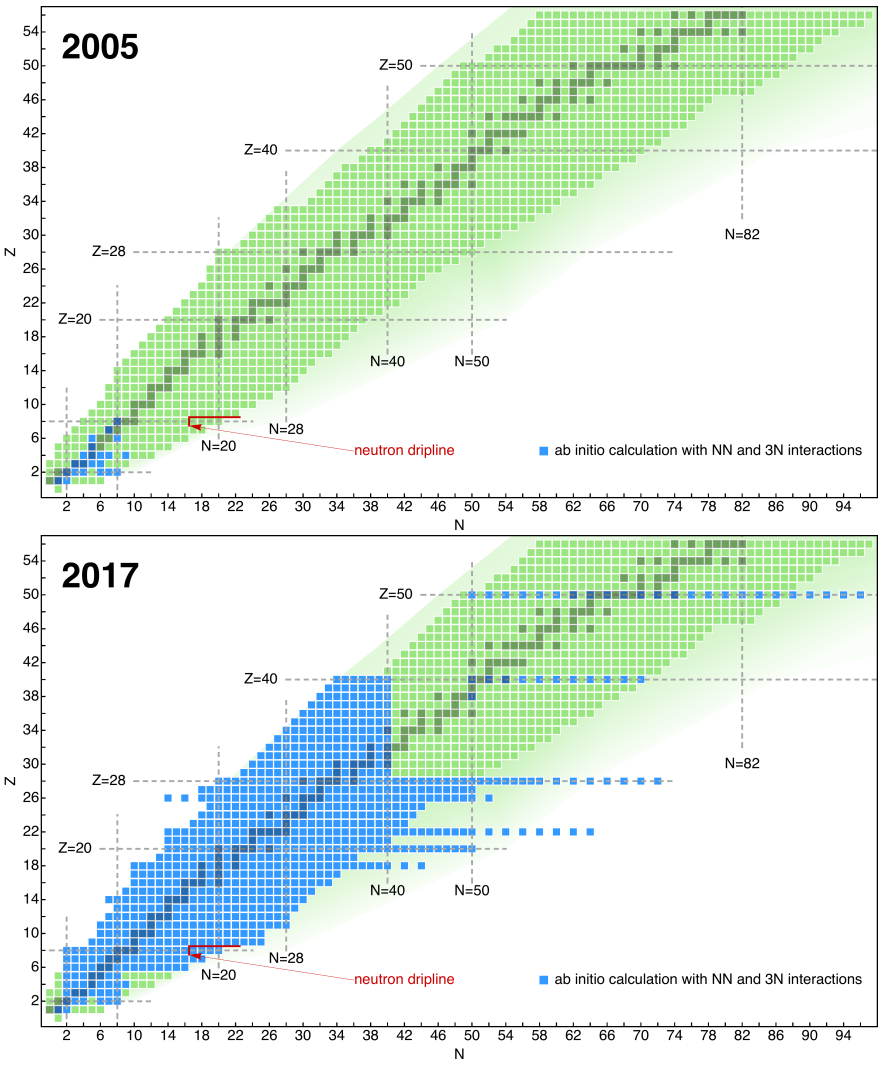


Figure 1.1: Nuclear chart of nuclei with ground-state energies which have been calculated with ab-initio methods and NN+3N interactions. Figure taken from [47].

QCD of the strong nuclear force. Second was the application of renormalization group (RG) methods to the nuclear force [12, 72]. This procedure can "soften" the NN interaction, to decouple the high- and low-momentum components of the nuclear force and generate less-correlated systems that can be calculated at a reasonable computational cost. These major changes to nuclear structure theory made it possible to merge the field with the progress of quantum chemistry and open a new area for additional developments in ab-initio descriptions of many-fermion systems, see Fig. 1.1.

Along with exponential improvements to high-performance computing, these novel techniques have allowed modern many-body methods to extend their reach and deepen their applicability across the nuclear chart, see Fig. 1.2. The no-core shell model (NCSM), a quasi-exact method, has been able to reach the *sd* shell and useful in calculating the radii, transition strengths, and effective interactions of light nuclei [63, 64, 5]. Another quasi-exact technique which follows a completely different methodology than NCSM, quantum Monte Carlo (QMC), has also progressed and is now capable of calculating properties of light nuclei with modern chiral forces [68, 67, 20]. In addition to these exponentially scaling techniques' successes with lighter nuclei, polynomially scaling techniques–such as the in-medium similarity renormalization group (IMSRG) [92, 93, 45, 10, 46, 44, 83, 82], self-consistent Green's functions (SCGF) [79, 80, 81], and coupled cluster theory [99, 100, 51, 52, 40, 56, 38, 8]–have been able to reach open-shell nuclei through the pf shell and even up to the chain of even tin isotopes with equations-of-motion and multi-reference techniques.

1.2 Electroweak Theory and Nuclear Structure

Nuclear structure is implicated in performing and analyzing experiments to probe fundamental symmetries and physics beyond the Standard Model. One example is determining the V_{ud} component of the Cabbibo-Kobayashi-Maskawa (CKM) matrix, which relates quark eigenstates of the weak interaction to their mass eigenstates [19, 54]. This matrix element can be determined from by measuring the half-lives of superallowed Fermi beta decays [87] and applying a nucleus-dependent structure correction [88, 91, 90, 4, 53]. The value of $|V_{ud}|$ is used to test the unitarity of the CKM matrix and the conserved-vector current hypothesis, which relates the ft-values of superallowed Fermi beta decays of different nuclei, both predicted by the standard model [41].

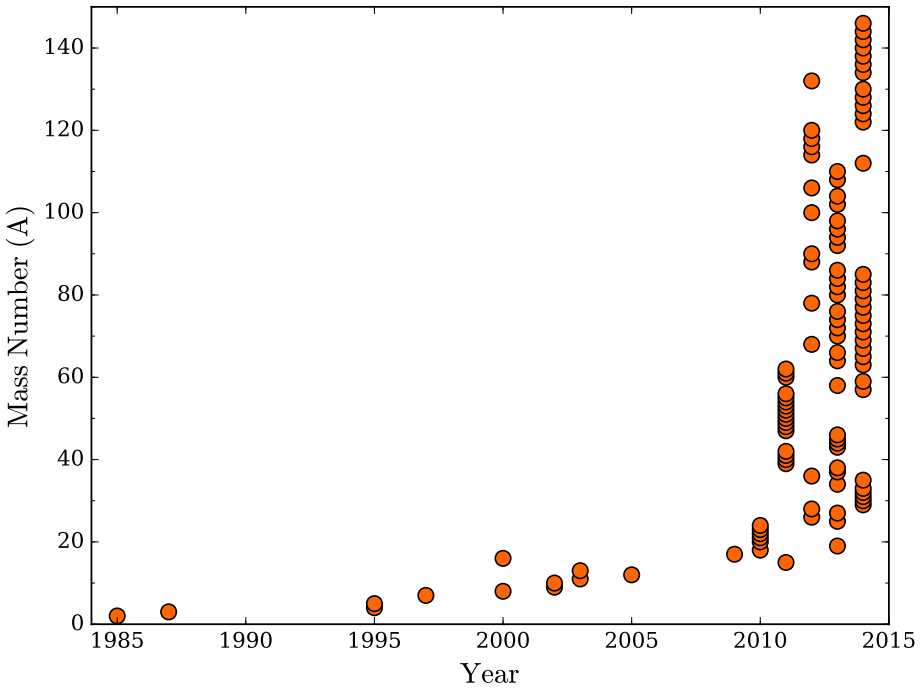


Figure 1.2: Progress of ab-initio nuclear structure from calculations of ground-state energies with NN+3N interactions. Early progress was approximately linear as the problem size scaled with Moore's law while more recent progress has taken advantage of new algorithms which have outpaced Moore's law. Data taken from [47].

Another example of physics beyond the standard model is the neutrinoless double-beta decay ($0\nu\beta\beta$) [84, 2]. The extremely-rare, two-neutrino double-beta decay ($2\nu\beta\beta$) has been observed in many experiments [30, 61], which has motivated the search for its neutrinoless counterpart, in which two Majorana neutrinos–being their own antiparticles–annihilate one another, which is not possible in the standard electro-weak theory. The long half-lives of these theoretical decays depend on a phase-space factor, which is highly dependent on the decay Q-value, and a nuclear matrix element. The Q-value can be determined from high-precision mass measurements of the relevant nuclei [59, 39, 71, 18], while the nuclear matrix element, which contributes the largest source of uncertainty, must be calculated with a sufficient many-body theory.

