INTRODUCTION TO THE SINGLE-REFERENCE MANY-BODY PERTURBATION THEORY AND ITS DIAGRAMMATIC REPRESENTATION

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U.S. DEPARTMENT OF ENERGY | Office of Science

Office of Basic Energy Sciences
Chemical Sciences, Geosciences
& Biosciences Division

MICHIGAN STATE UNIVERSITY

Workshop of the *Espace de Structure et de Réactions Nucléaires Théorique* on “Many-Body Perturbation Theories in Modern Quantum Chemistry and Nuclear Physics”, March 26-30, 2018, CEA Saclay, Gif-sur-Yvette, France

MANY THANKS TO ALEXANDER TICHAI, EMMANUEL GINER, AND THOMAS DUGUET FOR THE INVITATION

MANY-PARTICLE SCHRÖDINGER EQUATION

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QUANTUM CHEMISTRY: THE ELECTRONIC SCHRÖDINGER EQUATION

$$\boxed{H_e \Psi_K(\mathbf{X};\mathbf{R}) = E_K(\mathbf{R}) \Psi_K(\mathbf{X};\mathbf{R})}$$

$$H_e = Z + V = \sum_{i=1}^{N} z(\mathbf{x}_i) + \sum_{i>j=1}^{N} v(\mathbf{x}_i, \mathbf{x}_j)$$

$$z(\mathbf{x}_i) = -\tfrac{1}{2}\Delta_i + \sum_{A=1}^{M} \frac{Z_A}{R_{Ai}}, \qquad v(\mathbf{x}_i, \mathbf{x}_j) = \frac{1}{r_{ij}}$$

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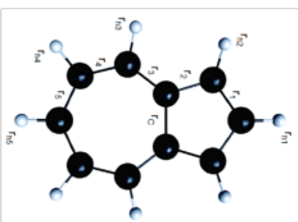

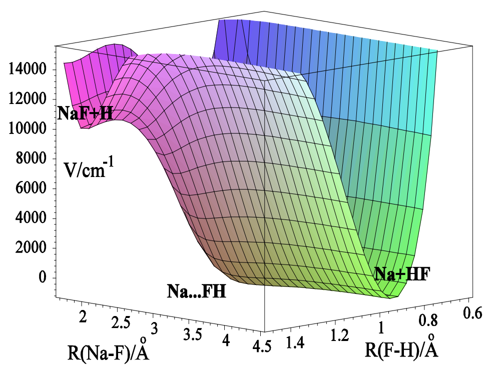

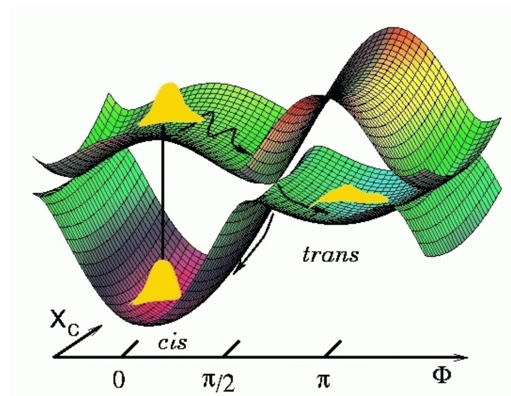

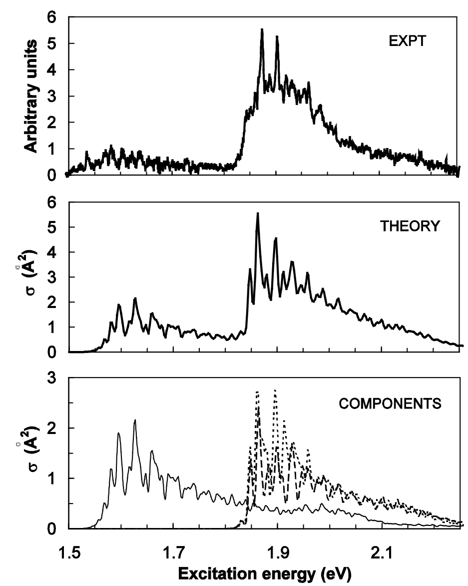

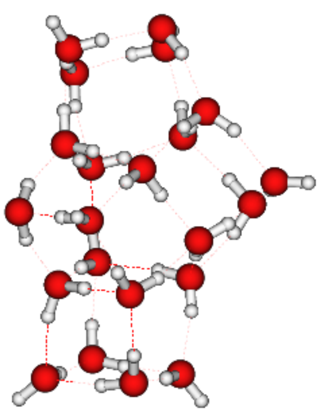

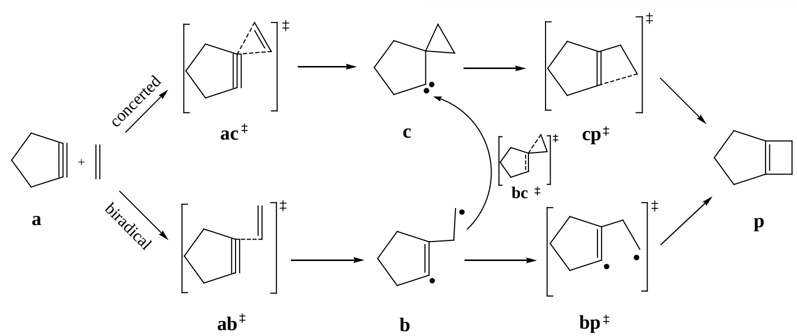

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NUCLEAR PHYSICS: THE NUCLEAR SCHRÖDINGER EQUATION

$$\boxed{H_n \Psi_\mu(\mathbf{X}) = E_\mu \Psi_\mu(\mathbf{X})}$$

$$H_n = Z + V_2 + V_3(+???) = \sum_{i=1}^{N} z(\mathbf{x}_i) + \sum_{i>j=1}^{N} v_2(\mathbf{x}_i, \mathbf{x}_j) + \sum_{i>j>k=1}^{N} v_3(\mathbf{x}_i, \mathbf{x}_j, \mathbf{x}_k)(+???)$$

$$z(\mathbf{x}_i) = \frac{p_i^2}{2m_i}, \qquad \left.\begin{aligned} &v_2(\mathbf{x}_i, \mathbf{x}_j) = ?\ (\text{Argonne } v_{18}, \text{ CD Bonn, Idaho-A, etc.}), \\ &v_3(\mathbf{x}_i, \mathbf{x}_j, \mathbf{x}_k) = ?\ (\text{Tucson-Melbourne, Urbana IX, etc.}) \end{aligned}\right\}$$

or NLO, N^2LO, N^3LO, etc.

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MANY-BODY TECHNIQUES DEVELOPED IN ONE AREA SHOULD BE APPLICABLE TO OTHER AREAS

SOLVING THE MANY-PARTICLE SCHRÖDINGER EQUATION

- Define a basis set of single-particle functions (e.g., LCAO-type molecular spin-orbitals in quantum chemistry obtained by solving mean-field equations or harmonic oscillator basis in nuclear physics)

$$V \equiv \left\{ \varphi_r(\mathbf{x}), r = 1, \ldots, \dim V \right\}$$

Exact case : $\dim V = \infty$,   in practice : $\dim V < \infty$

- Construct all possible Slater determinants that can be formed from these spin-particle states

$$\Phi_{r_1 \ldots r_N}(\mathbf{x}_1, \ldots, \mathbf{x}_N) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \varphi_{r_1}(\mathbf{x}_1) & \cdots & \varphi_{r_1}(\mathbf{x}_N) \\ \vdots & \ddots & \vdots \\ \varphi_{r_N}(\mathbf{x}_1) & \cdots & \varphi_{r_N}(\mathbf{x}_N) \end{vmatrix}$$

SOLVING THE MANY-PARTICLE SCHRÖDINGER EQUATION

- The exact wave function can be written as a linear combination of all Slater determinants

$$\Psi_\mu(\mathbf{x}_1,\ldots,\mathbf{x}_N) = \sum_{r_1<\cdots<r_N} c^\mu_{r_1\ldots r_N}\Phi_{r_1\ldots r_N}(\mathbf{x}_1,\ldots,\mathbf{x}_N)$$

$$= \sum_I c^\mu_I \Phi_I(\mathbf{x}_1,\ldots,\mathbf{x}_N)$$

- Determine the coefficients *c* and the energies E_μ by solving the matrix eigenvalue problem:

$$\mathbf{HC}^\mu = E_\mu \mathbf{C}^\mu$$

where the matrix elements of the Hamiltonian are

$$H_{IJ} = \left\langle \Phi_I \middle| \hat{H} \middle| \Phi_J \right\rangle = \int d\mathbf{x}_1 \ldots d\mathbf{x}_N \Phi^*_I(\mathbf{x}_1,\ldots,\mathbf{x}_N)\hat{H}\Phi_J(\mathbf{x}_1,\ldots,\mathbf{x}_N)$$

- This procedure, referred to as the full configuration interaction approach (FCI), yields the exact solution within a given single-particle basis set

THE PROBLEM WITH FCI

THE PROBLEM WITH FCI

Dimensions of the full CI spaces for many-electron systems

	Number of correlated electrons			
Orbitals	6	8	10	12
20	379×10^3	5.80×10^6	52.6×10^6	300×10^6
30	4.56×10^6	172×10^6	4.04×10^9	62.5×10^9
100	6.73×10^9	3.20×10^{12}	9.94×10^{14}	2.16×10^{17}

Dimensions of the full shell model spaces for nuclei

Nucleus	4 shells	7 shells
^{4}He	4E4	9E6
^{8}B	4E8	5E13
^{12}C	6E11	4E19
^{16}O	3E14	9E24

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- Alternative approaches are needed in order to study the majority of many-body systems of interest

The key to successful description of atoms, molecules, condensed matter systems, and nuclei is an accurate determination of the MANY-PARTICLE CORRELATION EFFECTS. INDEPENDENT-PARTICLE-MODEL APPROXIMATIONS, such as the Hartree-Fock method, ARE USUALLY INADEQUATE

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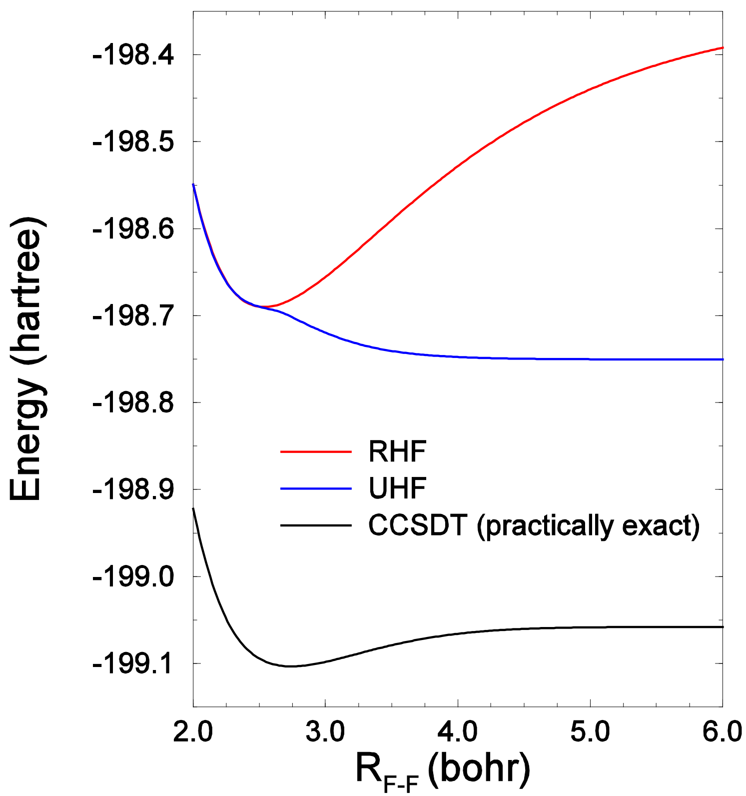
ELECTRONIC STRUCTURE:

Bond breaking in F_2



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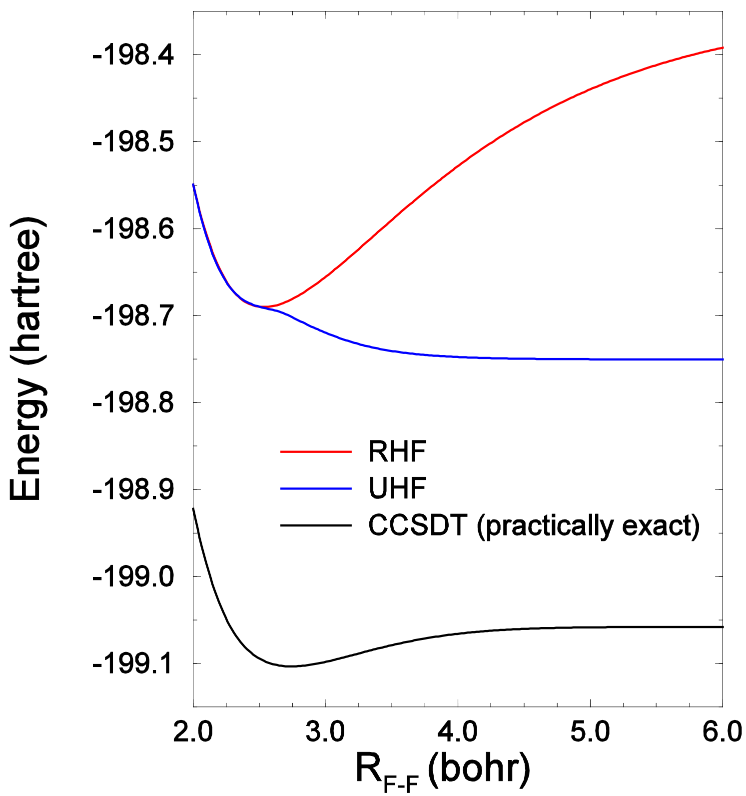


NUCLEAR STRUCTURE:

Binding energy of ^{4}He (4 shells)

Method	Energy (MeV)
$\langle \Phi_{osc} \| H' \| \Phi_{osc} \rangle$	-7.211
$\langle \Phi_{HF} \| H' \| \Phi_{HF} \rangle$	-10.520
CCSD	-21.978
CR-CCSD(T)	-23.524
Full Shell Model (Full CI)	-23.484

DESCRIPTION OF MANY-PARTICLE CORRELATION EFFECTS BY SINGLE-REFERENCE MANY-BODY PERTURBATION THEORY (MBPT)

This is a short course on single-reference MBPT aimed at the following content:

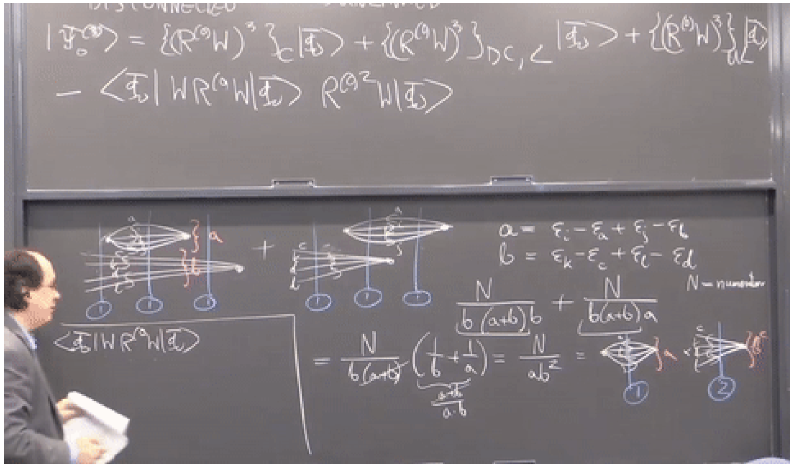
1. Rayleigh-Schrödinger perturbation theory, wave, reaction, and reduced resolvent operators
2. Eigenfunction and eigenvalue expansions, renormalization terms, and bracketing technique
3. Diagrammatic representation, rules for MBPT diagrams
4. MBPT diagrams in low orders (second-, third-, and fourth-order energy corrections; first- and second-order wave function contributions)
5. Linked, unlinked, connected, and disconnected diagrams; diagram cancellations in fourth-order energy and third- and fourth-order wave function corrections
6. Exclusion Principle Violating (EPV) diagrams
7. Factorization Lemma
8. Linked Cluster Theorem
9. Connected-Cluster Theorem

DESCRIPTION OF MANY-PARTICLE CORRELATION EFFECTS BY SINGLE-REFERENCE MANY-BODY PERTURBATION THEORY (MBPT)

This will be a brief course on single-reference MBPT based on the following materials:

1. **Lecture notes that will be provided to you in a PDF format.**

2. The online lecture series entitled "Algebraic and Diagrammatic Methods for Many-Fermion Systems," available at
https://pages.wustl.edu/ppiecuch/course-videos
and on YouTube at
https://www.youtube.com/results?search_query=Chem+580&sp=CAI%253D,
recorded during my visit at Washington University in St. Louis in 2016, consisting of 44 videos (MBPT starts in lecture 28, with introductory remarks at the end of lecture 27).



3. Lecture notes by Professor Josef Paldus, which can be downloaded from www.math.uwaterloo.ca/~paldus/resources.html.

DESCRIPTION OF MANY-PARTICLE CORRELATION EFFECTS BY SINGLE-REFERENCE MANY-BODY PERTURBATION THEORY (MBPT)

Although the use of perturbation theory to analyze the many-electron correlation problem dates back to the seminal 1934 work by Møller and Plesset, the Møller and Plesset work is limited to the second order and does not use second quantization.

OCTOBER 1, 1934 PHYSICAL REVIEW VOLUME 46

Note on an Approximation Treatment for Many-Electron Systems

CHR. MØLLER AND M. S. PLESSET,* *Institut for teoretisk Fysik, Copenhagen*
(Received July 14, 1934)

A perturbation theory is developed for treating a system of n electrons in which the Hartree-Fock solution appears as the zero-order approximation. It is shown by this development that the first order correction for the energy and the charge density of the system is zero. The expression for the second-order correction for the energy greatly simplifies because of the special property of the zero-order solution. It is pointed out that the development of the higher approximation involves only calculations based on a definite one-body problem.

THE Hartree-Fock method[1] for treating a system of n electrons in a given external field consists in making the approximation of assigning to the system a wave function of the determinantal form

$$\Phi^\circ = \frac{1}{(n!)^{\frac{1}{2}}} \begin{vmatrix} \varphi_1(q_1) & \varphi_1(q_2) & \cdots & \varphi_1(q_n) \\ \varphi_2(q_1) & \cdot & \cdots & \cdot \\ \vdots & & & \vdots \\ \varphi_n(q_1) & \cdot & \cdots & \varphi_n(q_n) \end{vmatrix}, \quad (1)$$

where the variables q_i represent space and spin coordinates, and the n functions $\varphi_r(q)$ are a set of orthogonal normalized solutions of the equation

$$i\hbar(\partial/\partial t)\varphi_r(q) = (H_0 + B - A)\varphi_r(q). \quad (2)$$

In (2) H_0 is the Hamiltonian for an electron in the external field, and the matrix elements of B and A in the q-representation are given by[2]

$$(q|B|q') = \int\int (qq''|V|q'q''')dq''dq'''(q'''|\rho|q''), \quad (3)$$

$$(q|A|q') = \int\int (qq''|V|q'''q')dq''dq'''(q'''|\rho|q''), \quad (4)$$

where the matrix of ρ is defined by

$$(q|\rho|q') = \sum_{r=1}^{n} \varphi_r(q)\varphi_r^*(q'), \quad (5)$$

and V is the interaction energy for a pair of electrons.

As follows from the definition (5) the density matrix ρ is Hermitean and obeys the equation $\rho^2 = \rho$; (5) together with (2) give the equation of motion for ρ

$$i\hbar\dot{\rho} = (H_0 + B - A)\rho - \rho(H_0 + B - A). \quad (6)$$

As Dirac has emphasized, all probabilities can be expressed by means of this density matrix ρ;[3] in particular the charge density at q is given by $(q|\rho|q)$.

It is supposed throughout the following that H_0 does not contain the time explicitly. We may then consider solutions of (2) and (6) which belong to a stationary state μ so that our equations become

$$F_\mu\varphi_r^{(\mu)}(q) \equiv (H_0 + B_\mu - A_\mu)\varphi_r^{(\mu)}(q) = \lambda_r^{(\mu)}\varphi_r^{(\mu)}(q); \quad (7)$$

$$F_\mu\rho_\mu - \rho_\mu F_\mu = 0. \quad (8)$$

It is clear that the form of the operator F_μ depends on the stationary state considered. The energy of the system is, in the present approximation, given by

$$W_\mu^\circ = D\{\rho(H_0 + \tfrac{1}{2}B_\mu - \tfrac{1}{2}A_\mu)\}, \quad (9)$$

where D denotes the diagonal sum. The corresponding wave function for a stationary state of the whole system is an eigenfunction of the operator

$$G_\mu = \sum_{i=1}^{n}\{H_0^{(i)} + B_\mu^{(i)} - A_\mu^{(i)}\} = \sum_{i=1}^{n} F_\mu^{(i)}, \quad (10)$$

* National Research Fellow.
[1] V. Fock, Zeits. f. Physik **61**, 126 (1930); P. A. M. Dirac, Proc. Camb. Phil. Soc. **26**, Part III, 376 (1930).
[2] $\int\cdots dq$ is always understood to include summation over the spin coordinate.
[3] Dirac, Proc. Camb. Phil. Soc. **27**, Part II, 240 (1930).

DESCRIPTION OF MANY-PARTICLE CORRELATION EFFECTS BY SINGLE-REFERENCE MANY-BODY PERTURBATION THEORY (MBPT)

They key original papers most relevant to this presentation of MBPT are:

after these corrections and that for compound nucleus contribution a similar discrepancy yet remains, it is in the sense to correspond to a greater reduced width for neutrons (in C^{13}) than for protons (in N^{13}); i.e., "the neutrons stick out further than the protons." Such an effect has been suggested for heavier nuclei, though it would be very surprising to find it holding for so light a nucleus as $A=13$.

An estimate of the course of the cross section for the reaction $C^{12}(d,t)C^{11}$ was made on the basis of compound nucleus formation by assuming, as before, that the whole of the cross section for $C^{12}(d,n)N^{13}$ at low deuteron energies involves compound nucleus formation. On the assumption that the reduced width for triton emission is as great as that for neutron emission (the assumption of "preformed" tritons), we predict the dashed line of Fig. 2—in which the coming into play of successive residual states of C^{11} has been allowed for and the associated irregularities smoothed out. It is seen that even under the very unplausible assumption of the existence of preformed tritons, compound nucleus theory fails by an order of magnitude to explain the observed C^{11} formation. We are forced then to assume that this (d,t) reaction proceeds by some pickup mechanism and that we are indeed measuring the relative probability of the deuteron's losing a nucleon to the nucleus and removing one from it. As yet no sufficiently reliable theory of (d,t) pickup exists to warrant a comparison being made with these results. It is interesting to note that, at $E_d=3.3$ Mev, the angular distribution of the reaction $C^{13}(d,t)C^{12}$ is such as to suggest that a direct mechanism already predominates.[4]

It is interesting to compare these results with those of Cohen and Handley[9] on (p,t) reactions. These authors suggest that triton emission from a compound nucleus state has an inherent probability comparable with that for single nucleon emission. They base this argument on the rather flat angular distributions sometimes obtained which, they remark, tell against a pickup process. However, this conclusion is no longer valid when the energy of one or both the charged particles concerned is of the order of or below the Coulomb barrier; here a direct mechanism can give a sensibly isotropic angular distribution. It appears that considerable interest attaches to the resolution of this question of the mechanism by which tritons and similar complicated particles are emitted from nuclei in events of moderate to high energy.

[9] B. L. Cohen and T. H. Handley, Phys. Rev. **93**, 514 (1954)

PHYSICAL REVIEW VOLUME 100, NUMBER 1 OCTOBER 1, 1955

Many-Body Problem for Strongly Interacting Particles. II. Linked Cluster Expansion*

K. A. Brueckner
Indiana University, Bloomington, Indiana
(Received April 28, 1955)

An approximation method developed previously to deal with many particles in strong interaction is examined in further detail. It is shown that the series giving the interaction energy is a development in a sequence of linked or irreducible cluster terms each of which gives a contribution to the energy proportional to the total number of particles. Consequently the convergence of the expansion is independent of the total number of particles. The origin of this simple feature is illustrated by showing that a similar situation exists in the expansion of standard perturbation theory. The numerical convergence of the expansion is quantitatively discussed for the nuclear problem where it is shown that the correction arising from the first cluster term involving three particles is less than the leading term by a factor of about 10^{-4}. The smallness of the correction is largely a result of the action of the exclusion principle.

I. INTRODUCTION

In a previous paper[1] (to be referred to as I) we have given a method for reducing approximately the many body problem for strongly interacting particles to a problem of self-consistent fields. Some of the physical content and origin of the method were discussed there and the nature of certain correction terms which can be neglected for very many particles was discussed. We shall in this paper examine the structure of another type of correction term which arises from interaction of clusters of particles and in so doing exhibit the general structure of the expansion involved. This will also allow us to draw some general conclusions about the convergence and accuracy of the method.

In Sec. II, we shall briefly summarize the relevant formulas from I and describe some difficulties which appear in high-order terms in the expansion for the energy which can be removed by a simple modification of the many-body propagation function. In Sec. III, we show how similar terms appear to arise in the usual perturbation theory but that they cancel identically, in a manner simply related to the cancellation discussed in Sec. II. In Sec. IV, we summarize these results and show how they may be generalized into a simple pre-

* Supported in part by a grant from the National Science Foundation.

[1] K. A. Brueckner and C. A. Levinson, Phys. Rev. **97**, 1344 (1955).

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* Supported in part
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[1] K. A. Brueckner an
(1955).

Derivation of the Brueckner many-body theory

By J. Goldstone

Trinity College, University of Cambridge‡

(*Communicated by N. F. Mott, F.R.S.—Received* 24 *August* 1956)

An exact formal solution is obtained to the problem of a system of fermions in interaction. This solution is expressed in a form which avoids the problem of unlinked clusters in many-body theory. The technique of Feynman graphs is used to derive the series and to define linked terms. The graphs are those appropriate to a system of many fermions and are used to give a new derivation of the Hartree–Fock and Brueckner methods for this problem.

1. Introduction

The Hartree–Fock approximation for the many-body problem uses a wave function which is a determinant of single-particle wave functions—that is, an independent-particle model. The single-particle states are eigenstates of a particle in a potential V, which is determined from the two-body interaction v by a self-consistent calculation. The Brueckner theory (Brueckner & Levinson 1955; Bethe 1956; Eden 1956) gives an improved method of defining V and shows why the residual effects of v not allowed for by V can be small. In particular, in the nuclear problem the corrections to the energy are small, even though the corrections to the wave function are large. The theory thus gives a reconciliation of the shell model, the strong two-nucleon interactions, and the observed two-body correlations in the nucleus. The smallness of the corrections is due to the operation of the exclusion principle. Bethe (1956) has shown that this same exclusion effect makes even the Hartree–Fock approximation good for quite strong interactions, such as an exponential potential fitted to low-energy nucleon-nucleon scattering.

The first problem on which calculations have been made is that of 'nuclear matter', that is, a very large nucleus with surface effects neglected (Brueckner 1955*a*; Wada & Brueckner 1956). In this problem the aim is to show that at a fixed density the energy is proportional to the number of particles, and that as the density is varied the energy per particle has a minimum at the observed density of large nuclei, and that this minimum value gives the observed volume energy of large nuclei. The single-particle wave functions are plane waves, and the potential V is diagonal in momentum space (in contrast to the ordinary Hartree potential which is diagonal in configuration space). The independent-particle model state is a 'Fermi gas' state with all the one-particle states filled up to the Fermi momentum k_F which depends only on the density.

Brueckner & Levinson's derivation, and that of Eden, is based on the multiple scattering formalism of Watson (Watson 1953). The proportionality of the energy of nuclear matter of a given density to the number of particles follows at once from the theory provided certain terms which represent several interactions occurring

‡ Author's present address: Institut for Teoretisk Fysik, Blegdamevej 17, Copenhagen.

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They key original papers most relevant to this presentation of MBPT are:

The description of collective motions in terms of many-body perturbation theory

By J. Hubbard

Atomic Energy Research Establishment, Harwell, Didcot, Berkshire

(*Communicated by R. E. Peierls, F.R.S.—Received* 2 *February* 1957)

In this and a succeeding paper it is shown how a theory equivalent to the Bohm & Pines collective motion theory of the electron plasma can be derived directly from a perturbation series which gives in principle an exact solution of the many-body problem. This result is attained by making use of a diagrammatic method of analysis of the perturbation series. By a process analogous to the elimination of photon self-energy parts from the electrodynamic S matrix it is found possible to simplify the perturbation series, introducing a modified interaction between the particles. A useful integral equation for this modified interaction can be set up, and it is shown how the energy of the system can be expressed in terms of the modified interaction. The close connexion between this approach and the dielectric theory of plasma oscillations is indicated.

1. Introduction

Within recent years much attention has been given in the study of the quantum mechanical many-body problem to the collective modes of motion which may be present (Bohm & Pines 1953; Tomonaga 1955; Bohr & Mottelson 1953). Two main theories of collective motion have been developed, that of Tomonaga (1955), and the superfluous co-ordinate type of theory introduced by Bohm & Pines (1953). In the Tomonaga theory a transformation of variables is made in such a way that some of the new co-ordinates are directly related to the collective modes of motion, whilst the remaining new co-ordinates are associated with internal modes of motion. In the superfluous co-ordinate treatment certain auxiliary variables are introduced together with an equal number of subsidiary conditions to preserve the correct number of degrees of freedom, and a transformation is made in such a way that the new auxiliary variables are related to the collective motion, whilst the original co-ordinates when transformed are related to the internal motion. If the collective modes being studied have real physical significance, then it will be found in both these methods that the Hamiltonian is, to a good approximation, separable in the new co-ordinates, and a separation of the collective motion is thereby obtained.

Though these methods are quite successful, they have certain unsatisfactory features. In the Tomonaga method it is generally found that when the Hamiltonian has been separated the problem of finding the eigenvalues of the internal motion part is very difficult. In the superfluous co-ordinate treatment one does not meet with this difficulty but with an equivalent one; this is that it is difficult to find eigenfunctions satisfying the subsidiary conditions. In addition, both theories suffer from the difficulty of not being able to treat very easily the interaction between the collective and internal modes of motion, or the intimately related problem of the damping of the collective motion; where the damping is small this is not a very

DESCRIPTION OF MANY-PARTICLE CORRELATION EFFECTS BY SINGLE-REFERENCE MANY-BODY PERTURBATION THEORY (MBPT)

They key original papers most relevant to this presentation of MBPT are:

Hugenholtz, N. M.
1957

Physica XXIII
481–532

PERTURBATION THEORY
OF LARGE QUANTUM SYSTEMS

by N. M. HUGENHOLTZ

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Synopsis

The time-independent perturbation theory of quantum mechanics is studied for the case of very large systems, *i.e.* systems with large spatial dimensions (large volume Ω), and a large number of degrees of freedom. Examples of such systems are met with in the quantum theory of fields, solid state physics, the theory of imperfect gases and in the theory of nuclear matter. Only systems at or near the ground state (*i.e.*, systems at zero temperature) are treated in this paper. In the application of the conventional perturbation theory to such large quantum systems one encounters difficulties which are connected with the fact that even small perturbations produce large changes of the energy and wave function of the whole system. These difficulties manifest themselves through the occurrence of terms containing arbitrarily high powers of the volume Ω in the perturbation expansion of physical quantities. An extremely bad convergence of the perturbation expansion is the result.

For the analysis of the Ω-dependence of the terms in the expansion a new formulation of the time-independent perturbation theory is used, which was introduced by Van Hove. Making extensive use of diagrams to represent the different contributions to matrix elements it is possible to locate and separate the Ω-dependent terms, and to carry out partial summations in the original expansion. These separations and summations solve the above difficulties completely. Improved perturbation theoretical expressions are obtained for energies and wave functions of stationary states, as well as for the life-times of metastable states. All terms in these expressions are, in the limit of large Ω, either independent of Ω or proportional to Ω, corresponding to intensive or extensive physical quantities. The convergence of the improved perturbation expansions is no longer affected by the large magnitude of Ω.

CHAPTER I. INTRODUCTION

1. *The problem.* This paper is devoted to the perturbation theory of large quantum systems *i.e.*, quantum systems which have large spatial dimensions and a large number of degrees of freedom. The systems met with in the quantum theory of fields are, as is well known, of this type. Also in other branches of physics, such as quantum statistics and the Fermi gas model of heavy nuclei, one has to deal with such large systems. We shall in this paper only be interested in systems at or near the ground state. Our results are, therefore, only applicable to quantum systems at zero temperature.

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MANY-BODY BASIS FOR THE OPTICAL MODEL

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Received 1 October 1959

Abstract: A formal expression is derived for an optical model potential based on an assumed two-body interaction between nucleons, which provides an exact description of the elastic scattering of a single nucleon by a closed shell (or closed shell ± 1) nucleus. A second-quantized description is used for the many-fermion system, the true state vector being expanded in terms of a complete set of single-particle model wave functions. Elimination of the variables of all but the scattered nucleon yields a weighting function which satisfies a one-body Schrödinger equation, whose S-matrix elements are identical with those of the true S-matrix between states corresponding to elastic scattering. The effective optical model potential is identified from this Schrödinger equation, and is found, of course, to be complex and non-local. It contains all the effects of the exclusion principle, and is in the form of a linked-cluster perturbation expansion, so that the spurious divergence of Brillouin-Wigner perturbation theory for a large number of nucleons is absent.

1. Introduction

In this paper a derivation of the optical-model potential will be presented starting from the Brueckner-Bethe-Goldstone treatment [1,2,3]) of the nuclear many-body problem. The rigorous equivalence of the optical-model and many-body descriptions of elastic scattering of a nucleon by a nucleus has previously been shown by others [4]). A different approach is adopted here, which results in an explicit prescription for calculating the optical potential by the use of Goldstone diagrams. This prescription involves a linked-cluster (Rayleigh-Schrödinger) expansion similar to that used by Brueckner *et al.* in calculating properties of static nuclei [1]). The exclusion principle is taken fully into account, and it will be seen that one of its effects on the qualitative nature of the optical potential is immediately evident from the formal expression for the potential. Specifically, the optical potential contains a projection operator which makes the optical wave function orthogonal to the occupied states of the nucleus, as described by a suitably chosen independent-particle model. On the basis of this property of the optical potential it has already been suggested that a modification be made in the usual scattering analysis by means of phenomenological optical-model potentials [5]).

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†† Supported by the National Science Foundation.

DESCRIPTION OF MANY-PARTICLE CORRELATION EFFECTS BY SINGLE-REFERENCE MANY-BODY PERTURBATION THEORY (MBPT)

They key original papers most relevant to this presentation of MBPT are:

Formulae for Non-degenerate Rayleigh–Schrödinger Perturbation Theory in any order

By R. Huby

Department of Theoretical Physics, University of Liverpool

MS. received 13*th February* 1961

Abstract. It is shown that Bloch's solution for the nth order perturbation of the energy and the eigenvector in the Rayleigh–Schrödinger perturbation theory of non-degenerate, discrete levels can be expressed in a different form, of a kind suggested by Brueckner, and some advantages of the latter form are presented.

§ 1. Introduction

The many-body problem has stimulated interest in the systematic formulation of the higher order terms in Rayleigh–Schrödinger perturbation theory for discrete energy levels, i.e. the determination of the discrete eigenstates and eigenvalues of a Hamiltonian:

$$H = H_0 + H' \qquad \ldots\ldots(1)$$

(the sum of an unperturbed operator H_0 and a perturbing one H') in the form of series in ascending powers of H'. The case most studied has been that of a system of many particles the interactions between which constitute H', and important perturbation developments appropriate to this particular case have been made (e.g. Goldstone 1957). However, some attention has also been paid to the formulation of the solution to the general problem (1). Bloch (1958) has presented an elegant formulation, which leads to a quite simple expression for the nth order energy or state vector when the problem is 'non-degenerate' (i.e. when we study the shift of a non-degenerate unperturbed energy level). A different prescription for writing down the energy shifts in the first few perturbation orders (again for the non-degenerate problem) had been suggested by Brueckner (1955), but it was not clear how this was to be generalized correctly to any arbitrary order. The purpose of this paper is to show that the prescription of Brueckner for the energy can in fact, with small modifications, be extended up to any arbitrary order; and that it can also be adapted to yield formulae for the state vectors to any order. This is achieved by showing that the formulae proved by Bloch can be expressed alternatively in Brueckner's form.

Brueckner's type of formula has some advantage in the ease with which it can be visualized and applied.

§ 2. Bloch's Formulation

Let us first summarize the relevant results of Bloch (see also Messiah 1960). We consider some unperturbed, discrete eigenvalue of H_0, say E_0, which in the first instance may perhaps be degenerate, its eigenvectors spanning a g-dimensional

DESCRIPTION OF MANY-PARTICLE CORRELATION EFFECTS BY SINGLE-REFERENCE MANY-BODY PERTURBATION THEORY (MBPT)

They key original papers most relevant to this presentation of MBPT are:

- K. A. Brueckner, *Phys. Rev.* **100**, 36 (1955).
- J. Goldstone, *Proc. R. Soc. Lond., Ser A* **239**, 267 (1957).
- J. Hubbard, *Proc. R. Soc. Lond., Ser. A* **240**, 539 (1957).
- N. M. Hugenholtz, *Physica* **23**, 481 (1957).
- L. M. Frantz and R. L. Mills, *Nucl. Phys.* **15**, 16 (1960).
- R. Huby, *Proc. Phys. Soc*. **78**, 529 (1961).

The discussion of the Rayleigh-Schrödinger perturbation theory and reduced resolvents, especially in the video lecture series, is taken from P. O. Löwdin, in Perturbation Theory and Its Applications in Quantum Mechanics, edited by C. H. Wilcox (John Wiley & Sons, New York, 1966), pp. 255-294, and references therein.

KEY THEOREMS OF MBPT

Linked cluster (diagram) theorem (Brueckner, 1955; Goldstone, 1957)

MBPT

$$\begin{aligned}\Psi^{(k)} &= (R_0 W)^k \Phi_0 + \text{renormalization terms} \\ &= \left[(R_0 W)^k\right]_{\text{linked}} \Phi_0\,, \quad (k = 1, 2, \ldots),\end{aligned}$$

$$\begin{aligned}\Delta E^{(k+1)} &= \langle \Phi_0 | W (R_0 W)^k | \Phi_0 \rangle + \text{renormalization terms} \\ &= \langle \Phi_0 | \left[W (R_0 W)^k\right]_{\text{connected}} | \Phi_0 \rangle\,, \quad (k = 1, 2, \ldots).\end{aligned}$$

Connected cluster theorem (Hubbard, 1957; Hugenholtz, 1957)

$$\Psi = e^T \Phi, \quad T = \sum_{k=1}^{\infty} \sum_{C} \{(R_0 W)^k\}_C$$

$$C \Leftrightarrow \text{connected diagrams (including EPV terms)}$$

- **Finite-order MBPT calculations lead to a size extensive description of many-fermion systems, so that no loss of accuracy occurs if the system is made larger.**
- **One can generate the entire infinite-order MBPT series via the exponential wave function ansatz of coupled-cluster theory, which is size extensive and which can be made size consistent if the reference determinant is separable.**

Lecture notes for the introductory talk on the single-reference many-body perturbation theory prepared by Piotr Piecuch for the Workshop of the *Espace de Structure et de Réactions Nucléaires Théorique* on "Many-Body Perturbation Theories in Modern Quantum Chemistry and Nuclear Physics," March 26-30, 2018, CEA Saclay, Gif-sur-Yvette, France.

MANY-BODY PERTURBATION THEORY (SINGLE-REFERENCE CASE).

1. Introductory remarks.

We will use the Rayleigh-Schrödinger perturbation theory (RSPT) for a non-generate ground state to solve the many-particle (many-fermion) Schrödinger equation,

$$H|\Psi_0\rangle = E_0|\Psi_0\rangle, \qquad (1)$$

where the correlated ground state $|\Psi_0\rangle$ can be obtained by perturbing the independent-particle-model (IPM) single-determinantal state $|\Phi_0\rangle$ that will also serve as a Fermi vacuum. We will assume that our Hamiltonian H consists of one- and two-body components, Z and V, respectively, so that

$$H = Z + V, \qquad (2)$$

where

$$Z = \sum_{p,q} \langle p|\hat{z}|q\rangle X_p^{\dagger} X_q \qquad (3)$$

and

$$V = \frac{1}{2}\sum_{pq,rs} \langle pq|\hat{v}|rs\rangle X_p^{\dagger} X_q^{\dagger} X_s X_r \tag{4}$$

$$= \frac{1}{4}\sum_{pq,rs} \langle pq|\hat{v}|rs\rangle_{A} X_p^{\dagger} X_q^{\dagger} X_s X_r ,$$

with

$$\langle pq|\hat{v}|rs\rangle_{A} = \langle pq|\hat{v}|rs\rangle - \langle pq|\hat{v}|sr\rangle \tag{5}$$

representing the antisymmetrized matrix elements. Here, $X_p^{\dagger}$ (X_p) are the creation (annihilation) operators associated with single-particle states (in quantum chemistry, spin-orbitals) $|p\rangle$.