The weak interaction and nuclear structure can also be exploited for supernova neutrino

detection and spectroscopy. While these original detectors were based on electron-neutrino scattering [48, 9], more recent experiments utilize correlated nucleon effects of large nuclei to enhance the scattering cross section and therefore the ability to resolve energies and distinguish neutrino flavors [42, 24, 33, 58]. Supernova models predict distinct distributions for different neutrino flavors based on the temperatures at which they are emitted [55, 6]. With nuclear structure calculations that include sufficient nuclear correlations, these high-resolution detectors can be used to verify specific models.

1.3 Ab-Initio Descriptions of Beta Decay

Since Enrico Fermi's originally rejected paper describing β decay in 1934 [34, 98], theorists have worked to refine this description within the ever-growing library of knowledge concerning the nature of the weak force, the characteristics of the neutrino, and the structure of nuclei. With the success of ab-initio calculations for nuclear properties such as masses, radii, and electromagnetic phenomena, these techniques also seem promising ways to calculate relevant quantities involved in nuclear β decay. Because the kinematics of the decay and the underlying weak process are well understood, the remaining task for nuclear theory to tackle is calculating the transition amplitudes between the initial and final nuclei.

Modern calculations of these β-decay matrix elements were originally performed using phenomenological interactions in the shell model framework [97, 15, 95, 65]. Also, predecessors to current ab-initio techniques like the random-phase approximation (RPA) [89] included core-correlation effects in these early descriptions. These methods were able to successfully reproduce experimental lifetime data and address technical issues such as the quenching of the axial-vector coupling constant. More recently, the success of the shell model has inspired an extension to the new method, known as the ab-initio shell model, where an effective in-

teraction is constructed within a certain valence space using a many-body method such as CC [29] or IMSRG [11]. However, these techniques are computationally expensive and cannot currently reach heavy nuclei of interest. The most common method used in their place is known as the quasiparticle random-phase approximation (QRPA) [85, 31]. While these calculations can be performed for heavy nuclei in large spaces, they also rely on phenomenological effective interactions. Therefore, there is a demand for computationally-economical, ab-initio techniques that can capture the relevant many-body correlations needed to accurately describe the nuclear structure aspects of electro-weak processes.

1.4 Thesis Structure

The main goal of this work is to explore the ab-initio description of nuclear beta decay within the coupled-cluster theory framework of EOM-CCSD using renormalized chiral NN and 3N interactions. The organization of the thesis builds from a general description of the many-body problem of quantum mechanics in chapter 2. Then, in chapter **??**, this many-body framework is applied within the coupled-cluster theory an applied to various systems including atomic nuclei. In chapter **??**, coupled-cluster theory is extended to the equations-of-motion method to describe open-shell systems. Chapter **??** outlines the procedure to express observables as effective coupled-cluster operators and how to calculate those observables in the equations-of-motion framework. Then, in chapter **??**, the ability to calculate effective operators is applied to Fermi- and Gamow-Teller- beta-decay operators and relevant quantities are determined for various nuclei. Lastly, conclusions and future perspectives are given in chapter **??** while technical details concerning the formalism and implementation are given in the appendix **??**.

Chapter 2

Many-Body Quantum Mechanics

Ab-initio structure calculations of many-fermion systems such as those in nuclear and electronic structure aim to describe emergent phenomena from the constituent particles subject to the underlying microscopic Hamiltonian. This amounts to finding the solution to the many-body Schrödinger equation. However, a calculation of the exact solution needs to account for all possible correlations among the particles and thus scales factorially. This motivates the need for approximations to the exact solution that account for the most important correlations. This chapter first establishes the formalism neccesary to define the many-body problem then illustrates several successive approximations to its solution. Because the type of fermions and the underlying Hamiltonian can be kept generic until specific systems are considered, the formalism and many-body methods can be kept generic as well.

2.1 Independent-Particle Model

The nonrelativistic A-body quantum problem begins with the Schrödinger equation,

$$\hat{H}\Psi_\nu\left(\mathbf{r}_1,\cdots,\mathbf{r}_A\right) = E_\nu\Psi_\nu\left(\mathbf{r}_1,\cdots,\mathbf{r}_A\right), \tag{2.1}$$

for the correlated wave function $\Psi_\nu\left(\mathbf{r}_1,\cdots,\mathbf{r}_A\right)$ and the corresponding energy E_ν. The Hamiltonian can be written generically as a sum of k-body pieces which, in principle, can

contain up to A-body interactions,

$$\begin{aligned}\hat{H} &= {}^{(1)}\hat{H} + {}^{(2)}\hat{H} + {}^{(3)}\hat{H} + \cdots \\ &= \sum_{i}^{A} {}^{(1)}\hat{H}(\mathbf{r}_i) + \sum_{i<j}^{A} {}^{(2)}\hat{H}\big(\mathbf{r}_i, \mathbf{r}_j\big) + \sum_{i<j<k}^{A} {}^{(3)}\hat{H}\big(\mathbf{r}_i, \mathbf{r}_j, \mathbf{r}_k\big) + \cdots . \end{aligned} \tag{2.2}$$

Regardless of the system, the one-body term contains the kinetic energy operator $\frac{-\hbar^2}{2m}\nabla_i^2$, while the higher-order terms result from inter-particle interactions.

An intuitive way to formulate the solution to the many-body Schrödinger equation is to express the collective wave function in terms of independent single-particle wave functions, or orbitals $\phi(\mathbf{r})$. In this *independent-particle model*, a selection of single-particle wave functions, known as the single-particle basis, are constructed by solving the Schrödinger equation for a single particle in some mean-field potential, for bound systems, or in free space, for infinite systems. Then a many-body wave function is constructed as a product of these single-particle orbits. This simple model is justified because it becomes exact when inter-particle interactions are completely suppressed and is useful because it provides an intuitive way to interpret complicated m any-body dynamics as processes involving few single-particle wave functions.

A many-body wave function of fermions must be anti-symmetric with respect to particle exchange so that the Pauli exclusion principle is followed, such that no single-particle wave function is occupied by more than one fermion. This condition is satisfied by a wave function

in the form of a *Slater determinant* [78],

$$\Phi\left(\mathbf{r}_1, \cdots, \mathbf{r}_A\right) = \frac{1}{\sqrt{A!}} \begin{vmatrix} \phi_1\left(\mathbf{r}_1\right) & \phi_1\left(\mathbf{r}_2\right) & \cdots & \phi_1\left(\mathbf{r}_A\right) \\ \phi_2\left(\mathbf{r}_1\right) & \phi_2\left(\mathbf{r}_2\right) & \cdots & \phi_2\left(\mathbf{r}_A\right) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_A\left(\mathbf{r}_1\right) & \phi_A\left(\mathbf{r}_2\right) & \cdots & \phi_A\left(\mathbf{r}_A\right) \end{vmatrix}, \tag{2.3}$$

where A is the number of particles in the system and $\phi_p\left(\mathbf{r}_\mu\right)$ is the p-th orbital filled with the μ-th particle.

If the orbitals are constructed from an appropriate phenomenological potential, a Slater determinant composed of the A lowest orbitals can represent a fairly good approximations to the ground state for a closed-shell system, where the lowest-energy Slater determinant can be uniquely determined. The set of all Slater determinants in a certain model space of single-particle wave functions defines a complete A-body Hilbert space such that a generic wave function can be written as a linear combination of Slater determinants,

$$\Psi_\nu\left(\mathbf{r}_1, \cdots, \mathbf{r}_A\right) = \sum_{\mu=1}^{\mathcal{N}} C_\nu^\mu \Phi_\mu\left(\mathbf{r}_1, \cdots, \mathbf{r}_A\right), \tag{2.4}$$

where $C_\nu^\mu = \langle \Psi\left(\mathbf{r}_1, \cdots, \mathbf{r}_A\right) | \Phi_\nu^\mu\left(\mathbf{r}_1, \cdots, \mathbf{r}_A\right) \rangle$. The number of Slater determinants $\mathcal{N}$ in an A-body Hilbert space with N orbits is given by,

$$\mathcal{N} = \binom{N}{A} = \frac{N!}{A!(N-A)!}, \tag{2.5}$$

which shows the factorial scaling of the exact problem. However, to reduce the size of the problem, progressively more significant Slater determinants can be chosen to systematically

refine approximations to the full solution.