To facilitate our considerations, where it will be assumed that $|\Psi_0\rangle$ is obtained by perturbing the IPM Fermi vacuum state $|\Phi_0\rangle$ ($|\Phi_0\rangle$ could, for example, be a Hartree-Fock determinant, although other choices are certainly possible), we will focus on the Schrödinger equation written as

$$H_N|\Psi_0\rangle = \Delta E_0|\Psi_0\rangle, \tag{6}$$

where

$$H_N = H - \langle\Phi_0|H|\Phi_0\rangle \tag{7}$$

is the Hamiltonian in the normal-ordered form (we will return to this later) and

$$\Delta E_0 = E_0 - \langle \Phi_0 | H | \Phi_0 \rangle . \qquad (8)$$

If $|\Phi_0\rangle$ is a Hartree-Fock state, ΔE_0 is the conventional correlation energy. We will be seeking the solutions of Eq. (6), where we know that the exact $|\Psi_0\rangle$ can be written as

$$|\Psi_0\rangle = |\Phi_0\rangle + \sum_{i,a} c_a^i |\Phi_i^a\rangle + $$
$$+ \sum_{i<j,a<b} c_{ab}^{ij} |\Phi_{ij}^{ab}\rangle + \dots$$
$$= |\Phi_0\rangle + \sum_{n=1}^{N} \sum_{\substack{i_1<\dots<i_n \\ a_1<\dots<a_n}} c_{a_1 \dots a_n}^{i_1 \dots i_n} |\Phi_{i_1 \dots i_n}^{a_1 \dots a_n}\rangle \qquad (9)$$

where

$$|\Phi_i^a\rangle = X_a^\dagger X_i |\Phi_0\rangle \equiv E_i^a |\Phi_0\rangle,$$
$$|\Phi_{ij}^{ab}\rangle = X_a^\dagger X_i X_b^\dagger X_j |\Phi_0\rangle = E_{ij}^{ab} |\Phi_0\rangle,$$
$$\dots \qquad (10)$$
$$|\Phi_{i_1 \dots i_n}^{a_1 \dots a_n}\rangle = \prod_{g=1}^{n} X_{a_g}^\dagger X_{i_g} |\Phi_0\rangle$$
$$= \prod_{g=1}^{n} E_{i_g}^{a_g} |\Phi_0\rangle = E_{i_1 \dots i_n}^{a_1 \dots a_n} |\Phi_0\rangle$$

one-particle–one-hole

are the 1p-1h, 2p-2h, ..., np-nh excited determinants, in the form of a perturbative expansion,

$$|\Psi_0\rangle = |\Psi_0^{(0)}\rangle + |\Psi_0^{(1)}\rangle + |\Psi_0^{(2)}\rangle + \ldots$$
$$= \sum_{n=0}^{\infty} |\Psi_0^{(n)}\rangle , \qquad (11)$$

in which $|\Psi_0^{(0)}\rangle \equiv |\Phi_0\rangle$ and $|\Psi_0^{(n)}\rangle$ with $n \geq 1$ are the corrections to the zeroth-order state $|\Phi_0\rangle$. The corresponding correlation energy (defined as E_0 minus $\langle\Phi_0|H|\Phi_0\rangle$) will be represented as

$$\Delta E_0 \equiv \Delta E_0^{(0)} + \Delta E_0^{(1)} + \Delta E_0^{(2)} + \ldots$$
$$= \sum_{n=0}^{\infty} \Delta E_0^{(n)} , \qquad (12)$$

where, quite obviously and as we will see, $\Delta E_0^{(0)} = 0$ and $\Delta E_0^{(1)} = 0$. We will use the RSPT approach to determine expansions (11) and (12). Before doing this, let us discuss key elements of RSPT for a generic Hermitian eigenvalue problem,

$$K|\Psi_0\rangle = k_0|\Psi_0\rangle \qquad (13)$$

for a non-degenerate state $|\Psi_0\rangle$.

2. Rayleigh-Schrödinger perturbation theory for a nondegenerate eigenvalue problem.

We want to solve

$$K|\Psi_0\rangle = k_0|\Psi_0\rangle . \quad (14)$$

In RSPT, we assume that we can split K into the unperturbed part K_0 and perturbation W,

$$K = K_0 + W, \quad (15)$$

such that we know all eigenvalues $\mathcal{E}_n$ and all eigenstates $|\Phi_n\rangle$ of K_0,

$$K_0|\Phi_n\rangle = \mathcal{E}_n|\Phi_n\rangle, \quad n=0,1,2,\ldots . \quad (16)$$

K_0 is Hermitian, so states $|\Phi_n\rangle$ form an orthonormal basis in the Hilbert space,

$$\langle\Phi_m|\Phi_n\rangle = \delta_{mn} , \quad (17)$$

and $\mathcal{E}_n$'s are real numbers. We seek the solution of Eq. (14) in the form

$$|\Psi_0\rangle = \Omega|\Phi_0\rangle,$$

~~where~~

where Ω is the so-called <u>wave operator</u>, using intermediate normalization,

$$\langle \Phi_0 | \Psi_0 \rangle = \langle \Phi_0 | \Omega | \Phi_0 \rangle = \langle \Phi_0 | \Phi_0 \rangle$$
$$= 1 . \qquad (18)$$

We obtain,

project both sides on $\langle \Phi_0 |$

$$\langle \Phi_0 | \, (K_0 + W) | \Psi_0 \rangle = k_0 | \Psi_0 \rangle ,$$

$$\underbrace{\langle \Phi_0 | K_0}_{\varkappa_0 \langle \Phi_0 |} | \Psi_0 \rangle + \langle \Phi_0 | W | \Psi_0 \rangle = k_0 \langle \Phi_0 | \Psi_0 \rangle = k_0$$

$$k_0 = \varkappa_0 + \langle \Phi_0 | W | \Psi_0 \rangle$$
$$= \varkappa_0 + \langle \Phi_0 | W \Omega | \Phi_0 \rangle$$
$$= \varkappa_0 + \langle \Phi_0 | \tau | \Phi_0 \rangle , \qquad (19)$$

where

$$\tau = P W \Omega ,$$

with

$$P = | \Phi_0 \rangle \langle \Phi_0 | \qquad (20)$$

representing the projection operator on the P-space spanned by $|\Phi_0\rangle$, is the so-called reaction operator.

Ω maps $|\Phi_0\rangle$ onto $|\Psi_0\rangle$, but without knowing how it acts on the remaining basis states $|\Phi_n\rangle$, with $n \geq 1$, it is not uniquely defined. RSPT is one of the infinitely many possibilities of finding Ω. The key quantity for setting up the RSPT series is the

REDUCED RESOLVENT.

To define the reduced resolvent, we decompose the Hilbert space $\mathcal{H}$ into the P space spanned by $|\Phi_0\rangle$, $\mathcal{H}_P$, and the orthogonal complement called the Q space, $\mathcal{H}_Q$, so that

$$\mathcal{H} = \mathcal{H}_P \oplus \mathcal{H}_Q . \qquad (21)$$

The corresponding projection operators are P, Eq. (20), and

$$Q = 1 - P = \sum_{n=1}^{\infty} |\Phi_n\rangle\langle\Phi_n| . \qquad (22)$$

The reduced resolvent of operator K_0, which is parametrized by $\varkappa$, is formally defined as

[$\varkappa$ - real variable]

$$\mathcal{R}_\varkappa(K_0) = Q\left[\alpha P + Q(\varkappa - K_0)Q\right]^{-1} Q , \qquad (23)$$

where $\alpha \neq 0$. It is easy to show that the matrix representation of $\mathcal{R}_\varkappa(K_0)$ in a basis set defined by $|\Phi_n\rangle$, $n = 0, 1, 2, \ldots$, is

$$\begin{array}{rc} \begin{array}{r} P\text{ space} \Rightarrow \\ \\ Q\text{ space} \Rightarrow \end{array} & \left(\begin{array}{c|c} 0 & \underline{\underline{0}} \\ \hline \underline{\underline{0}} & (x\mathbb{1}_Q - QK_0Q)^{-1} \end{array}\right) \\ & \begin{array}{cc} \uparrow P\text{-space} & \uparrow Q\text{-space} \end{array} \end{array}. \quad (24)$$

The spectral representation of $R_x(K_0)$ is

$$R_x(K_0) = \sum_{n=1}^{\infty} \frac{|\Phi_n\rangle\langle\Phi_n|}{x - x_n}. \quad (25)$$

eigenvalues of QKQ

Thus, $R_x(K_0)$ becomes singular for $x = x_1, x_2, \ldots$, but not for $x = x_0$, since x_0 is non-degenerate (by assumption).

Properties of P, Q, and $R_x(K_0)$:

- $P^2 = P$, $P^\dagger = P$, $Q^2 = Q$, $Q^\dagger = Q$, $PQ = QP = 0$.
  (idempotent) (hermitian)
- $R_x(K_0) = R_x(K_0)^\dagger$ (for real x),
- $R_x(K_0)P = PR_x(K_0) = 0$.
- $QR_x(K_0) = R_x(K_0)Q = R_x(K_0)$.

this is why sometimes we write $R_x(K_0) = \frac{Q}{x - K_0}$

- $$Q(x - K_0)\,R_x(K_0) = R_x(K_0)(x - K_0)Q = Q\,. \quad (26)$$

There are other. The last one is particularly important, and we can prove it as follows:

$$Q(x - K_0)\,R_x(K_0) = Q \sum_{n=1}^{\infty} \frac{(x - K_0)|\Phi_n\rangle\langle\Phi_n|}{x - x_n} = Q \sum_{n=1}^{\infty} \frac{\cancel{(x - x_n)}|\Phi_n\rangle\langle\Phi_n|}{\cancel{x - x_n}} = Q \cdot Q = Q\,. \quad (27)$$

Equipped with the above definitions, we define the reduced resolvent of K_0 at $x = x_0$, which I will call the unperturbed reduced resolvent,

$$R^{(0)} \equiv R_{x=x_0}(K_0) = Q\left[\alpha P + Q(x_0 - K_0)Q\right]^{-1} Q = \sum_{n=1}^{\infty} \frac{|\Phi_n\rangle\langle\Phi_n|}{x_0 - x_n}\,. \quad (28)$$

We can use it to develop the RSPT series in the following few steps:

(i) We know that

$$|\Psi_0\rangle = (P + Q)|\Psi_0\rangle = |\Phi_0\rangle\underbrace{\langle\Phi_0|\Psi_0\rangle}_{=1} + Q|\Psi_0\rangle = |\Phi_0\rangle + Q|\Psi_0\rangle\,. \quad (29)$$

We consider the following expression:

$$(x_0 - K_0)\,\underline{Q|\Psi_0\rangle} = Q(x_0 - K_0)|\Psi_0\rangle$$
$$= Q(x_0 - K + W)|\Psi_0\rangle$$
$$= Q(x_0 - K_0 + W)|\Psi_0\rangle, \qquad (30)$$

where we used the fact that $[Q, K_0] = 0$ (obvious). Let us define

$$W' = W - (K_0 - x_0). \qquad (31)$$

We obtain,

$$(x_0 - K_0)\,\underline{Q|\Psi_0\rangle} = Q W'|\Psi_0\rangle. \qquad (32)$$

(ii) We know that (see Eq. (26))

$$Q(x_0 - K_0)R^{(0)} = R^{(0)}(x_0 - K_0)Q$$
$$= Q. \qquad (33)$$

Thus, from Eqs. (32) and (33), we obtain,

$$\underbrace{R^{(0)}(x_0 - K_0)Q}_{\text{Eq.(33)} \to Q}|\Psi_0\rangle = \underbrace{R^{(0)}Q}_{\text{see p.8 (bottom)} \to R^{(0)}} W'|\Psi_0\rangle, \qquad (34)$$

$$Q|\Psi_0\rangle = R^{(0)}W'|\Psi_0\rangle, \quad (35)$$

$$|\Psi_0\rangle = |\Phi_0\rangle + Q|\Psi_0\rangle$$
$$= |\Phi_0\rangle + R^{(0)}W'|\Psi_0\rangle. \quad (36)$$

(iii) Iterating the last relationship, we obtain,

$$|\Psi_0\rangle = |\Phi_0\rangle + R^{(0)}W'\left(|\Phi_0\rangle + R^{(0)}W'|\Psi_0\rangle\right)$$
$$= |\Phi_0\rangle + (R^{(0)}W')|\Phi_0\rangle + (R^{(0)}W')^2|\Psi_0\rangle$$
$$= \ldots = \sum_{n=0}^{\infty} (R^{(0)}W')^n|\Phi_0\rangle. \quad (37)$$

Thus,
$$|\Psi_0\rangle = \sum_{n=0}^{\infty} (R^{(0)}W')^n|\Phi_0\rangle, \quad (38)$$

where W' is given by Eq. (31).

Using Eq. (19), we obtain

$$k_0 = \varepsilon_0 + \langle\Phi_0|W|\Psi_0\rangle = \varepsilon_0 + \sum_{n=0}^{\infty} \langle\Phi_0|W(R^{(0)}W')^n|\Phi_0\rangle. \quad (39)$$

We can make further slight simplifications,

$$|\Psi_0\rangle = \sum_{n=0}^{\infty} (R^{(0)}W')^n |\Phi_0\rangle$$

$$= |\Phi_0\rangle + \sum_{n=1}^{\infty} (R^{(0)}W')^n |\Phi_0\rangle$$

$$= |\Phi_0\rangle + \sum_{n=0}^{\infty} (R^{(0)}W')^n (R^{(0)}W')|\Phi_0\rangle$$

$$= |\Phi_0\rangle + \sum_{n=0}^{\infty} (R^{(0)}W')^n (R^{(0)}W)|\Phi_0\rangle, \quad (40)$$

since

$$R^{(0)}W'|\Phi_0\rangle = R^{(0)}W|\Phi_0\rangle + R^{(0)}(\mathcal{E}_0 - k_0)|\Phi_0\rangle$$

$$= R^{(0)}W|\Phi_0\rangle \quad (41)$$

$(R^{(0)}|\Phi_0\rangle = R^{0}P|\Phi_0\rangle = 0)$.

Similarly, and using Eqs. (19) and (40),

$$k_0 = \mathcal{E}_0 + \langle\Phi_0|W|\Psi_0\rangle = \mathcal{E}_0 + \langle\Phi_0|W|\Phi_0\rangle + \sum_{n=0}^{\infty} \langle\Phi_0|W(R^{0}W')^n R^{0}W|\Phi_0\rangle. \quad (42).$$

Summary:

$$|\Psi_0\rangle = |\Phi_0\rangle + \sum_{n=0}^{\infty} (R^{(0)}W')^n R^{(0)} W |\Phi_0\rangle \tag{43a}$$

$$k_0 = \varepsilon_0 + \langle\Phi_0|W|\Phi_0\rangle + \sum_{n=0}^{\infty} \langle\Phi_0|W(R^{(0)}W')^n R^{(0)}W|\Phi_0\rangle \tag{43b}$$

or, using the wave and reaction operators,

$$|\Psi_0\rangle = \Omega|\Phi_0\rangle, \tag{44}$$

where

$$\Omega = P + \sum_{n=0}^{\infty} (R^{(0)}W')^n R^{(0)} W P, \tag{45}$$

and

$$k_0 = \varepsilon_0 + \langle\Phi_0|\tau|\Phi_0\rangle, \tag{46}$$

where

$$\tau = PW\Omega = PWP + \sum_{n=0}^{\infty} P(R^{(0)}W')^n R^{(0)} W P, \tag{47}$$

with

$$W' = W - (k_0 - \varepsilon_0).$$

Ω used in the above equations is an example of Bloch wave operator, which satisfies

$$\Omega P = \Omega, \quad P\Omega = P, \quad \Omega^2 = \Omega, \tag{48}$$

(or $\Omega Q = \Omega(1-P) = 0$)

Ω is idempotent

The property $P\Omega = P$ is an intermediate normalization condition, since

$$\langle\Phi_0|\Psi_0\rangle = \langle\Phi_0|\Omega|\Phi_0\rangle = \underbrace{\langle\Phi_0|P}_{\langle\Phi_0|}\Omega|\Phi_0\rangle$$

$$\overset{(48)}{\underset{P\Omega=P}{=}} \langle\Phi_0|P|\Phi_0\rangle = \langle\Phi_0|\Phi_0\rangle = 1. \tag{49}$$

Because of $\Omega^2 = \Omega$, Ω is sometimes called the non-orthogonal projector and we obtain this property as

$$\Omega^2 = (\Omega P)(\Omega P) = \Omega(P\Omega)P = \Omega P^2 = \Omega P$$
$$= \Omega \quad (\text{non-orthogonal, since } \Omega \neq \Omega^\dagger). \tag{50}$$

target space

model or reference space

$$\begin{tikzcd} \mathcal{M}_0 \arrow[r, bend left, "\Omega"] & \mathcal{M} \arrow[l, bend left, "P"] \end{tikzcd}$$

$\Omega|\Phi_0\rangle = |\Psi_0\rangle$

$P|\Psi_0\rangle = |\Phi_0\rangle$

$\Omega|_{\mathcal{M}_0} = (P|_{\mathcal{M}})^{-1}$

$\Omega|_{\mathcal{M}_0^\perp} = 0$

($\Omega Q = 0$)

$\mathcal{M}_0 = \mathrm{Span}\{|\Phi_0\rangle\}$ $\quad$ $\mathcal{M} = \mathrm{Span}\{|\Psi_0\rangle\}$

When $\mathcal{M}_0$ is multi-dimensional, we obtain multireference theories, such as MR MBPT. In that case, $\mathcal{M} = \mathrm{Span}\{|\Psi_\mu\rangle\}_{\mu=1}^{M}$.

In RSPT we define PT orders according to powers of W (zeroth-order: W^0, 1st order: W^1, second order: W^2, etc.). As a result,

$$|\Psi_0\rangle = \sum_{n=0}^{\infty} |\Psi_0^{(n)}\rangle,$$

$$k_0 = \sum_{n=0}^{\infty} k_0^{(n)}, \qquad (51)$$

$$\Omega = \sum_{n=0}^{\infty} \Omega^{(n)},$$

$$\tau = \sum_{n=0}^{\infty} \tau^{(n)} = \sum_{n=1}^{\infty} \tau^{(n)}, \text{ since}$$

$$\tau^{(n+1)} = PW\Omega^{(n)} \quad (\tau^{(0)} = 0).$$

In generating the above expansions, we must keep in mind that

[W' contain 1st and higher-order terms]

$$W' = W - (k_0 - \varepsilon_0) = W - \sum_{m=1}^{\infty} k_0^{(m)},$$

since $k_0^{(0)} = \varepsilon_0$. [THIS IS WHY WE HAVE RENORMALIZATION TERMS IN RSPT] (52)

Using Eqs. (43) - (47) and Eq. (52), we obtain:

<u>0th order:</u> $|\Psi_0^{(0)}\rangle = |\Phi_0\rangle \quad (\Omega^{(0)} = P),$

as anticipated $\quad k_0^{(0)} = \varepsilon_0 \quad (\tau^{(0)} = 0).$ (53)

1st order: $$|\Psi_0^{(1)}\rangle = R^{(0)}W|\Phi_0\rangle \quad (\Omega^{(1)} = R^{(0)}WP),$$
$$k_0^{(1)} = \langle\Phi_0|W|\Phi_0\rangle \quad (\tau^{(1)} = PWP). \tag{54}$$

2nd order:
$$\begin{aligned}
|\Psi_0^{(2)}\rangle &= \overbrace{R^{(0)}(W-k_0^{(1)})}^{\text{from } n=1 \text{ in (43a)}} R^{(0)}W|\Phi_0\rangle \\
&= (R^{(0)}W)^2|\Phi_0\rangle - k_0^{(1)} R^{(0)^2} W|\Phi_0\rangle \\
&= (R^{(0)}W)^2|\Phi_0\rangle - \langle\Phi_0|W|\Phi_0\rangle R^{(0)^2} W|\Phi_0\rangle,
\end{aligned} \tag{55}$$
$$k_0^{(2)} = \langle\Phi_0|W R^{(0)} W|\Phi_0\rangle. \quad \text{(from } n=0 \text{ in (43b))}$$

3rd order:
$$\begin{aligned}
|\Psi_0^{(3)}\rangle &= \Big[\overbrace{R^{(0)}(W-k_0^{(1)})}^{\text{from } n=2 \text{ in (43a)}}\Big]^2 R^{(0)}W|\Phi_0\rangle \\
&\quad - k_0^{(2)} R^{(0)^2} W|\Phi_0\rangle \quad \left(\text{from } n=1 \text{ in (43a)}, \; k_0^{(2)} \text{ from } W'\right) \\
&= (R^{(0)}W)^3|\Phi_0\rangle - \langle\Phi_0|W|\Phi_0\rangle \\
&\quad \times \left(R^{(0)^2} W R^{(0)} W|\Phi_0\rangle + R^{(0)} W R^{(0)^2} W|\Phi_0\rangle \right) \\
&\quad + \langle\Phi_0|W|\Phi_0\rangle^2 R^{(0)^3} W|\Phi_0\rangle \\
&\quad - \langle\Phi_0|W R^{(0)} W|\Phi_0\rangle R^{(0)^2} W|\Phi_0\rangle,
\end{aligned} \tag{56}$$

 from n=1 in (43b)

$$k_0^{(3)} = \langle \Phi_0 | W\, R^{(0)}(W - k_0^{(1)})\, R^{(0)} W | \Phi_0 \rangle$$
$$= \langle \Phi_0 | W (R^{(0)} W)^2 | \Phi_0 \rangle$$
$$- \langle \Phi_0 | W | \Phi_0 \rangle \langle \Phi_0 | W R^{(0)2} W | \Phi_0 \rangle,$$

etc. We should note that

$$k_0^{(n+1)} = \langle \Phi_0 | \tau^{(n+1)} | \Phi_0 \rangle$$
$$= \langle \Phi_0 | P W \Omega^{(n)} | \Phi_0 \rangle$$
$$= \langle \Phi_0 | W | \Psi_0^{(n)} \rangle, \quad (57)$$

since $\Omega^{(n)} | \Phi_0 \rangle = | \Psi_0^{(n)} \rangle$. Thus, we obtain $k_0^{(n+1)}$ by attaching $\langle \Phi_0 | W$ to $| \Psi_0^{(n)} \rangle$.

For example,

$$k_0^{(4)} = \langle \Phi_0 | W | \Psi_0^{(3)} \rangle = \langle \Phi_0 | W (R^{(0)} W)^3 | \Phi_0 \rangle$$
$$- \langle \Phi_0 | W | \Phi_0 \rangle \Big(\langle \Phi_0 | W R^{(0)2} W R^{(0)} W | \Phi_0 \rangle$$
$$+ \langle \Phi_0 | W R^{(0)} W R^{(0)2} W | \Phi_0 \rangle \Big)$$
$$+ \langle \Phi_0 | W | \Phi_0 \rangle^2 \langle \Phi_0 | W R^{(0)3} W | \Phi_0 \rangle$$
$$- \langle \Phi_0 | W R^{(0)} W | \Phi_0 \rangle \langle \Phi_0 | W R^{(0)2} W | \Phi_0 \rangle . \quad (58)$$

It is easy to show that the above equations combined with the spectral representation of $R^{(0)}$ give the well-known RSPT corrections, for example,

$$|\Psi_0^{(1)}\rangle = \sum_{n=1}^{\infty} \frac{|\Phi_n\rangle\langle\Phi_n|}{\mathcal{E}_0-\mathcal{E}_n} W|\Phi_0\rangle$$

$$= \sum_{n=1}^{\infty} \frac{\langle\Phi_n|W|\Phi_0\rangle}{\mathcal{E}_0-\mathcal{E}_n} |\Phi_n\rangle, \qquad (59)$$

$$K_0^{(2)} = \langle\Phi_0|W\sum_{n=1}^{\infty} \frac{|\Phi_n\rangle\langle\Phi_n|}{\mathcal{E}_0-\mathcal{E}_n} W|\Phi_0\rangle$$

$$= \sum_{n=1}^{\infty} \frac{\langle\Phi_0|W|\Phi_n\rangle\langle\Phi_n|W|\Phi_0\rangle}{\mathcal{E}_0-\mathcal{E}_n}, \text{ etc.} \qquad (60)$$

In general,

$$|\Psi_0^{(n)}\rangle = \underbrace{(R^{(0)}W)^n|\Phi_0\rangle}_{\text{principal term}} + \text{renormalization terms}$$

$$K_0^{(n+1)} = \overbrace{\langle\Phi_0|W(R^{(0)}W)^n|\Phi_0\rangle}^{\text{principal term}} + \text{renormalization terms.} \qquad (61)$$

One can generate the renormalization terms using the Brueckner-Huby bracketing technique.

The idea is to insert non-straddling bracket pairs $\langle \dots \rangle$ representing $\langle \varphi_0 | \dots | \varphi_0 \rangle$ into the principal term and doing it such that the following rules are satisfied:

- no two brackets can touch
- bracketing operation including the rightmost and, in the case of eigenvalue corrections, the leftmost W are not allowed,
- each bracket must have W on each side (as in $\langle W \dots W \rangle$)

We assign the sign $(-1)^r$ to a term with r inserted bracket pairs.

Examples:

- $$k_0^{(3)} = \langle W (R^{(0)} W)^2 \rangle + \text{renorm. terms}$$

Principal term:

$$\langle W R^{(0)} W R^{(0)} W \rangle .$$

Renormalization terms (term, only one here):

$$\langle W R^{(0)} \langle W \rangle R^{(0)} W \rangle$$

$$= \langle W \rangle \langle W R^{(0)2} W \rangle . \quad \text{Sign } (-1)^1 = -1 .$$
$(r=1)$

$$k_0^{(3)} = \langle W (R^{(0)} W)^2 \rangle - \langle W \rangle \langle W R^{(0)2} W \rangle .$$

- $k_0^{(4)} = \langle W (R^{(0)} W)^3 \rangle$ + renorm. terms.

Principal term:

$$\langle W R^{(0)} W R^{(0)} W R^{(0)} W \rangle .$$

Renormalization terms:

$$\langle W R^{(0)} \langle W \rangle R^{(0)} W R^{(0)} W \rangle \qquad (r=1)$$

$$\langle W R^{(0)} W R^{(0)} \langle W \rangle R^{(0)} W \rangle \qquad (r=1)$$

$$\langle W R^{(0)} \langle W \rangle R^{(0)} \langle W \rangle R^{(0)} W \rangle \qquad (r=2)$$

$$\langle W R^{(0)} \langle W R^{(0)} W \rangle R^{(0)} W \rangle \qquad (r=1)$$

$$\begin{aligned}
k_0^{(4)} = {} & \langle W (R^{(0)} W)^3 \rangle \\
& - \langle W \rangle \langle W R^{(0)2} W R^{(0)} W \rangle \\
& - \langle W \rangle \langle W R^{(0)} W R^{(0)2} W \rangle \\
& + \langle W \rangle^2 \langle W R^{(0)3} W \rangle \\
& - \langle W R^{(0)} W \rangle \langle W R^{(0)2} W \rangle .
\end{aligned}$$

- $$|\Psi_0^{(2)}\rangle = (R^{(0)}W)^2|\Phi_0\rangle + \text{renorm. terms}$$

$$= R^{(0)}WR^{(0)}W|\Phi_0\rangle$$
$$- R^{(0)}\langle W\rangle R^{(0)}W|\Phi_0\rangle$$
$$= (R^{(0)}W)^2|\Phi_0\rangle - \langle W\rangle R^{(0)2}W|\Phi_0\rangle,$$

etc.

Back to MBPT.

3. Unperturbed and perturbed operators in MBPT.

We are interested in using RSPT to solve

$$K|\Psi_0\rangle = k_0|\Psi_0\rangle, \quad (62)$$

where

$$K = H_N = H - \langle\Phi_0|H|\Phi_0\rangle$$

$$(63)$$

and

$$k_0 = \Delta E_0 = E_0 - \langle\Phi_0|H|\Phi_0\rangle.$$

$|\Phi_0\rangle$ is the normalized IPM state defining the Fermi vacuum. Let us reorder the single-particle states such that the first N of them correspond to states occupied in $|\Phi_0\rangle$ (hole states) and single-particle states $N+1, N+2, \ldots$ are unoccupied (particle states). We will also use the standard notation for single-particle states:

- $i, j, \ldots$ – hole states (occupied in $|\Phi_0\rangle$)
- $a, b, \ldots$ – particle states (unoccupied in $|\Phi_0\rangle$)
- $p, q, \ldots$ – generic states (occupied or unoccupied)

Thus,

$$i = 1, 2, 3, \ldots, N,$$

where N is the number of fermions in the system, and

$$a = N+1, N+2, \ldots .$$

With this notation,

$$|\Phi_0\rangle = X_1^\dagger \ldots X_N^\dagger |0\rangle = \prod_{i=1}^{N} X_i^\dagger |0\rangle,$$

where $|0\rangle$ is the true vacuum state.

3.1. Unperturbed problem.

We must define K_0 and a single-particle basis such that

$$|\Phi_0\rangle = \prod_{i=1}^{N} X_i^{\dagger}|0\rangle \qquad (64)$$

is an eigenstate of K_0. To do this, we recall that

[we could, in principle, use Z as an unperturbed operator, but then V is usually too big to obtain convergence of RSPT]

$$H = Z + V. \qquad (65)$$

Let us approximate the two-body part of H by a one-body operator U and define

$$H_0 = Z + U, \qquad (66)$$

where

$$U = \sum_{pq} \langle p|\hat{u}|q\rangle X_p^{\dagger} X_q$$ (in 1st quantization, $U = \sum_{i=1}^{N} \hat{u}(x_i)$).

↑ coordinates of fermion i

We obtain

$$H_0 = \sum_{pq} \langle p|\hat{z}+\hat{u}|q\rangle X_p^{\dagger} X_q. \qquad (67)$$

Let us further assume that $\hat{u}$ is chosen such that we know how to solve the one-particle eigenvalue (or pseudoeigenvalue if $\hat{u} = \hat{g} = \hat{f} - \hat{z}$, where $\hat{f}$ is a Fock operator) problem,

$$(\hat{z} + \hat{u})|p\rangle = \varepsilon_p |p\rangle . \qquad (68)$$

With this choice of single-particle basis, we can write

$$H_0 = \sum_p \varepsilon_p X_p^\dagger X_p . \qquad (69)$$

It is easy to show that any Slater determinant

$$|\Phi_{q_1 \cdots q_N}\rangle \equiv |\{q_1 \cdots q_N\}\rangle \qquad (70)$$
$$= X_{q_1}^\dagger \cdots X_{q_N}^\dagger |0\rangle$$

is an eigenstate of H_0 with an eigenvalue $\varepsilon_{q_1} + \dots + \varepsilon_{q_N}$. For example, in 1st quantization,

antisymmetrizer $\frac{1}{\sqrt{N!}} \sum_{P \in S_N} (-1)^P P$

$$H_0 |\Phi_{q_1 \cdots q_N}\rangle = \sum_{i=1}^{N} [\hat{z}(x_i) + \hat{u}(x_i)] \mathcal{A} \Big(\prod_{r=1}^{N} \varphi_{q_r}(x_r) \Big)$$

$\langle x_r | q_r \rangle$

$$\overset{[\mathcal{A}, H_0] = 0}{=} \mathcal{A} \sum_{i=1}^{N} \underbrace{[\hat{z}(x_i) + \hat{u}(x_i)] \varphi_{q_i}(x_i)}_{\varepsilon_{q_i} \varphi_{q_i}(x_i)}$$
$$\times \varphi_{q_1}(x_1) \cdots \varphi_{q_{i-1}}(x_{i-1}) \varphi_{q_{i+1}}(x_{i+1}) \cdots \varphi_{q_N}(x_N)$$

$$= \left(\sum_{i=1}^{N} \varepsilon_{q_i}\right) \mathcal{A}\left(\prod_{r=1}^{N} \chi_{q_r}(x_r)\right)$$

$$= \left(\sum_{i=1}^{N} \varepsilon_{q_i}\right) |\Phi_{q_1 \cdots q_N}\rangle . \qquad (71).$$

In particular,

$$H_0|\Phi_0\rangle = E_0^{(0)}|\Phi_0\rangle,$$

where

$$E_0^{(0)} = \sum_{i=1}^{N} \varepsilon_i . \qquad (72)$$

Let us then look at the remaining Slater determinants organized as particle-hole excitations from $|\Phi_0\rangle$. For example,

(i->a)

$$H_0|\Phi_i^a\rangle = (\varepsilon_1 + \dots + \varepsilon_{i-1} + \varepsilon_a + \varepsilon_{i+1} + \dots + \varepsilon_N)|\Phi_i^a\rangle$$

$$= [(\varepsilon_a - \varepsilon_i) + (\varepsilon_1 + \dots + \varepsilon_{i-1} + \varepsilon_i + \varepsilon_{i+1} + \dots + \varepsilon_N)]|\Phi_i^a\rangle$$

$$= [(\varepsilon_a - \varepsilon_i) + E_0^{(0)}]|\Phi_i^a\rangle . \qquad (73)$$

Similarly,

$$H_0|\Phi_{ij}^{ab}\rangle = [(\varepsilon_a - \varepsilon_i + \varepsilon_b - \varepsilon_j) + E_0^{(0)}]|\Phi_{ij}^{ab}\rangle, \quad (74)$$

$$H_0 | \Phi^{a_1 \dots a_n}_{i_1 \dots i_n} \rangle = \left[\sum_{g=1}^{n} (\varepsilon_{a_g} - \varepsilon_{i_g}) + E_0^{(0)} \right] | \Phi^{a_1 \dots a_n}_{i_1 \dots i_n} \rangle \quad (75)$$

Keeping the above in mind, we define the unperturbed operator K_0 used in MBPT as

$$K_0 = H_0 - \langle \Phi_0 | H_0 | \Phi_0 \rangle$$
$$= H_0 - E_0^{(0)}, \quad (76)$$

where $E^{(0)}$ is given by Eq. (72).

We obtain,

$$K_0 | \Phi_0 \rangle = 0 = x_0 | \Phi_0 \rangle,$$
$$K_0 | \Phi_i^a \rangle = x_i^a | \Phi_i^a \rangle, \quad (77)$$
$$\dots$$
$$K_0 | \Phi^{a_1 \dots a_n}_{i_1 \dots i_n} \rangle = x^{a_1 \dots a_n}_{i_1 \dots i_n} | \Phi^{a_1 \dots a_n}_{i_1 \dots i_n} \rangle, \ (n=1,\dots,N)$$

where

$$x_0 = 0,$$
$$x_i^a = \varepsilon_a - \varepsilon_i, \quad (78)$$
$$\dots$$
$$x^{a_1 \dots a_n}_{i_1 \dots i_n} = \sum_{g=1}^{n} (\varepsilon_{a_g} - \varepsilon_{i_g}), \ n=1,\dots,N.$$

Determinants $|\Phi_0\rangle$, $|\Phi_i^a\rangle$, ... form our unperturbed states $|\Phi_n\rangle$ and $\mathcal{E}_0$, $\mathcal{E}_i^a$, ... form the corresponding unperturbed eigenvalues $\mathcal{E}_n$.

The many-body structure of K_0 is

$$K_0 = Z + U - \langle \Phi_0 | Z + U | \Phi_0 \rangle$$
$$= Z_N + U_N \text{, where} \quad (79)$$

$$Z_N = \sum_{p,q} \langle p | \hat{z} | q \rangle N[X_p^\dagger X_q] \quad (80)$$

and

$$U_N = \sum_{p,q} \langle p | \hat{u} | q \rangle N[X_p^\dagger X_q] \quad (81)$$

are the normal-ordered forms of Z and U, respectively. We can also write

$$K_0 = \sum_p \varepsilon_p N[X_p^\dagger X_p]. \quad (82)$$

We recall that $N[\ldots]$ means: move the particle-hole creation operators $(X_a^\dagger, X_i)$ to the left with respect to the corresponding (p-h) p-h annihilation operators $(X_a, X_i^\dagger)$ and multiply by the sign of the corresponding permutation needed for operator rearrangement.

$Z = Z_N + \langle \Phi_0 | Z | \Phi_0 \rangle$, since, using Wick's theorem,

$$Z = \sum_{pq} \langle p | \hat{z} | q \rangle X_p^\dagger X_q$$
$$= \sum_{pq} \langle p | \hat{z} | q \rangle N[X_p^\dagger X_q] \qquad (83)$$
$$+ \sum_{pq} \langle p | \hat{z} | q \rangle N[\overbrace{X_p^\dagger X_q}]$$
$$= Z_N + \sum_{pq} \langle p | \hat{z} | q \rangle \, \alpha(p) \, \delta_{pq} \,,$$

where

$$\alpha(p) = 1 \text{ if } \underset{\text{(occupied } p\text{)}}{p = i} \text{ and } 0 \text{ if } \underset{\text{(unoccupied } p\text{)}}{p = a}.$$

This gives,

$$Z = Z_N + \sum_i \langle i | \hat{z} | i \rangle = Z_N + \langle \Phi_0 | Z | \Phi_0 \rangle \qquad (84)$$

Similarly for U_N (and any one-body operator).

3.2. Perturbation

We want to write $K = H_N$ as

$$K = K_0 + W.$$

Then,

$$W = K - K_0 = \left(H - \langle \Phi_0 | H | \Phi_0 \rangle\right)$$
$$- \left(H_0 - \langle \Phi_0 | H_0 | \Phi_0 \rangle\right)$$
$$= (H - H_0) - \langle \Phi_0 | H - H_0 | \Phi_0 \rangle$$
$$= \cancel{Z} + V - (\cancel{Z} + U) - \langle \Phi_0 | \cancel{Z} + V - (\cancel{Z} + U) | \Phi_0 \rangle$$
$$= V - U - \langle \Phi_0 | V - U | \Phi_0 \rangle \qquad (85)$$
$$= V - \langle \Phi_0 | V | \Phi_0 \rangle - \left(U - \langle \Phi_0 | U | \Phi_0 \rangle\right)$$

We already know that $U - \langle \Phi_0 | U | \Phi_0 \rangle = U_N$.

Using Wick's theorem, we can easily show that

$$V = \frac{1}{2} \sum_{pq,rs} \langle pq | \hat{v} | rs \rangle X_p^\dagger X_q^\dagger X_s X_r \qquad (86)$$

$$= V_N + G_N + \langle \Phi_0 | V | \Phi_0 \rangle, \text{ where}$$

$$V_N = \frac{1}{2}\sum_{pq,rs} \langle pq|\hat{v}|rs\rangle N[X_p^\dagger X_q^\dagger X_s X_r]$$

$$= \frac{1}{2}\sum_{pq,rs} \langle pq|\hat{v}|rs\rangle N[X_p^\dagger X_r X_q^\dagger X_s]$$

$$\left(\text{or } \frac{1}{4} \cdots \langle pq|\hat{v}|rs\rangle_A \cdots\right), \quad (87)$$

$$G_N = \sum_{pq} \langle p|\hat{g}|q\rangle N[X_p^\dagger X_q], \quad (88)$$

with $\langle p|\hat{g}|q\rangle = \sum_{i=1}^{N} \langle pi|\hat{v}|qi\rangle_A$

(mean field one-body potential created by $|\Phi_0\rangle$)

$$\langle\Phi_0|V|\Phi_0\rangle = \frac{1}{2}\sum_{i,j} \langle ij|\hat{v}|ij\rangle_A \ . \quad (89),$$

Thus,

$$W = V_N + G_N - U_N = W_1 + W_2, \quad (90)$$

where

$$W_1 = G_N - U_N \equiv \mathcal{Q}_N \quad (91)$$

and

$$W_2 = V_N . \quad (92)$$

Note that the one-body perturbation,

$$W_1 = Q_N = \sum_{p,q} \langle p|\hat{g} - \hat{u}|q\rangle N[X_p^\dagger X_q] \qquad (93)$$

$$= \sum_{p,q} \langle p|\overset{\text{Fock operator } \hat{f}}{(\hat{z}+\hat{g})} - \underbrace{(\hat{z}+\hat{u})|q\rangle}_{\varepsilon_q |q\rangle} N[X_p^\dagger X_q]$$

$$= \sum_{p,q} \left[\langle p|\hat{f}|q\rangle - \varepsilon_p \delta_{pq}\right] N[X_p^\dagger X_q],$$

measures the departure of the single-particle basis from the Hartree-Fock case. Indeed, when $|p\rangle$'s are H-F states,

$$W_1 = Q_N = 0, \text{ since in the H-F}$$

case we use $\hat{u} = \hat{g}$ (or $(\hat{z}+\hat{u}) = \hat{f}$).

In general though,

$$W_1 = \hat{Q}_N = \sum_{r,s} \langle r|\hat{q}|s\rangle N[X_r^\dagger X_s], \quad (94)$$

where $\hat{q} = \hat{g} - \hat{u}$, and

$$W_2 = V_N . \quad (95)$$

3.3. Reduced resolvent in MBPT

We know that $R^{(0)} = \sum_{n>0} \frac{|\Phi_n\rangle\langle\Phi_n|}{\mathcal{E}_0 - \mathcal{E}_n}$.