2.2 Second Quantization

Even with the simplification of the independent-particle model, the many-body Schrödinger equation is an unwieldy and complex system of coupled differential equations. A useful reformulation of this equation is to promote the single-particle orbits to operators in a step known as *second quantization* (see e.g., [75, 35]). In this framework, a Slater determinant is represented by a string of occupied orbitals,

$$\Phi\left(\mathbf{r}_1, \cdots, \mathbf{r}_A\right) \equiv \mathcal{A}\left(\phi_{p_1}\ \phi_{p_2}\ \phi_{p_3} \cdots \phi_{p_N}\right) \equiv |p_1\ p_2\ p_3 \cdots p_N\rangle, \tag{2.6}$$

where $\mathcal{A}$ represents a permutation and normalization operator to correspond with Eq. (2.3). These second-quantized Slater determinants can be constructed with the use of operators that correspond to specific orbitals. A *creation* operator, $\hat{a}_p^\dagger$, places a particle in the p orbital, and an *annihilation* operator, $\hat{a}_p$, removes a particle from the p orbital,

$$\hat{a}_p^\dagger|0\rangle = |p\rangle \qquad\qquad \hat{a}_p|p\rangle = |0\rangle, \tag{2.7}$$

where $|0\rangle$ represents the true vacuum, a state void of any particles. Because there must be a correspondence between the original first quantization and second quantization, these creation an annihilation operators obey the following anticommutation relations ($[\hat{A}, \hat{B}]_+ = \hat{A}\hat{B} + \hat{A}\hat{B}$),

$$[\hat{a}_p^\dagger, \hat{a}_q]_+ = \delta_{pq} \qquad [\hat{a}_p^\dagger, \hat{a}_q^\dagger]_+ = [\hat{a}_p, \hat{a}_q]_+ = 0, \tag{2.8}$$

which guarantee that wave functions comprised of these operators obey antisymmetry and the Pauli exclusion principle required of fermionic systems.

The Hamiltonian in the form of Eq. (2.2) can be written with second-quantized operators as,

$$\hat{H} = \sum_{pq} {}^{(1)}H_q^p \; \hat{a}_p^\dagger \hat{a}_q + \frac{1}{4} \sum_{pqrs} {}^{(2)}H_{rs}^{pq} \; \hat{a}_p^\dagger \hat{a}_q^\dagger \hat{a}_s \hat{a}_r + \frac{1}{36} \sum_{pqrstu} {}^{(3)}H_{stu}^{pqr} \; \hat{a}_p^\dagger \hat{a}_q^\dagger \hat{a}_r^\dagger \hat{a}_u \hat{a}_t \hat{a}_s + \cdots , \quad (2.9)$$

where the prefactors account for the double counting of particle-particle interactions, and the matrix elements represent integrals over the relevant single-particle wave functions,

$$\begin{aligned} {}^{(1)}H_q^p &\equiv \int d\mathbf{r}_1 \; \phi_p^* (\mathbf{r}_1) \, {}^{(1)}\hat{H}(\mathbf{r}_1) \, \phi_q (\mathbf{r}_1) \\ {}^{(2)}H_{rs}^{pq} &\equiv \int d\mathbf{r}_1 d\mathbf{r}_2 \; \phi_p^* (\mathbf{r}_1) \, \phi_q^* (\mathbf{r}_2) \, {}^{(2)}\hat{H}(\mathbf{r}_1, \mathbf{r}_2) \left[\phi_r (\mathbf{r}_1) \, \phi_s (\mathbf{r}_2) - \phi_s (\mathbf{r}_1) \, \phi_r (\mathbf{r}_2) \right] \\ &\vdots \end{aligned} \quad (2.10)$$

Matrix elements involving two or more particles include exchange terms which guarantee that they are also antisymmetric,

$$\begin{aligned} {}^{(2)}H_{rs}^{pq} &= -{}^{(2)}H_{rs}^{qp} = -{}^{(2)}H_{sr}^{pq} = {}^{(2)}H_{sr}^{qp} \\ {}^{(3)}H_{stu}^{pqr} &= -{}^{(3)}H_{stu}^{qpr} = -{}^{(3)}H_{tsu}^{pqr} = {}^{(3)}H_{tsu}^{qpr} = \cdots \end{aligned} \quad (2.11)$$

These definitions apply regardless of the form of the Hamiltonian, and thus this formalism remains generic to the particular system. Second quantization is a crucial step in simplifying the many-body Schrödinger equation because it reduces the complexity of the spatial and spin degrees of freedom within the single-particle wave functions and interactions into precomputed matrix elements. The remaining effort is reduced to algebraic expressions in-

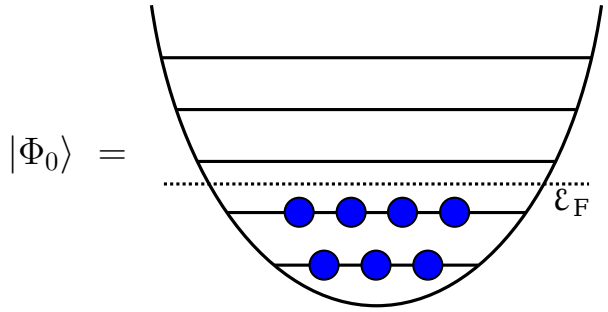


Figure 2.1: A depiction of the closed-shell reference state in the independent particle model. Each horizontal line represents a shell of single-particle orbits, and the dotted line represents the Fermi level which separates *particle* states from *hole* states.

volving creation and annihilation operators.

2.3 Normal Ordering

It's convenient to define an A-particle reference state, where states are filled from the true vacuum up to a closed shell, known as the Fermi level. This reference state must be uniquely determined from the number of particles in the system and therefore nondegenerate with other Slater determinants,

$$|\Phi_0\rangle = \left\{ \prod_i^A \hat{a}_i^\dagger \right\} |0\rangle. \tag{2.12}$$

This reference determinant defines a new *Fermi vacuum*. States above the Fermi vacuum are called *particle* states and will be denoted with the indices $a, b, c, d...$ while states below the Fermi vacuum are called *hole* states and will be denoted with the indices $i, j, k, l....$ Generic states above or below the Fermi vacuum will be denoted with the indices $p, q, r, s....$

Any other Slater determinant can be constructed relative to this reference state by adding particles and/or removing holes. A Slater determinant with A particles added and B holes

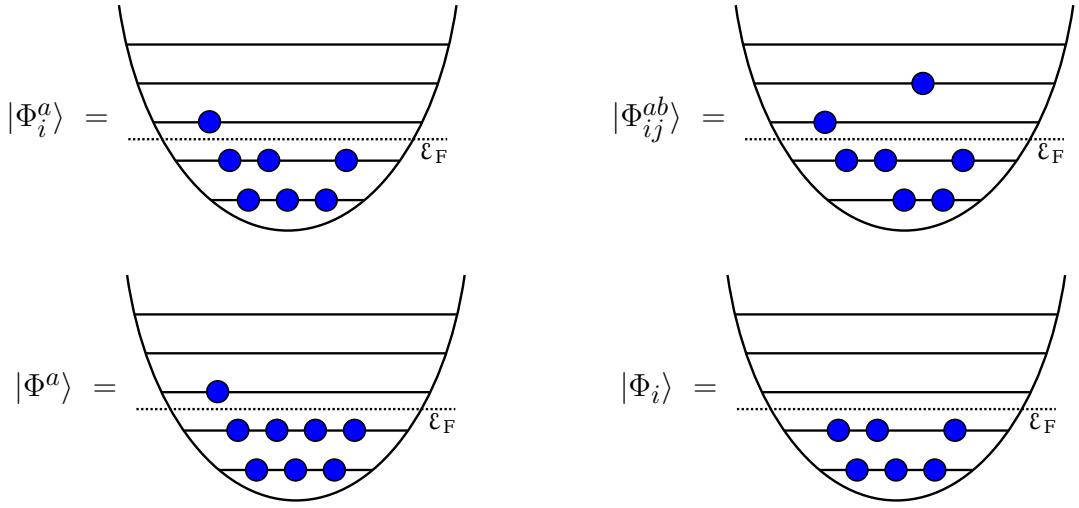


Figure 2.2: A depiction of $1p$-$1h$, $2p$-$2h$, $1p$-$0h$, and $0p$-$1h$ Slater determinants defined relative to the reference state in the independent particle model.

removed from reference state is known as a Ap-Bh excitation.

$$
\begin{aligned}
|\Phi_i^a\rangle &\equiv \hat{a}_a^\dagger \hat{a}_i |\Phi\rangle \\
|\Phi_{ij}^{ab}\rangle &\equiv \hat{a}_a^\dagger \hat{a}_b^\dagger \hat{a}_j \hat{a}_i |\Phi\rangle \\
|\Phi^a\rangle &\equiv \hat{a}_a^\dagger |\Phi\rangle \\
|\Phi_i\rangle &\equiv \hat{a}_i |\Phi\rangle
\end{aligned}
\tag{2.13}
$$

Using these definitions, hole-creation and particle-annihilation operators vanish when acting on the Fermi vacuum from the left, $\hat{a}_i^\dagger |\Phi_0\rangle = \hat{a}_a |\Phi_0\rangle = 0$. Conversely, hole-annihilation and particle-creation operators vanish when acting on the Fermi vacuum from the right, $\langle\Phi_0|\hat{a}_i = \langle\Phi_0|\hat{a}_a^\dagger = 0$.

These results can be exploited to simplify expressions involving strings of creation and annihilation operators by a procedure called *normal ordering* with respect to the Fermi vacuum. Denoted by $\{\cdots\}$, normal ordering permutes a string of creation and annihilation operators so that hole-annihilation and particle-creation operators are to the left of hole-

creation and particle-annihilation operators, which guarantees that normal ordered operators vanish on the Fermi vacuum, $\langle\Phi_0|\,\{\cdots\} = 0$ and $\{\cdots\}\,|\Phi_0\rangle = 0$.

$$\left\{\hat{a}_j^\dagger \cdots \hat{a}_i \cdots \hat{a}_b \cdots \hat{a}_a^\dagger\right\} = (-1)^\sigma \hat{a}_i \cdots \hat{a}_a^\dagger \cdots \hat{a}_j^\dagger \cdots \hat{a}_b, \tag{2.14}$$

where σ is the number of two-state permutations required to do the normal ordering.

2.4 Wick's Theorem

At this point, the many-body problem has been reduced to computing long strings of creation and annihilation operators between the normal-ordered Hamiltonian and the correlated wave function using Eq. (2.8). Instead of using a brute-force approach by permuting over and over, a further simplification known as *Wick's theorem* [96] can be introduced. A Wick contraction of two operators with respect to the reference state is defined as

$$\hat{A}\hat{B} = \hat{A}\hat{B} - \left\{\hat{A}\hat{B}\right\}. \tag{2.15}$$

Which, given the definition in Eq. (2.14) and the anticommutation relations int Eq. (2.8), means that the only nonzero contractions are of the form,

$$\hat{a}_i^\dagger \hat{a}_j = \delta_{ij} \qquad \text{and} \qquad \hat{a}_a \hat{a}_b^\dagger = \delta_{ab}. \tag{2.16}$$

Because contracted operators simply represent a Kronecker delta, they can be removed from a normal ordered product by permuting the product σ times so that the contracted operators

are next to each other,

$$\{\hat{A}\cdots\overbrace{\hat{B}\cdots\hat{C}}\cdots\hat{D}\} = (-1)^{\sigma}\{\hat{A}\cdots\overbrace{\hat{B}\hat{C}}\cdots\hat{D}\} = (-1)^{\sigma}\overbrace{\hat{B}\hat{C}}\{\hat{A}\cdots\hat{D}\}. \tag{2.17}$$

These different definitions for operator manipulation come together to define the time-independent Wick's theorem, which reformulates a product of operators as the sum of its normal-ordered form and all possible contractions of its normal-ordered form.

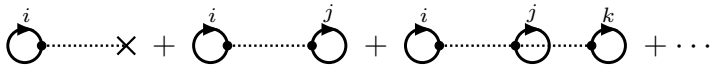
$$\hat{A}\hat{B}\hat{C}\cdots = \left\{\hat{A}\hat{B}\hat{C}\cdots\right\} + \sum_{\substack{\text{one-}\\\text{contractions}}}\{\overbrace{\hat{A}\hat{B}\hat{C}\cdots}\} + \sum_{\substack{\text{two-}\\\text{contractions}}}\{\overbrace{\hat{A}\hat{B}\hat{C}\cdots}\} + \cdots + \sum_{\substack{\text{all-}\\\text{contractions}}}\{\overbrace{\hat{A}\hat{B}\hat{C}\cdots}\} \tag{2.18}$$

Wick's theorem is incredibly useful in many-body techniques because complicated expressions of operators can be expressed as diagrams that are easy to compute with simple diagrammatic rules which correspond to Eqs. (2.8),(2.16), and (2.17). These diagrammatic techniques are an integral component to deriving expressions used in this work, and their underlying rules are summarized in **??** and are extensively discussed in [75].

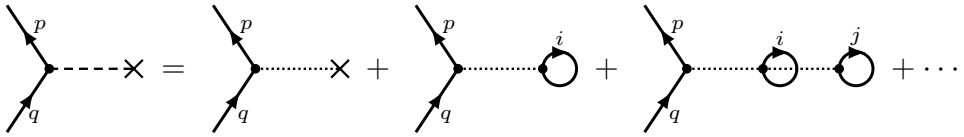
A powerful application of Wick's theorem is to rewrite the Hamiltonian in normal-ordered form.

$$\hat{H} = E_0 + \sum_{pq} f^p_q \left\{\hat{a}^\dagger_p \hat{a}_q\right\} + \frac{1}{4}\sum_{pqrs} \mathrm{V}^{pq}_{rs} \left\{\hat{a}^\dagger_p \hat{a}^\dagger_q \hat{a}_s \hat{a}_r\right\} + \frac{1}{36}\sum_{pqrstu} \mathrm{W}^{pqr}_{stu} \left\{\hat{a}^\dagger_p \hat{a}^\dagger_q \hat{a}^\dagger_r \hat{a}_u \hat{a}_t \hat{a}_s\right\} + \cdots, \tag{2.19}$$

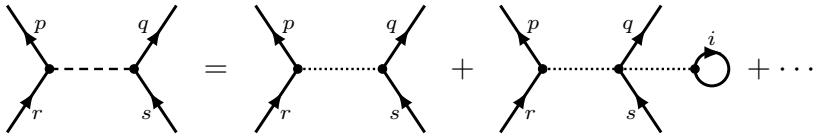
where the newly defined normal-ordered Hamiltonian terms are defined as,

$E_0 =$  $+ \cdots$

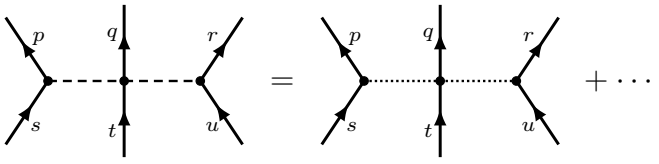
$$= \sum_i {}^{(1)}H_i^i + \frac{1}{2}\sum_{ij} {}^{(2)}H_{ij}^{ij} + \frac{1}{6}\sum_{ijk} {}^{(3)}H_{ijk}^{ijk} \cdots \tag{2.20}$$



$$f_q^p = {}^{(1)}H_q^p + \sum_i {}^{(2)}H_{qi}^{pi} + \frac{1}{2}\sum_{ij} {}^{(3)}H_{qij}^{pij} + \cdots \tag{2.21}$$



$$\mathrm{V}_{rs}^{pq} = {}^{(2)}H_{rs}^{pq} + \sum_i {}^{(3)}H_{rsi}^{pqi} + \cdots \tag{2.22}$$



$$\mathrm{W}_{stu}^{pqr} = {}^{(3)}H_{stu}^{pqr} + \cdots \tag{2.23}$$

This has the effect of shuffling higher-order interactions into lower-order terms, and makes it feasible to include computationally expensive many-body interactions as normal-ordered few-body interactions. Also, it reorganizes many-body correlations into the reference state so that additional correlations around the Fermi surface can be treated as a perturbation. Therefore, from this point forward, the many-body problem will be formulated in terms of the normal-ordered Hamiltonian, and the bare interactions will be truncated beyond the three-body level for computational feasibility. Electronic systems are naturally truncated at the two-body Coulomb force, while nuclear systems can be successfully described with the two-body normal-ordered piece of the three-body force.