In our case, $|\Phi_n\rangle$'s are $|\Phi_0\rangle, |\Phi_i^a\rangle, \ldots$.

Thus,

$$R^{(0)} = \sum_{n=1}^{N} \sum_{\substack{i_1<\ldots<i_n \\ a_1<\ldots<a_n}} \frac{|\Phi_{i_1\ldots i_n}^{a_1\ldots a_n}\rangle\langle\Phi_{i_1\ldots i_n}^{a_1\ldots a_n}|}{\mathcal{E}_0 - \mathcal{E}_{i_1\ldots i_n}^{a_1\ldots a_n}}, \quad (96)$$

where $\mathcal{E}_0 = 0$ and $\mathcal{E}_{i_1\ldots i_n}^{a_1\ldots a_n} = \sum_{\gamma=1}^{n} (\varepsilon_{a_\gamma} - \varepsilon_{i_\gamma})$.

This allows us to write

$$R^{(0)} = \sum_{n=1}^{N} R_n^{(0)}, \quad (97)$$

where the n-body component of $R^{(0)}$ is

$$R_n^{(0)} = \sum_{\substack{i_1 < \dots < i_n \\ a_1 < \dots < a_n}} \frac{|\Phi_{i_1 \dots i_n}^{a_1 \dots a_n}\rangle\langle\Phi_{i_1 \dots i_n}^{a_1 \dots a_n}|}{\omega_{i_1 \dots i_n}^{a_1 \dots a_n}}$$

$$= \left(\frac{1}{n!}\right)^2 \sum_{\substack{i_1 \neq \dots \neq i_n \\ a_1 \neq \dots \neq a_n}} \frac{|\Phi_{i_1 \dots i_n}^{a_1 \dots a_n}\rangle\langle\Phi_{i_1 \dots i_n}^{a_1 \dots a_n}|}{\omega_{i_1 \dots i_n}^{a_1 \dots a_n}}$$

ALLOWING EPV determinants which are zero here

$$\left(\frac{1}{n!}\right)^2 \sum_{\substack{i_1, \dots, i_n \\ a_1, \dots, a_n}} \frac{E_{i_1 \dots i_n}^{a_1 \dots a_n}|\Phi_0\rangle\langle\Phi_0|E_{a_1 \dots a_n}^{i_1 \dots i_n}}{\omega_{i_1 \dots i_n}^{a_1 \dots a_n}} \qquad (98)$$

MBPT denominator

with

$$\omega_{i_1 \dots i_n}^{a_1 \dots a_n} = \sum_{g=1}^{n} (\varepsilon_{i_g} - \varepsilon_{a_g}), \qquad (99)$$

$$E_{i_1 \dots i_n}^{a_1 \dots a_n} = \prod_{g=1}^{n} X_{a_g}^{\dagger} X_{i_g}, \qquad (100)$$

$$E_{a_1 \dots a_n}^{i_1 \dots i_n} = \left(E_{i_1 \dots i_n}^{a_1 \dots a_n}\right)^{\dagger} = \prod_{g=1}^{n} X_{i_g}^{\dagger} X_{a_g}$$

In RSPT, we need powers of $R^{(0)}$ as well, (101).

because of orthonormality of $|\Phi_n\rangle$ s, all that changes is power of $(\mathcal{E}_0-\mathcal{E}_n)$

$$\left(R^{(0)}\right)^k = \sum_{n>0} \frac{|\Phi_n\rangle\langle\Phi_n|}{(\mathcal{E}_0-\mathcal{E}_n)^k}, \quad (102).$$

In our case, because of orthonormality of Slater determinants,

$$\left(R^{(0)}\right)^k = \sum_{n=1}^{N} \left(R^{(0)}_n\right)^k, \quad (103)$$

where

$$\left(R^{(0)}_n\right)^k = \left(\frac{1}{n!}\right)^2 \sum_{\substack{i_1,\ldots,i_n \\ a_1,\ldots,a_n}} \frac{E^{a_1\ldots a_n}_{i_1\ldots i_n}|\Phi_0\rangle\langle\Phi_0|E^{i_1\ldots i_n}_{a_1\ldots a_n}}{\left(\omega^{a_1\ldots a_n}_{i_1\ldots i_n}\right)^k} \quad (104)$$

k-th power of the MBPT denominator

3.4. MBPT energy and wave function corrections.

We know that $K = K_0 + W$ $(K = H_N)$, $K_0 = Z_N + U_N$, and $W = W_1 + W_2$, where $W_1 = Q_N$ and $W_2 = \cancel{W}_N$ are both in the normal product form. Because of the latter observation,

$\langle \Phi_0 | N[\ldots] | \Phi_0 \rangle = 0$

$$k_0^{(1)} = \langle \Phi_0 | W | \Phi_0 \rangle = 0. \qquad (105).$$

This simplifies the MBPT analysis using $K = H_N$. We obtain ($\langle \ldots \rangle$ means $\langle \Phi_0 | \ldots | \Phi_0 \rangle$),

$$\Delta E_0^{(1)} \equiv k_0^{(1)} = \langle \Phi_0 | W | \Phi_0 \rangle \equiv \langle W \rangle = 0,$$

$$\Delta E_0^{(2)} \equiv k_0^{(2)} = \langle W R^{(0)} W \rangle,$$

$$\Delta E_0^{(3)} \equiv k_0^{(3)} = \langle W (R^{(0)} W)^2 \rangle - \underbrace{\langle W \rangle}_{= k_0^{(1)}} \langle W R^{(0)2} W \rangle$$

$$= \langle W (R^{(0)} W)^2 \rangle$$ ← no renormalization terms yet!

the 1st occurrence of renormalization terms →

$$\Delta E_0^{(4)} \equiv k_0^{(4)} \underset{\substack{\text{after eliminating} \\ \text{the } k_0^{(1)} \text{ terms}}}{=} \langle W (R^{(0)} W)^3 \rangle - \langle W R^{(0)} W \rangle \times \langle W R^{(0)2} W \rangle, \qquad (106)$$

etc.

IMPORTANT FOR DIAGRAM CANCELLATION ANALYSIS THAT LEADS TO LINKED CLUSTER THEOREM

Similarly,

$$|\Psi_0^{(1)}\rangle = R^{(0)} W |\Phi_0\rangle ,$$

$$|\Psi_0^{(2)}\rangle = (R^{(0)} W)^2 |\Phi_0\rangle - \langle W\rangle R^{(0)^2} W |\Phi_0\rangle$$

$$= (R^{(0)} W)^2 |\Phi_0\rangle ,$$

$$|\Psi_0^{(3)}\rangle = (R^{(0)} W)^3 |\Phi_0\rangle - \langle W R^{(0)} W\rangle R^{(0)^2} W |\Phi_0\rangle ,$$

etc.

1st occurrence of renormalization terms (important for linked cluster theorem)

(107)

Finally,

$$k_0 = \Delta E_0 = E_0 - \langle\Phi_0|H|\Phi_0\rangle \qquad (108)$$

$$= \varepsilon_0 + k_0^{(1)} + k_0^{(2)} + \ldots$$

$\varepsilon_0 = 0$, $k_0^{(1)} = 0$ $\rightarrow$

$$= k_0^{(2)} + \ldots = \sum_{n=2}^{\infty} k_0^{(n)} = \sum_{n=2}^{\infty} \Delta E_0^{(n)} .$$

<u>Correlation energy starts in the second order.</u>

This is easy to understand. If we used H rather than H_N and $H_0 = Z + U$ rather than the shifted $K_0 = H_0 - \langle\Phi_0|H_0|\Phi_0\rangle$, we would have

$$K = H = \tilde{K}_0 + \tilde{W}, \text{ where}$$

$$\tilde{K}_0 = Z + U \text{ and } \tilde{W} = V - U.$$

In that case, the energy E_0 (in $H|\Psi_0\rangle = E_0|\Psi_0\rangle$) would become

$$E_0 = E_0^{(0)} + E_0^{(1)} + E_0^{(2)} + \ldots,$$

where

$$E_0^{(0)} = \langle\Phi_0|\overbrace{Z+U}^{\tilde{K}_0}|\Phi_0\rangle = \sum_{i=1}^{N} \varepsilon_i,$$

$$E_0^{(1)} = \langle\Phi_0|V-U|\Phi_0\rangle = \langle\Phi_0|\tilde{W}|\Phi_0\rangle,$$

etc. Now, $E_0^{(0)} + E_0^{(1)} = \langle\Phi_0|\tilde{K}_0 + \tilde{W}|\Phi_0\rangle$

$$= \langle\Phi_0|(Z+U)+(V-U)|\Phi_0\rangle$$

$$= \langle\Phi_0|H|\Phi_0\rangle \Longrightarrow \text{mean-field energy; no correlations!}$$

Thus, $$E_0 = \underbrace{\overbrace{\langle \Phi_0 | H | \Phi_0 \rangle}^{\text{reference energy}}}_{\text{0th + 1st order}} + \underbrace{\overbrace{E_0^{(2)}}^{\text{correlation.}}}_{\text{2nd order}} + \ldots .$$

---

4. Diagrammatic representation of MBPT energy and wave function corrections.

In order to evaluate MBPT expressions for the energy and wave function corrections, we need to evaluate quantities of the following types:

$$\langle \Phi_0 | W (R^{(0)})^{n_1} W (R^{(0)})^{n_2} W \ldots (R^{(0)})^{n_\gamma} W | \Phi_0 \rangle \tag{109}$$

(energy corrections)

and $$(R^{(0)})^{n_1} W (R^{(0)})^{n_2} W \ldots (R^{(0)})^{n_\gamma} W | \Phi_0 \rangle \tag{110}$$

(wave function corrections),

where $n_1, n_2, \ldots, n_\gamma \geq 1$ and $W = W_1 + W_2$.

If we want to do it diagrammatically, we must come up with a diagrammatic representation of W_1, W_2, and $(R_n^{(0)})^k$ and then follow the diagrammatic rules to determine the final formulas.

QUICK SUMMARY OF DIAGRAMMATIC CALCULATIONS

Diagrammatic formalism allows us to calculate expressions of the following form:

$$K_A \ldots K_Z = \prod_C K_C , \qquad (111)$$

where each K_C is a many-body operator in the standard or normal product form. We could, of course, do this algebraically, using Wick's theorem, but Wick's theorem often produces multiple copies of the same term, which we have to manually recognize and collect. Diagrams are nicer in this regard, since one only has to determine the non-equivalent admissible resulting diagrams relevent to the problem of interest. All of the redundancies are taken care of by the so-called topological weights. Here, because of time constraints we will focus on Hugenholtz diagrams, which are used to represent many-body operators employing antisymmetrized matrix elements. For example the O k-body operator in the normal-product form

$$\hat{O}_k = \left(\frac{1}{k!}\right)^2 \sum_{\substack{p_1,\ldots,p_k \\ q_1,\ldots,q_k}} \langle p_1 \ldots p_k | \hat{o}_k | q_1 \ldots q_k \rangle_A$$

$$\times N[X^{\dagger}_{p_1} \ldots X^{\dagger}_{p_k} X_{q_k} \ldots X_{q_1}]$$

$$= \left(\frac{1}{k!}\right)^2 \sum_{\substack{p_1,\ldots,p_k \\ q_1,\ldots,q_k}} \langle p_1 \ldots p_k | \hat{o}_k | q_1 \ldots q_k \rangle_A$$

$$\times N[X^{\dagger}_{p_1} X_{q_1} \ldots X^{\dagger}_{p_k} X_{q_k}], \quad (112)$$

where

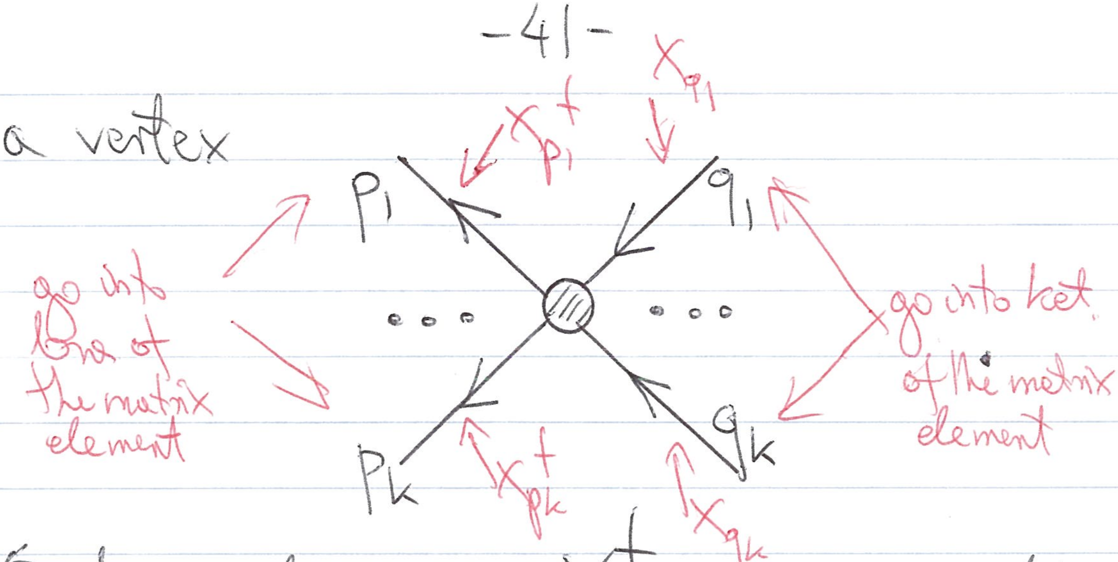
$$\langle p_1 \ldots p_k | \hat{o}_k | q_1 \ldots q_k \rangle_A = \sum_{R \in S_k} (-1)^R$$

$$\times \langle p_1 \ldots p_k | \hat{o}_k | q_{R_1} \ldots q_{R_k} \rangle_A, \quad (113)$$

with

$$R = \begin{pmatrix} 1 & \ldots & k \\ R_1 & \ldots & R_k \end{pmatrix} \quad (114)$$

representing the index permutation, is represented by a vertex



(115)

Outgoing lines are X^{+}, incoming lines are X, the

$$\left(\frac{1}{k!}\right)^2$$

factor is taken care of by the equivalences among fermion lines $p_1, \ldots, p_k$ and $q_1, \ldots, q_k$.

The vertex is always drawn in a way specific to the operator of interest. We will show the W_1, W_2, and $(R_n^{(0)})^{+}$ operators diagrammatically in a moment.

Once we represent operators $K_A, \ldots, K_Z$ on the left-hand side of Eq. (111), we proceed as follows (we will assume that all fermion lines carry free labels, which are summed over):

(1) Draw the nonoriented (no arrows) Hugenholtz skeletons corresponding to $K_A, \ldots, K_Z$ along the fictitious time line (axis), going in this presentation from left to right, and form the nonequivalent resulting Hugenholtz skeletons (or their subset relevant to the calculation of interest; cf. below)

Formation of the resulting diagrams is accomplished by connecting fermion lines. Such connections represent contractions of X and $X^\dagger$ operators, as in Wick's theorem,

$$
\begin{aligned}
M_1 \ldots M_m &= N[M_1 \ldots M_m] + \sum_{\mu<\nu} N[M_1 \ldots \overbracket{M_\mu \ldots M_\nu} \ldots M_m] \\
&+ \sum_{\substack{\mu_1<\nu_1,\\ \mu_2<\nu_2,\ \mu_1<\mu_2,\\ \nu_1\neq\nu_2}} N[M_1 \ldots M_{\mu_1} \ldots M_{\mu_2} \ldots M_{\nu_1} \ldots M_{\nu_2} \ldots M_m] \\
&+ \ldots \qquad (116)
\end{aligned}
$$

(2) Add arrows to fermion lines in all possible allowed ways (for example, k lines have arrows toward ⊘ and k lines leave ⊘ in (115)). Lines that remain uncontracted must carry the same orientation as on the left-hand side of Eq. (111), unless a particular expression forces a modification.

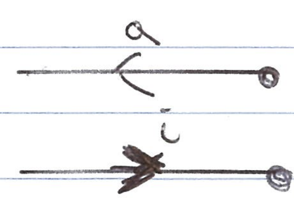
(3) Add the appropriate spin-orbital or single-particle choices to each line in the resulting Hugenholtz diagrams. For the internal lines going from left to right, use hole choices, e.g.,

$$\bullet \xrightarrow{\;i\;} \bullet \qquad \left(\overbracket{X_i^\dagger X_j} = \delta_{ij}\right)$$

For the internal lines going from right to left, use particle indices, e.g.,

$(\overset{\sqcap}{X_a X_b^{\dagger}} = \delta_{ab})$

Uncontracted external fermion lines retain their character from the left-hand side of Eq. (111), unless the actual expression forces some adjustment. For example, in MBPT, all external lines will extend to the left, since $X_a|\Phi_0\rangle = X_i^{\dagger}|\Phi_0\rangle = 0$. and the normal ordering places X_a and $X_i^{\dagger}$ in the rightmost positions, allowing direct action on $|\Phi_0\rangle$. In MBPT, operator products always act on $|\Phi_0\rangle$. In other words, in MBPT we can only have external lines of the following two types:



$= X_a^{\dagger}$

$= X_i$

As shown below, $R^{(0)}$ in wave function corrections enforces the same.

(4) Read the resulting Hugenholtz diagrams.

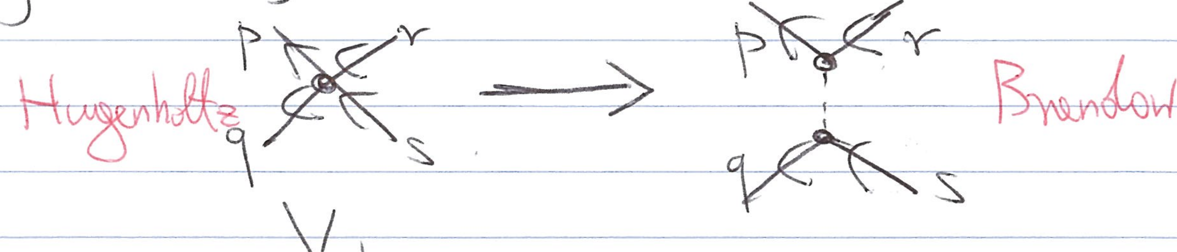
The last step is executed as follows:

(a) Determine the topological weight

$$W_R^{(H)}$$

based on the equivalences among fermion lines in the oriented Hugenholtz skeleton (diagram stripped of free indices labeling fermion lines) corresponding to a given resulting diagram R.

(b) Draw the Brandow representative (one of the Goldstone diagrams corresponding to Hugenholtz diagram R) by expanding Hugenholtz vertices to their Goldstone-like form, e.g.



Assign the scalar factor $d^{(B)}_{X_R', X_R''}$, being a product of ANTISYMMETRIZED matrix elements, labeled by appropriate internal (X_R') and external (X_R'') indices at various fermion lines, as seen in the Brandow diagram representing R.

Assign the sign $(-1)^{l_R^{(B)}+h_R^{(B)}}$, where $l_R^{(B)}$ and $h_R^{(B)}$ are the numbers of closed loops and internal hole lines in the Brandow diagram.

$\leftarrow s_R^{(B)}$ (sign factor)

Assign, if relevant, the operator expression

$$\hat{O}^{(B)}_{\chi_R''} = N\left[\prod_{r=1}^{m_R^{(B)}} X^{\dagger}_{p_r} X_{q_r}\right]$$

to the diagram, where $X^{\dagger}_{p_r}$ and X_{q_r} correspond to external lines p_r and q_r exiting and entering open path r in Brandow diagram R ($m_R^{(B)}$ is the total number of open paths). In MBPT, p_r must be a particle line and q_r must be a hole line, as explained above. The final formula for $K_A \dots K_Z$ is

$$K_A \dots K_Z = \sum_R K_R \, , \tag{117}$$

where the summation on the right-hand side involves only the non-equivalent resulting diagrams (relevant to the problem of interest; cf. below) and

$$K_R = (-1)^{l_R^{(B)}+h_R^{(B)}} w_R^{(H)} \sum_{\chi_R', \chi_R''} d^{(B)}_{\chi_R', \chi_R''} \hat{O}^{(B)}_{\chi_R''}$$

indices of external lines

indices of internal lines

In MBPT, we only have two situations:

- energy diagrams that correspond to Eq. (109), meaning resulting diagrams with no external lines, so that

$$K_R = (-1)^{l_R^{(B)} + h_R^{(B)}} \, w_R^{(H)} \sum_{\chi_R'} d^{(B)}_{\chi_R'} \qquad (118)$$

- have function diagrams that correspond to Eq. (110), where all external lines extend to the left, as in $\xleftarrow{a}\!\bullet = X_a^\dagger$ and $\xrightarrow{i}\!\bullet = X_i$, so that

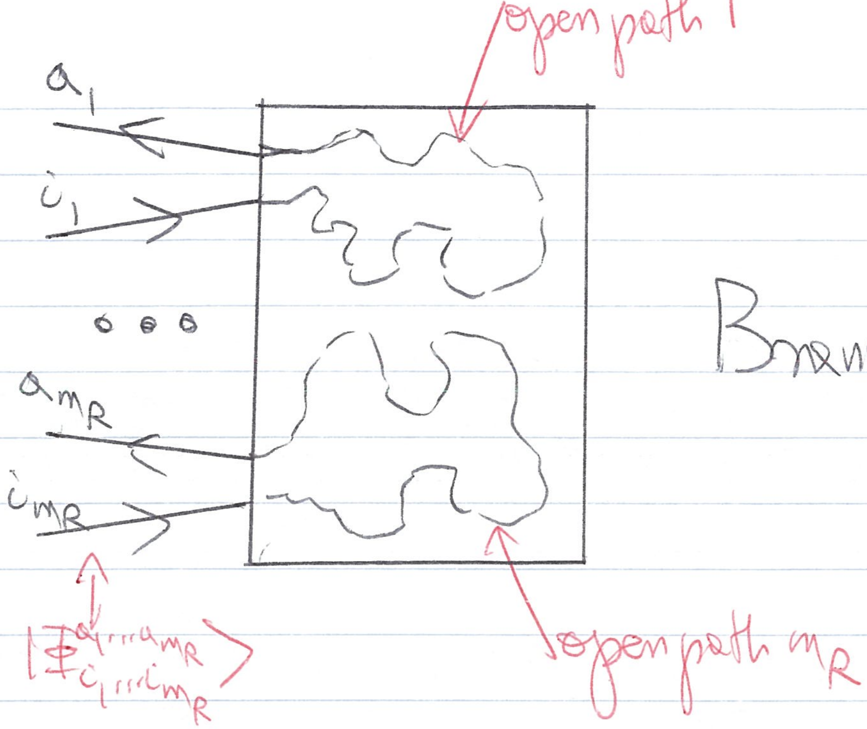
$$K_R = (-1)^{l_R^{(B)} + h_R^{(B)}} \, w_R^{(H)}$$

indices of external lines in open paths

$$\times \sum_{\chi_R', a_1,\ldots,a_{m_R}, i_1,\ldots,i_{m_R}} d^{(B)}_{\chi_R', a_1,\ldots,a_{m_R}, i_1,\ldots,i_{m_R}}$$

indices of internal lines

$$\times \underbrace{N[X_{a_1}^\dagger X_{i_1} \ldots X_{a_{m_R}}^\dagger X_{i_{m_R}}] |\Phi_0\rangle}_{|\Phi_{i_1 \ldots i_{m_R}}^{a_1 \ldots a_{m_R}}\rangle} \qquad (119)$$



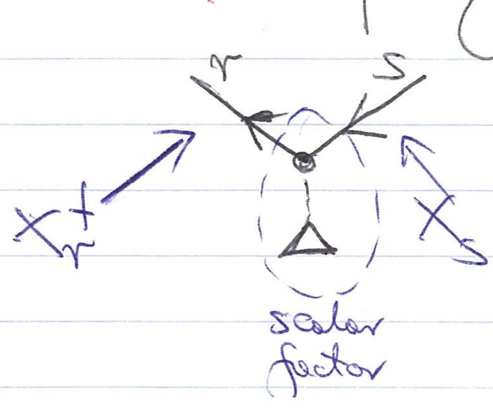
Brandow diagram R. (120)

The requirement that all external lines must extend to the left is also enforced by the presence of the reduced resolvent in the leftmost position of Eq. (110).

Now, we introduce Hugenholtz and Brandow vertices representing $W_1 = Q_N$, $W_2 = V_N$, and $R_n^{(0)}$:

- $$W_1 \equiv Q_N = \sum_{r,s} \langle r|\hat{q}|s\rangle N[X_r^\dagger X_s], \text{ where}$$
  $$\hat{q} = \hat{g} - u.$$

Hugenholtz and Brandow look identical since W_1 is one-body



$W^{(H)}_{Q_N} = 1$

outgoing

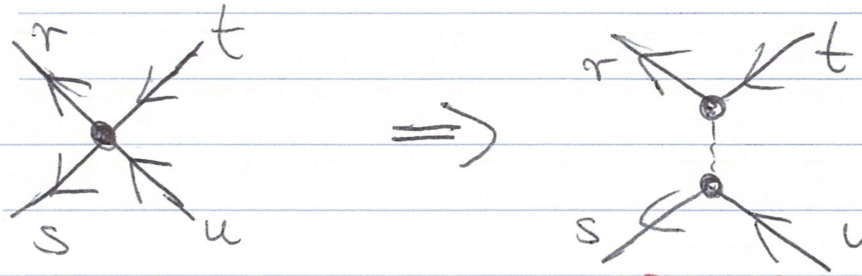
$d^{(B)}_{rs} = \langle r|\hat{q}|s\rangle$

incoming

$\hat{O}^{(B)}_{rs} = N[X_r^\dagger X_s]$

$$W_1 = w^{(H)}_{\mathcal{Q}_N} \sum_{r,s} d^{(B)}_{rs}\, \hat{O}^{(B)}_{rs} \qquad \left(l^{(B)}_{\mathcal{Q}_N}=0,\ h^{(B)}_{\mathcal{Q}_N}=0\right)$$

- $$W_2 \equiv V_N = \underset{\uparrow \left(\frac{1}{2!}\right)^2}{\frac{1}{4}} \sum_{rs,tu} \langle rs|\hat{o}|tu\rangle_A \times N[X_r^\dagger X_t X_s^\dagger X_u]$$



Hugenholtz

Brandow (Goldstone representative)

$$w^{(H)}_{V_N} = \frac{1}{4}$$

$$d^{(B)}_{rstu} = \langle \overset{\text{outgoing}}{rs}|\hat{o}|\overset{\text{incoming}}{tu}\rangle_A$$

$$\hat{O}^{(B)}_{rstu} = N[\underbrace{X_r^\dagger X_t}_{\text{open path}}\ \underbrace{X_s^\dagger X_u}_{\text{open path}}]$$

$$W_2 = w^{(H)}_{V_N} \sum_{rstu} d^{(B)}_{rstu}\, \hat{O}^{(B)}_{rstu} \qquad \left(l^{(B)}_{V_N}=0,\ h^{(B)}_{V_N}=0\right).$$

- Reduced resolvent, focus on k-th power of the n-body component $\left(R_n^{(0)}\right)^k$.

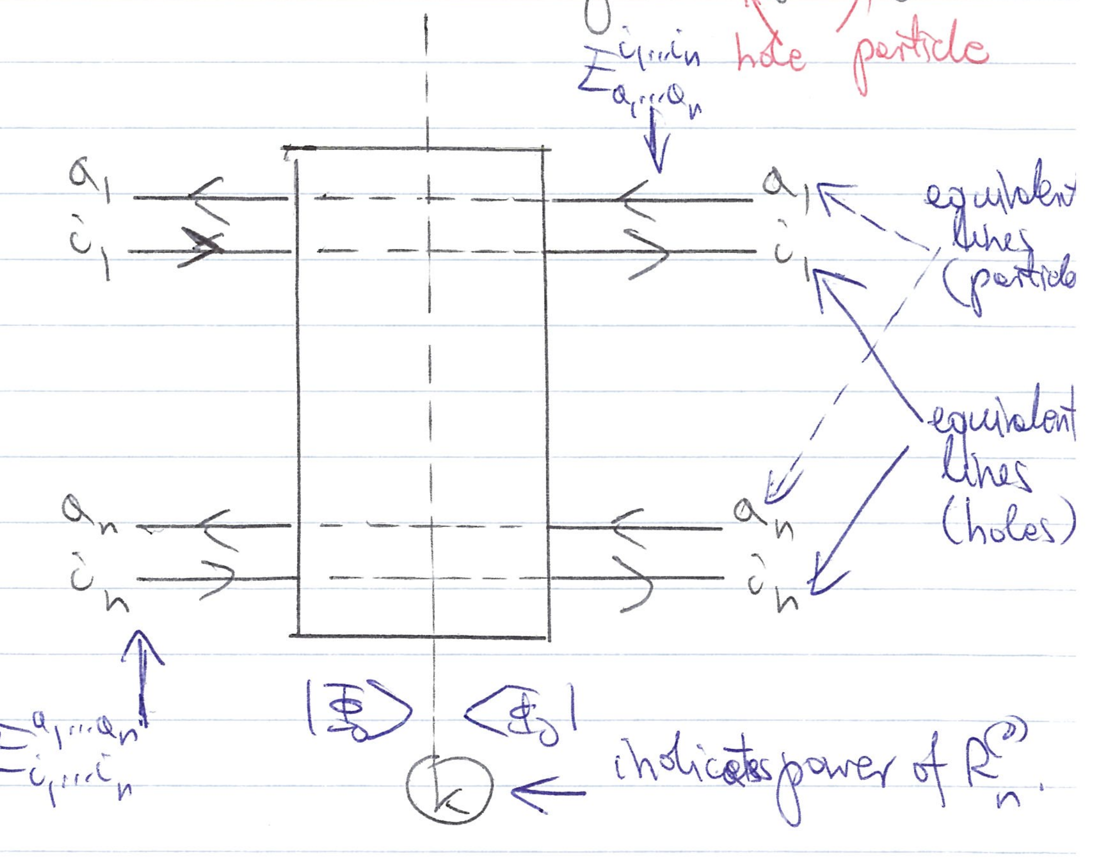
$$\left(R_n^{(0)}\right)^k = \left(\frac{1}{n!}\right)^2 \sum_{\substack{i_1,\dots,i_n \\ a_1,\dots,a_n}} \frac{E^{a_1,\dots,a_n}_{i_1,\dots,i_n} |\Phi_0\rangle\langle\Phi_0| E^{i_1,\dots,i_n}_{a_1,\dots,a_n}}{\left(\omega^{a_1,\dots,a_n}_{i_1,\dots,i_n}\right)^k}$$

$$E^{a_1,\dots,a_n}_{i_1,\dots,i_n} \equiv N[X^\dagger_{a_1} X_{i_1} \dots X^\dagger_{a_n} X_{i_n}]$$

$$E^{i_1,\dots,i_n}_{a_1,\dots,a_n} = \left(E^{a_1,\dots,a_n}_{i_1,\dots,i_n}\right)^\dagger = N[X^\dagger_{i_1} X_{a_1} \dots X^\dagger_{i_n} X_{a_n}]$$

$$\omega^{a_1,\dots,a_n}_{i_1,\dots,i_n} = -\delta^{a_1,\dots,a_n}_{i_1,\dots,i_n} = \sum_{\gamma=1}^{n} \left(\varepsilon_{i_\gamma} - \varepsilon_{a_\gamma}\right)$$

hole particle



$$W^{(H)}_{R_n^{(0)}} = \left(\frac{1}{n!}\right)^2$$

$$d^{(B)}_{i_1,\ldots,i_n,a_1,\ldots,a_n} = \left(\omega^{a_1\ldots a_n}_{i_1\ldots i_n}\right)^{-k}$$

$$= \left[\sum_{g=1}^{n} \left(\varepsilon_{i_g} - \varepsilon_{a_g}\right)\right]^{-k}$$

lines "sliced" by

$$\hat{O}^{(B)}_{i_1\ldots i_n,a_1\ldots a_n} = E^{a_1\ldots a_n}_{i_1\ldots i_n} |\Phi_0\rangle\langle\Phi_0| E^{i_1\ldots i_n}_{a_1\ldots a_n}$$

$$\left(R_n^{(0)}\right)^k = W^{(H)}_{R_n^{(0)}} \sum_{\substack{i_1\ldots i_n\\ a_1\ldots a_n}} d^{(B)}_{i_1\ldots i_n,a_1\ldots a_n} \hat{O}^{(B)}_{i_1\ldots i_n,a_1\ldots a_n}$$

We can see now the $R_n^{(0)}$ in the leftmost position in wave function expressions enforces the requirement that external lines extend to the left representing

$$E^{a_1\ldots a_n}_{i_1\ldots i_n} = N\left[\prod_{g=1}^{n} X^{\dagger}_{a_g} X_{i_g}\right]$$ acting

on $|\Phi_0\rangle$.

Equipped with the above information, let us examine the second-order correction to energy,

$$K_0^{(2)} = \langle \Phi_0 | W R^{(0)} W | \Phi_0 \rangle$$

$$= \langle \Phi_0 | Q_N R^{(0)} Q_N | \Phi_0 \rangle + \langle \Phi_0 | Q_N R^{(0)} V_N | \Phi_0 \rangle$$

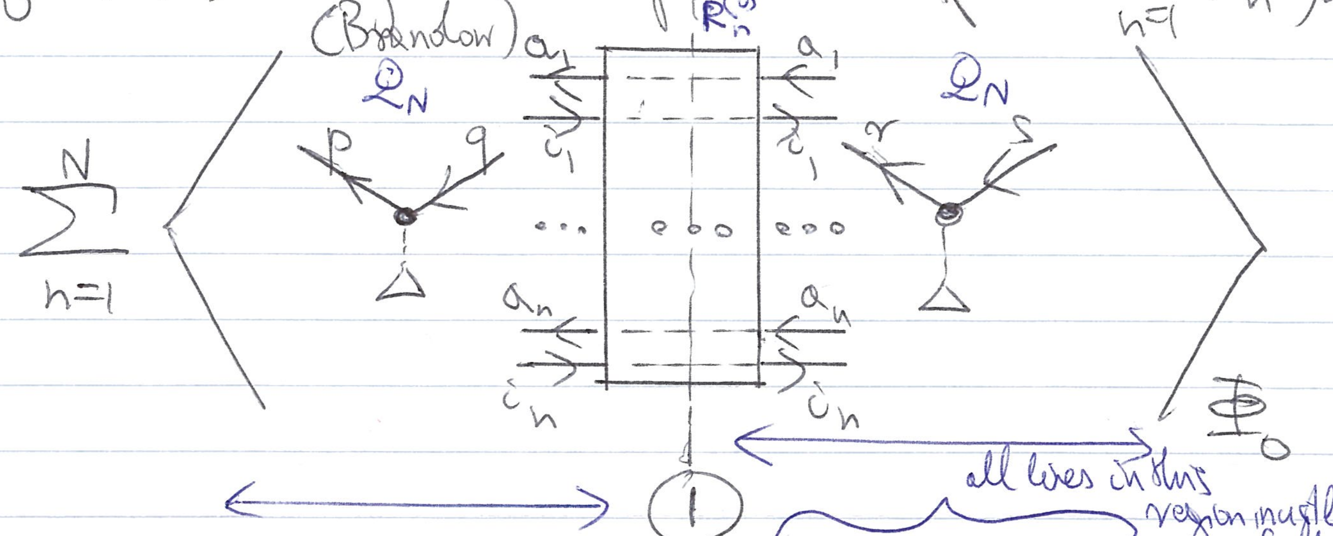
$W = W_1 + W_2$
$= Q_N + V_N$

$$+ \langle \Phi_0 | V_N R^{(0)} Q_N | \Phi_0 \rangle + \langle \Phi_0 | V_N R^{(0)} V_N | \Phi_0 \rangle$$

$$= K_0^{(2)}(A) + K_0^{(2)}(X_1) + K_0^{(2)}(X_2) + K_0^{(2)}(B) \qquad (121)$$

$K_0^{(2)}(A)$ in Hugenholtz representation $\left(R^{(0)} = \sum_{n=1}^{N} R_n^{(0)}\right)$:

(Brandow)



all lines in this region must be fully contracted

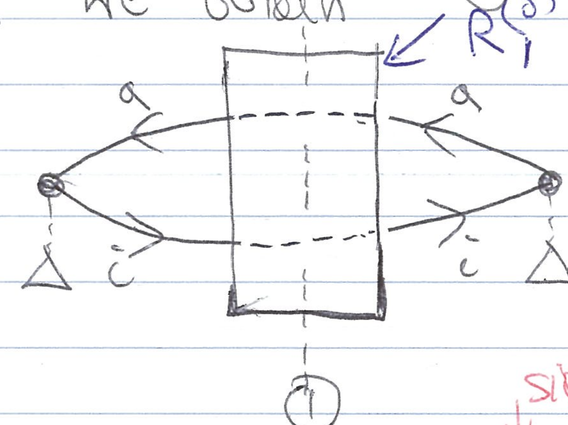
$$\underbrace{\langle \Phi_0 | \ \ldots \ | \Phi_0 \rangle}\langle \Phi_0 | \ \ldots \ | \Phi_0 \rangle$$

all lines in this region must be fully contracted

central part of $\hat{O}^{(B)}_{i_1 \ldots i_n a_1 \ldots a_n}$ in $R_n^{(0)}$

one cannot contract lines on Q_N due to normal ordering or a lines with i lines

Thus, we must fully contract (connect) p and q lines with $a_1, \ldots, a_n, i_1, \ldots, i_n$ lines to the left of the dashed slicing line. Similarly, r and s must be connected (fully) to lines $a_1, \ldots, a_n, i_1, \ldots, i_n$ extending to the right relative to the dashed slicing line. This can only be done when $n=1$! We obtain



In this case,

$$W_A^{(H)} = 1, \quad S_A^{(B)} = (-1)^{\overset{1\,(\text{or }2)}{l_A^{(B)}} + \overset{1\,(\text{or }2)}{h_A^{(B)}}} = +1,$$

sign factor

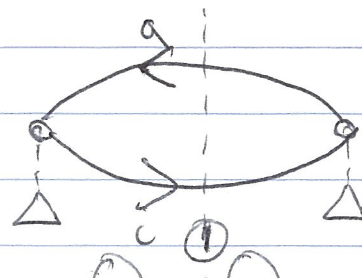
$$d_{ia}^{(B)} = \langle i|\hat{q}|a\rangle\langle a|\hat{q}|i\rangle\,(\varepsilon_i - \varepsilon_a)^{-1}.$$

$(\omega_i^a)^{-1}$

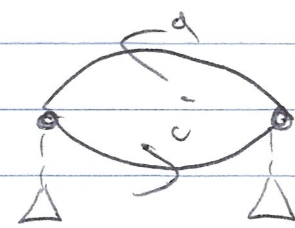
Thus,

$$K_0^{(2)}(A) = \sum_{i,a} \frac{\langle i|\hat{q}|a\rangle\langle a|\hat{q}|i\rangle}{\varepsilon_i - \varepsilon_a} \tag{122}$$

Please note that we could obtain this result by drawing



or even



obtained from $Q_N \overset{1}{} Q_N$ only if we agreed on an additional denominator convention that with each pair of neighboring W (Q_N or V_N) vertices we associate the energy denominator obtained by assigning

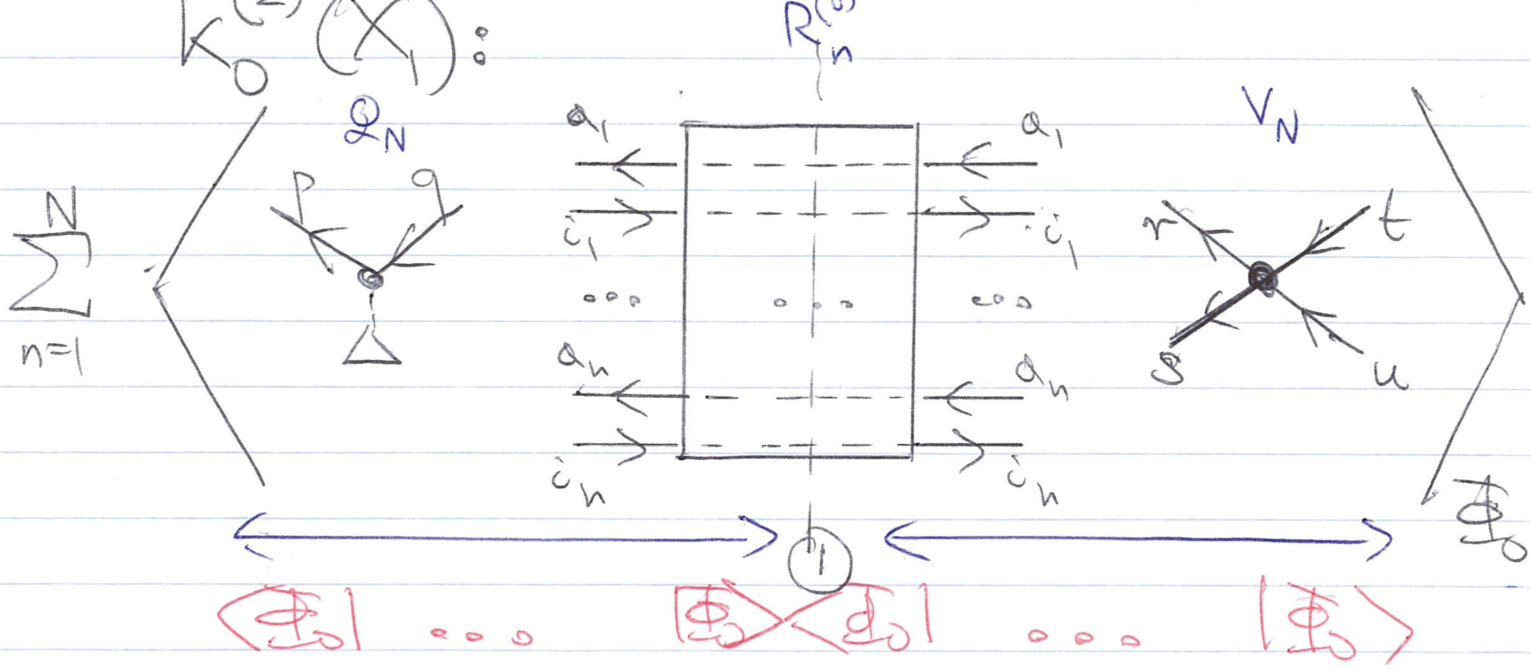
$$\left[(\varepsilon_{i_1}-\varepsilon_{a_1})+\dots+(\varepsilon_{i_n}-\varepsilon_{a_n})\right]^{-k}$$

to lines

in the region between the neighboring Ws where there is $[R_n^{(0)}]^k$.