In this form, the Hamiltonian is written is as a sum of the *reference energy*, E_0, which is the fully-contracted expectation value of the Hamiltonian with respect to the reference state,

$$E_0 = \langle \Phi | \hat{H} | \Phi \rangle, \tag{2.24}$$

and the remaining normal-ordered pieces of the Hamiltonian, $\hat{H}_{\mathrm{N}}$. Rewriting the many-body Schrödinger equation for the ground state, $|\Psi\rangle$, and using this partition gives,

$$\begin{aligned} \hat{H}|\Psi\rangle &= (E_0 + \hat{H}_{\mathrm{N}})|\Psi\rangle = E|\Psi\rangle \\ \longrightarrow \quad \hat{H}_{\mathrm{N}}|\Psi\rangle &= (E - E_0)|\Psi\rangle = \Delta E|\Psi\rangle, \end{aligned} \tag{2.25}$$

where ΔE is known as the *correlation energy*.

Now that the many-body quantum problem has been formulated, different approaches to solving that problem can be proposed and analyzed. Because taking account of correlations from all particles simultaneously is a demanding–and for some systems, computationally impossible–endeavor, methods for solving the many-body Schrödinger equation should be

systematically improvable. Successful methods with this quality incorporate the most dominant correlations in lower-order solutions and approach the exact solution when more and more orders are included.

2.5 Hartree–Fock Method

A successful, first-order approximation to any many-body method comes from noticing that each individual particle feels a mean-field potential from the cumulative interactions with all the other particles. The *Hartree-Fock* (HF) method [43, 36] aims to transform the original single-particle basis to a Hartree-Fock basis where each orbital is the eigenfunction of its corresponding mean-field. Because the transformation of a single orbital changes its effect on every other particle, this process must be performed iteratively until self-consistency between all the orbitals is reached, which is why this method is also known as the *Self-Consistent Field* (SCF) method.

This mean-field picture results from the following procedure. It begins by minimizing the reference energy with respect to the reference state. This functional is just the zero-body piece of the normal-ordered Hamiltonian,

$$E_{\mathrm{HF}}\left[\Phi_0\right] = \langle\Phi_0|\,\hat{H}|\Phi_0\rangle = \sum_i {}^{(1)}H_i^i + \frac{1}{2}\sum_{ij} {}^{(2)}H_{ij}^{ij} + \frac{1}{6}\sum_{ijk} {}^{(3)}H_{ijk}^{ijk}. \tag{2.26}$$

Transforming the reference determinant can be accomplished by rotating the state within the single-particle basis by use of the *Thouless theorem* [86], which states that any Slater determinant can be written as the product of any other Slater determinant and an exponentiated

single-excitation operator,

$$|\Phi'\rangle = e^{\hat{C}_1}|\Phi_0\rangle, \qquad \text{where} \;\; \hat{C}_1 = \sum_{ai} C_i^a \left\{\hat{a}_a^\dagger \hat{a}_i\right\}. \tag{2.27}$$

If the difference between the two Slater determinants is dominated by single excitations, this transformation can be approximated by expanding the exponential and ignoring higher-order terms,

$$|\Phi'\rangle \simeq \left(1 + \sum_{ai} C_i^a \left\{\hat{a}_a^\dagger \hat{a}_i\right\}\right)|\Phi_0\rangle. \tag{2.28}$$

The reference energy functional can now be written as a sum of the original reference state and new terms that incorporate the single-excitation variation,

$$E_{\mathrm{HF}}\left[\Phi'\right] = \langle\Phi'|\hat{H}|\Phi'\rangle \simeq E_{\mathrm{HF}}\left[\Phi_0\right] + \sum_{ai} C_i^a \langle\Phi_0|\hat{H}|\Phi_i^a\rangle + \sum_{ai} C_i^{a*}\langle\Phi_i^a|\hat{H}|\Phi_0\rangle. \tag{2.29}$$

The minimum of this functional is found by differentiating the expression with respect to the coefficients C_i^a and setting the result to zero,

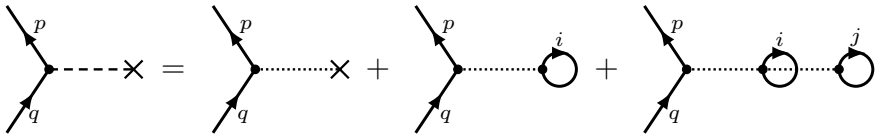
$$\delta E_{\mathrm{HF}}\left[\Phi'\right] \simeq \sum_{ai} \delta C_i^a \langle\Phi_0|\hat{H}|\Phi_i^a\rangle + \sum_{ai} \delta C_i^{a*}\langle\Phi_i^a|\hat{H}|\Phi_0\rangle = 0 \tag{2.30}$$

Because this expression is Hermitian, both terms must vanish independently so that,

$$\langle\Phi_0|\hat{H}|\Phi_i^a\rangle = \langle\Phi_i^a|\hat{H}|\Phi_0\rangle = 0. \tag{2.31}$$

This condition is the result of the *Brillouin theorem* [14], which states that the Hamiltonian matrix element must vanish between an optimized Hartree-Fock ground state and any single excitation from it. The Brillouin condition is satisfied by diagonalizing the one-body piece

of the normal-ordered Hamiltonian f_q^p, known as the *Fock* operator, such that off-diagonal pieces like $\langle\Phi_0|\hat{H}|\Phi_i^a\rangle = f_a^i$ and $\langle\Phi_i^a|\hat{H}|\Phi_0\rangle = f_i^a$ vanish.



$$f_q^p = {}^{(1)}H_q^p + \sum_i {}^{(2)}H_{qi}^{pi} + \frac{1}{2}\sum_{ij} {}^{(3)}H_{qij}^{pij} \quad \longrightarrow \quad \varepsilon_q^p \delta_{pq}, \tag{2.32}$$

where ε_q^p is the eigenvalue of the Fock operator.

A practical way of solving this system of equations is to express each new orbital in the unknown Hatree-Fock basis, $|p'\rangle \equiv \phi_{p'}(\mathbf{r})$, denoted with primed labels, as a linear combination of the known single-particle basis states, $|p\rangle \equiv \phi_p(\mathbf{r})$, denoted without primed labels.

$$|p'\rangle = \sum_p \langle p|p'\rangle\,|p\rangle = \sum_p C_{p'}^p\,|p\rangle \tag{2.33}$$

Then the Fock matrix can be written in terms of the Hartree-Fock basis,

$$\begin{aligned} f_{q'}^{p'} &= {}^{(1)}H_{q'}^{p'} + \sum_{i'} {}^{(2)}H_{q'i'}^{p'i'} + \frac{1}{2}\sum_{i'j'} {}^{(3)}H_{q'i'j'}^{p'i'j'} \\ = \sum_{pq} C_p^{p'*}{}^{(1)}H_q^p C_{q'}^q &+ \sum_{\substack{i' \\ prqs}} C_p^{p'*} C_r^{i'*}{}^{(2)}H_{qs}^{pr} C_{q'}^q C_{i'}^s + \frac{1}{2}\sum_{\substack{i'j' \\ prsqtu}} C_p^{p'*} C_r^{i'*} C_s^{j'*}{}^{(3)}H_{qtu}^{prs} C_{q'}^q C_{i'}^t C_{j'}^u. \end{aligned} \tag{2.34}$$

Defining the first-order density matrix γ_q^p as the product of expansion coefficients, summed over all shared hole states,

$$\gamma_q^p = \sum_{i'} C_{i'}^p C_q^{i'*}, \tag{2.35}$$

Eq. (2.5) is simplified to,

$$f^{p'}_{q'} = \sum_{pq} C^{p'*}_{p} \left[{}^{(1)}H^{p}_{q} + \sum_{rs} \gamma^{r}_{s}{}^{(2)}H^{pr}_{qs} + \frac{1}{2} \sum_{rstu} \gamma^{r}_{t} \gamma^{s}_{u}{}^{(3)}H^{prs}_{qtu} \right] C^{q}_{q'} \quad \longrightarrow \quad \varepsilon^{p'}_{q'} \delta_{p'q'}. \tag{2.36}$$

Therefore, the Hartree-Fock equations are ultimately expressed as an eigenvalue problem where the matrix to diagonalize is the Fock matrix in the form,

$$\hat{F}^{p}_{q}\left(\hat{C}\right) = {}^{(1)}H^{p}_{q} + \sum_{rs} \gamma^{s}_{r}{}^{(2)}H^{pr}_{qs} + \frac{1}{2} \sum_{rstu} \gamma^{t}_{r} \gamma^{u}_{s}{}^{(3)}H^{prs}_{qtu}, \tag{2.37}$$

and the matrix of coefficients, $\hat{C} = C^{p}_{p'}$, is the unitary operator that transforms the matrix to a diagonal form,

$$\sum_{pq} C^{p'*}_{p} F^{p}_{q}\left(\hat{C}\right) C^{q}_{q'} = \varepsilon^{p'}_{q'} \delta_{p'q'} \tag{2.38}$$

The iterative nature of the solution comes from the dependence of the Fock matrix on the transformation coefficients. These Hartree-Fock equations are solved numerically by using an iterative algorithm where the Fock matrix is built using a known set of coefficients and diagonalized to obtain an updated set of coefficients. This process is repeated until the unitary set of coefficients is unchanged within a certain tolerance. For most calculations, using the identity matrix as an initial guess for the coefficients is sufficient. To improve the rate of convergence, techniques such as the direct inversion of the iterative subspace (DIIS) [70, 69] or Broyden's method [16] can be implemented. And, to avoid any oscillatory behavior around the solution, techniques such as the level-shifting method or *ad hoc* linear mixing can be implemented to dampen the large changes between iterations.

To make use of the HF solution as the reference state for post-HF calculations, the Hamiltonian matrix elements must be transformed to the new basis and the normal-ordered

version redefined to account for the additional reordering of one-particle correlations into the HF energy.

$$f^{p'}_{q'} = \varepsilon^{p'}_{q'}\delta_{p'q'} \tag{2.39}$$

$$\mathrm{V}^{p'q'}_{r's'} = \sum_{pqrs} C^{p'*}_{p} C^{q'*}_{q} \left({}^{(2)}H^{pq}_{rs} + {}^{(3)}H^{pqt}_{rsu}\gamma^{u}_{t} \right) C^{r}_{r'} C^{s}_{s'} \tag{2.40}$$

$$\begin{aligned} E_0 &= \sum_{i'} {}^{(1)}H^{i'}_{i'} + \frac{1}{2}\sum_{i'j'} {}^{(2)}H^{i'j'}_{i'j'} + \frac{1}{6}\sum_{i'j'k'} {}^{(3)}H^{i'j'k'}_{i'j'k'} \\ &= \sum_{i'} \varepsilon^{i'}_{i'} - \frac{1}{2}\sum_{i'j'} \mathrm{V}^{i'j'}_{i'j'} + \frac{1}{6}\sum_{i'j'k'} {}^{(3)}H^{i'j'k'}_{i'j'k'} \end{aligned} \tag{2.41}$$

Additionally, any operators that are constructed in the original basis must be transformed in a similar manner. For example, a one-body operator $\hat{O}$ in the Hartree-Fock basis is,

$$\begin{aligned} \hat{O} = \sum_{p'q'} O^{p'}_{q'} \left\{ \hat{a}^{\dagger}_{p'} \hat{a}_{q'} \right\} &= \sum_{p'q'pq} C^{p'*}_{p} O^{p}_{q} C^{q}_{q'} \left\{ \hat{a}^{\dagger}_{p'} \hat{a}_{q'} \right\} \\ \longrightarrow \quad O^{p'}_{q'} &= \sum_{pq} C^{p'*}_{p} O^{p}_{q} C^{q}_{q'}. \end{aligned} \tag{2.42}$$

Because the Hartree-Fock basis is diagonal in the one-body piece of the Hamiltonian, any terms that include off-diagonal elements automatically vanish, greatly simplifying any post-Hartree-Fock methods. From this point, any calculations will use the Hartree-Fock basis unless stated otherwise, and prime symbols will be omitted.

2.6 Configuration-Interaction

The most generic way to write a correlated wave function in a given basis is as a linear combination of all possible Slater determinants. In normal-ordered form, this expansion

can, in principle, consist of the $0p$-$0h$ reference state and all possible Np-Nh excitations up to Ap-Ah excitations,

$$|\Psi_\nu\rangle = \sum_{\nu_i}^{\mathcal{N}} C_{\nu_i} |\Phi_{\nu_i}\rangle = C_0|\Phi_0\rangle + \sum_{N=1}^{A} \left(\frac{1}{N!}\right)^2 \sum_{\substack{a_1 \cdots a_N \\ i_1 \cdots i_N}} C_{i_1 \cdots i_N}^{a_1 \cdots a_N} |\Phi_{i_1 \cdots i_N}^{a_1 \cdots a_N}\rangle. \tag{2.43}$$

Using this form of the wave function in Eq. (2.43), the Schrödinger equation can be reformulated as a standard matrix eigenvalue problem,

$$\begin{aligned} \hat{H}_{\mathrm{N}}|\Psi_\nu\rangle = \Delta E_\nu |\Psi_\nu\rangle \quad &\longrightarrow \quad \langle\Psi_\mu|\hat{H}_{\mathrm{N}}|\Psi_\nu\rangle = \Delta E_\nu \langle\Psi_\mu|\Psi_\nu\rangle \\ = \sum_{\mu_i\nu_i} C_{\mu_i}^* \langle\Phi_{\mu_i}|\hat{H}_{\mathrm{N}}|\Phi_{\nu_i}\rangle C_{\nu_i} &= \Delta E_\nu \sum_{\mu_i\nu_i} C_{\mu_i}^* C_{\nu_i} \delta_{\mu_i\nu_i} \\ \longrightarrow \quad \mathbf{C}_\mu^{\mathrm{T}} \left(\langle\Phi_{\mu_i}|\hat{H}_{\mathrm{N}}|\Phi_{\nu_i}\rangle - \Delta E_\nu \mathbf{I}\right) \mathbf{C}_\nu &= 0. \end{aligned} \tag{2.44}$$

In this case, the matrix elements are Hamiltonian terms that connect two Slater determinants, and the eigenvectors are the ground and excited states in the form of Eq. (2.43). The matrix elements can be found with the help of the Slater-Condon rules [78, 28] which, because the Hamiltonian is restricted to one- and two-body terms, require that any terms connecting Slater determinants which differ by more than two single-particle states vanish. Also, because the one-body Hamiltonian is diagonal in the Hatree-Fock basis, it only contributes to diagonal elements the CI matrix. Some examples of these matrix elements

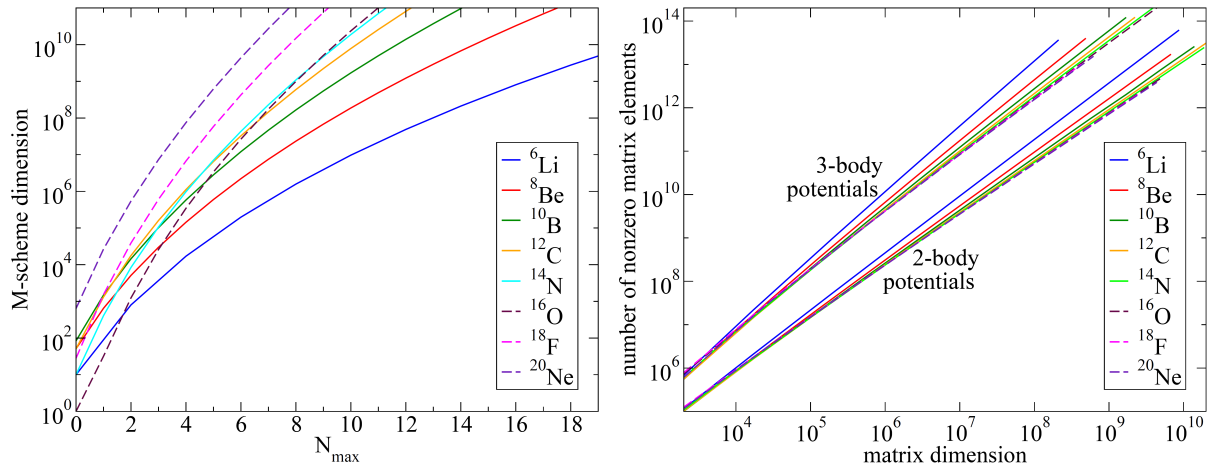


Figure 2.3: Scaling of the matrix size and number of non-zero matrix elements for nuclear CI calculations of light nuclei. Even for modest $N_{\max}$, the memory requirements approach the limit of petascale supercomputers (10^{10}). Figure taken from [74].

are,

$$\langle \Phi_i^a | \hat{H} | \Phi_i^a \rangle = \varepsilon_a - \varepsilon_i - \mathrm{V}_{ia}^{ia} \tag{2.45}$$

$$\langle \Phi_{ij}^{ab} | \hat{H} | \Phi_{ij}^{cd} \rangle = \mathrm{V}_{cd}^{ab} \tag{2.46}$$

$$\langle \Phi_{ijk}^{abc} | \hat{H} | \Phi_{ijl}^{abd} \rangle = -\mathrm{V}_{kd}^{lc} \tag{2.47}$$

Because the configuration-interaction method exhaustively captures all the correlations of a many-body system, it is considered an "exact" method within a certain model space and becomes truly exact as the number of single-particle states is increased to infinity. However, there is a price to pay for this exactness. The number of Slater determinants, $\mathcal{N}$, in model space scales factorially according to Eq. (2.5) and the configuration-interaction matrix scales as $\mathcal{N}^2$. For sufficiently-sized model spaces, the memory required for this matrix quickly becomes unmanigable even for the largest supercomputers.