Let us examine the remaining contributions to $K_0^{(2)}$.

$K_0^{(2)}(X_1)$:

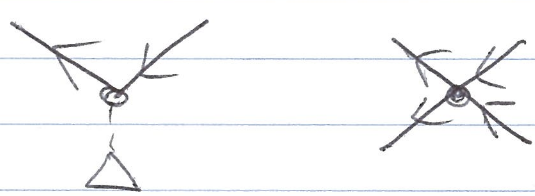


$\langle\Phi_0| \dots |\Phi_0\rangle\langle\Phi_0| \dots |\Phi_0\rangle$

Again, we must connect lines p, q with lines $a_1, i_1, \dots, a_n, i_n$ extending to the left of the dashed line slicing the reduced resolvent. We also must fully contract lines r, s, t, u with lines $a_1, i_1, \dots, a_n, i_n$ extending to the right of the slicing dashed line. The former means $n=1$, the latter $n=2$. We cannot have it both ways, so

$$K_0^{(2)}(X_1) = 0. \quad (123)$$

Note that we do not need diagrams representing $R^{(0)}$ to come up with such a result, since we cannot produce a diagram without external lines from



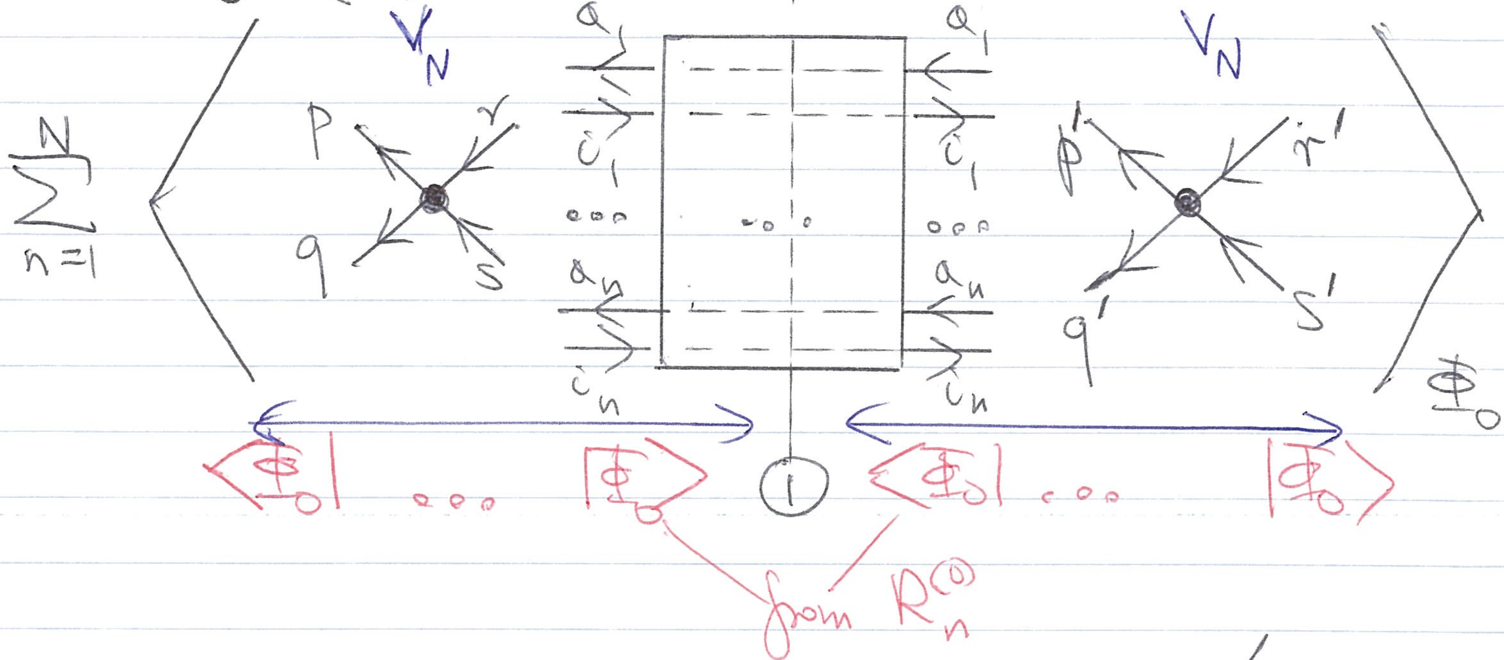
$Q_N^{(1)}$ $\qquad$ V_N

(we are not allowed to contract lines on V_N since V_N is in the normal ordered form $\rightarrow$ $\rightarrow$ generalized Wick's theorem).

Similarly,

$$K_0^{(2)}(X_2) = 0. \quad (124)$$

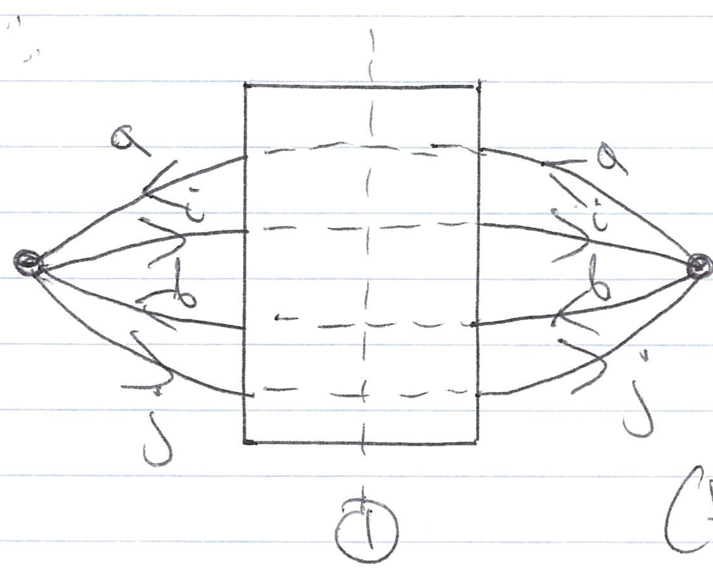
$K_0^{(2)}$(B):



We must fully contract lines between $\Big\langle$ and $|\Phi_0\rangle$ (or ①) and between $\langle\Phi_0|$ (or ①) and $\Big\rangle$.

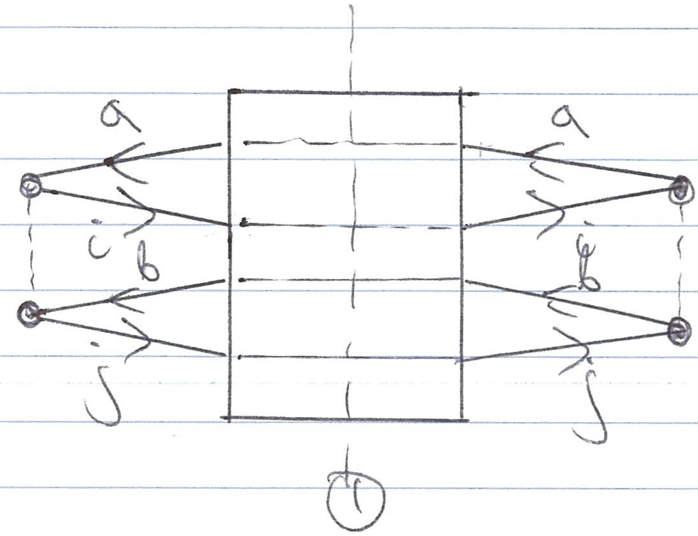
This is only possible when $n=2$ (we cannot contract lines on the same V_N due to normal ordering).

We obtain:



(Hugenholtz diagram)

The corresponding Brandow diagram looks as follows:



We obtain,

$$w_B^{(H)} = \frac{1}{4} \quad (a, b \text{ equivalent; } i, j \text{ equivalent}),$$

$$S_B^{(B)} = (-1)^{l_B^{(B)} + h_B^{(B)}} = +1, \quad \left(l_B^{(B)} = 2 \,(\text{or } 4);\ h_B^{(B)} = 2\,(\text{or } 4) \right)$$

$$d_{ijab}^{(B)} = \langle ij|\hat{v}|ab\rangle_A \langle ab|\hat{v}|ij\rangle_A \times \left(\varepsilon_i - \varepsilon_a + \varepsilon_j - \varepsilon_b \right)^{-1},$$

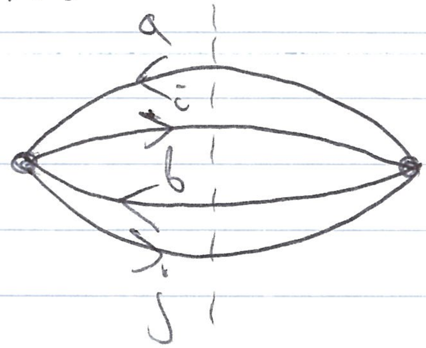
$(\omega_{ij}^{ab})^{-1}$

$$K_0^{(2)}(B) = \frac{1}{4} \sum_{ijab} \frac{\langle ij|\hat{v}|ab\rangle_A \langle ab|\hat{v}|ij\rangle_A}{\varepsilon_i - \varepsilon_a + \varepsilon_j - \varepsilon_b} \quad (125)$$

Once again, the only role of the reduced resolvent is to introduce the denominator

$$\left(\varepsilon_i - \varepsilon_a + \varepsilon_j - \varepsilon_b\right)^{-1},$$

obtained by slicing the lines between V_N vertices in a Hugenholtz diagram obtained for $V_N \cdot V_N$,

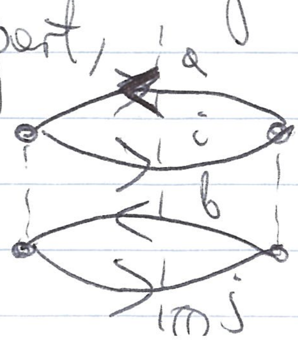


(126)

Lines i going from left to right contributes ε_i, line a going from right to left contributes $-\varepsilon_a$, for a total of $(\varepsilon_i - \varepsilon_a)$ contributions for this pair of lines. The rest of the expression, i.e.,

$$\frac{1}{4}\langle ij|\hat{v}|ab\rangle_A \langle ab|\hat{v}|ij\rangle_A$$

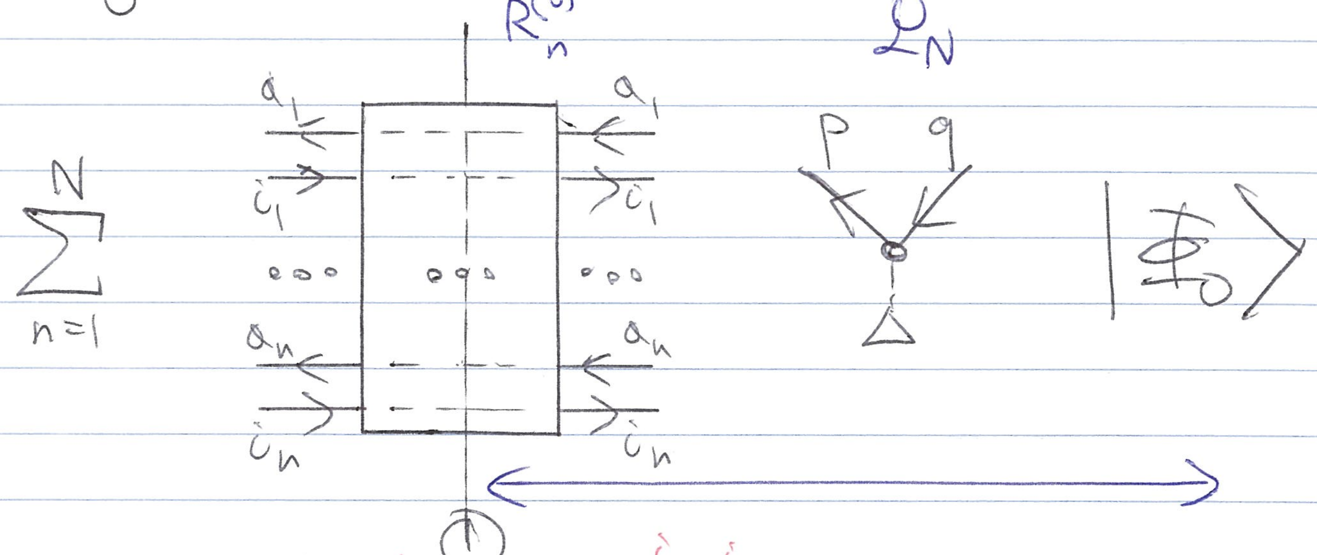
can be read from diagram (126) and its Brandow counterpart,



We see similar patterns in wave function expressions in first order,

$$
\begin{aligned}
|\Psi_0^{(1)}\rangle &= R^{(0)} W |\Phi_0\rangle \\
&= R^{(0)} Q_N |\Phi_0\rangle + R^{(0)} V_N |\Phi_0\rangle \\
&= |\Psi_0^{(1)}(A)\rangle + |\Psi_0^{(1)}(B)\rangle .
\end{aligned} \tag{127}
$$

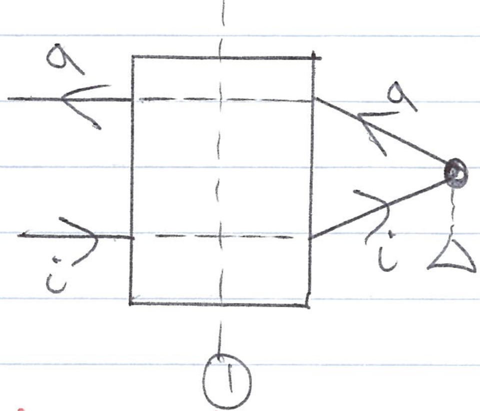
$|\Psi_0^{(1)}(A)\rangle$:



$$E^{a_1 \ldots a_n}_{i_1 \ldots i_n} |\Phi_0\rangle \underbrace{\langle \Phi_0 | E^{i_1 \ldots i_n}_{a_1 \ldots a_n} \quad \ldots \quad |\Phi_0\rangle}_{\text{all lines must be fully contracted between } \langle\Phi_0| \text{ and } |\Phi_0\rangle.}$$

This means that $n = 1$.

We obtain,



$= \sum_{ia} \frac{\langle a|\hat{q}|i\rangle}{\varepsilon_i - \varepsilon_a} |\Phi_i^a\rangle$

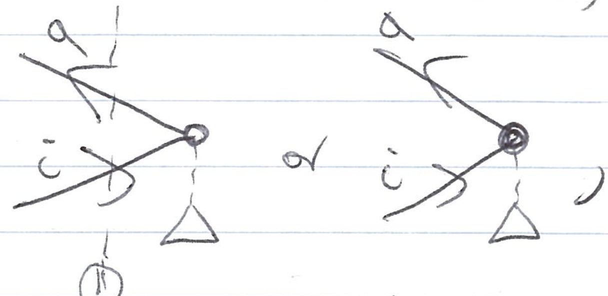
ω_i^a

$N[X_a^\dagger X_i] |\Phi_0\rangle$

$E_i^a |\Phi_0\rangle \equiv |\Phi_i^a\rangle$

(128)

We could obtain this from



,

if we adopted the additional denominator convention for lines sliced by the resolvent line.

1

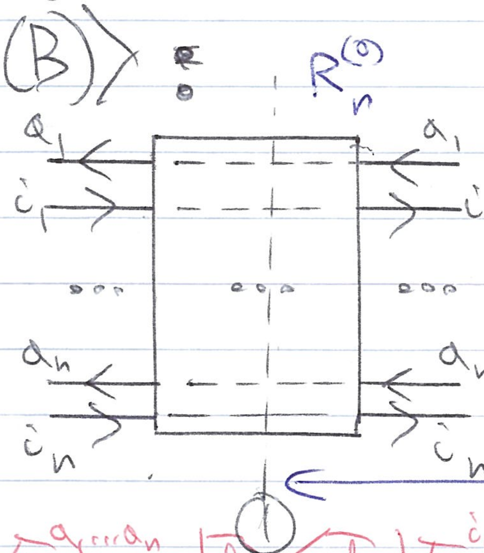
Similarly,

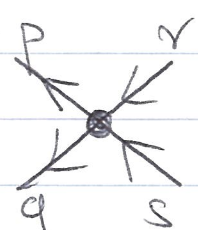
$|\Psi_0^{(1)}(B)\rangle$:

$R_n^{(0)}$

V_N

$\sum_{n=1}^{N}$





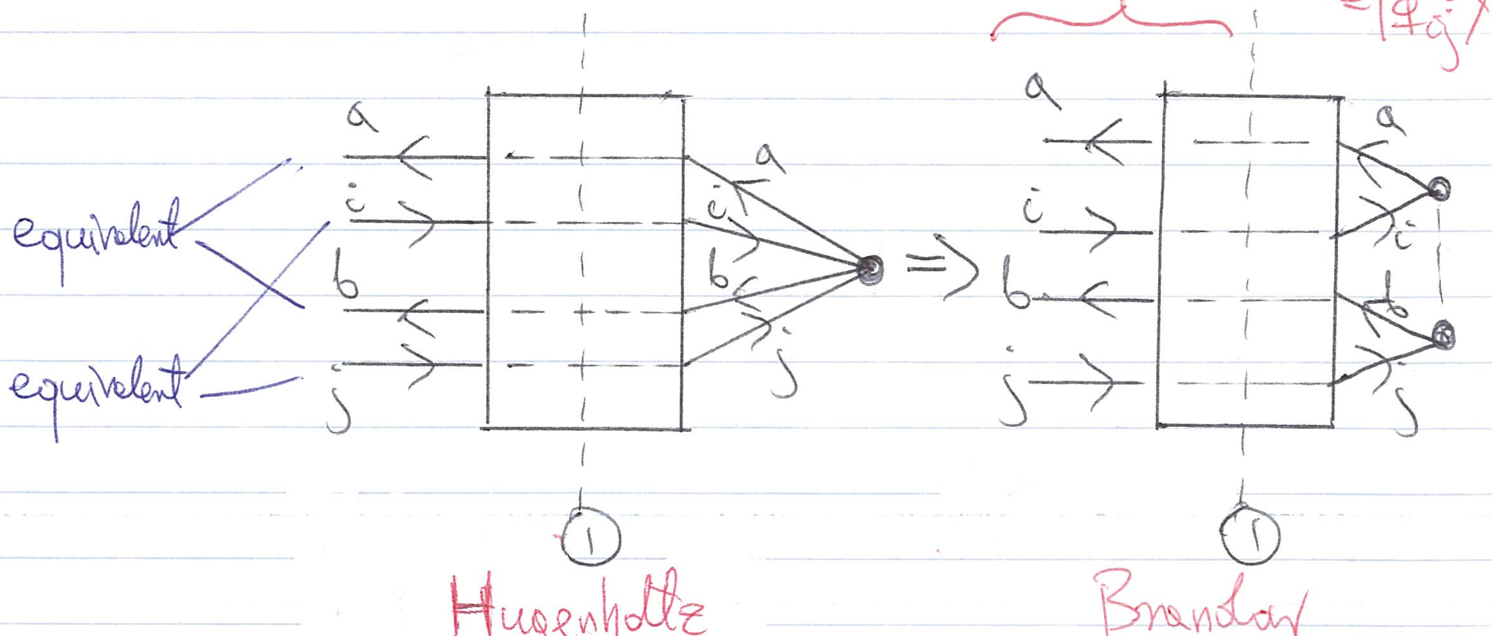
$|\Phi_0\rangle$

to connect fully here, n must be 2

$E_{i_1 \ldots i_n}^{a_1 \ldots a_n} |\Phi_0\rangle\langle\Phi_0| E_{a_1 \ldots a_n}^{i_1 \ldots i_n} \ldots$ $|\Phi_0\rangle_n$

We obtain

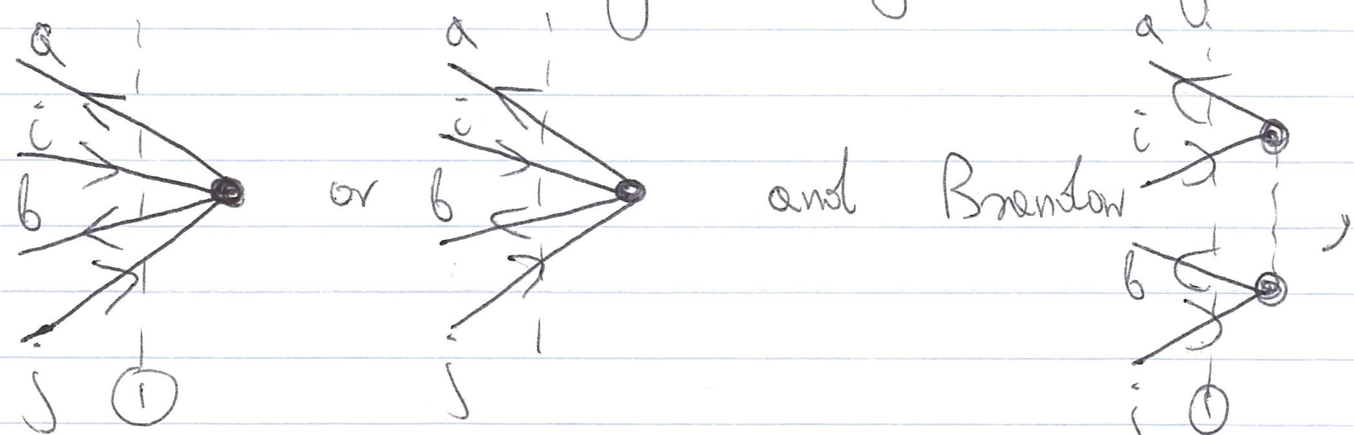
$E_i^a E_j^b |\Phi_0\rangle = E_{ij}^{ab}|\Phi_0\rangle = |\Phi_{ij}^{ab}\rangle$



$$= \frac{1}{4} \sum_{ijab} \frac{\langle ab|\hat{v}|ij\rangle_A}{\varepsilon_i - \varepsilon_a + \varepsilon_j - \varepsilon_b} |\Phi_{ij}^{ab}\rangle . \tag{129}$$

ω_{ij}^{ab}

We could obtain this from a Hugenholtz diagram

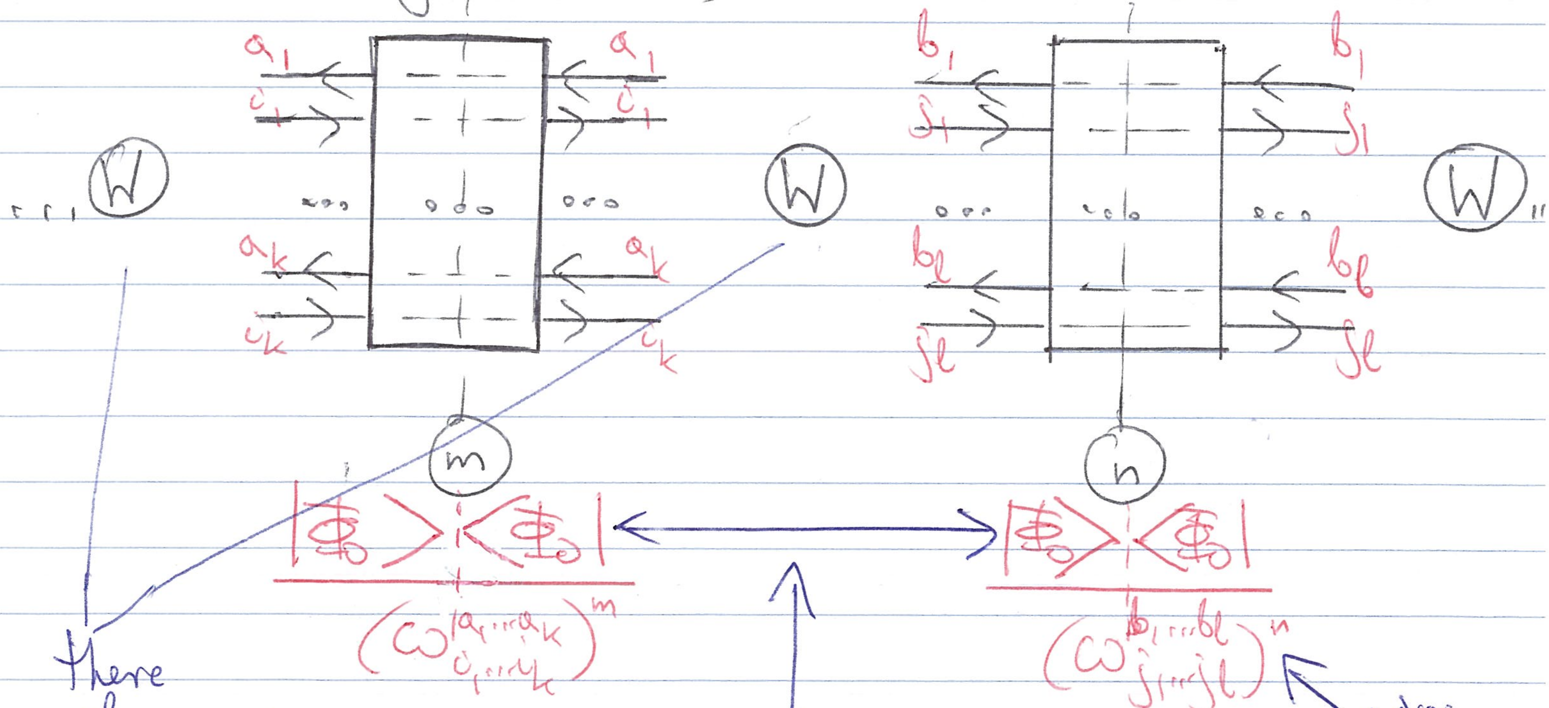


if we adopted the denominator convention.

The denominator convention of reading denominators from lines sliced between the neighboring Ws and the external lines originates from the observation that, in general, every MBPT expression has a structure

$$\cdots \underset{Q_N \text{ or } V_N}{W} \left(R^{(0)}\right)^m \underset{Q_N \text{ or } V_N}{W} \left(R^{(0)}\right)^n \underset{Q_N \text{ or } V_N}{W} \cdots$$

or, diagrammatically (schematically),

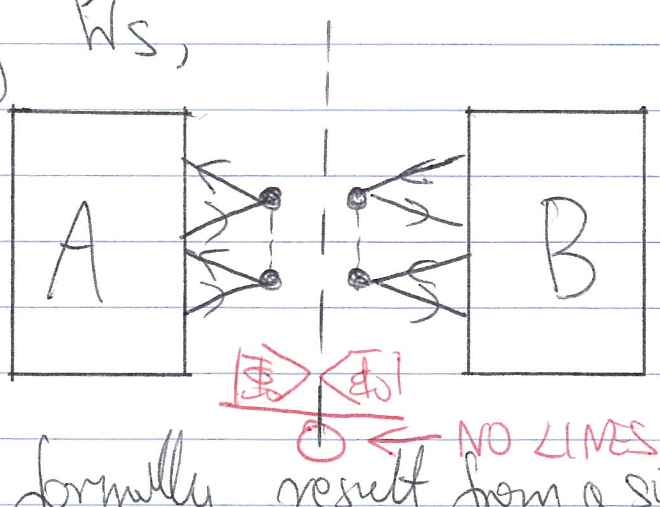


there always are lines between neighboring Ws

ALL LINES IN THIS REGION (between $\langle\Phi_0|$ and $|\Phi_0\rangle$) or between $(R^{(0)})^m$ and $(R^{(0)})^n$) MUST BE FULLY CONTRACTED

gives MBPT denominator

In other words, we do not need to draw diagrams representing reduced resolvents and can use the standard rules of constructing the resulting energy and wave function corrections from W vertices only, as if $R^{(0)}$'s were not present, if we adopt the denominator convention, i.e. the incorporation of denominators corresponding to fermion lines between the neighboring W vertices with the powers corresponding to powers of resolvents between theses Ws. The energy diagrams have no external lines and the wave function diagrams have lines extending to the left (representing excited determinants). The leftmost external lines in the wave function diagrams are also accompanied by the denominators corresponding to $(R^{(0)})^k$ showing up in the leftmost position in $|\Psi_0^{(n)}\rangle$. The denominator convention automatically excludes diagrams with "dangerous denominators", where there are no lines between neighboring Ws,



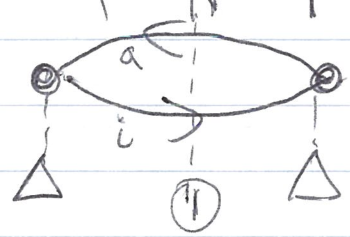
which would formally result from a singular expression $\dfrac{|\Phi_0\rangle\langle\Phi_0|}{\mathcal{E}_0-\mathcal{E}_0}$. We have learned that

$$\Delta E_0^{(2)} \equiv K_0^{(2)} = K_0^{(2)}(A) + K_0^{(2)}(B), \qquad (130)$$

where

$$K_0^{(2)}(A) = \langle\Phi_0|\mathcal{Q}_N R^{(0)} \mathcal{Q}_N|\Phi_0\rangle$$

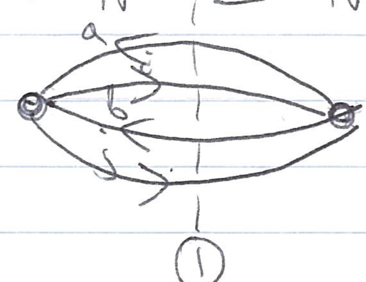
$$= \langle\Phi_0|\mathcal{Q}_N R_1^{(0)} \mathcal{Q}_N|\Phi_0\rangle$$

$=$ 

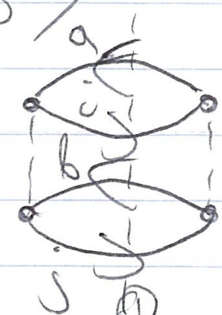
$$= \sum_{ia} \frac{\langle i|\hat{q}|a\rangle\langle a|\hat{q}|i\rangle}{\varepsilon_i-\varepsilon_a}, \qquad (131)$$

$$K_0^{(2)}(B) = \langle\Phi_0|V_N R^{(0)} V_N|\Phi_0\rangle$$

$$= \langle\Phi_0|V_N R_2^{(0)} V_N|\Phi_0\rangle$$

$=$ 

Hugenholtz

or 

Brandow

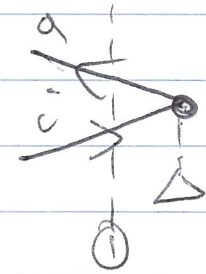
$$= \frac{1}{4} \sum_{ijab} \frac{\langle ij|\hat{v}|ab\rangle_A \langle ab|\hat{v}|ij\rangle_A}{\varepsilon_i - \varepsilon_a + \varepsilon_j - \varepsilon_b}$$

$$= \frac{1}{2} \sum_{ijab} \frac{\langle ij|\hat{v}|ab\rangle \langle ab|\hat{v}|ij\rangle_A}{\varepsilon_i - \varepsilon_a + \varepsilon_j - \varepsilon_b} . \quad (132)$$

$$|\Psi_0^{(1)}\rangle = |\Psi_0^{(1)}(A)\rangle + |\Psi_0^{(1)}(B)\rangle , \quad (133)$$

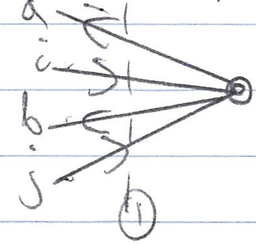
where

$$|\Psi_0^{(1)}(A)\rangle = R^{(0)} Q_N |\Phi_0\rangle = R_1^{(0)} Q_N |\Phi_0\rangle$$

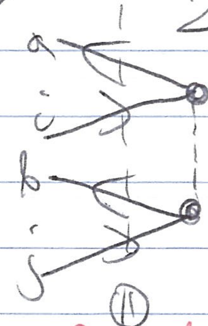
=


$$= \sum_{ia} \frac{\langle a|\hat{q}|i\rangle}{\varepsilon_i - \varepsilon_a} |\Phi_i^a\rangle , \quad (134)$$

$$|\Psi_0^{(1)}(B)\rangle = R^{(0)} V_N |\Phi_0\rangle = R_2^{(0)} V_N |\Phi_0\rangle$$

=


or



(135)

Hugenholtz Brandow

$$= \frac{1}{4} \sum_{ijab} \frac{\langle ab|\hat{v}|ij\rangle_A}{\varepsilon_i - \varepsilon_a + \varepsilon_j - \varepsilon_b} |\Phi_{ij}^{ab}\rangle = \frac{1}{2} \sum_{ijab} \frac{\langle ab|\hat{v}|ij\rangle}{\varepsilon_i - \varepsilon_a + \varepsilon_j - \varepsilon_b} |\Phi_{ij}^{ab}\rangle$$

In the following, we will sometimes use the notation,

$$\Delta^{(k)}(i_1,\ldots,i_n;a_1,\ldots a_n) = \left(\omega^{a_1\ldots a_n}_{i_1\ldots i_n}\right)^{-k}$$
$$= \left[\sum_{g=1}^{n}(\varepsilon_{i_g}-\varepsilon_{a_g})\right]^{-k}. \qquad (136)$$

Then, for example,

$$k_0^{(2)} = \sum_{i,a} \langle i|\hat{q}|a\rangle\langle a|\hat{q}|i\rangle \Delta^{(1)}(i;a)$$
$$+ \frac{1}{4}\sum_{i,j,a,b} \langle ij|\hat{v}|ab\rangle_A \langle ab|\hat{v}|ij\rangle_A$$
$$\times \Delta^{(1)}(i,j;a,b) \qquad (137)$$

$$|\Psi_0^{(1)}\rangle = \sum_{i,a}\langle a|\hat{q}|i\rangle \Delta^{(1)}(i;a)|\Phi_i^a\rangle$$
$$+ \frac{1}{4}\sum_{i,j,a,b}\langle ab|\hat{v}|ij\rangle_A \Delta^{(1)}(i,j;a,b)|\Phi_{ij}^{ab}\rangle$$
$$(138)$$

Note that in the H-F case ($\hat{q}=0$), there is no contribution from 1p-1h excitations to $|\Psi_0^{(1)}\rangle$ and $k_0^{(2)}$. 2p-2h excitations appear already in MBPT(2) energy and MBPT(1) wave function (not a surprise for H with 2-body interactions). The question is how far do we have to go to see 3p-3h, 4p-4h, etc. excitations.

5. Third-order MBPT correction to the energy

$$\Delta E_0^{(3)} \equiv K_0^{(3)} = \langle \Phi_0 | W R^{(0)} W R^{(0)} W | \Phi_0 \rangle$$

$$W = W_1 + W_2 = Q_N + V_N . \qquad (139)$$

There are the following groups of terms:

$$K_0^{(3)}(A) = \langle \Phi_0 | V_N R^{(0)} V_N R^{(0)} V_N | \Phi_0 \rangle, \qquad (140)$$

$$K_0^{(3)}(B) = \langle \Phi_0 | V_N R^{(0)} V_N R^{(0)} Q_N | \Phi_0 \rangle$$
$$+ \langle \Phi_0 | V_N R^{(0)} Q_N R^{(0)} V_N | \Phi_0 \rangle$$
$$+ \langle \Phi_0 | Q_N R^{(0)} V_N R^{(0)} V_N | \Phi_0 \rangle, \qquad (141)$$

$$K_0^{(3)}(C) = \langle \Phi_0 | Q_N R^{(0)} Q_N R^{(0)} V_N | \Phi_0 \rangle$$
$$+ \langle \Phi_0 | Q_N R^{(0)} V_N R^{(0)} Q_N | \Phi_0 \rangle$$
$$+ \langle \Phi_0 | V_N R^{(0)} Q_N R^{(0)} Q_N | \Phi_0 \rangle, \qquad (142)$$

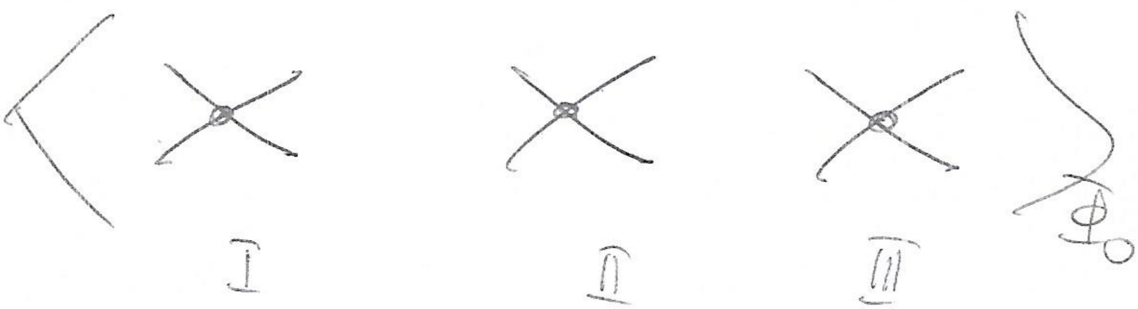
$$K_0^{(3)}(D) = \langle \Phi_0 | Q_N R^{(0)} Q_N R^{(0)} Q_N | \Phi_0 \rangle. \qquad (143)$$

We begin with the A term (the only term in the Hartree-Fock case; $Q_N = 0$).

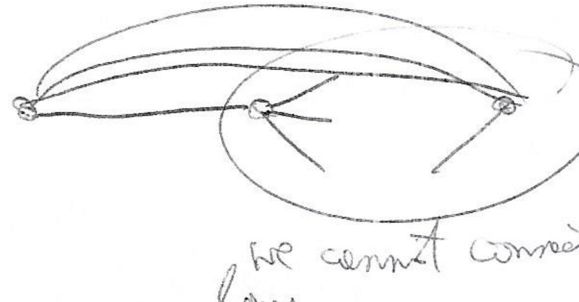
$$k_0^{(3)}(A) = \langle \Phi_0 | V_N R^{(0)} V_N R^{(0)} V_N | \Phi_0 \rangle . \quad (144)$$

We have to draw all nonequivalent resulting diagrams, with no external lines and without disappearing denominators, from three V_N vertices (remembering about the denominator convention):

Nonoriented Hugenholtz skeletons:

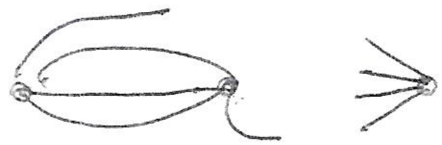


There are 4 lines at I. If none of the lines of I goes to II, all lines of I go to III and II is left not connected. Thus, at least 1 line of I has to be connected with II. If the remaining 3 lines of I are connected with III, we get

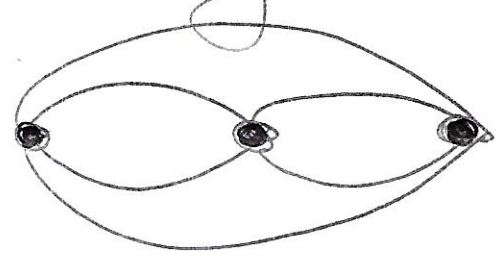


we cannot connect all these lines.