However, for a reference state that is a good approximation to the true ground state, few-body excitations generally dominate the wave functions for low-lying states [76]. This

can be exploited by truncating the expansion in Eq. (2.43). Owing to the two-body nature of the interaction, the lowest appropriate truncation is also at the two-body level, known as configuration interaction with singles and doubles (CISD),

$$|\Psi_\nu\rangle = C_0|\Phi_0\rangle + \sum_{ai} C_i^a |\Phi_i^a\rangle + \frac{1}{4}\sum_{abij} C_{ij}^{ab}|\Phi_{ij}^{ab}\rangle. \tag{2.48}$$

This is a very straightforward and tractable way to approximate the many-body Schrödinger equation, and it can be systematically improved by adding more excitations such as triples (CISDT) or triples and quadruples (CISDTQ). But the drawback to this simplicity is that any truncated CI method is not size-extensive such that any extensive property of a system, like the energy, would scale with the size of the system. A desirable many-body method will be both systematically improvable and size-extensive while maintaining computational feasibility.

2.7 Many-Body Perturbation Theory

One many-body method that is both size-extensive and systematically improvable treats particle-particle interactions as a perturbation to the mean-field potential and is known as many-body perturbation theory (MBPT) [62, 49, 50, 75]. The Hamiltonian is partitioned into a diagonal piece and the interaction piece,

$$\begin{aligned} \hat{H} &= \hat{H}_0 + \hat{V}, \quad \text{with} \\ \hat{H}_0 &= E_0 + \sum_p f_p^p \left\{\hat{a}_p^\dagger \hat{a}_p\right\} \quad \text{and} \\ \hat{V} &= \frac{1}{4}\sum_{pqrs} \mathrm{V}_{rs}^{pq} \left\{\hat{a}_p^\dagger \hat{a}_q^\dagger \hat{a}_s \hat{a}_r\right\} \end{aligned} \tag{2.49}$$

When not in the Hartree-Fock basis, the interaction piece has the additional off-diagonal Fock term, $\sum_{p\neq q} f_q^p \left\{\hat{a}_p^\dagger \hat{a}_q\right\}$. This means that the reference state is an eigenstate of the zero-order piece of the Hamiltonian,

$$\hat{H}_0|\Phi_0\rangle = \left(E_0 + \sum_i f_i^i \left\{\hat{a}_i^\dagger \hat{a}_i\right\}\right)|\Phi_0\rangle = \left(E_0 + \sum_i \varepsilon_i\right)|\Phi_0\rangle = E_0^{(0)}|\Phi_0\rangle \tag{2.50}$$

.

Using *intermediate normalization*, which sets $\langle\Phi_0|\Psi\rangle = 1$, the Schrödinger equation, Eq. (2.1) for the ground state, becomes,

$$\begin{aligned}\langle\Phi_0|\,(\hat{H}_0 + \hat{V})|\Psi\rangle &= \langle\Phi_0|\hat{H}_0|\Psi\rangle + \langle\Phi_0|\hat{V}|\Psi\rangle = E\langle\Phi|\Psi\rangle \\ &= E^{(0)}\langle\Phi|\Psi\rangle + \langle\Phi_0|\hat{V}|\Psi\rangle = E^{(0)} + \langle\Phi_0|\hat{V}|\Psi\rangle = E.\end{aligned} \tag{2.51}$$

Next, the projection operators $\hat{P}$ and $\hat{Q}$ can be introduced,

$$\hat{P} = |\Phi_0\rangle\langle\Phi_0|, \tag{2.52}$$

$$\hat{Q} = \sum_{n\neq 0} |\Phi_n\rangle\langle\Phi_n| = 1 - |\Phi_0\rangle\langle\Phi_0|. \tag{2.53}$$

The $\hat{P}$ operator isolates the reference-state component of any Slater determinant while the $\hat{Q}$ operator isolates all components *except* the reference-state component out of any Slater determinant. Both these operators are idempotent, which means that $\hat{P}^2 = \hat{P}$ and $\hat{Q}^2 = \hat{Q}$, and because of intermediate normalization, the correlated wave function can be written as $|\Psi\rangle = (\hat{P} + \hat{Q})|\Psi\rangle = |\Phi\rangle + \hat{Q}|\Psi\rangle$. Also, both operators commute with the unperturbed part of the Hamiltonian, $\hat{H}_0\hat{P} = \hat{P}\hat{H}_0$ and $\hat{H}_0\hat{Q} = \hat{Q}\hat{H}_0$. These identities can be applied to an alternate version of the Schrödinger equation which defines a particular version of perturba-

tion theory known as Raleigh-Schrödinger perturbation theory (RSPT). In this version, the zeroth-order energy $E^{(0)}$ is added to both sides of the Schrödinger equation. Acting with $\hat{Q}$ and rearranging terms gives,

$$\begin{aligned}\hat{Q}\,(E^{(0)}-\hat{H}_0)|\Psi\rangle &= \hat{Q}\,(E^{(0)}+\hat{V}-E)|\Psi\rangle \\ \hat{Q}\,(E^{(0)}-\hat{H}_0)\,\hat{Q}|\Psi\rangle &= \hat{Q}\,(\hat{V}-\Delta E_0)|\Psi\rangle,\end{aligned} \tag{2.54}$$

where $\Delta E_0 \equiv E - E^{(0)} = \langle\Phi_0|\hat{V}|\Psi\rangle$. The operator $\hat{Q}\,(E^{(0)}-\hat{H}_0)\,\hat{Q}$ is invertible because $(E^{(0)}-\hat{H}_0)^{-1}$ is never singular in Q-space. Therefore, the operator $\hat{R}_0 = \hat{Q}\,(E^{(0)}-\hat{H}_0)^{-1}\,\hat{Q}$, known as the *resolvant*, can be applied to both sides to result in the generating equation for RSPT,

$$\begin{aligned}\hat{Q}\,(E^{(0)}-\hat{H}_0)^{-1}\,(E^{(0)}-\hat{H}_0)\,\hat{Q}|\Psi\rangle &= \hat{Q}\,(E^{(0)}-\hat{H}_0)^{-1}\,\hat{Q}\,(\hat{V}-\Delta E_0)|\Psi\rangle \\ \hat{Q}|\Psi\rangle &= \hat{R}_0\,(\hat{V}-\Delta E_0)|\Psi\rangle \\ |\Psi\rangle &= |\Phi\rangle + \hat{R}_0\,(\hat{V}-\Delta E_0)|\Psi\rangle\end{aligned} \tag{2.55}$$

This equation can be iterated infinitely to give the solution for the fully correlated wave function which can, in turn, be used to solve for the energy with Eq. (2.51),

$$|\Psi\rangle = \sum_{n=0}^{\infty}\left[\hat{R}_0\,(\hat{V}-\Delta E_0)\right]^n|\Phi_0\rangle, \tag{2.56}$$

$$\Delta E_0 = \langle\Phi_0|\hat{V}|\Psi\rangle = \sum_{n=0}^{\infty}\langle\Phi_0|\hat{V}\left[\hat{R}_0\,(\hat{V}-\Delta E_0)\right]^n|\Phi_0\rangle \tag{2.57}$$

The immediate problem with this equation is that the right-hand side of the equations contain the target energy difference ΔE_0 for which these equations are meant to solve. This