Thus, at least 2 lines of I have to be connected with II. If ≥ 3 lines of I are connected with II, we get

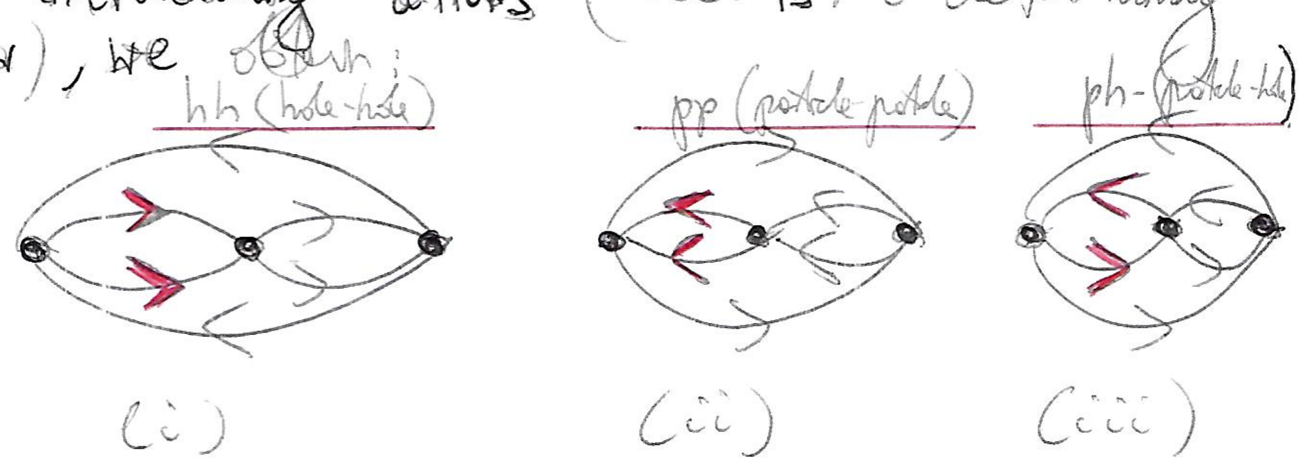


, from which we cannot get a diagram with no external lines (remember, Φ_N is in the N-product form). Thus, exactly 2 lines must connect I and II and exactly 2 lines must connect II and III. We end up with only one resulting skeleton:



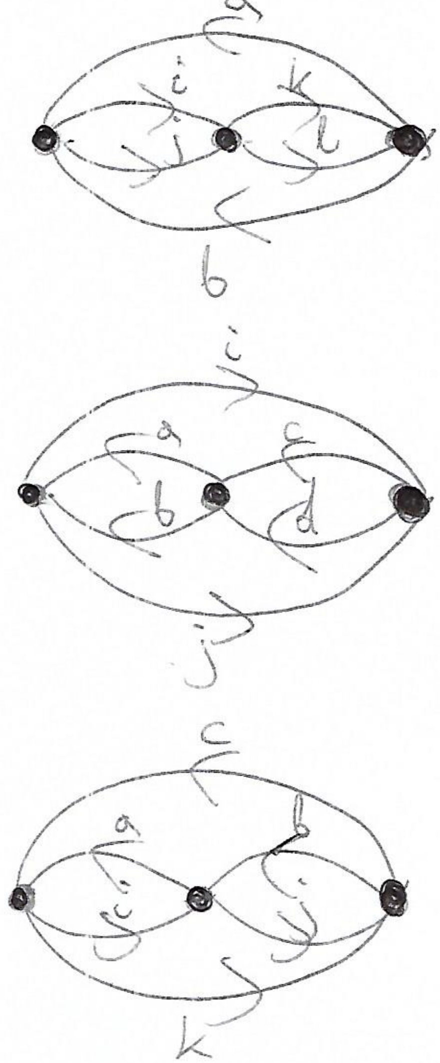
Oriented Hugenholtz diagrams.

By introducing arrows (red is the determining arrow), we obtain:

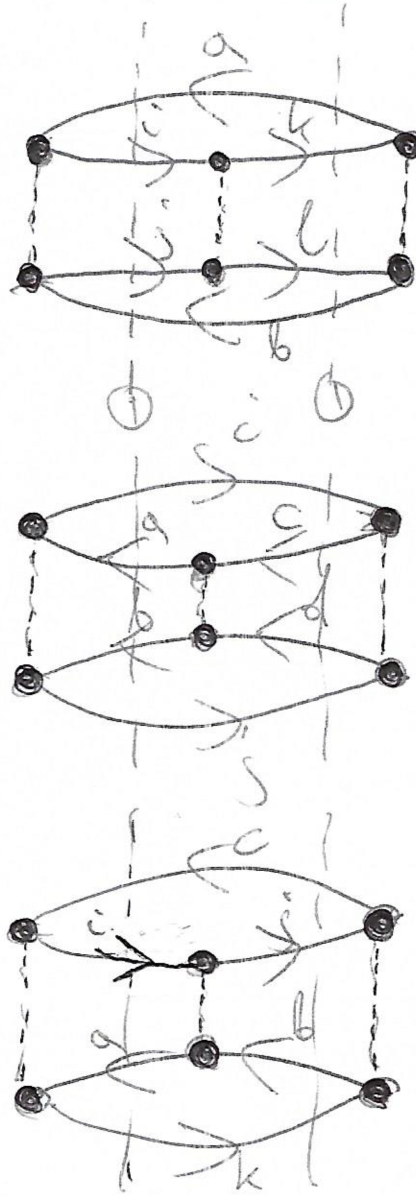


denominators from reduced resolvents

We obtain:



Hugenholtz



$W = \frac{1}{8}$

$S = +1$

$(\ell = 2, h = 4)$

$W = \frac{1}{8}$

$S = 1$

$(\ell = 2, h = 2)$

$W = 1$

$S = -1$

$(\ell = 2, h = 3)$

Brandow

We get the following result:

$$k_0^{(3)}(A) = k_0^{(3)}(hh) + k_0^{(3)}(pp) + k_0^{(3)}(ph), \qquad (145)$$

where

$$k_0^{(3)}(hh) = \frac{1}{8} \sum_{ab,ijkl} \langle ab|\hat{v}|kl\rangle_A \langle kl|\hat{v}|ij\rangle_A \times \langle ij|\hat{v}|ab\rangle_A \times \Delta^{(1)}(i,j;a,b)\Delta^{(1)}(k,l;a,b), \tag{146}$$

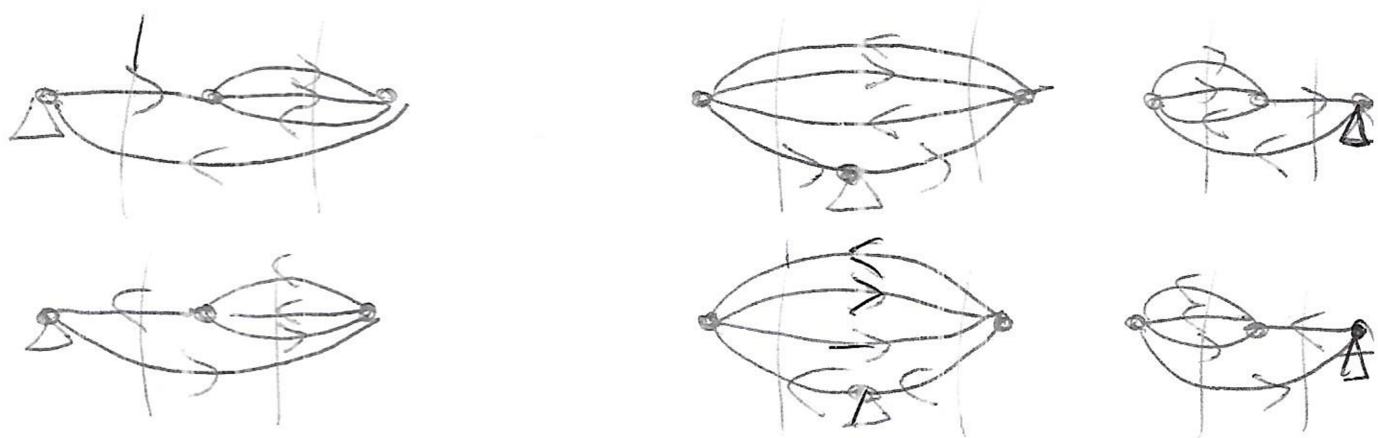
$$k_0^{(3)}(pp) = \frac{1}{8} \sum_{abcd,ij} \langle ij|\hat{v}|ab\rangle_A \langle ab|\hat{v}|cd\rangle_A \times \langle cd|\hat{v}|ij\rangle_A \times \Delta^{(1)}(i,j;a,b)\Delta^{(1)}(i,j;c,d), \tag{147}$$

$$k_0^{(3)}(ph) = -\sum_{abc,ijk} \langle bc|\hat{v}|kj\rangle_A \langle ja|\hat{v}|ib\rangle_A \times \langle ik|\hat{v}|ca\rangle_A \times \Delta^{(1)}(i,k;a,c)\Delta^{(1)}(j,k;b,c), \tag{148}$$

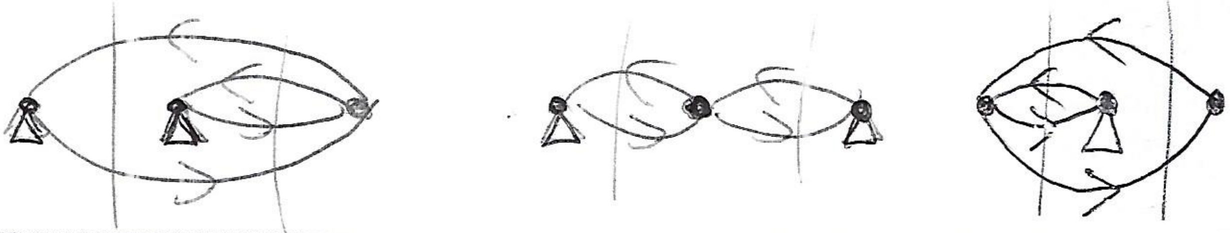
Other terms contributing to $K_0^{(3)}$ are:

$$K_0^{(3)}(B) = \langle \Phi_0 | Q_N R^{(0)} V_N R^{(0)} V_N | \Phi_0 \rangle$$
$$+ \langle \Phi_0 | V_N R^{(0)} Q_N R^{(0)} V_N | \Phi_0 \rangle$$
$$+ \langle \Phi_0 | V_N R^{(0)} V_N R^{(0)} Q_N | \Phi_0 \rangle ; \quad (149)$$

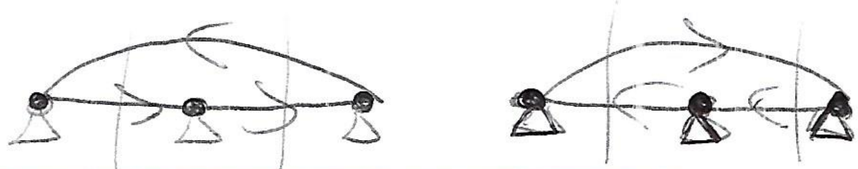
Hugenholtz diagrams:



$$K_0^{(3)}(C) = \langle \Phi_0 | Q_N R^{(0)} Q_N R^{(0)} V_N | \Phi_0 \rangle$$
$$+ \langle \Phi_0 | Q_N R^{(0)} V_N R^{(0)} Q_N | \Phi_0 \rangle$$
$$+ \langle \Phi_0 | V_N R^{(0)} Q_N R^{(0)} Q_N | \Phi_0 \rangle ; \quad (150)$$

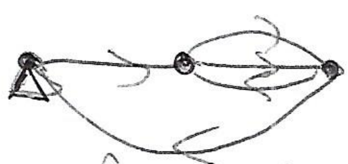


$$k_0^{(3)}(D) = \langle \Phi_0 | \hat{Q}_N R^{(0)} \hat{Q}_N R^{(0)} \hat{Q}_N | \Phi_0 \rangle \; ; \quad (151)$$

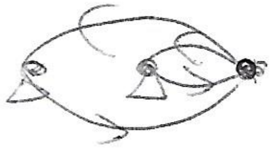


Please note that all of these diagrams containing at least one $\hat{Q}_N$ vertex can be grouped together..

Diagrams in the B group can be all obtained from



by allowing the $\hat{Q}_N$ and V_N vertices to be permuted.

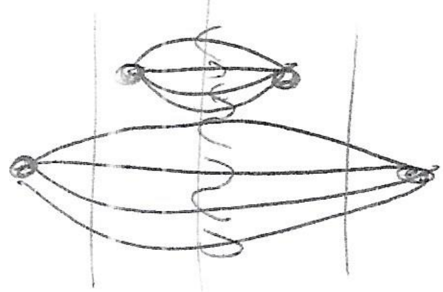
Similar applies to diagrams in the C group (can all be obtained from )

and in the D group (the  diagram can be obtained from ).

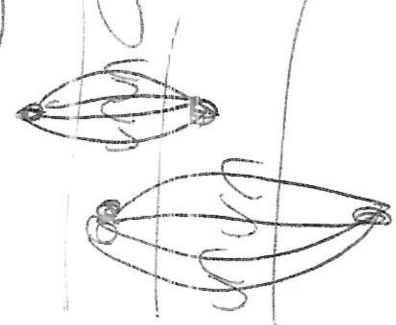
The diagrams that can be transformed into one another by topological transformations that do not break lines, but which do not preserve the order of operators along the horizontal time axis, are referred to as the TIME VERSIONS of the same diagram.

We distinguish between:

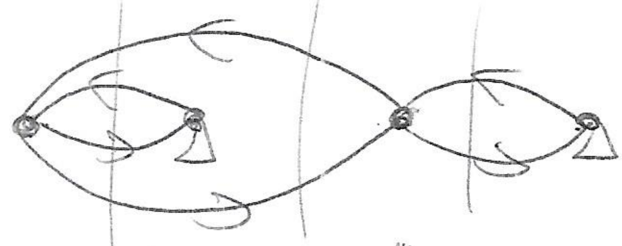
— time versions of the first level: vertices are permuted without changing the particle-hole character of any fermion line.



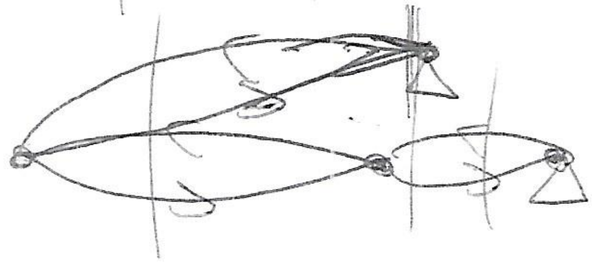
vs.



or



vs.



- time versions of the second kind: vertices are permuted along the time axis and at least one line changes its p-h character.

  Diagrams in each of the three groups B-D are in this category.

Time versions of the first kind are very important for proving the linked cluster theorem.

In terms of physics, $K_0^{(3)}$ does not bring information about higher than 2p-2h excitations. For example, $K_0^{(3)}(A)$, which survives any type of single-particle basis, describes the 3rd-order contribution to 2p-2h excitations, since the only reduced resolvents involved are the two-body $R_2^{(0)}$ components. This can be easily understood if we realise that the two-body interaction V_N cannot couple $|\Phi_0\rangle$ to higher than 2p-2h excitations,

m, n must be 2 $\Rightarrow$ $\langle\Phi_0|V_N R_m^{(0)} V_N R_n^{(0)} V_N|\Phi_0\rangle$.

We need to go to higher orders to see 3p-3h and other higher-order terms.

The remaining pages are taken directly from the lecture notes for CEM 993 class on "Algebraic and Diagrammatic Methods for Many-Fermion Systems," taught by Piotr Piecuch at Michigan State University. The page numbers are consecutive, but they do not continue from the last page number in the preceding lecture notes prepared for the Workshop of the *Espace de Structure et de Réactions Nucléaires Théorique* on "Many-Body Perturbation Theories in Modern Quantum Chemistry and Nuclear Physics," March 26-30, 2018, CEA Saclay, Gif-sur-Yvette, France.

Fourth-order MBPT energy contributions:

$$E_0^{(4)} = \langle \Phi_0 | W R^{(0)} W R^{(0)} W R^{(0)} W | \Phi_0 \rangle - \langle \Phi_0 | W R^{(0)} W | \Phi_0 \rangle \langle \Phi_0 | W R^{(0)2} W | \Phi_0 \rangle ,$$

where $W = V_N + \mathcal{L}_N$.

Let us look at the purely V_N terms:

$$\langle \Phi_0 | V_N (R^{(0)} V_N)^3 | \Phi_0 \rangle \quad \text{(principal term)}$$

$$- \underbrace{\langle \Phi_0 | V_N R^{(0)} V_N | \Phi_0 \rangle}_{E_0^{(2)}} \langle \Phi_0 | V_N R^{(0)2} V_N | \Phi_0 \rangle . \quad \text{(renorm. term)}$$

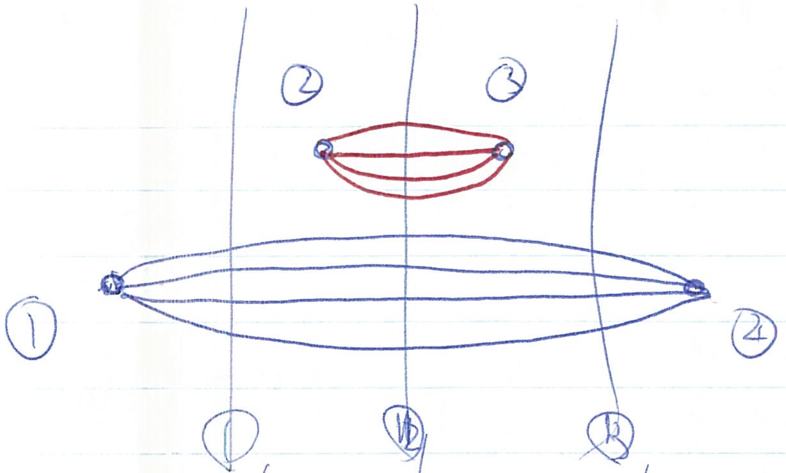
Principal term:

Nonorien. skels

← we will obtain skeletons by combining; 0, 1, 2, 3, 4 lines between ① and ②.

V2

I



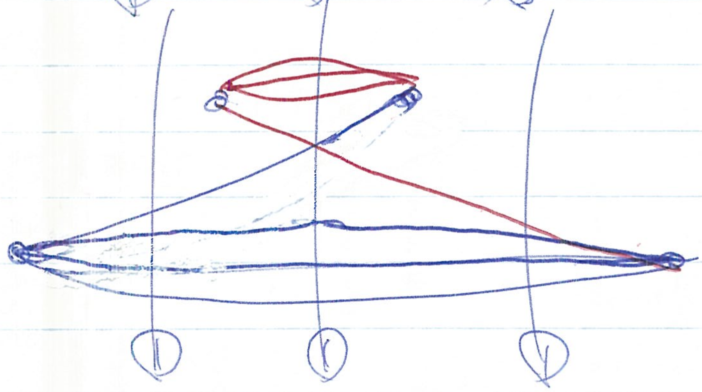
no lines between 1 and 2

[4 between 1 & 4]

|||

4+0

II

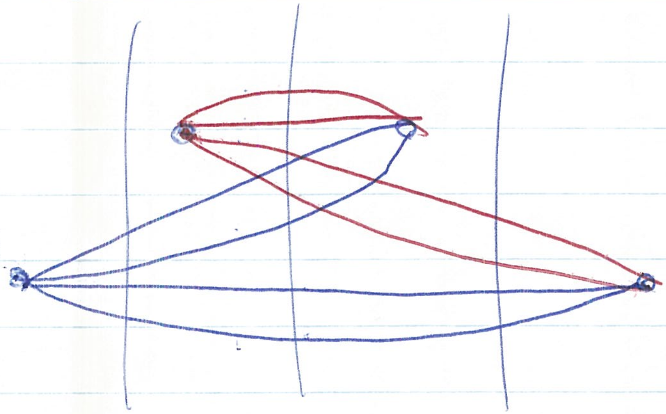


[3 between 1 & 4 and 1 between 1 and 3]

|||

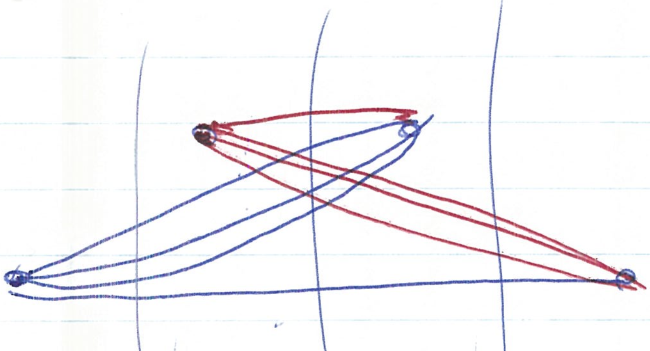
3+1

III



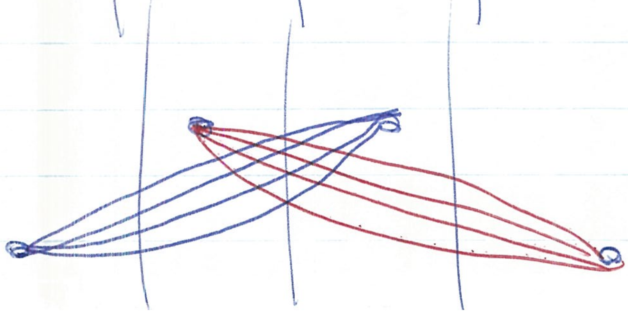
2+2

IV



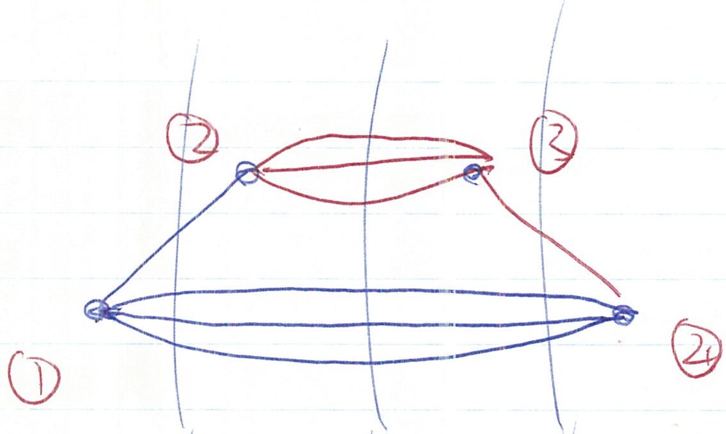
1+3

V



0+4

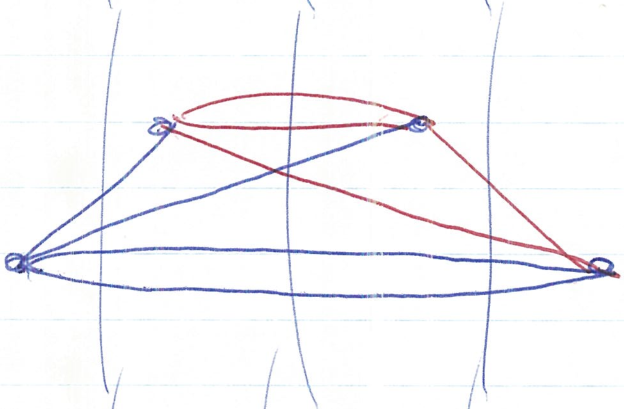
VI



1 line between 1 and 2

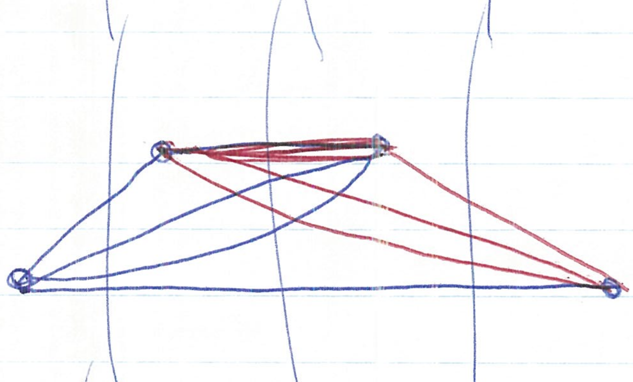
3 between 1 and 4
[3+0]

VII



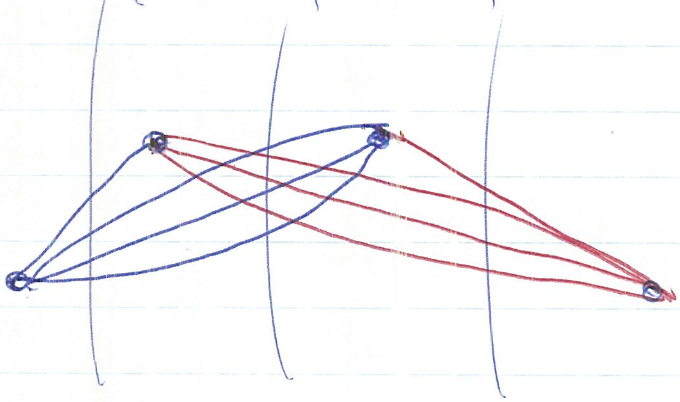
2+1

VIII



1+2

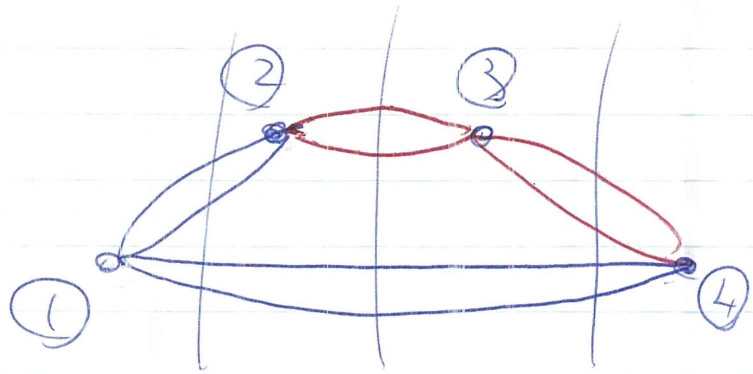
IX



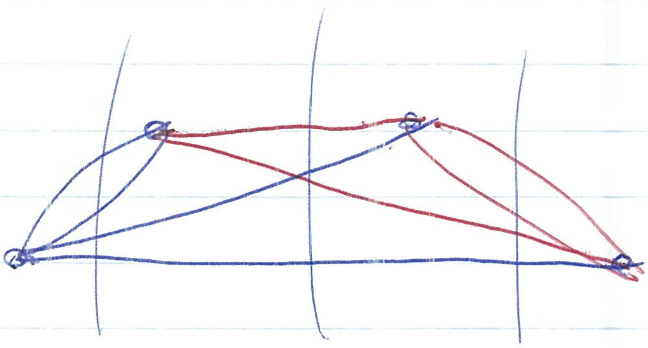
0+3

2 lines between 1 and 2

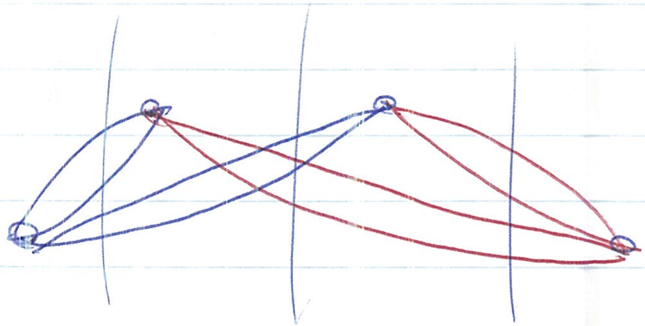
X



XI

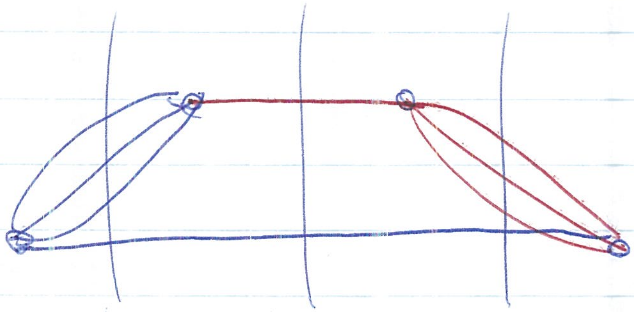


XII

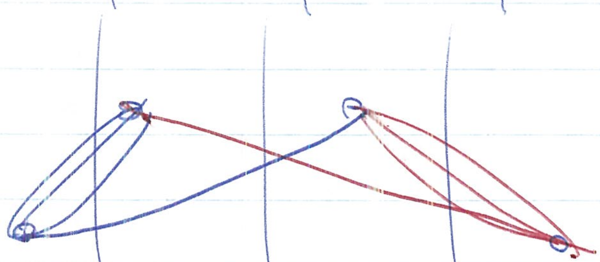


3 lines between 1 and 2

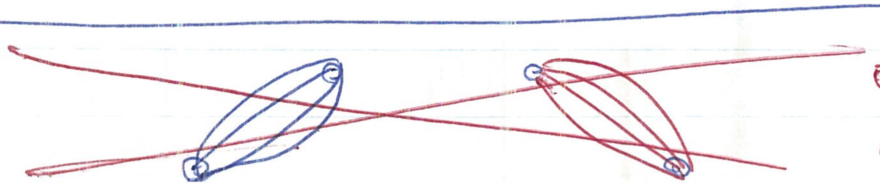
XIII



XIV



4 lines between 1 and 2



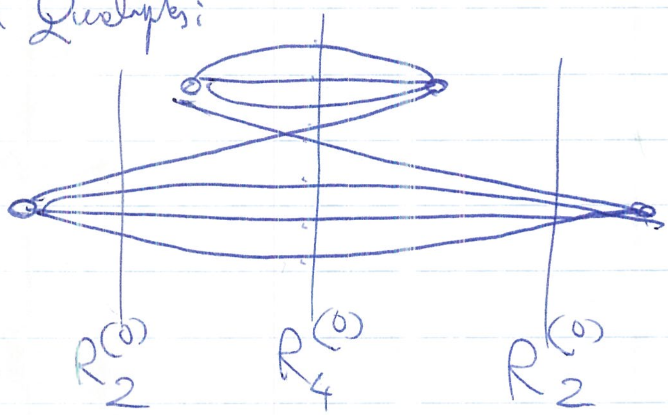
dangerous denominator.

Thus, we get the following diagrams in the principal term;

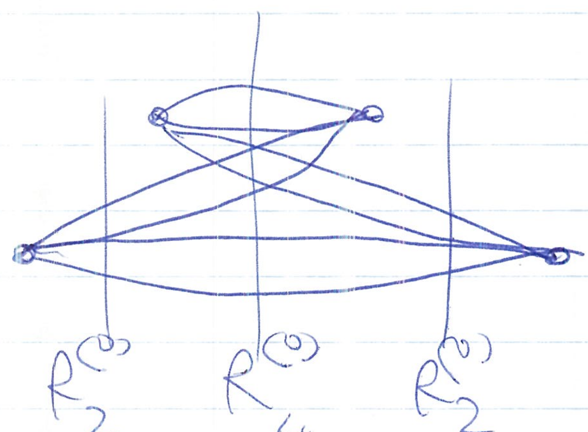
CONNECTED DIAGRAMS:

Intermediate Quadruples:

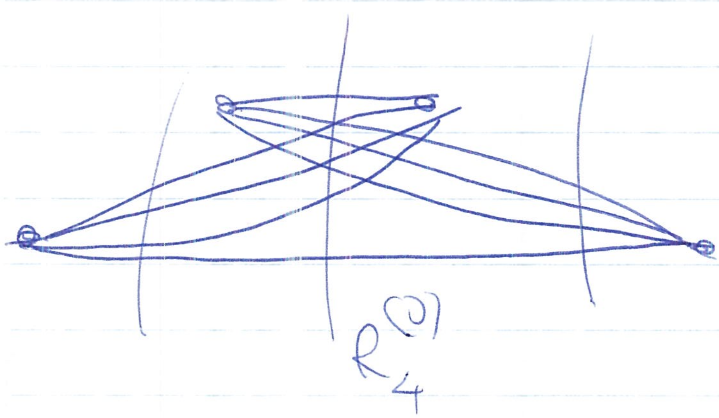
II



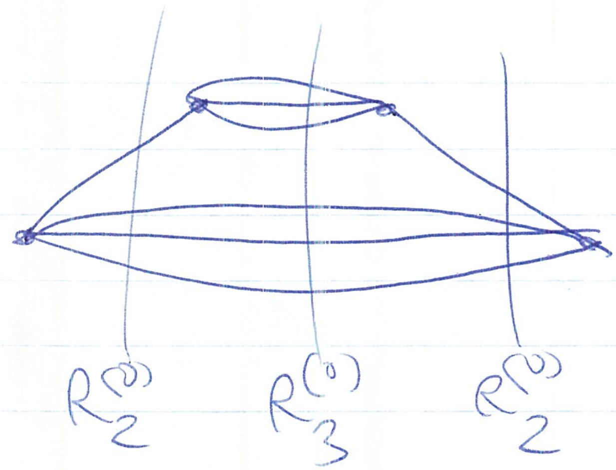
III



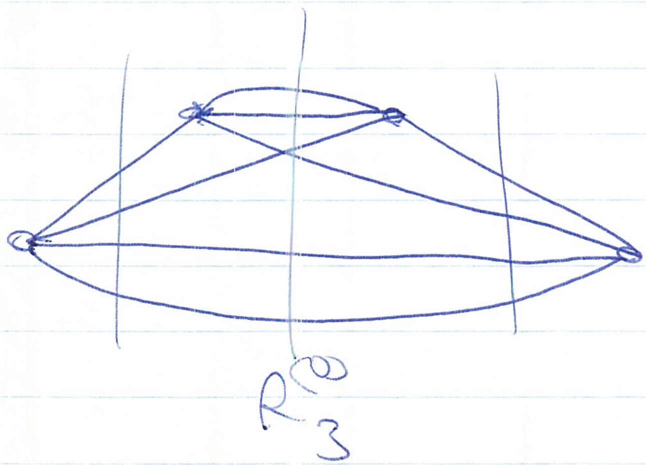
IV



Intermediate topologies

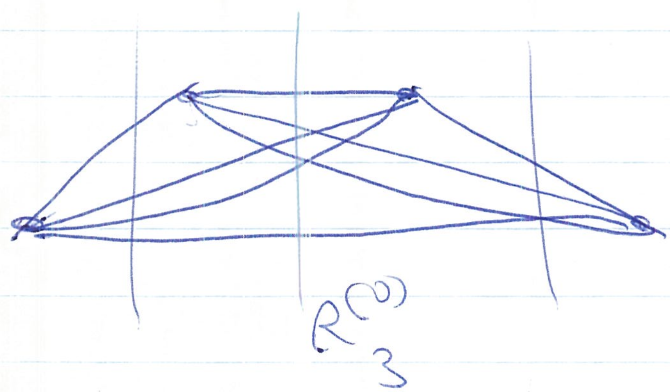


VI

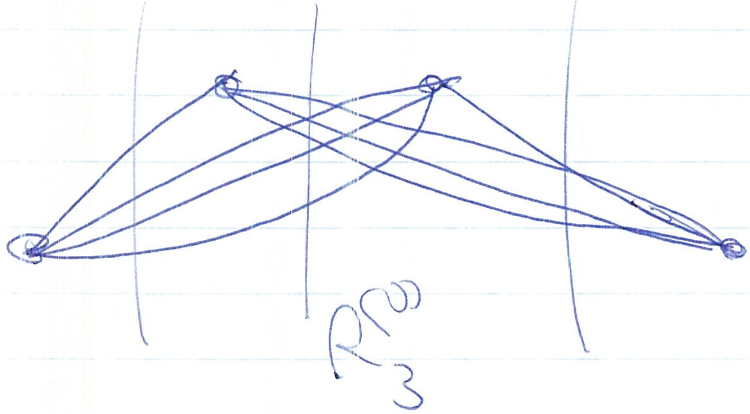


VII

VIII

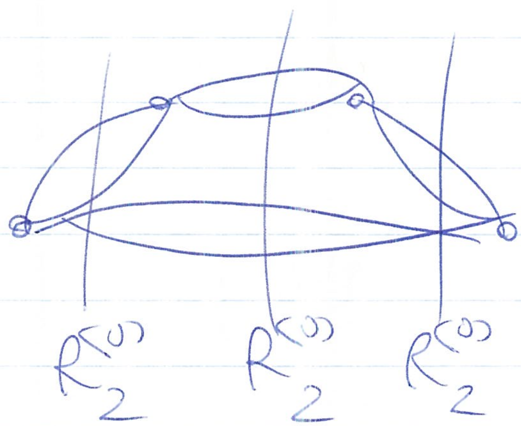


IX

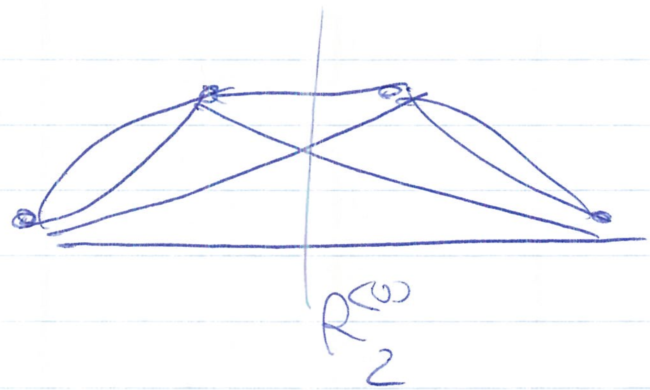


Intermediate doubles;

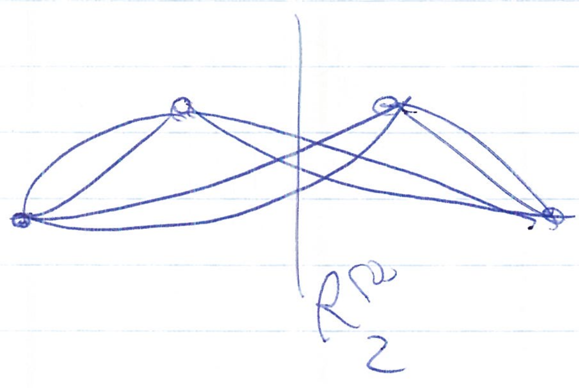
X



XI

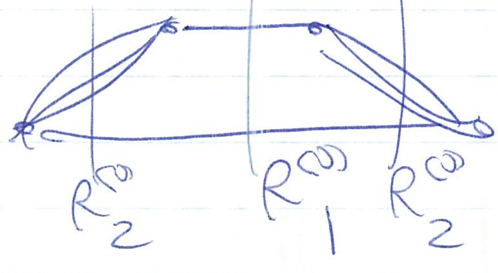


XII

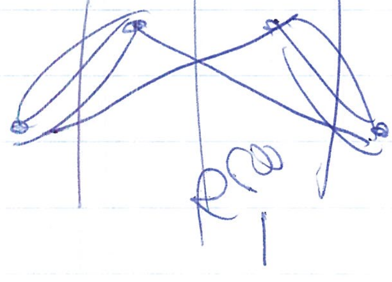


Intermediate singles;

XIII

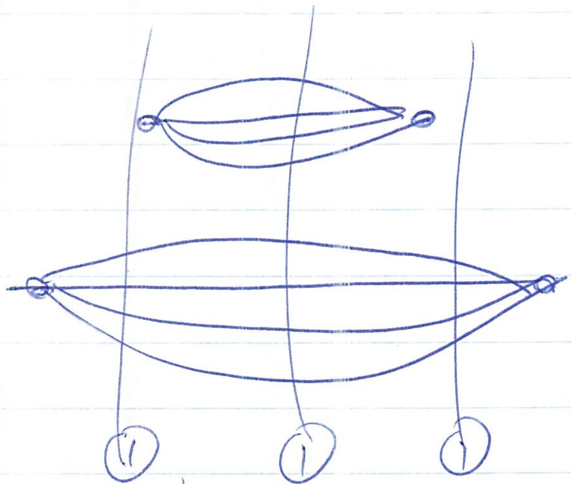


XIV

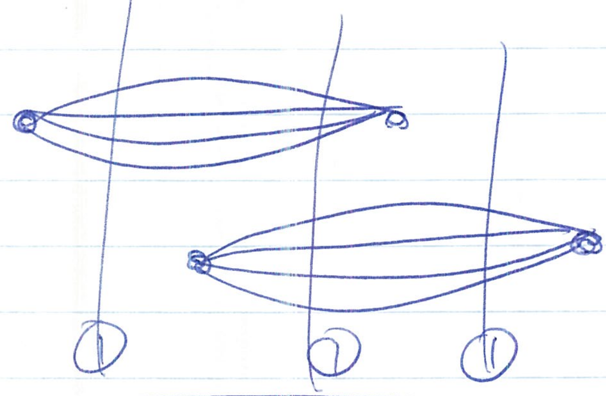


DISCONNECTED D-MS in the principal term:

I

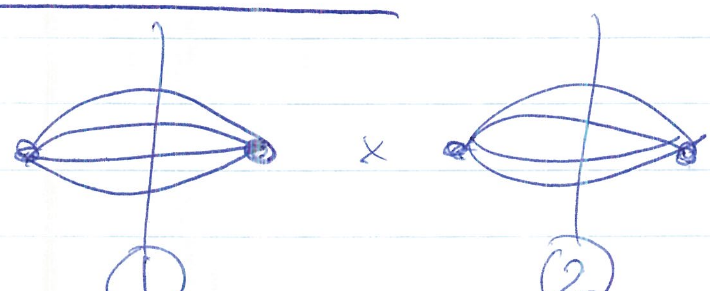


V



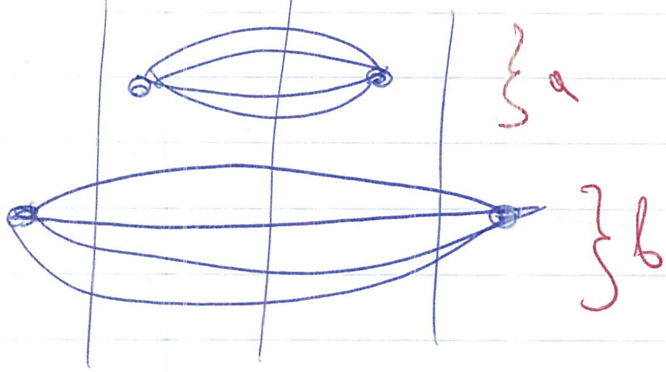
Renormalization terms:

$-$



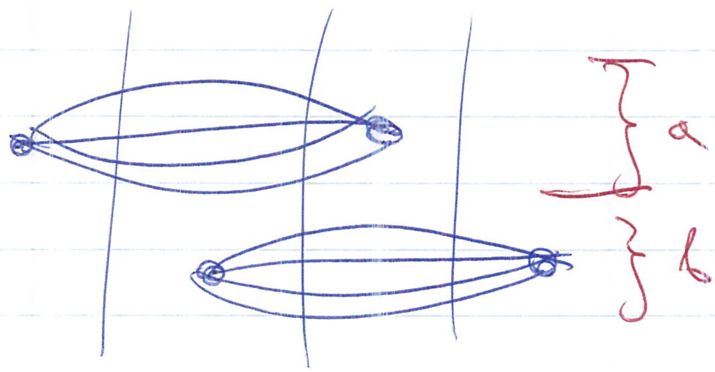
$\uparrow K_0^{(2)}$ $\qquad$ $\uparrow \langle\Phi_0|V_N R^{(0)^2} V_N|\Phi_0\rangle$

Let us see what happens with the disconnected terms from the principal term:

I 

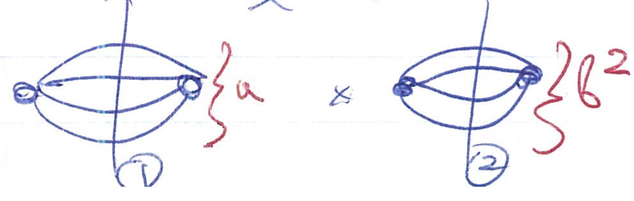
$$\mathrm{I} = \frac{N}{b(a+b)\,b}$$ ← numerator

(summed over the relevant spin orbital choices)

II 

$$\mathrm{II} = \frac{N}{a(a+b)\,b}$$ ← the same numerator

$$\mathrm{I} + \mathrm{II} = \frac{N}{(a+b)\,b}\left(\frac{1}{a} + \frac{1}{b}\right) = \frac{N}{\cancel{(a+b)}\,b}\,\frac{\cancel{(a+b)}}{ab}$$

$$= \frac{N}{ab^2} =$$ 

As we can see, the disconnected terms from the principal term cancel the renormalization terms:

$$K_0^{(4)} = \langle \Phi_0 | W (R^{(0)} W)^3 | \Phi_0 \rangle - \langle \Phi_0 | W R^{(0)} W | \Phi_0 \rangle$$
$$\times \langle \Phi_0 | W R^{(0)2} W | \Phi_0 \rangle$$
$$= \underbrace{\langle \Phi_0 | \{ W (R^{(0)} W)^3 \}_C | \Phi_0 \rangle}_{\text{connected}} +$$
$$+ \cancel{\underbrace{\langle \Phi_0 | \{ W (R^{(0)} W)^3 \}_{DC} | \Phi_0 \rangle}_{\text{disconnected}}}$$
$$- \cancel{\langle \Phi_0 | W R^{(0)} W | \Phi_0 \rangle \langle \Phi_0 | W R^{(0)2} W | \Phi_0 \rangle}$$

$$\boxed{K_0^{(4)} = \langle \Phi_0 | \{ W (R^{(0)} W)^3 \}_C | \Phi_0 \rangle}$$

This is an example of a cancellation that takes place in every order and which is summarized by the linked-cluster theorem which states that

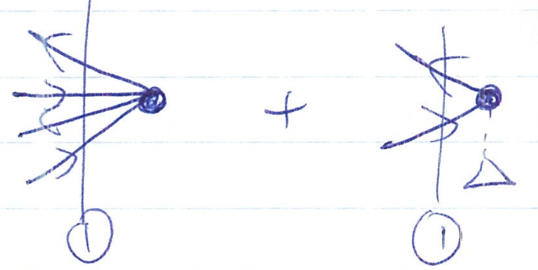
$$K_0^{(n+1)} = \langle \Phi_0 | \{ W (R^{(0)} W)^n \}_C | \Phi_0 \rangle .$$

A similar cancellation occurs in the wave function contributions. To understand this cancellation in wave function corrections, let us look at a few low order contributions to $|\Psi_0\rangle$.