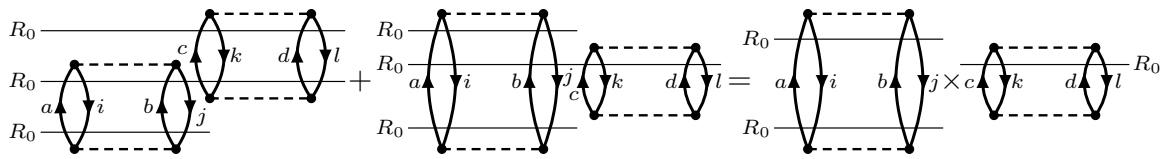
can be remedied by expanding the right-hand sides and rearranging terms. Using the fact that $\hat{R}_0 \Delta E_0 |\Phi_0\rangle = \Delta E_0 \hat{R}_0 |\Phi_0\rangle = 0$, the first-order energy $E^{(1)} = \langle \Phi_0 | \hat{V} | \Phi_0 \rangle$, and the shifted term $\widetilde{V} \equiv \hat{V} - E^{(1)}$, these simplify to,

$$\begin{aligned} |\Psi\rangle - |\Phi_0\rangle &= \hat{R}_0 \hat{V} |\Phi_0\rangle + \hat{R}_0 \widetilde{V} \hat{R}_0 \hat{V} |\Phi_0\rangle \\ &\quad + \hat{R}_0 \widetilde{V} \hat{R}_0 \widetilde{V} \hat{R}_0 \hat{V} |\Phi_0\rangle - \langle \Phi_0 | \hat{V} \hat{R}_0 \hat{V} |\Phi_0\rangle \hat{R}_0^2 \hat{V} |\Phi_0\rangle + \cdots \qquad (2.58) \\ \Delta E_0 &= \langle \Phi_0 | \hat{V} | \Phi_0 \rangle + \langle \Phi_0 | \hat{V} \hat{R}_0 \hat{V} |\Phi_0\rangle + \langle \Phi_0 | \hat{V} \hat{R}_0 \widetilde{V} \hat{R}_0 \hat{V} |\Phi_0\rangle \\ &\quad + \langle \Phi_0 | \hat{V} \hat{R}_0 \widetilde{V} \hat{R}_0 \widetilde{V} \hat{R}_0 \hat{V} |\Phi_0\rangle - \langle \Phi_0 | \hat{V} \hat{R}_0 \hat{V} |\Phi_0\rangle \langle \Phi_0 | \hat{V} \hat{R}_0^2 \hat{V} |\Phi_0\rangle + \cdots \qquad (2.59) \end{aligned}$$

The order of each term can be easily identified by counting the numbers of times that $\hat{V}$ or $\widetilde{V}$ appears. At the third order in the wave function and the fourth order in the energy, *renormalization* terms make their first appearance. These terms contain separated and closed factors in the form of lower-order energy terms, such as $\langle \Phi_0 | \hat{V} \hat{R}_0 \hat{V} |\Phi_0\rangle \equiv E^{(2)}$. Terms that do not contain normalization factors are known as *principle* terms.

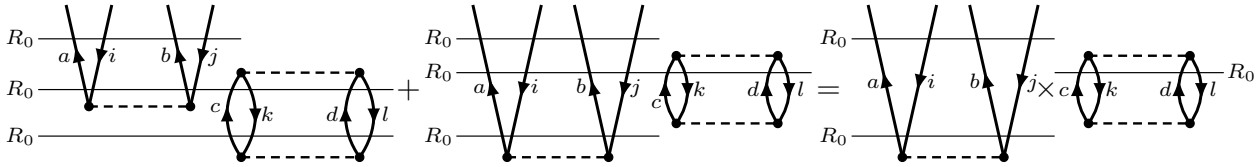
A powerful application of diagrammatic techniques known as the *factorization theorem* [50, 37, 13] can immediately be used to simplify these expansions. By factoring sums of *disconnected* diagrams from the principle terms, where two or more parts of a diagram are not connected with any lines, it can be shown that they exactly cancel with the renormalization

terms at each order.



$$\frac{1}{16}\sum_{\substack{abcd\\ijkl}}\frac{\mathrm{V}_{ab}^{ij}\mathrm{V}_{ij}^{ab}\mathrm{V}_{cd}^{kl}\mathrm{V}_{kl}^{cd}}{\varepsilon_{ij}^{ab}\varepsilon_{ijkl}^{abcd}\varepsilon_{kl}^{cd}}+\frac{1}{16}\sum_{\substack{abcd\\ijkl}}\frac{\mathrm{V}_{ab}^{ij}\mathrm{V}_{ij}^{ab}\mathrm{V}_{cd}^{kl}\mathrm{V}_{kl}^{cd}}{\varepsilon_{ij}^{ab}\varepsilon_{ijkl}^{abcd}\varepsilon_{ij}^{ab}}=\frac{1}{16}\sum_{\substack{abcd\\ijkl}}\mathrm{V}_{ab}^{ij}\mathrm{V}_{ij}^{ab}\mathrm{V}_{cd}^{kl}\mathrm{V}_{kl}^{cd}\frac{\varepsilon_{ij}^{ab}+\varepsilon_{kl}^{cd}}{\left(\varepsilon_{ij}^{ab}\right)^2\varepsilon_{ijkl}^{abcd}\varepsilon_{kl}^{cd}}$$

$$=\frac{1}{4}\sum_{abij}\frac{\mathrm{V}_{ab}^{ij}\mathrm{V}_{ij}^{ab}}{\left(\varepsilon_{ij}^{ab}\right)^2}\cdot\frac{1}{4}\sum_{cdkl}\frac{\mathrm{V}_{cd}^{kl}\mathrm{V}_{kl}^{cd}}{\varepsilon_{kl}^{cd}}=\langle\Psi_n^{(1)}|\Psi_n^{(1)}\rangle E_n^{(2)} \tag{2.60}$$



$$\frac{1}{16}\sum_{\substack{abcd\\ijkl}}\frac{\mathrm{V}_{ij}^{ab}\mathrm{V}_{cd}^{kl}\mathrm{V}_{kl}^{cd}}{\varepsilon_{kl}^{cd}\varepsilon_{ijkl}^{abcd}\varepsilon_{ij}^{ab}}|\Phi_{ij}^{ab}\rangle+\frac{1}{16}\sum_{\substack{abcd\\ijkl}}\frac{\mathrm{V}_{ij}^{ab}\mathrm{V}_{cd}^{kl}\mathrm{V}_{kl}^{cd}}{\varepsilon_{ij}^{ab}\varepsilon_{ijkl}^{abcd}\varepsilon_{ij}^{ab}}|\Phi_{ij}^{ab}\rangle=\frac{1}{16}\sum_{\substack{abcd\\ijkl}}\mathrm{V}_{ij}^{ab}\mathrm{V}_{cd}^{kl}\mathrm{V}_{kl}^{cd}\frac{\varepsilon_{ij}^{ab}+\varepsilon_{kl}^{cd}}{\left(\varepsilon_{ij}^{ab}\right)^2\varepsilon_{ijkl}^{abcd}\varepsilon_{kl}^{cd}}|\Phi_{ij}^{ab}\rangle$$

$$=\frac{1}{4}\sum_{abij}\frac{\mathrm{V}_{ij}^{ab}}{\left(\varepsilon_{ij}^{ab}\right)^2}|\Phi_{ij}^{ab}\rangle\cdot\frac{1}{4}\sum_{cdkl}\frac{\mathrm{V}_{cd}^{kl}\mathrm{V}_{kl}^{cd}}{\varepsilon_{kl}^{cd}}=\frac{|\Psi_n^{(1)}\rangle}{\varepsilon_n}E_n^{(2)} \tag{2.61}$$

The factorization theorem is also valid with off-diagonal Fock terms and applies to the MBPT expansions of both the wave function and energy. Therefore, these can be written in

terms of connected diagrams only,

$$|\Psi\rangle = \sum_{n=0}^{\infty} \left[\hat{R}_0 \left(\hat{V} - \Delta E_0\right)\right]^n |\Phi_0\rangle_{\mathrm{C}}, \tag{2.62}$$

$$\Delta E_0 = \sum_{n=0}^{\infty} \langle\Phi_0| \hat{V} \left[\hat{R}_0 \left(\hat{V} - \Delta E_0\right)\right]^n |\Phi_0\rangle_{\mathrm{C}}, \tag{2.63}$$

where "C" denotes connected diagrams. This result not only simplifies the MBPT expressions, but it guarantees the size-extensivity of the MBPT wave function at each order. Also, it is a useful step towards coupled-cluster theory which reorganizes the connected diagrams from MBPT such that certain classes can be summed to infinite order.

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