We have already analysed $|\Psi_0^{(1)}\rangle$:

$$|\Psi_0^{(1)}\rangle = R^{(0)} W |\Phi_0\rangle = R^{(0)} V_N |\Phi_0\rangle +$$

$$+ R^{(0)} Q_N |\Phi_0\rangle =$$

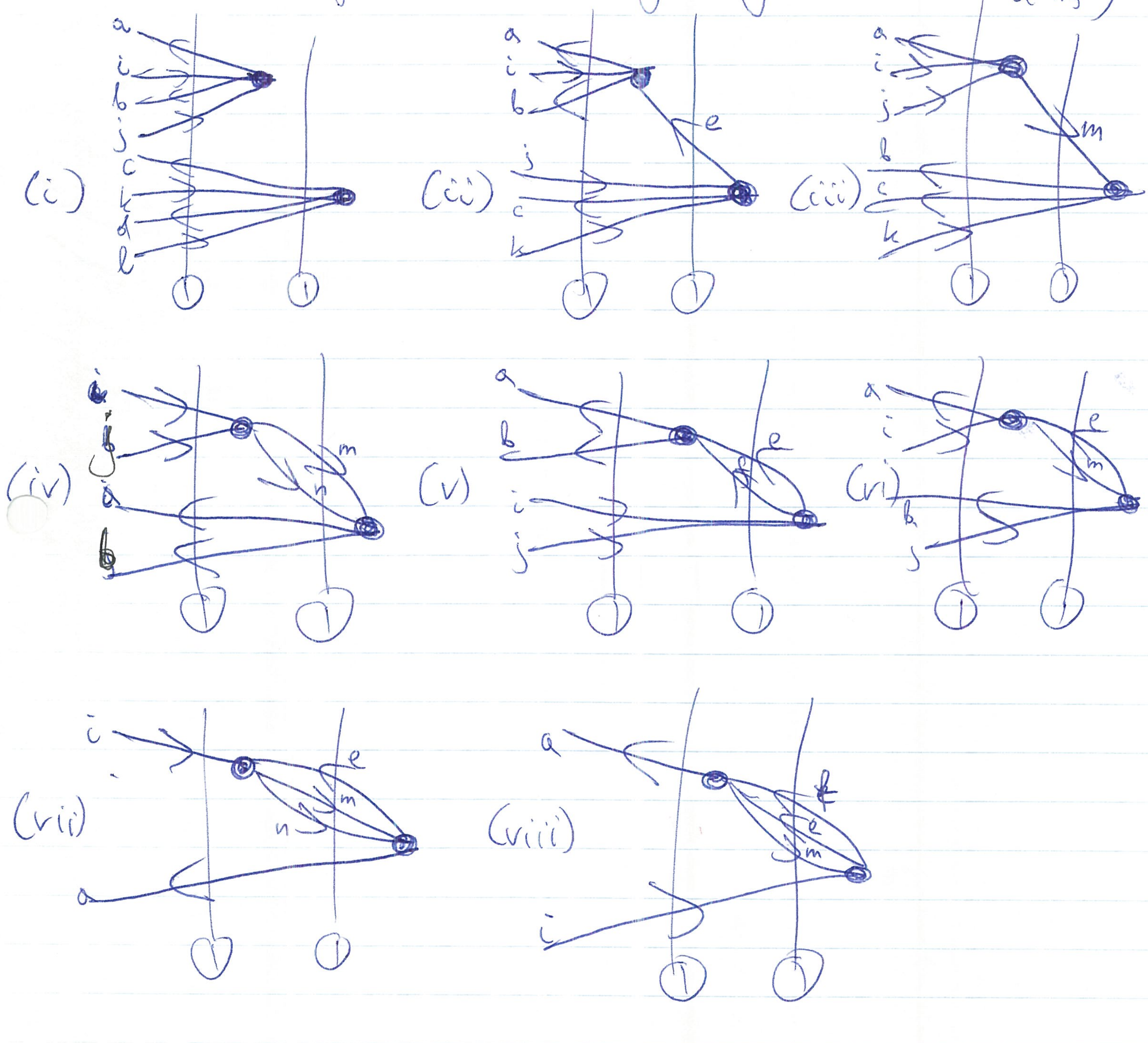


Nothing interesting happens here, both contributions to the wave function are CONNECTED.

Let us look at $|\Psi_0^{(2)}\rangle$:

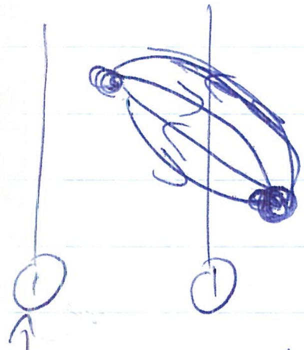
$$|\Psi_0^{(2)}\rangle = R^{(0)} W R^{(0)} W |\Phi_0\rangle$$ (there are no renormalization terms).

Let us analyze terms that originate from V_N (Hugenholtz d-ms):



(in all d-ms, all lines extend to the left)

Please note that we did not draw



this would be a "dangerous denominator".

Clearly, we must always have some external lines in each of the wave function diagrams (because of the leftmost $R^{(0)}$).

As we can see,

$$|\Psi_0^{(2)}\rangle = |\Psi_0^{(2)}(Q)\rangle + |\Psi_0^{(2)}(T)\rangle + |\Psi_0^{(2)}(D)\rangle + |\Psi_0^{(2)}(S)\rangle$$

quadruples $|\Phi_{ijkl}^{abcd}\rangle$ (disconnected)

triples $|\Phi_{ijk}^{abc}\rangle$

doubles $|\Phi_{ij}^{ab}\rangle$

singles $|\Phi_i^a\rangle$.

Triples and quadruples contribute for the first time in the second-order MBPT wave function. Singles contribute for the first time in $|\Psi_0^{(2)}\rangle$ if H-F orbitals are used.

Diagrams contributing to $|\Psi_0^{(2)}\rangle$ are of the two types: connected (diagrams (ii)-(viii)) and disconnected (term (i)). Thus, if there is a cancellation of diagrams in the wave function, the cancellation must involve some other diagrams than just disconnected.

Well, let us look at the 3rd order:

$$|\Psi_0^{(3)}\rangle = R^{(0)}WR^{(0)}WR^{(0)}W|\Phi_0\rangle$$

$$- \langle WR^{(0)}W\rangle R^{(0)2}W|\Phi_0\rangle.$$

Again, let us focus on the contributions originating from V_N terms; we will draw skeletons only:

$(R^{(0)}V_N)^3|\Phi_0\rangle$ TERM (principal term)

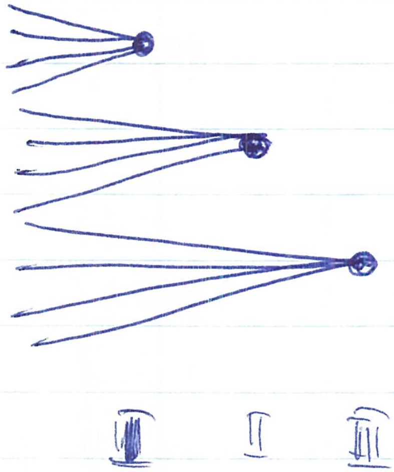
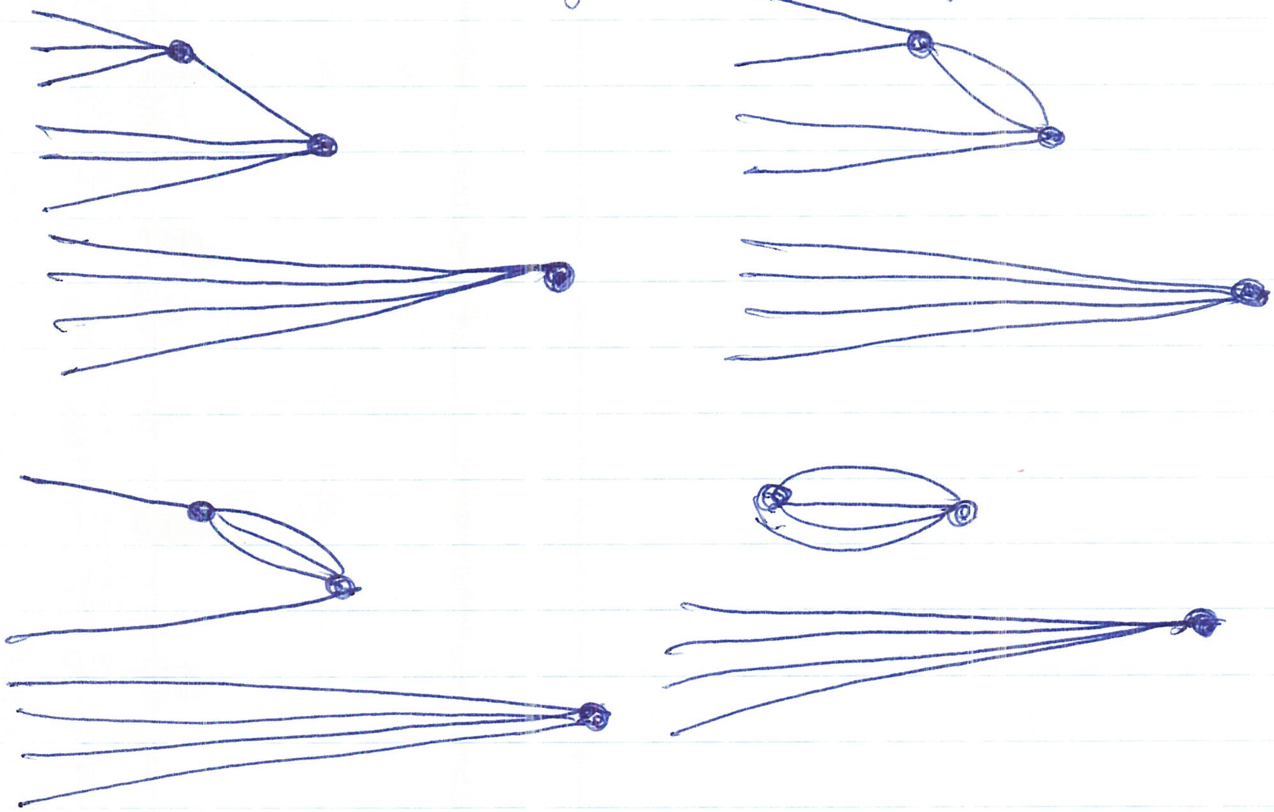
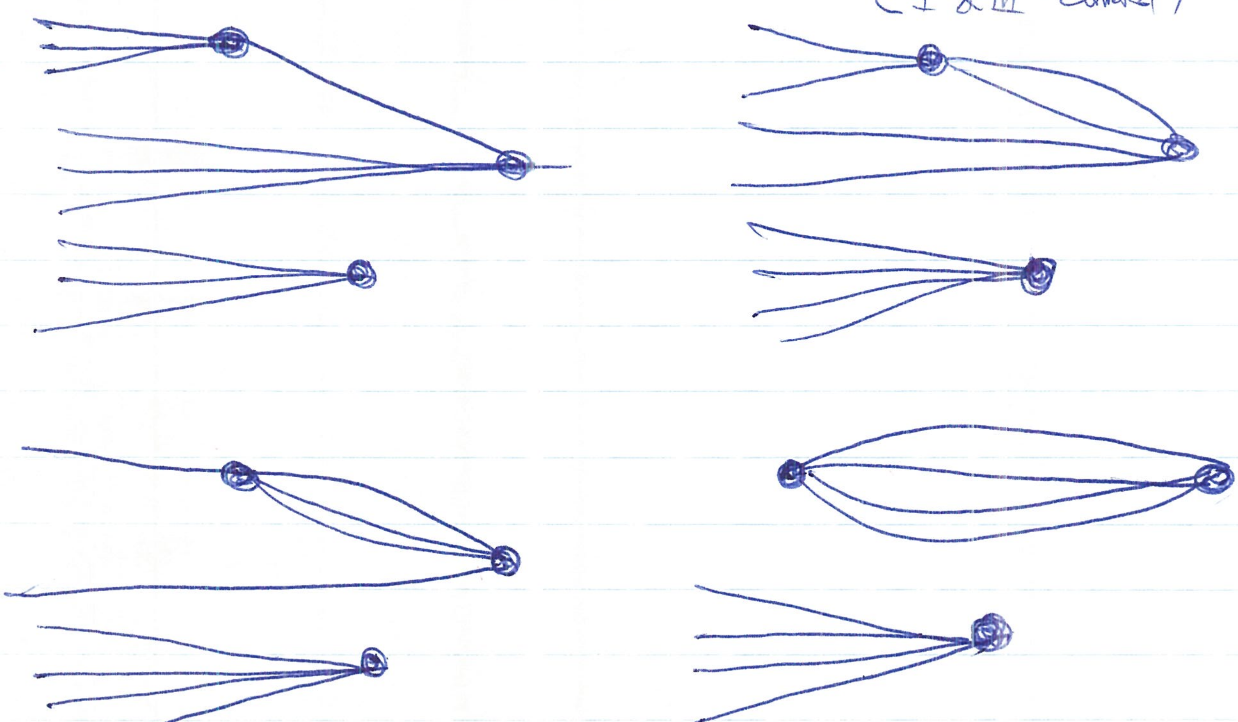


Diagram with 3 connected parts

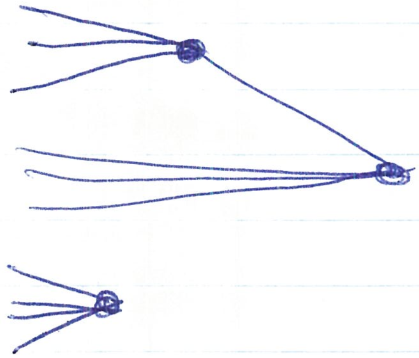
diagrams with 2 connected parts (III & II connected)

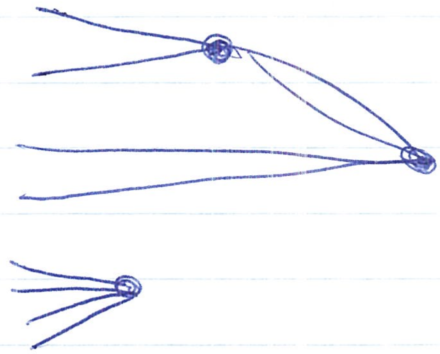


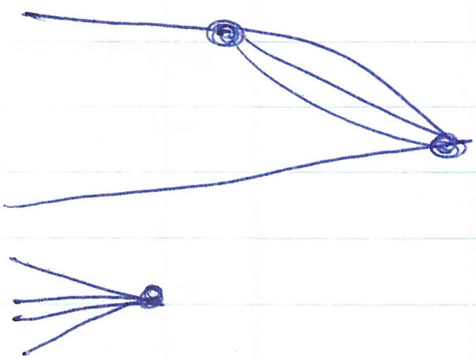
(I & III connected)

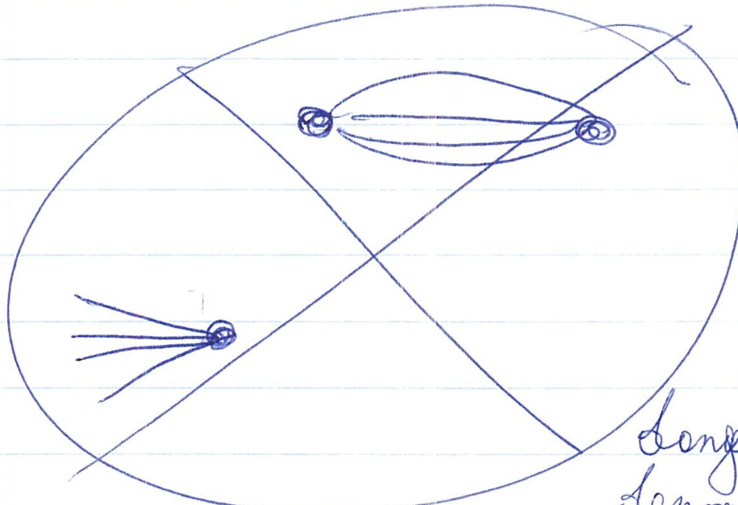


(II and III connected)



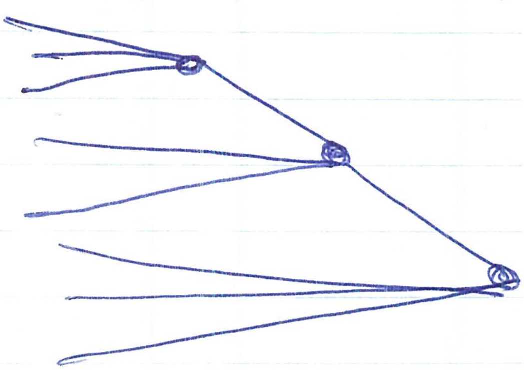


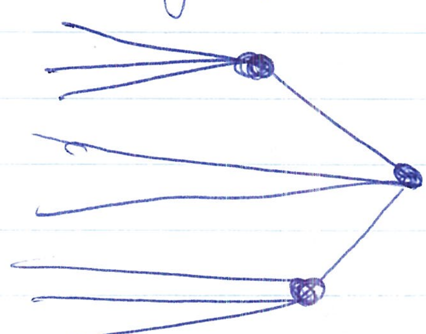


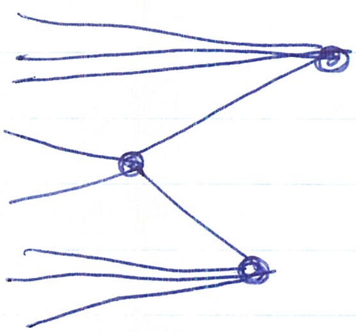


dangerous denominator

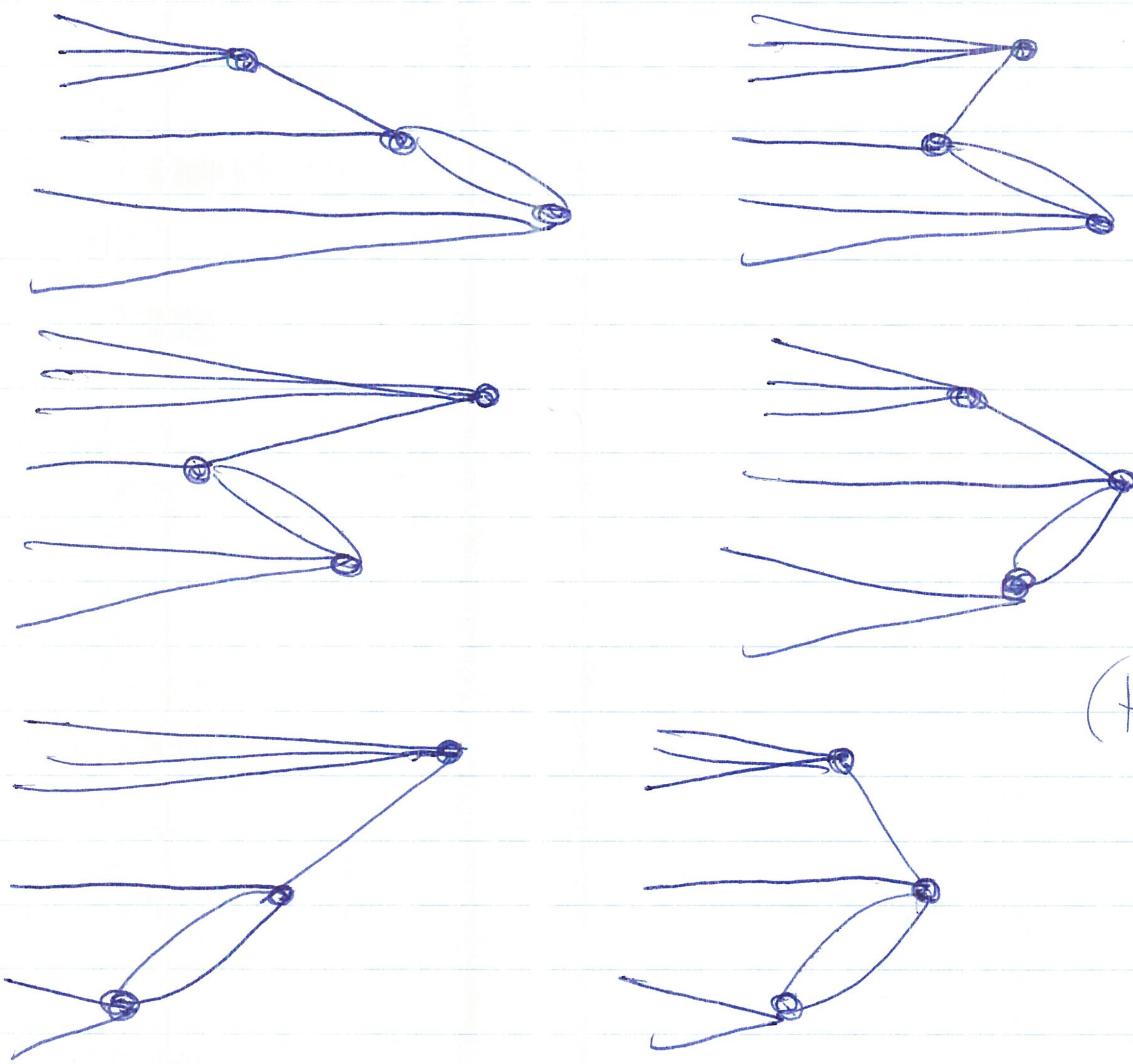
diagrams with one connected part
(connected diagrams)







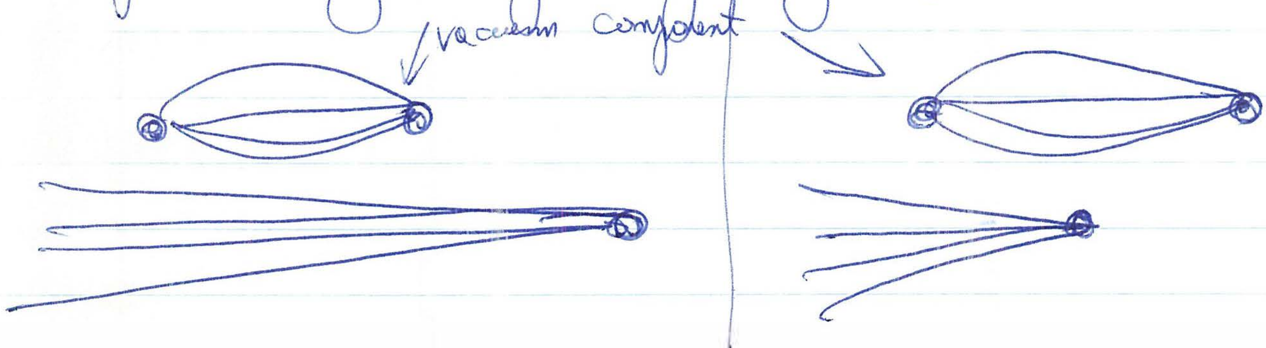
(time versions of the 2nd kind)

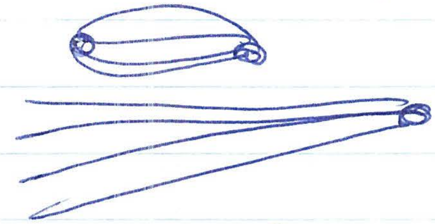


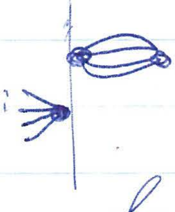
(time versions of the second kind)

etc.

Please notice the presence of two (disconnected) diagrams, which contain the closed (vacuum) component among diagrams forming $(R^{(0)}W)^{3+}(\Phi_0)$:
no ext. lines



These two diagrams are two time versions of the first term obtained from 

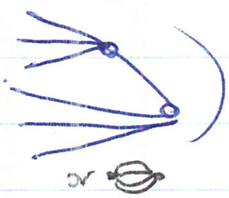
(The third time version:  is excluded, since it would lead to a dangerous denominator.

The above two diagrams are examples of the UNLINKED diagrams: In general, a disconnected diagram that has at least one disconnected vacuum component is called UNLINKED.

LINKED diagrams have no disconnected vacuum parts.

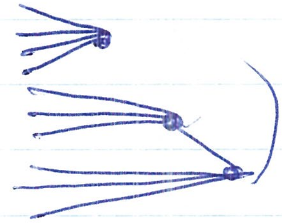
We have the following classification of diagrams:

CONNECTED → LINKED (e.g.



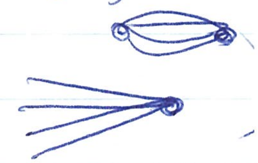
)

DISCONNECTED → LINKED (e.g.



)

DISCONNECTED → UNLINKED (e.g.



CONNECTED → LINKED

DISCONNECTED → LINKED

DISCONNECTED → UNLINKED

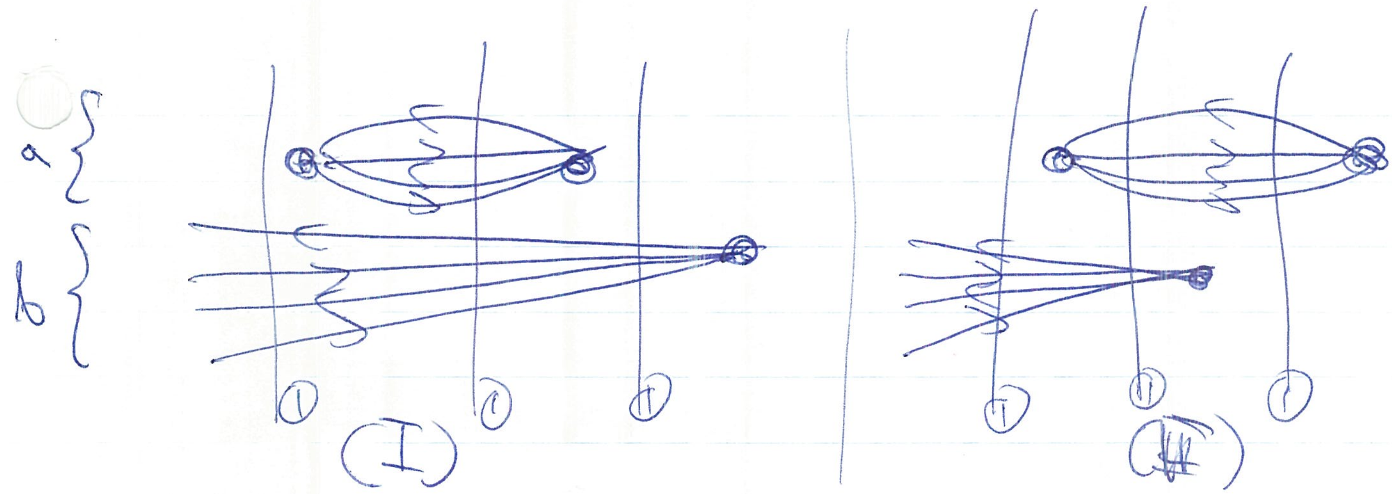
Any unlinked diagram is, by definition, disconnected. However, a linked diagram can be connected or disconnected.

We can write (referring to the $|\Psi_0^{(3)}\rangle$ case):

$$\left.\begin{array}{l} \left.\begin{array}{l} |\Psi_0^{(3)}\rangle = \{(R^{(0)}W)^3\}_C\,|\Phi_0\rangle \\[2ex] \quad + \{(R^{(0)}W)^3\}_{\underbrace{DC,L}_{\text{disconnected, linked}}}\,|\Phi_0\rangle \end{array}\right\} \Rightarrow \text{LINKED} \\[4ex] \quad + \{(R^{(0)}W)^3\}_{\underset{\text{unlinked}}{UL}}\,|\Phi_0\rangle \end{array}\right\} \text{principal term}$$

$$- \langle\Phi_0|WR^{(0)}W|\Phi_0\rangle\, R^{(0)2}W\,|\Phi_0\rangle \Big\}\ \text{renorm. term}$$

The $\{(R^{(0)}W)^3\}_{UL}|\Phi_0\rangle$ part is represented by two time versions of the first kind containing the vacuum part;



$$(\mathrm{I}) = \frac{N}{b(a+b)b}$$

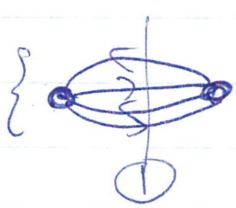
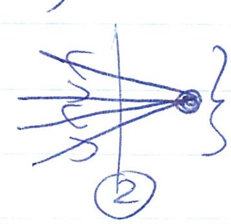
$$(\mathrm{II}) = \frac{N}{b(a+b)a}$$

← (summed over the relevant spin-orbital labels).

[N is the numerator, i.e. the product of the v matrix elements and $\psi^\dagger$ operators corresponding to external lines, signs, and weight factors]

$$\left\{\left(R^{(0)}W\right)^3\right\}_{UL}|\Phi_0\rangle = \frac{N}{b(a+b)b} + \frac{N}{b(a+b)a}$$

$$= \frac{N}{b(a+b)}\left(\frac{1}{b}+\frac{1}{a}\right) = \frac{N}{b\cancel{(a+b)}}\,\frac{\cancel{a+b}}{ab}$$

$$= \frac{N}{ab^2} =$$ a  ×  b

$$= \langle \Phi_0 | W R^{(0)} W | \Phi_0 \rangle \, R^{(0)^2} W | \Phi_0 \rangle .$$

Thus, the unlinked part of $|\Psi_0^{(3)}\rangle$ cancels the renormalization term and we obtain:

$$|\Psi_0^{(3)}\rangle = \{(R^{(0)}W)^3\}_C |\Phi_0\rangle$$

$$+ \{(R^{(0)}W)^3\}_{DC,L} |\Phi_0\rangle \equiv \underbrace{\{(R^{(0)}W)^3\}_L}_{\text{linked}} |\Phi_0\rangle$$

A very similar cancellation of unlinked principal and renormalization terms takes place in every order,

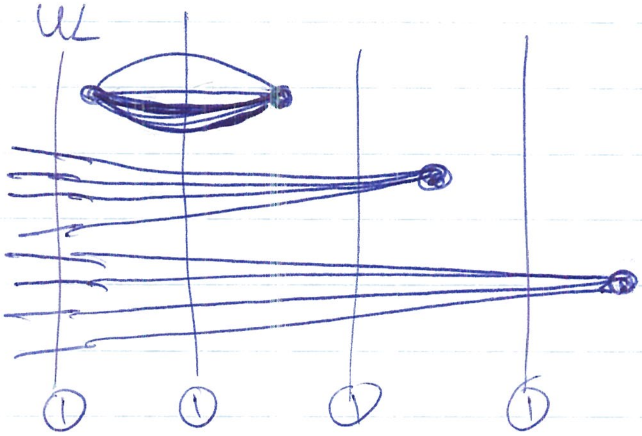
$$|\Psi_0^{(n)}\rangle = \underbrace{\{(R^{(0)}W)^n\}_L}_{\text{only linked diagrams}} |\Phi_0\rangle ,$$

For example, in the 4th order, the unlinked principal terms are:

$$\{(R^{(0)}W)^4\}|\Phi_0\rangle \Rightarrow$$

$\Rightarrow$

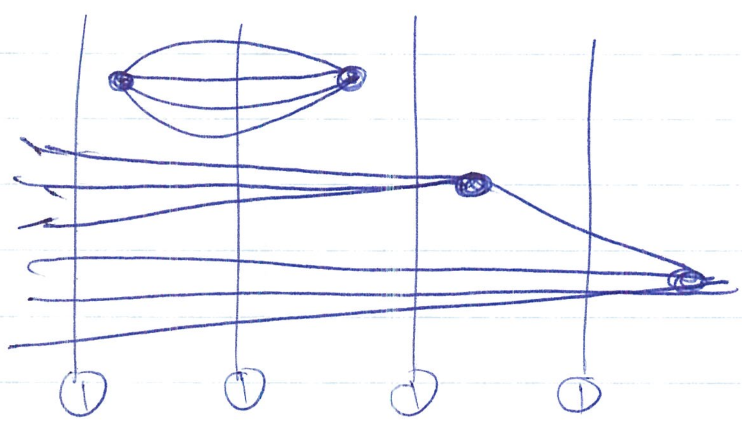
(i)



+ time versions of the 1st level

+

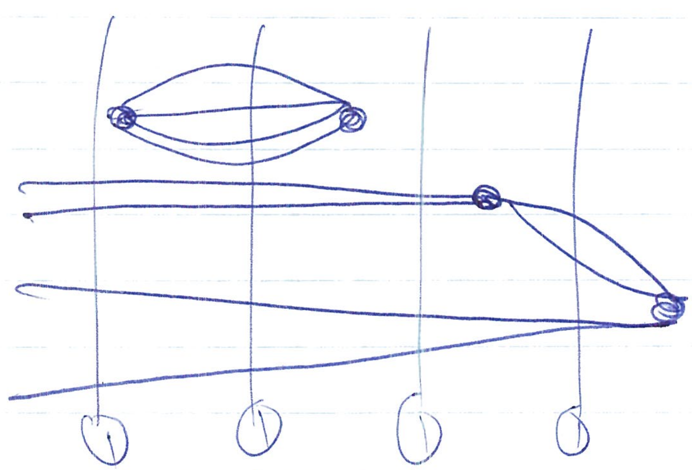
(ii)



+ time versions of the 1st level

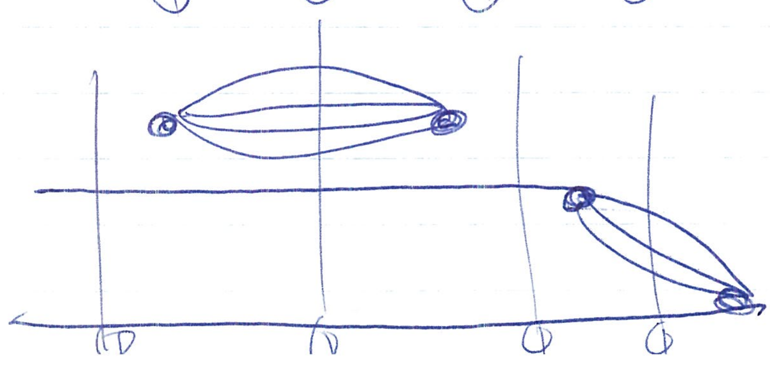
+

(iii)

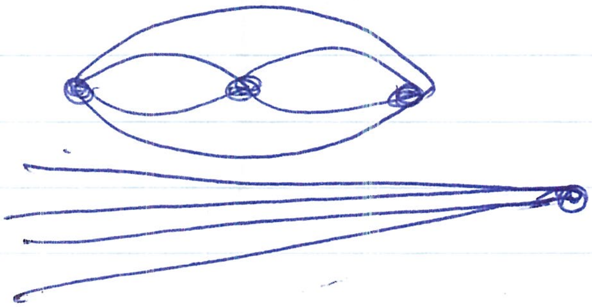


+ time versions of the 1st level

(iv) +

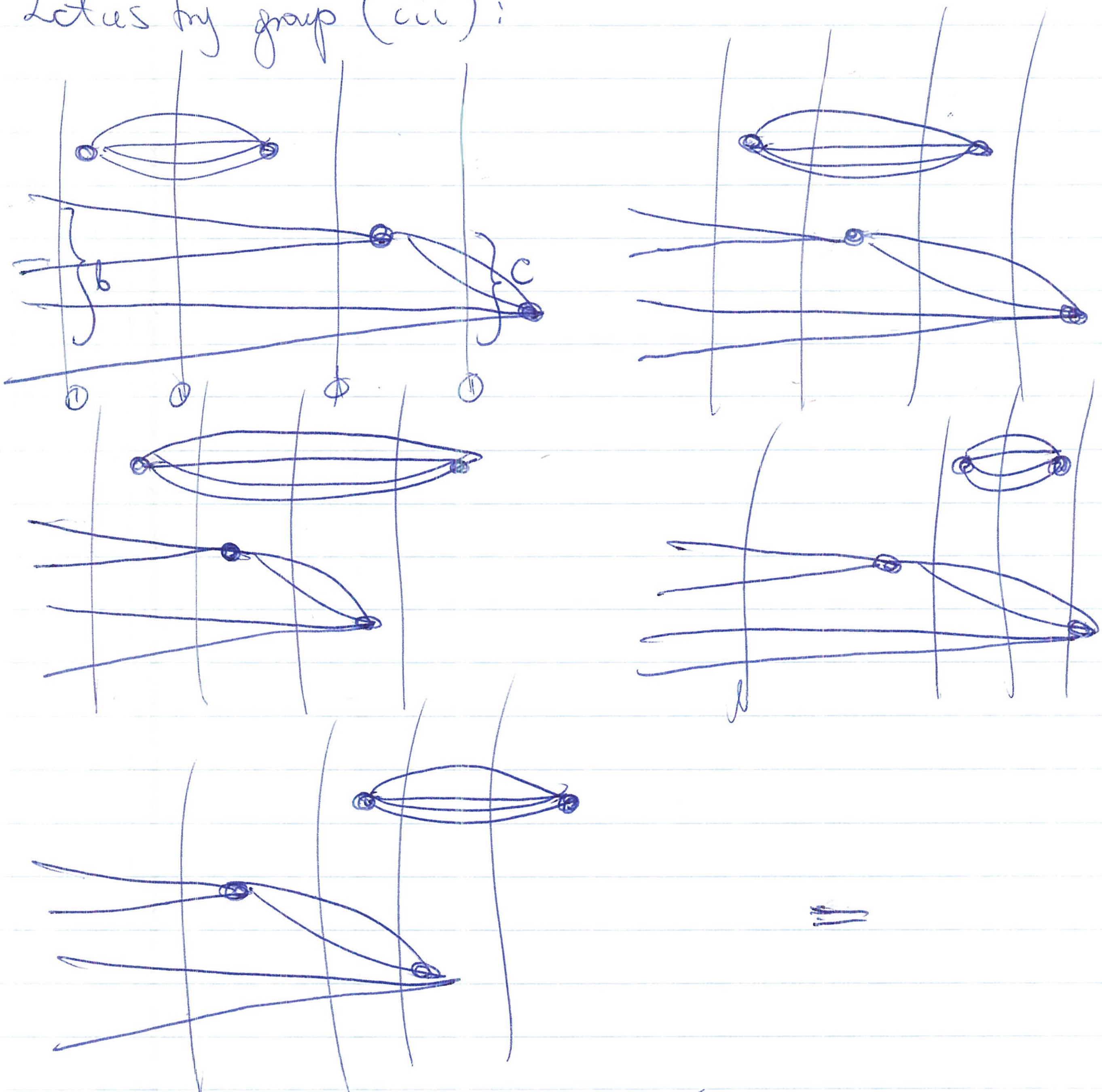


+ time versions of the 1st level

(v) +  + three versions of the 1st term.

Lotus for group (iii):

a)



$=$

$$= \frac{N}{b(a+b)bc} + \frac{N}{b(a+b)(a+c)c} + \frac{N}{b(a+b)(a+c)a}$$

$$+ \frac{N}{bc(a+c)c} + \frac{N}{bc(a+c)a} =$$

$$= \frac{N}{b(a+b)bc} + \frac{N}{b(a+b)(a+c)}\left(\frac{1}{c} + \frac{1}{a}\right)$$

$$+ \frac{N}{bc(a+c)}\left(\frac{1}{c} + \frac{1}{a}\right) =$$

$$= \frac{N}{b(a+b)bc} + \frac{N}{b(a+b)\cancel{(a+c)}} \frac{\cancel{(a+c)}}{ac}$$

$$+ \frac{N}{bc\cancel{(a+c)}} \frac{\cancel{(a+c)}}{ac} =$$

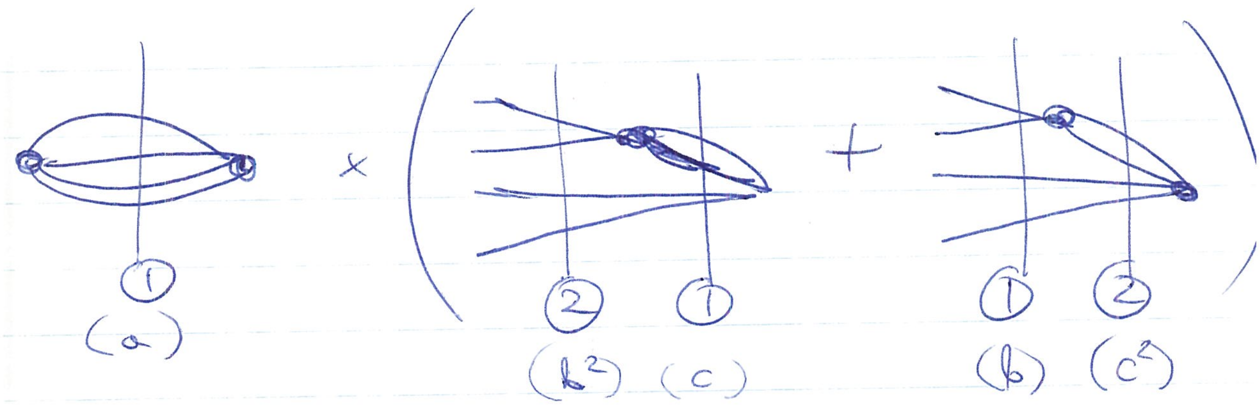
$$= \frac{N}{b(a+b)bc} + \frac{N}{b(a+b)ac} + \frac{N}{abc^2}$$

$$= \frac{N}{b(a+b)c}\left(\frac{1}{b} + \frac{1}{a}\right) + \frac{N}{abc^2}$$

$$= \frac{N}{b\cancel{(a+b)}c} \frac{\cancel{(a+b)}}{ab} + \frac{N}{abc^2}$$

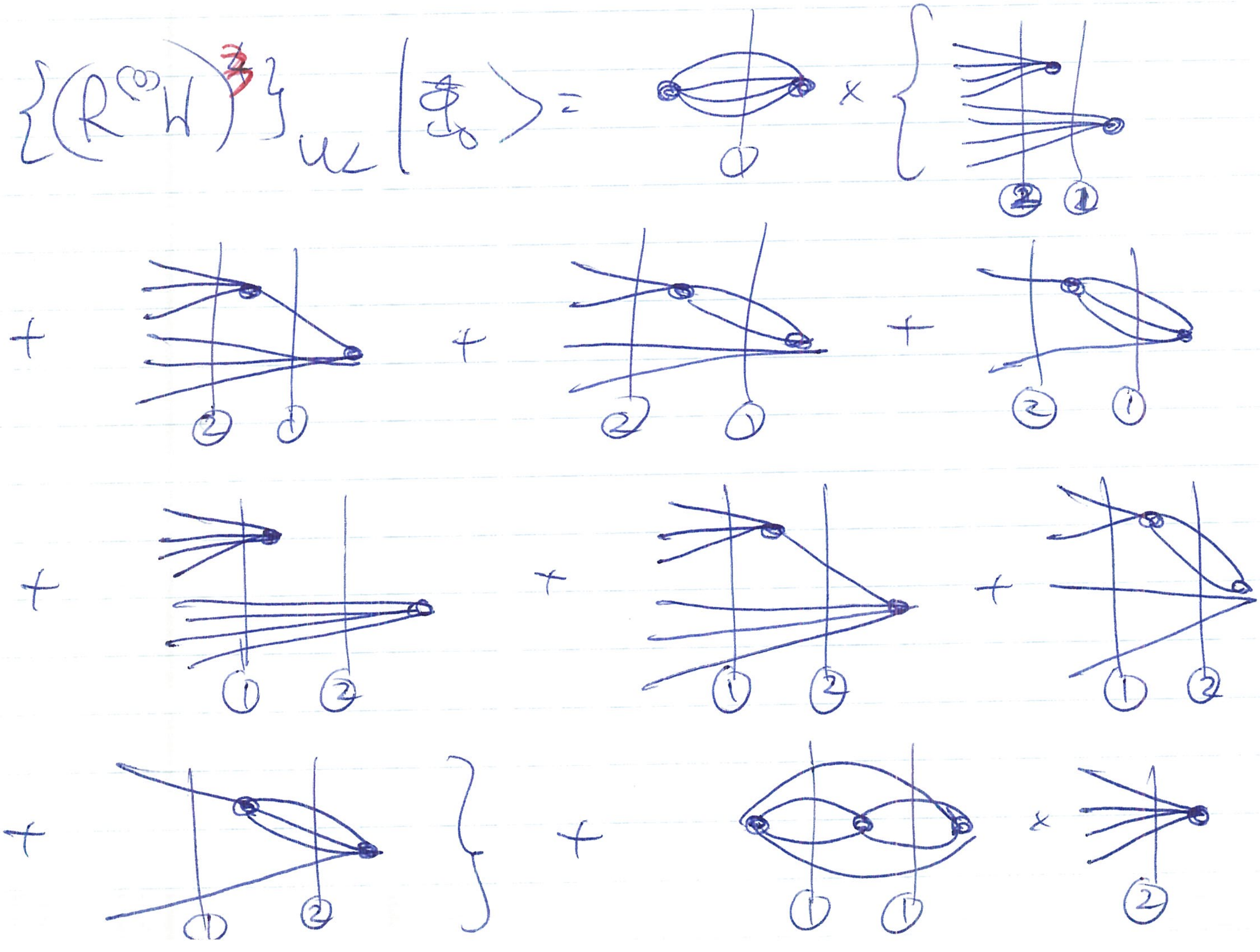
$$= \frac{N}{ab^2c} + \frac{N}{abc^2} =$$

=



By continuing a similar analysis for the remaining UL terms, we obtain:

$\{(R^{(0)}W)^3\}_{UL}|\Phi_0\rangle =$



$$= \langle W R^{(0)} W \rangle \left[R^{(0)2} W R^{(0)} W |\Phi_0\rangle \right.$$

$$\left. + R^{(0)} W R^{(0)2} W |\Phi_0\rangle \right]$$

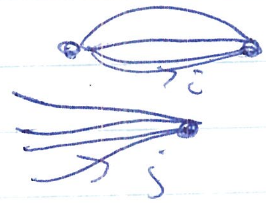
$$+ \langle W R^{(0)} W R^{(0)} W \rangle R^{(0)2} W |\Phi_0\rangle$$

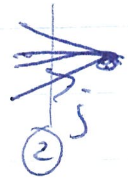
= renormalization terms in $|\Psi_0^{(4)}\rangle$!

Thus, again,

$$\underline{|\Psi_0^{(4)}\rangle = \{(R^{(0)}W)^4\}_L |\Phi_0\rangle}$$

Please note that in order for the above cancellations to take place, we must assume that all labels in the diagrams correspond to unrestricted summations. Indeed,

$\{(R^{(0)}W)^3\}_{UL} |\Phi_0\rangle = \sum_{\ldots i, j \ldots} \Big($  $+$  $\Big)$

$= \sum_{\ldots i, j \ldots}$  $\times$  $= \Big(\underbrace{\sum_{\ldots i \ldots}}_{\langle\Phi_0|W R^{(0)} W|\Phi_0\rangle}$  $\Big) \sum_{\ldots j \ldots}$  , Ah car

all i's all j's

$R^{(0)2} W |\Phi_0\rangle$

The renormalization term $-\langle W R^{(0)} W \rangle R^{(0)2} W|\Phi\rangle$.
These summations are unrestricted, since we replaced the original formula for $R^{(0)}$,

$$R^{(0)} = \sum_{n=1}^{N} R^{(0)}_n,$$

$$R^{(0)}_n = \sum_{\substack{i_1<\ldots<i_n \\ a_1<\ldots<a_n}} \frac{|\Phi^{a_1\ldots a_n}_{i_1\ldots i_n}\rangle\langle\Phi^{a_1\ldots a_n}_{i_1\ldots i_n}|}{-\cancel{\mathcal{D}}^{a_1\ldots a_n}_{i_1\ldots i_n}}$$

restricted
$i_1 \neq i_2 \neq \ldots \neq i_n$
$a_1 \neq a_2 \neq \ldots \neq a_n$

by

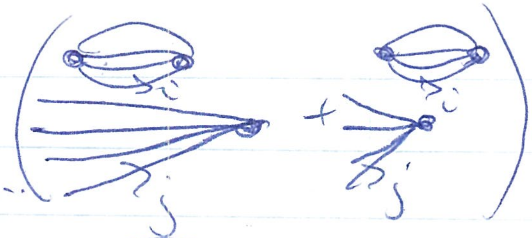
$$R^{(0)}_n = \left(\frac{1}{n!}\right)^2 \sum_{\substack{i_1\ldots i_n \\ a_1\ldots a_n}} \frac{|\Phi^{a_1\ldots a_n}_{i_1\ldots i_n}\rangle\langle\Phi^{a_1\ldots a_n}_{i_1\ldots i_n}|}{-\mathcal{D}^{a_1\ldots a_n}_{i_1\ldots i_n}}.$$

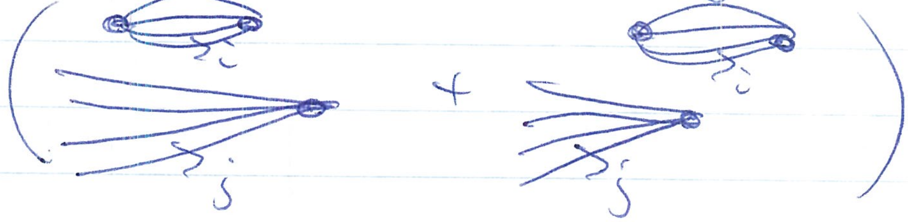
unrestricted
i_1 can be i_2, etc.

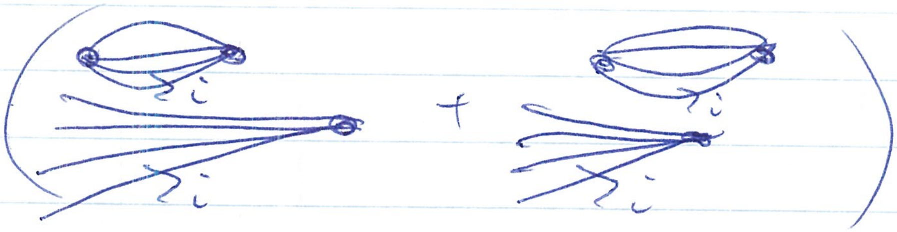
Clearly, all terms with $i_1 = i_2$ or $i_1 = i_3$, etc. in $R^{(0)}$ vanish, but when we form more complicated quantities using diagrams they will contribute (although, mutually cancel out in the original diagrams).

Suppose, we used
$$R^{(0)}_n = \left(\frac{1}{n!}\right)^2 \sum_{\substack{i_1\neq\ldots\neq i_n \\ a_1\neq\ldots\neq a_n}} \frac{|\Phi^{a_1\ldots a_n}_{i_1\ldots i_n}\rangle\langle\Phi^{a_1\ldots}_{i_1\ldots}}{-\mathcal{D}^{a_1\ldots a_n}_{i_1\ldots i_n}}$$

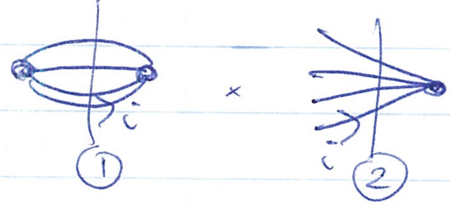
In the third order, we would get

$$\left\{ \left(R^{(0)}W\right)^3 \right\}_{u\,L\,(i\neq j)} |\Phi_0\rangle = \sum_{\cdots i \neq j \cdots}$$ 

$$= \sum_{\cdots i j \cdots}$$ 

$$- \sum_{\cdots i \cdots}$$  (← EPV terms)

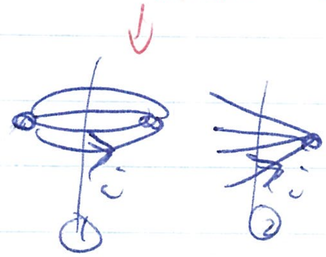
$$= \langle W R^{(0)} W \rangle R^{(0)2} W |\Phi_0\rangle -$$

$$- \sum_{\cdots i \cdots}$$  , so that

$$|\Psi_0^{(3)}\rangle = \left\{ \left(R^{(0)}W\right)^3 \right\}_{L(i\neq j)} |\Phi_0\rangle + \left\{ \left(R^{(0)}W\right)^3 \right\}_{uL(i\neq j)} |\Phi_0\rangle$$

$$- \langle W R^{(0)} W \rangle R^{(0)2} W |\Phi_0\rangle$$

unlinked EPV

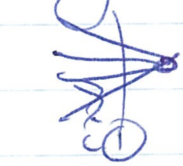
$$= \left\{ \left(R^{(0)}W\right)^3 \right\}_{L(i\neq j)} |\Phi_0\rangle + \sum_{\cdots i \cdots}$$ 

The latter term is unlinked and is left uncancelled, since we restricted the summations.

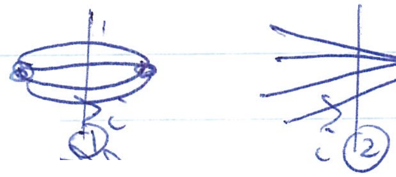
By adding back the $i = j$ terms to the linked term

$$\left\{\left(R^{(0)}W\right)^3\right\}_{L(i\neq j)} |\Phi_0\rangle ,$$

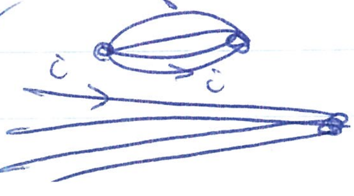
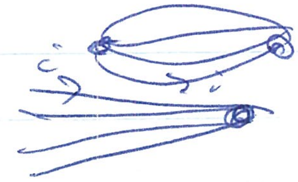
we can immediately eliminate the unlinked

$\sum_{\ldots i \ldots}$   term. Instead, by adding (and subtracting) $\left\{\left(R^{(0)}W\right)^3\right\}_{L(i=j)} |\Phi_0\rangle$ to $|\Psi_0^{(3)}\rangle$, we obtain:

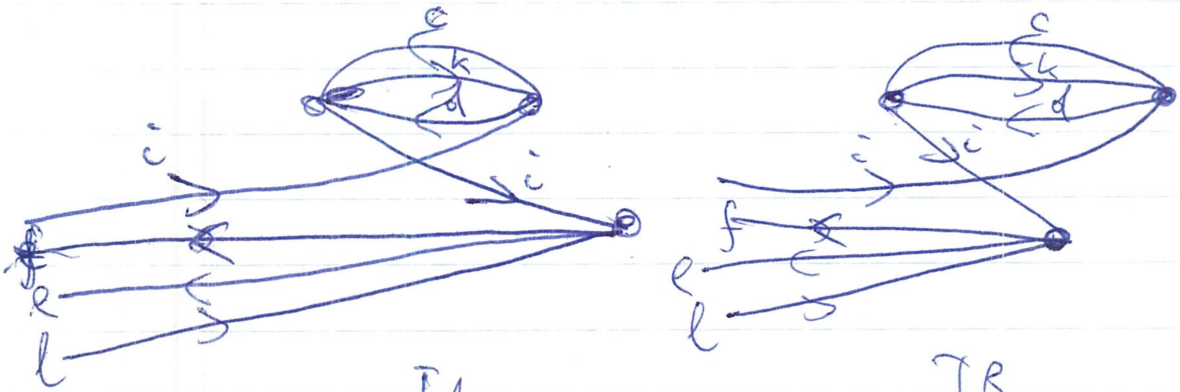
$$|\Psi_0^{(3)}\rangle = \left\{\left(R^{(0)}W\right)^3\right\}_{L\,\text{all}} |\Phi_0\rangle - \left\{\left(R^{(0)}W\right)^3\right\}_{L(i=j)} |\Phi_0\rangle$$

$- \sum_i$ 

will cancel each other

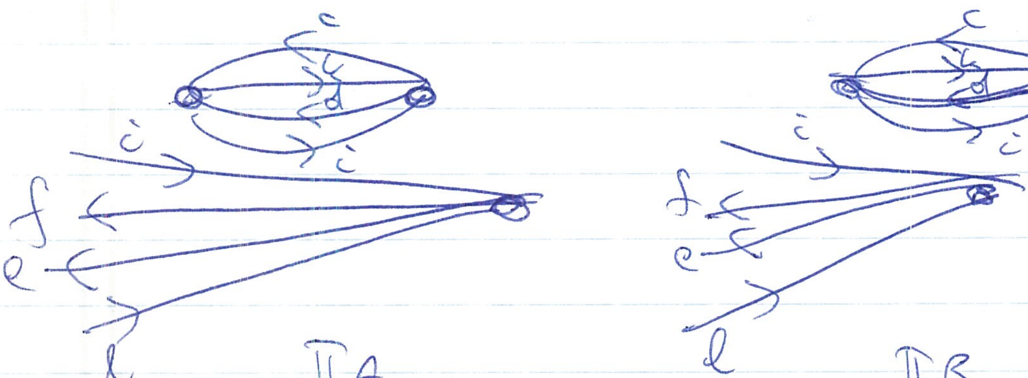
or ( + )

$\{(R^{(0)}W)^3\}_{L(i=j)}|\Phi_0\rangle$ contains



IA IB

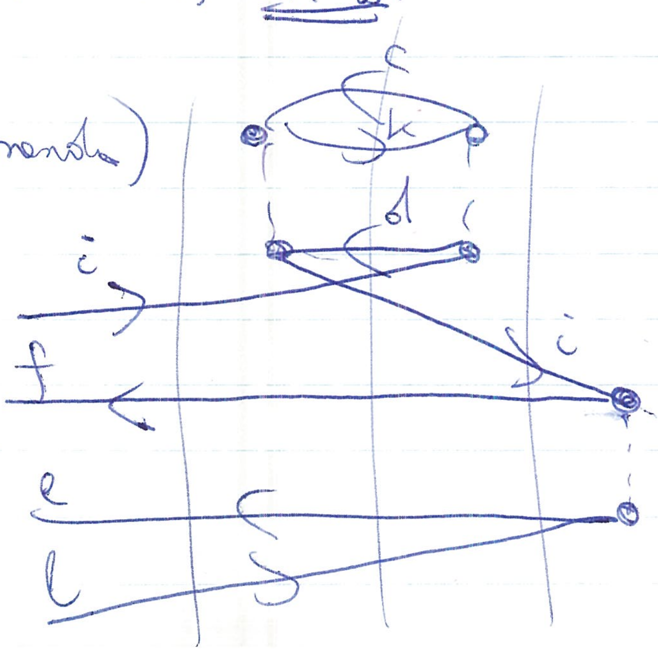
These terms cancel unlinked ~~renormalization~~ $i=j$ terms:



IIA IIB

Indeed, $(\mathrm{IA})_L$:

(Brandow)



$$-\frac{1}{4}\sum_{cd\,efkli}\langle ef|v|li\rangle_A \langle cd|v|ki\rangle_A$$

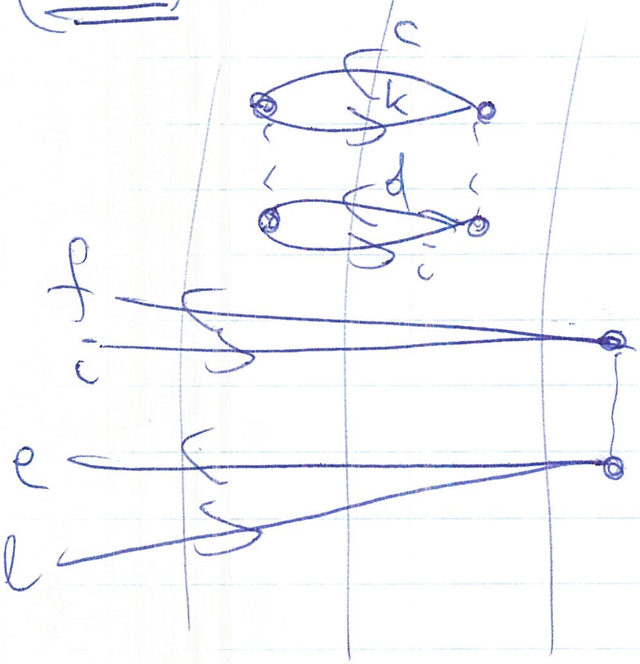
$$\times \langle ki|v|cd\rangle_A$$

$$\times \Delta^{(1)}(i,l;ef)$$

$$\times \Delta^{(1)}(i,k,l;c,d,e,f)$$

$$\times \Delta^{(1)}(i,l;ef)$$

(IIA)



$$\frac{1}{4} \sum_{cdefkli} \langle ef|\hat{v}|li\rangle_A \times \langle cd|\hat{v}|ki\rangle_A \langle ki|\hat{v}|cd\rangle_A \times \Delta^{(1)}(i,l;e,f)\,\Delta^{(2)}(i,i,k,l;c,d,e,f)\,\Delta^{(1)}(i,l;e,f)$$

Thus,

$$(IA) + (IIA) = 0.$$

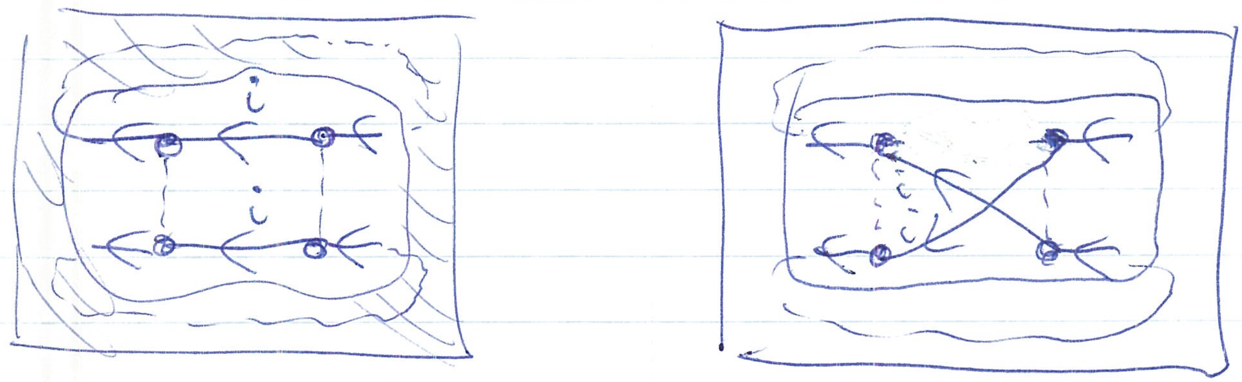
Similarly, $(IB) + (IIB) = 0.$

Thus, after adding and subtracting the "unlinked" $i=j$ terms,

$$|\Psi_0^{(3)}\rangle = \{(R^{(0)}W)^3\}_C |\Phi_0\rangle.$$

This example illustrates the need for considering the so-called exclusion principle violating (EPV) diagrams, in which a given spin-orbital state is occupied more than once (we have two identically labeled hole or particle lines).

In general, the EPV terms cancel out. Schematically,



EPV d-m another EPV d-m.
(number of loops changes by one here)

Clearly, the above diagrams cancel out. They do not have to vanish, but once all of the diagrams (in the principal & renorm. terms) including EPV, are considered, EPV terms mutually cancel out.
In some cases, EPV diagrams that cancel out are in the principal term. However, there are cases where one of the two EPV diagrams that cancel out is linked and another unlinked.
In the above example, EPV diagram (I A) is linked, EPV diagram (II A) is unlinked. Yet, they cancel out. If we did not allow the EPV terms, the above cancellations of unlinked principal and renormalization terms would not be complete. Thus, the linked cluster theorem will have a form;

-129-

$$|\Psi_0^{(n)}\rangle = \sum_{\cancel{}\ L,\text{ including EPV}} \left\{\left(R^{(0)}W\right)^n\right\}_{L,\text{ including EPV}} |\Phi_0\rangle$$

The unlinked terms including EPV diagrams cancel out. ~~Another~~ Other statements, such as:

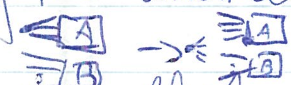
$$\boxed{|\Psi_0^{(n)}\rangle = \sum_{L,\text{ no EPV}} \left\{\left(R^{(0)}W\right)^n\right\}_{L,\text{ no EPV}} |\Phi_0\rangle}$$

are not true.

6.7. Factorization Lemma

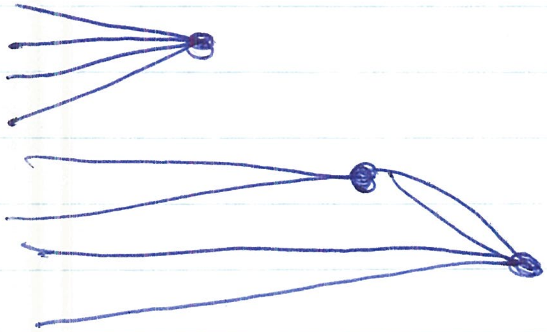
and the connected cluster theorem

Before proving the linked diagram (cluster) theorem, we have to prove the so-called Factorization Lemma (following the work of Frantz and Mills). This Lemma allows to factorize the disconnected, but linked diagrams, a factorization appearing in the proof of the linked cluster theorem. These diagrams are obtained in the ~~Let us illustrate the factorization Lemma by a few examples.~~ proof of the linked cluster theorem by removing the leftmost interaction vertex from the vacuum part ~~Suppose we have a~~ of the unlinked diagrams having precisely one vacuum part).

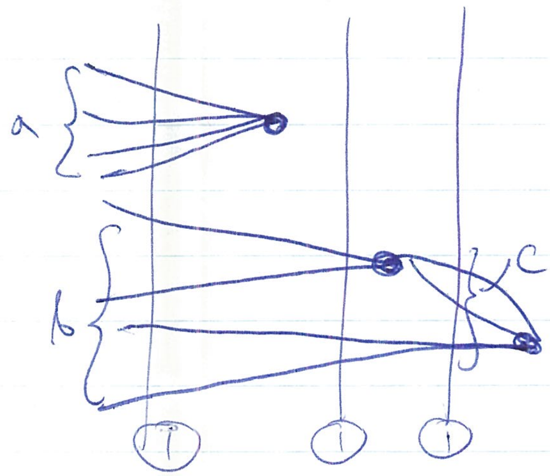


Let us illustrate the Factorization Lemma by a few examples:

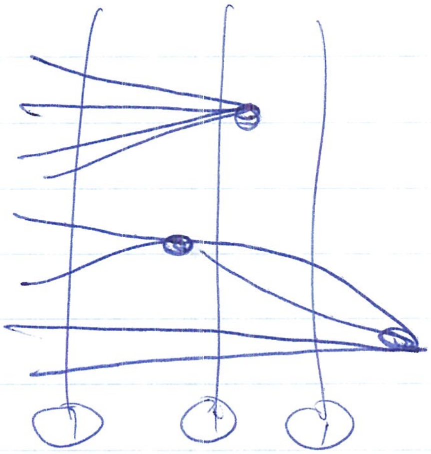
- disconnected linked diagrams having nonequivalent connected components:



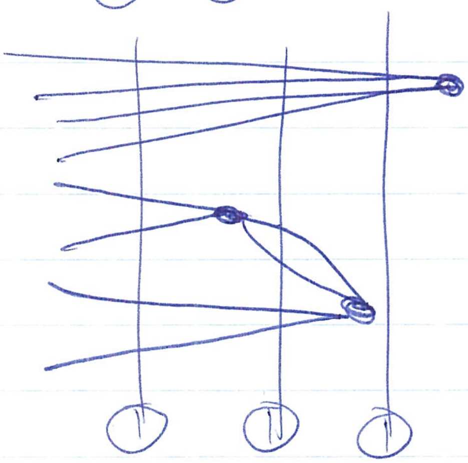
\+ all the nonequivalent versions of the first kind



+



+

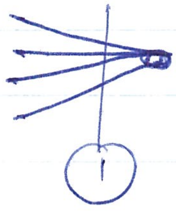


$$\frac{N}{(a+b)bc} + \frac{N}{(a+b)(a+c)c} + \frac{N}{(a+b)(a+c)a}$$

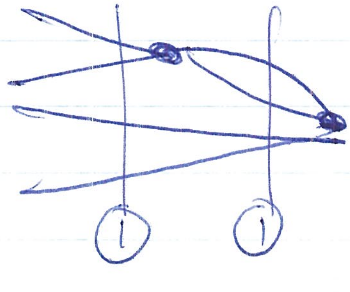
$$= \frac{N}{(a+b)bc} + \frac{N}{(a+b)(a+c)}\left(\frac{1}{a}+\frac{1}{c}\right)$$

$$= \frac{N}{(a+b)bc} + \frac{N}{(a+b)ac} = \frac{N}{(a+b)c}\left(\frac{1}{b}+\frac{1}{a}\right)$$

$$= \frac{N}{abc} =$$

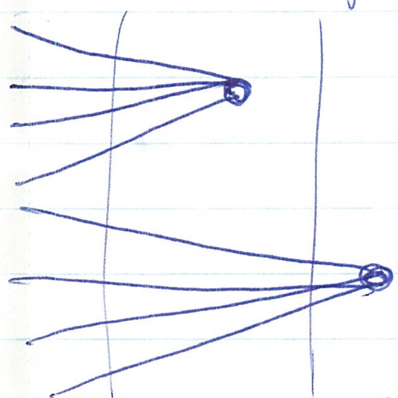


×

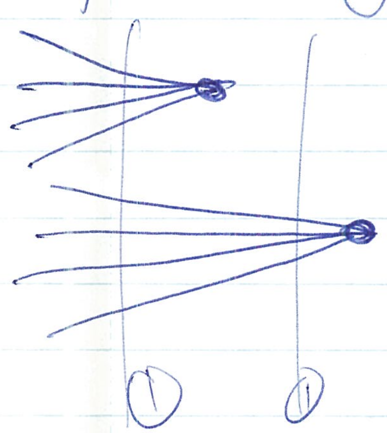


denominators in the first process

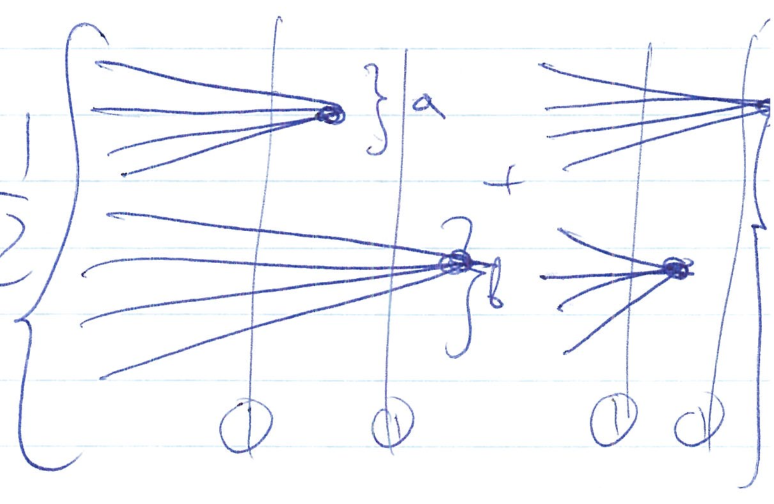
- disconnected linked diagrams having equivalent connected components:



This diagram does not ~~seem~~ have nonequivalent time versions, but we can obtain the same ~~diagram~~ contribution by writing the above diagram twice, as ~~...~~ two equivalent time versions (all spin-orbital labels are free), and by dividing the result by 2:



$= \frac{1}{2}$



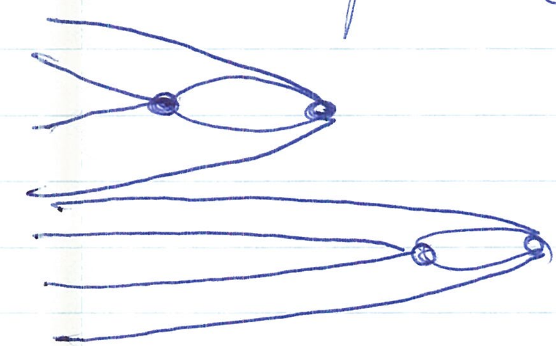
$$= \frac{1}{2}\left(\frac{N}{(a+b)\,b} + \frac{N}{(a+b)\,a}\right) = \frac{1}{2}\,\frac{N}{(a+b)}\left(\frac{1}{b}+\frac{1}{a}\right)$$

$$= \frac{1}{2}\,\frac{N}{ab}$$ agrees, the diagram on the first page

Thus, when we have two equivalent parts, we obtain a similar factorization as in the earlier example, but we also get a factor of $\frac{1}{2}$ associated with the fact that we have two equivalent parts. This is consistent with our rules for topological factors, since disconnected equivalent parts ~~[illegible]~~ can be permuted among themselves when treated and counted as independent components.

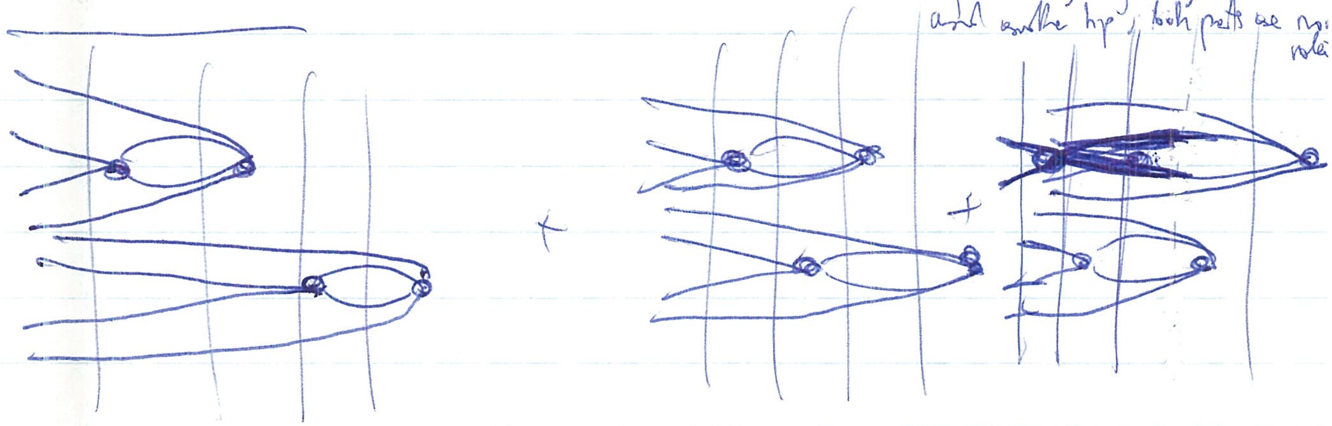
The above example was ~~somewhat~~ ~~simple~~ very simple, both connected parts were simple vertices. Let us try something more complicated:

@ disconnected contour diagrams having equivalent connected components (a more complicated example):



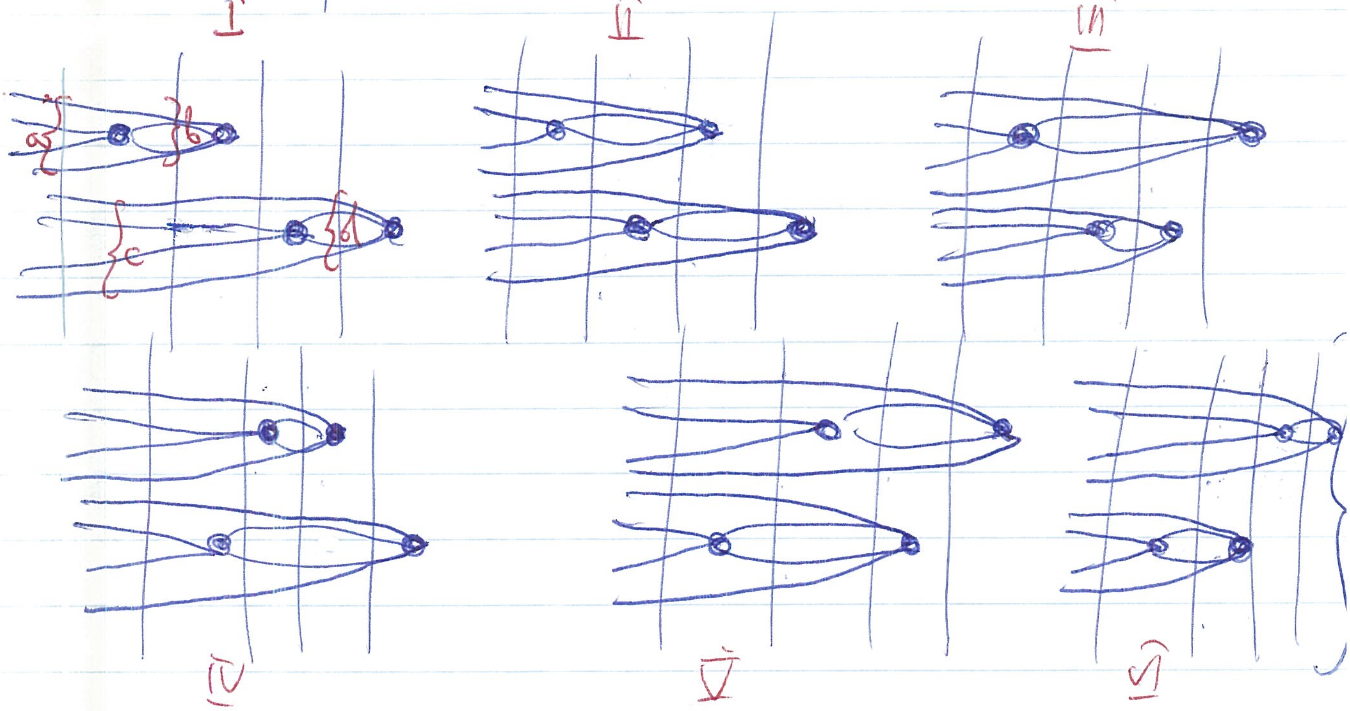
+ all nonequivalent time versions

(we must assume that both connected pieces have the same orientations of lines; say hh; if one is hh and another hp, both parts are no[illegible]



If we analyzed the above three diagrams, we would not achieve factorization. However, we can double the number of diagrams by considering all time versions of the 1st kind and dividing by a factor of 2:

$\frac{1}{2}$



$(\mathrm{I} = \mathrm{VI};\ \mathrm{II} = \mathrm{V};\ \mathrm{III} = \mathrm{IV}).$

$$= \frac{1}{2}\left\{ \frac{N}{(a+c)(b+c)d} + \frac{N}{(a+c)(b+c)(b+d)d} + \frac{N}{(a+c)(b+c)(b+d)b} \right.$$

$$+ \frac{N}{(a+c)(a+d)(b+d)d} + \frac{N}{(a+c)(a+d)(b+d)b}$$

$$\left. + \frac{N}{(a+c)(a+d)ab} \right\} =$$

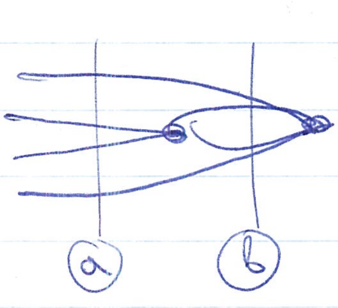
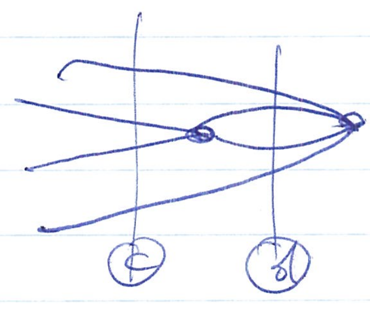
$$= \frac{1}{2}\left\{ \frac{N}{(a+c)(b+c)cd} + \frac{N}{(a+c)(b+c)bd} \right.$$

$$\left. + \frac{N}{(a+c)(a+d)bd} + \frac{N}{(a+c)(a+d)ab} \right\}$$

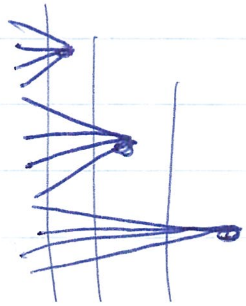
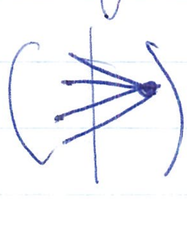
$$= \frac{1}{2}\left\{ \frac{N}{(a+c)d\,bc} + \frac{N}{(a+c)bad} \right\}$$

$$= \frac{1}{2}\frac{N}{(a+c)bd}\underbrace{\left(\frac{1}{c}+\frac{1}{a}\right)}_{=\frac{a+c}{ac}}$$

$$= \frac{1}{2}\frac{N}{abcd}$$

$= \frac{1}{2}$  $\times$ 

At home: examine ~~graphs~~ cases with more than 2 equivalent parts.

Show that  $= \frac{1}{6}\Big($  $\Big)^3$

Let us generalize the above result:

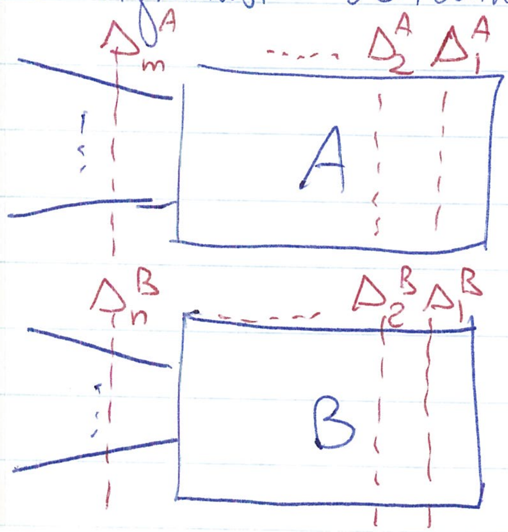
Consider all possible time versions of the first kind for a ~~LINKED DISCONNECTED~~ diagram consisting of two parts: A and B. These two parts are not necessarily connected, so this ~~proof~~ applies to ALL LINKED DISCONNECTED diagrams.

We designate the set of energy denominators for part A alone by

$$\Delta^{A}_{\mu}\ ,\ \mu=1,\dots,m\ ,\ \text{and for}$$

part B by:
$$\Delta^{B}_{\nu}\ ,\ \nu=1,\dots,n\ .$$

The denominators are numbered along the time axis, i.e., the rightmost denominators are Δ^{A}_{1} and Δ^{B}_{1}.



The denominator contribution from all possible time versions of the first kind, corresponding to all possible orderings of ~~energy~~ interaction vertices in parts A and B relative to one another (the numerator part is always identical for all time versions) can be written as:

$$D^{AB}_{mn} = \sum_{\{\alpha,\beta\}} \prod_{p=1}^{m+n} \left(\Delta^{A}_{\alpha(p)} + \Delta^{B}_{\beta(p)}\right)^{-1},$$

where the summation over α, β extends over all sets of $(m+n)$ integer pairs,

$$\Gamma_p = \left(\alpha(p), \beta(p)\right), \quad 0 \leq \alpha(p) \leq m, \quad 0 \leq \beta(p) \leq n,$$

defined as follows:

(i) $\Gamma_1 = (1, 0)$ or $(0, 1)$,

(ii) $\Gamma_{p+1} = \left(\alpha(p)+1, \beta(p)\right)$ or $\left(\alpha(p), \beta(p)+1\right)$,

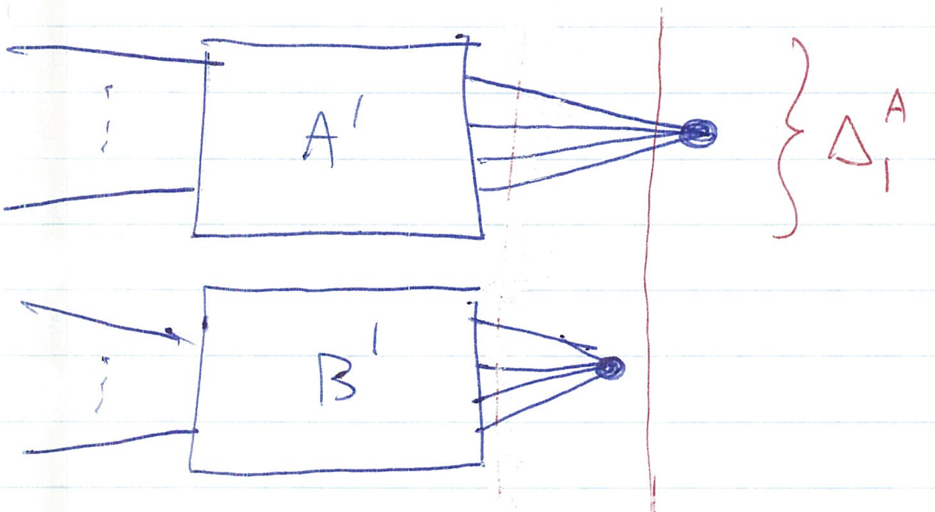
(iii) $\Gamma_{m+n} = (m, n)$.

We also define:

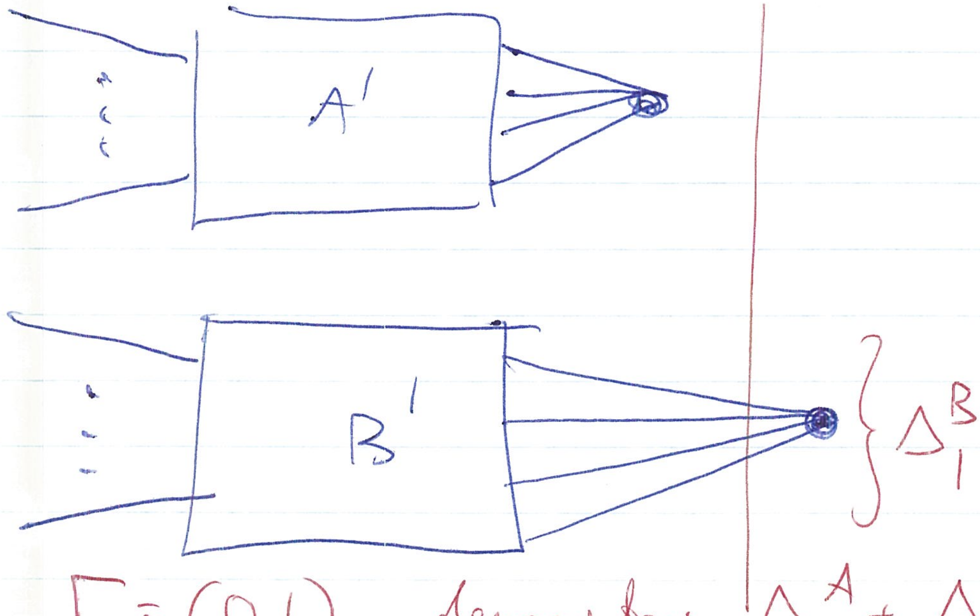
$$\Delta^{A}_{0} = \Delta^{B}_{0} \equiv 0.$$

Explanation:

(i) This condition reflects the obvious fact that the rightmost perturbation vertex is either from part A' [$\Gamma_1 = (1,0)$ case] or from part B' [$\Gamma_1 = (0,1)$];

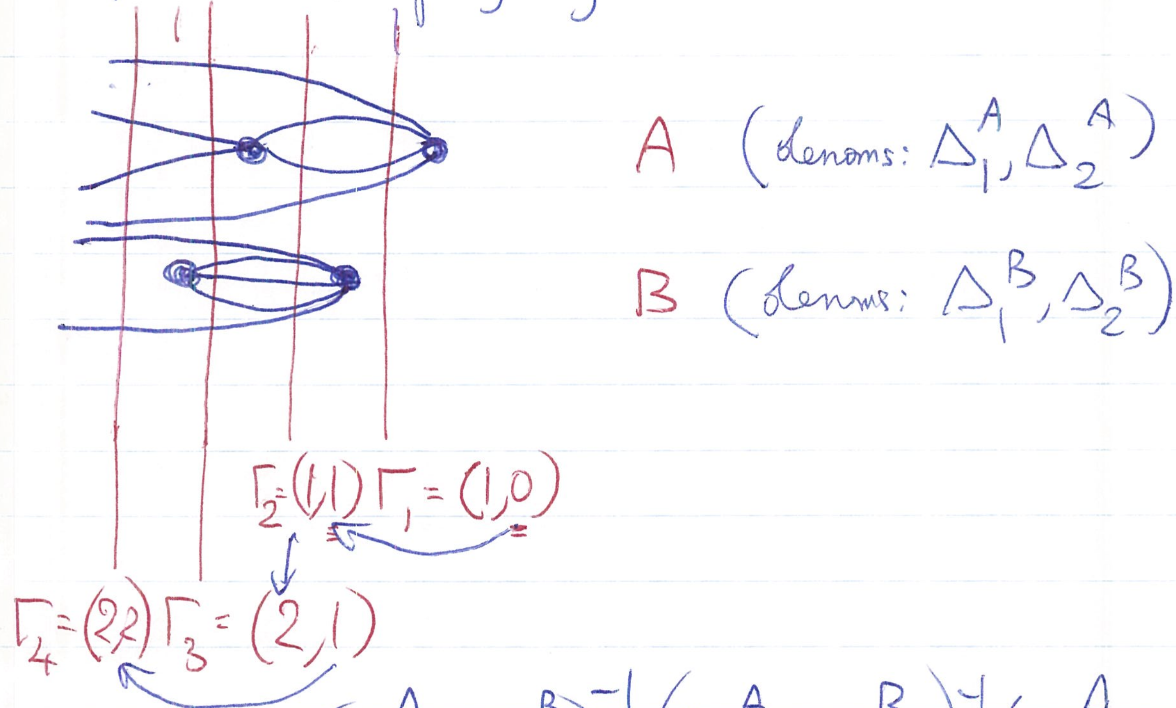


$\Gamma_1 = (1,0)$ denominator: $\Delta_1^A + \Delta_0^B = \Delta_1^A$



$\Gamma_1 = (0,1)$ denominator: $\Delta_0^A + \Delta_1^B = \Delta_1^B$

(ii) After going through the first p vertices, the next vertex can be either in the A part or in the B part, e.g.



Denominator:
$$\underbrace{\left(\Delta_1^A+\Delta_0^B\right)^{-1}}_{\Gamma_1}\underbrace{\left(\Delta_1^A+\Delta_1^B\right)^{-1}}_{\Gamma_2}\underbrace{\left(\Delta_2^A+\Delta_1^B\right)^{-1}}_{\Gamma_3}$$

$$\times\ \underbrace{\left(\Delta_2^A+\Delta_2^B\right)^{-1}}_{\Gamma_4}$$

(iii) The last (leftmost) denominator is
$$\left(\Delta_m^A+\Delta_n^B\right)^{-1}$$
(cf. the above example in (ii)).

For the separate parts A and B, the denominators are given by the products of Δ^A_μ and Δ^B_ν, respectively,

$$D^A_m = \prod_{\mu=1}^{m} \left(\Delta^A_\mu\right)^{-1},$$

$$D^B_n = \sum_{\nu=1}^{n} \left(\Delta^B_\nu\right)^{-1}.$$

Note that

$$D^A_m = D^{AB}_{m0}, \quad D^B_n = D^{AB}_{0n}.$$

Indeed:

$$D^{AB}_{m0} = \sum_{\{\alpha\beta\}} \prod_{p=1}^{m+0} \left(\Delta^A_{\alpha(p)} + \Delta^B_{\beta(p)}\right)^{-1}$$

$$= \sum_{\{\alpha,\beta\}} \prod_{p=1}^{m} \left(\Delta^A_{\alpha(p)} + \Delta^B_{\beta(p)}\right)^{-1}$$

$$= \left(0 \le \beta(p) \le n;\ \beta(p) = 0\ \forall_p \Rightarrow \Delta^B_{\beta(p)} = \Delta^B_0 \equiv 0\right)$$

$$= \sum_{\{\alpha\}} \prod_{p=1}^{m} \left[\Delta^A_{\alpha(p)}\right]^{-1}.$$ But,

since $\beta(p) = 0$,

$\Gamma_1 = (1, 0)$, so that $\alpha(1) = 1$,

$\Gamma_2 = (\alpha(1)+1, \beta(1)) = (1+1, 0) = (2, 0)$, so that $\alpha(2) = 2$,

$\Gamma_{p+1} = (\alpha(p)+1, \beta(p)) = (\alpha(p)+1, 0) = (\alpha(p+1), 0)$

so that $\alpha(p+1) = \alpha(p)+1$, which

means that $\alpha(p) = p$, $p = 1, \dots, m$,

which in turn implies that

$$D^{AB}_{m0} = \prod_{p=1}^{m} \left(\Delta^A_p\right)^{-1} = D^A_m .$$

Similarly for $D^B_n = D^{AB}_{0n}$.

We also define: $D^A_0 = D^B_0 = D^{AB}_{00} = 1$.

Factorization lemma states that

$$\boxed{D^{AB}_{mn} = D^A_m \, D^B_n}$$

all the versions

sum of the elementals from

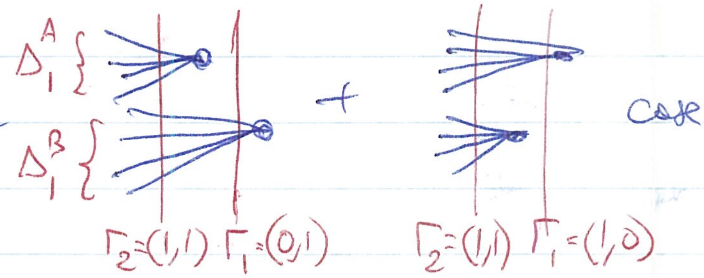
Proof: Mathematical induction:

$m=0$ or $n=0$:

$$D^{AB}_{m0} = D^{A}_{m} = D^{A}_{m} D^{B}_{0},$$

$$D^{AB}_{0n} = D^{B}_{n} = D^{A}_{0} D^{B}_{n}.$$

Check on D^{AB}_{11} (e.g. the



)

$$D^{AB}_{11} = \sum_{\{\alpha,\beta\}} \prod_{p=1}^{2} \left[\Delta^{A}_{\alpha(p)} + \Delta^{B}_{\beta(p)}\right]^{-1}$$

$$= \sum_{\{\alpha,\beta\}} \left[\Delta^{A}_{\alpha(1)} + \Delta^{B}_{\beta(1)}\right]^{-1} \left[\Delta^{A}_{\alpha(2)} + \Delta^{B}_{\beta(2)}\right]^{-1}$$

$$= \left(\Delta^{A}_{1} + \Delta^{B}_{0}\right)^{-1} \left(\Delta^{A}_{1} + \Delta^{B}_{1}\right)^{-1}$$

$$+ \left(\Delta^{A}_{0} + \Delta^{B}_{1}\right)^{-1} \left(\Delta^{A}_{1} + \Delta^{B}_{1}\right)^{-1}$$

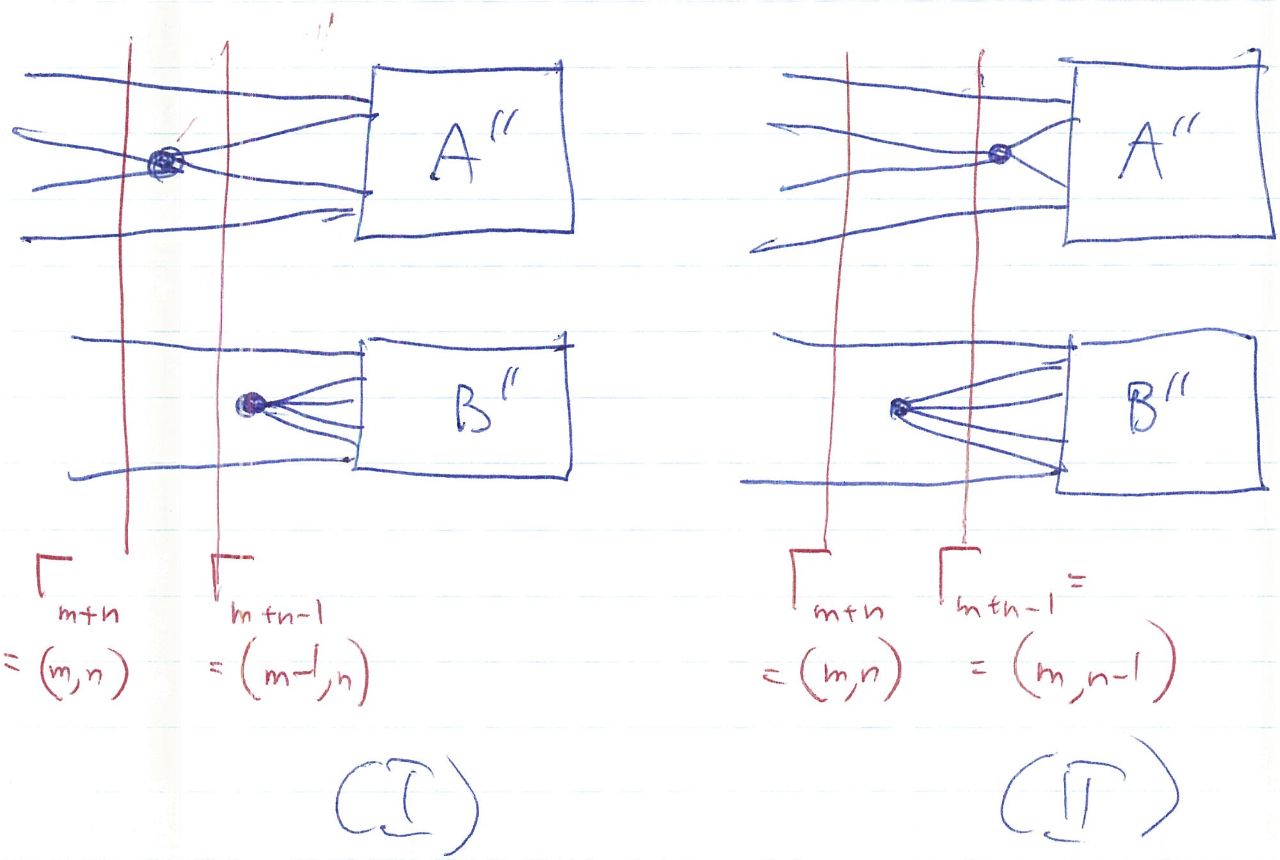
$$= \left[\left(\Delta^{A}_{1}\right)^{-1} + \left(\Delta^{B}_{1}\right)^{-1}\right] \left(\Delta^{A}_{1} + \Delta^{B}_{1}\right)^{-1} =$$

$$= \left(\Delta_1^A\right)^{-1}\left(\Delta_1^B\right)^{-1} \cancel{\left(\Delta_1^A+\Delta_1^B\right)\left(\Delta_1^A+\Delta_1^B\right)^{-1}}$$

$$= \left(\Delta_1^A\right)^{-1}\left(\Delta_1^B\right)^{-1} = D_1^A D_1^B \,.$$

Induction step:

Suppose the lemma holds for $M = m-1$, $N = n$ and $M = m$ and $N = n-1$; $m, n \geq 1$,
Let us consider that (m,n) case.
All terms in D^{AB}_{mn} can be divided into two disjoint classes depending on whether the leftmost interaction occurs in A or B; schematically,



The last denominator (the leftmost one) is (see (iii)):

$$\left(\Delta^A_m + \Delta^B_n\right)^{-1} \qquad \left(\Gamma_{m+n} = (m,n) \Rightarrow \Rightarrow \alpha(m+n) = m, \; \beta(m+n) = n\right).$$

The remaining part of D^{AB}_{mn} is either $D^{AB}_{m-1,n}$ (case I) or $D^{AB}_{m,n-1}$ (case II), since after pulling out $\left(\Delta^A_m + \Delta^B_n\right)^{-1}$ out the remaining denominator are identical to those obtained for the diagrams obtained by deleting the leftmost vertex. Thus,

$$D^{AB}_{mn} = \left(\Delta^A_m + \Delta^B_n\right)^{-1}\left[D^{AB}_{m-1,n} + D^{AB}_{m,n-1}\right]$$

From the induction assumption,

$$D^{AB}_{m-1,n} = D^A_{m-1} D^B_n ,$$

$$D^{AB}_{m,n-1} = D^{A}_{m} D^{B}_{n-1}.$$

Now,

$$D^{A}_{m} = D^{A}_{m-1} \left(\Delta^{A}_{m}\right)^{-1},$$

$$D^{B}_{n} = D^{B}_{n-1} \left(\Delta^{B}_{n}\right)^{-1}$$

Thus,

$$D^{AB}_{mn} = \left(\Delta^{A}_{m} + \Delta^{B}_{n}\right)^{-1} \left[D^{A}_{m-1} D^{B}_{n} + D^{AB}_{m,n-1} \right]$$

$$= \left(\Delta^{A}_{m} + \Delta^{B}_{n}\right)^{-1} \left[\Delta^{A}_{m} D^{A}_{m} D^{B}_{n} + \Delta^{B}_{n} D^{A}_{m} D^{B}_{n} \right]$$

$$= \cancel{\left(\Delta^{A}_{m} + \Delta^{B}_{n}\right)^{-1}} \cancel{\left(\Delta^{A}_{m} + \Delta^{B}_{n}\right)} D^{A}_{m} D^{B}_{n}$$

$$= D^{A}_{m} D^{B}_{n}.$$

This completes the proof.

LINKED CLUSTER THEOREM

We have already postulated the linked cluster theorem (based on examples) in the following way:

$$|\Psi_0^{(n)}\rangle = \{(R^{(0)}W)^n\}_L\,|\Phi_0\rangle$$

all linked diagrams, including EPV

This implies that

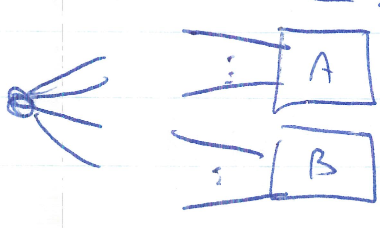
$$K_0^{(n+1)} = \langle\Phi_0|\,W\,|\Psi_0^{(n)}\rangle$$

$$= \langle\Phi_0|\,W\underbrace{\{(R^{(0)}W)^n\}_L}_{\text{no vacuum parts}}|\Phi_0\rangle$$

$$= \langle\Phi_0|\left(W\{(R^{(0)}W)^n\}_L\right)_{C_0}|\Phi_0\rangle$$

connected, no external lines, since

W has to connect to external lines of $\{(R^{(0)}W)^n\}_L$; if the $(R^{(0)}W)^n$ diagram is connected, we obviously get the C_0 terms; if $(R^{(0)}W)^n$ is linked but disconnected, we have



and all lines of A and B must be

connected with W, producing the connected diagrams.

Thus, $$K_0^{(n+1)} = \langle \Phi_0 | \{ W (R^{(0)} W)^n \}_{C_0} | \Phi_0 \rangle .$$

In other words:

$$\boxed{\begin{aligned} K_0 - \varepsilon_0 &= \sum_{n=0}^{\infty} K_0^{(n+1)} = \\ &= \sum_{n=0}^{\infty} \langle \Phi_0 | \{ W (R^{(0)} W)^n \}_{C_0} | \Phi_0 \rangle \\ |\Psi_0\rangle = \sum_{n=0}^{\infty} |\Psi_0^{(n)}\rangle &= \sum_{n=0}^{\infty} \{ (R^{(0)} W)^n \}_L | \Phi_0 \rangle \end{aligned}}$$

Proof of the linked cluster theorem:

We must show that

$$(K_0 + W) | \Psi_0 \rangle = K_0 | \Psi_0 \rangle$$

for $|\Psi_0\rangle$ and K_0 defined above.

Let us calculate

$$(\varkappa_0 - K_0)\,|\Psi_0\rangle \quad \text{(using } |\Psi_0\rangle \text{ defined by the linked terms):}$$

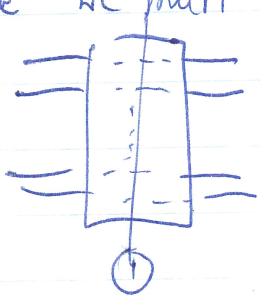
$$(\varkappa_0 - K_0)\,|\Psi_0\rangle =$$

$$= (\varkappa_0 - K_0)\left[\,|\Phi_0\rangle + \sum_{n=1}^{\infty}\left\{(R^{(0)}W)^n\right\}_L |\Phi_0\rangle\right]$$

$$= (\varkappa_0 - K_0) \sum_{n=1}^{\infty}\left\{(R^{(0)}W)^n\right\}_L |\Phi_0\rangle$$

$$= (\varkappa_0 - K_0)\, R^{(0)} \sum_{n=0}^{\infty}\left\{W\,(R^{(0)}W)^n\right\}_{L_{ext}} |\Phi_0\rangle$$

These L_{ext} are all linked diagrams with external lines. There must be external lines in $W(R^{(0)}W)^n$ since we must connect lines of $W(R^{(0)}W)^n$ with $R^{(0)} =$



($R^{(0)}$ has at least two lines extending to the right).

Recall that

$$(\varepsilon_0 - K_0) R^{(0)} = 1 - |\Phi_0\rangle\langle\Phi_0| .$$

Thus,

$$(\varepsilon_0 - K_0)|\Psi_0\rangle = \left(1 - |\Phi_0\rangle\langle\Phi_0|\right)$$

$$\times \sum_{n=0}^{\infty} \{W(R^{(0)}W)^n\}_{L_{ext}} |\Phi_0\rangle$$

$$= \sum_{n=0}^{\infty} \{W(R^{(0)}W)^n\}_{L_{ext}} |\Phi_0\rangle$$

$$- |\Phi_0\rangle \sum_{n=0}^{\infty} \underbrace{\langle\Phi_0|\{W(R^{(0)}W)^n\}_{L_{ext}}|\Phi_0\rangle}_{=0}\,,$$

0, since L_{ext} d-ms have external lines.

so that $$(\varepsilon_0 - K_0)|\Psi_0\rangle = \sum_{n=0}^{\infty} \{W(R^{(0)}W)^n\}_{L_{ext}} |\Phi_0\rangle$$

Clearly, we can only obtain the L_{ext} diagrams

$$\left\{W\left(R^{\infty}W\right)^{n}\right\}_{L_{ext}}|\Phi_0\rangle$$

from the linked diagrams

$$\left\{\left(R^{\infty}W\right)^{n}\right\}_{L}$$

(adding W to the UL diagram cannot produce the linked diagram).

Thus,

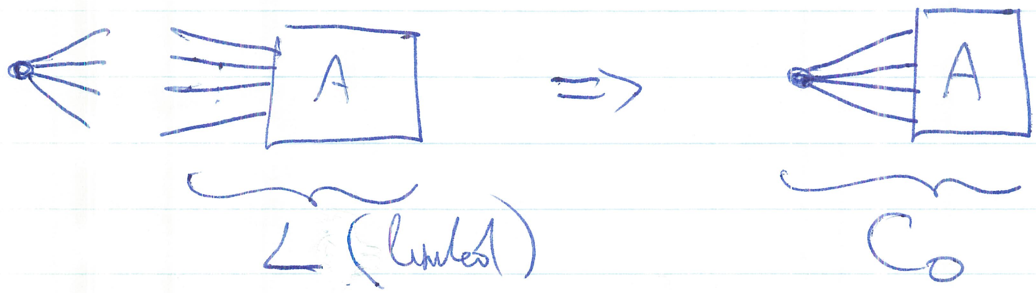
$$(\mathcal{H}_0 - K_0)|\Phi_0\rangle = \sum_{n=0}^{\infty}\Big\{W\underbrace{\left\{\left(R^{\infty}W\right)^{n}\right\}_{L}}_{\text{linked}}\Big\}_{\underbrace{ext}_{\text{linked with external lines}}}|\Phi_0\rangle$$

Let us analyze what we get by applying W to the $\left\{\left(R^{\infty}W\right)^{n}\right\}_{L}$ terms:

$$W\sum_{n=0}^{\infty}\left\{\left(R^{\infty}W\right)^{n}\right\}_{L}|\Phi_0\rangle =$$

$$=' \sum_{n=0}^{\infty} \left\{ W \left\{ \left(R^{(0)} W\right)^n \right\}_L \right\}_{C_0} |\Phi_0\rangle$$

W is used to close all the external lines of $\{(R^{(0)}W)^n\}_L$, as in

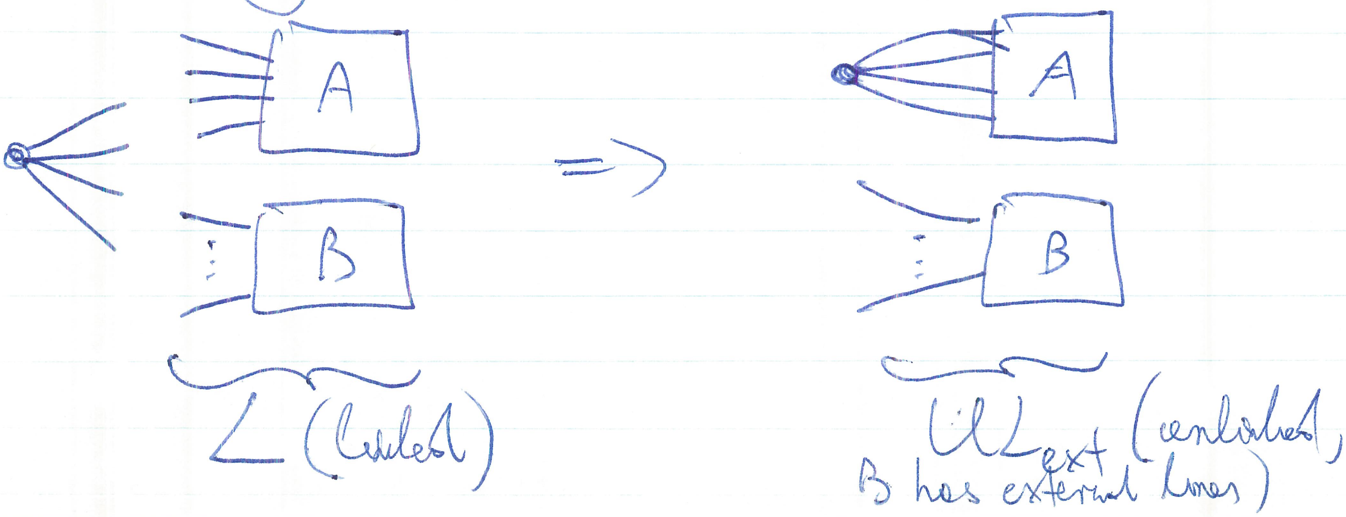


This must be connected, since $\boxed{A}$ does not have vacuum parts

$$+ \sum_{n=0}^{\infty} \left\{ W \left\{ \left(R^{(0)} W\right)^n \right\}_L \right\}_{U_{ext}} |\Phi_0\rangle$$

unlinked with external lines

W is closing the lines of one of the disconnected parts of $\{(R^{(0)}W)^n\}_L$ (producing the vacuum term), producing unlinked d-ms (having external lines)



$$+ \sum_{n=0}^{\infty} \left\{ W \left\{ (R^{(0)} W)^n \right\}_L \right\}_{L\,ext} |\Phi_0\rangle$$

$\uparrow$

W is not closing the lines of any of the parts of $\{(R^{(0)}W)^n\}_L$, leaving us with linked diagrams with some external lines.

This means that

$$(\mathcal{E}_0 - K_0)|\Psi_0\rangle = W \overbrace{\sum_{n=0}^{\infty} \left\{(R^{(0)}W)^n\right\}_L |\Phi_0\rangle}^{|\Psi_0\rangle}$$

$$- \sum_{n=0}^{\infty} \left\{ W \left\{ (R^{(0)} W)^n \right\}_L \right\}_{C_0} |\Phi_0\rangle$$

$$- \sum_{n=0}^{\infty} \left\{ W \left\{ (R^{(0)} W)^n \right\}_L \right\}_{UL\,ext} |\Phi_0\rangle$$

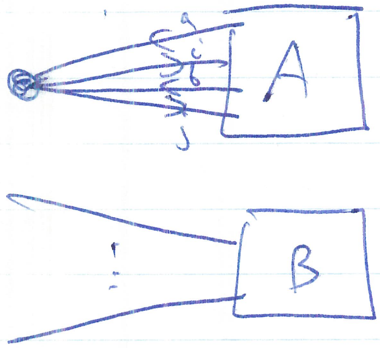
Now:

$$\sum_{n=0}^{\infty} \overbrace{\left\{ W \left\{ (R^{(0)} W)^n \right\}_L \right\}_{C_0}}^{\text{a number}} |\Phi_0\rangle$$

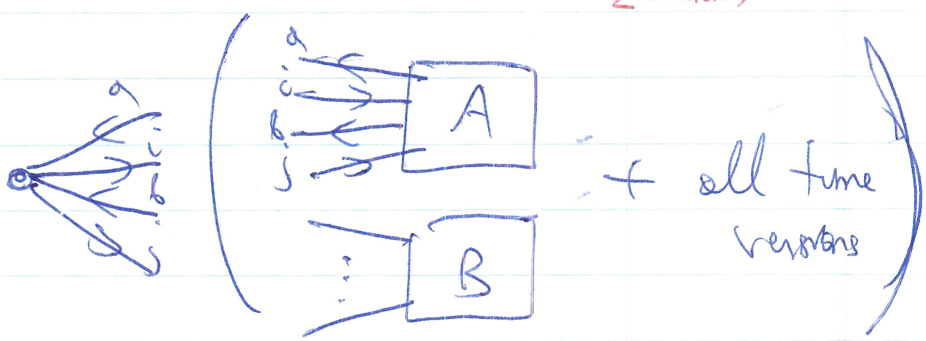
$$= \sum_{n=0}^{\infty} \left\{ W (R^{(0)} W)^n \right\}_{C_0} |\Phi_0\rangle = (K_0 - \mathcal{E}_0) \times |\Phi_0\rangle .$$

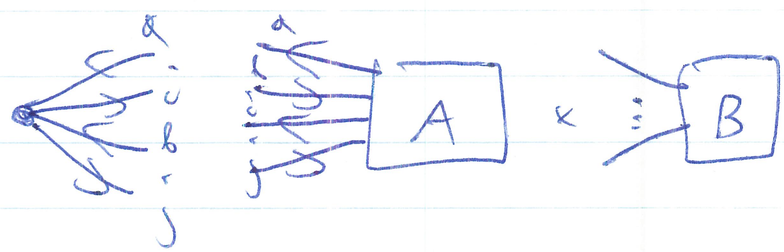
$$\sum_{n=0}^{\infty}\left\{W\left\{(R^{\infty}W)^{n}\right\}_{L}\right\}_{ULext}|\Phi_0\rangle =$$

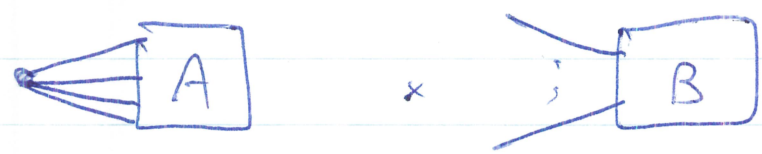
(in reality $n \geq 1$)

$\sum_{i,j,a,b}$  + all time versions

$\underbrace{\{(R^{\infty}W)^{n}\}}_{L_2 \text{(or more)}}$

$= \sum_{i,j,a,b}$  + all time versions

FACTORIZATION LEMMA $\sum_{i,j,a,b}$ 

$=$ 

Since we consider ALL ORDERS in

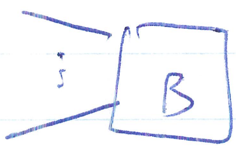
$$\sum_{n=0}^{\infty}\left\{W\left\{(R^{\infty}W)^{n}\right\}_{L}\right\}_{ULext}|\Phi_0\rangle ,$$

the  piece contains all linked terms $\{(R^{\infty}W)^{n}\}_{L}$ with $n \geq 1$, so that after correcting with W,  contains all CONNECTED vacuum diagrams of the $\{W\{(R^0W)^n\}\}_{C_0}$ type. In other words, all  terms give

$$(k_0 - \mathcal{E}_0).$$

Since we have all orders in

$$\sum_{n=0}^{\infty} \{W\{(R^0W)^n\}_L\}_{UL_{ext}} |\Phi_0\rangle,$$

the  pieces represents all linked terms with external lines, i.e.:

$$\sum_{n=1}^{\infty} \{(R^0W)^n\}_L |\Phi_0\rangle = |\Psi_0\rangle - |\Phi_0\rangle.$$

This implies that

$$\sum_{n=0}^{\infty} \{W\{(R^0W)^n\}_L\}_{UL_{ext}} |\Phi_0\rangle$$

$$= (k_0 - \mathcal{E}_0)\left(|\Psi_0\rangle - |\Phi_0\rangle\right).$$

From the above equations for

$$\sum_{n=0}^{\infty} \{W\{(R^{\infty}W)^n\}_L\}_{C_0}|\Phi_0\rangle \text{ and}$$

$$\sum_{n=0}^{\infty} \{W\{(R^{\infty}W)^n\}_L\}_{ULext}|\Phi_0\rangle \text{ terms, we}$$

obtain,

$$(\mathcal{H}_0 - K_0)|\Psi_0\rangle = W|\Psi_0\rangle - \cancel{(K_0-\mathcal{H}_0)|\Phi_0\rangle}$$

$$- (K_0-\mathcal{H}_0)\cancel{(|\Psi_0\rangle - |\Phi_0\rangle)} =$$

$$= W|\Psi_0\rangle - (K_0-\mathcal{H}_0)|\Psi_0\rangle$$

$$(\cancel{\mathcal{H}_0} - K_0)|\Psi_0\rangle = W|\Psi_0\rangle - (K_0 - \cancel{\mathcal{H}_0})|\Psi_0\rangle$$

$$(K_0+W)|\Psi_0\rangle = K_0|\Psi_0\rangle,$$

i.e., the $|\Psi_0\rangle = \sum_{n=0}^{\infty}\{(R^{\infty}W)^n\}_L|\Phi_0\rangle$ wave function satisfies the Schrödinger equation — This completes the proof!

We proved the linked cluster (diagram) theorem, which states that

$$|\Psi_0^{(n)}\rangle = \{(R^{(0)}W)^n\}_L |\Phi_0\rangle ,$$

$$k_0^{(n+1)} = \langle\Phi_0|\{W(R^{(0)}W)^n\}_C|\Phi_0\rangle .$$

Let us analyze the significance of these statements for the size extensivity of the calculated energies, understood as the proper dependence of the energy on the size of the system in the limit of noninteracting fragments.

Let us analyse what happens with the general connected quantity of the

$$\langle\Phi_0|\{W(R^{(0)}W)^n\}_C|\Phi_0\rangle$$

or

$$\{(R^{(0)}W)^n\}_C|\Phi_0\rangle \quad \text{type}$$

(let us call this quantity Λ), when a given system separates into non-interacting fragments

$$A, B, \ldots .$$

$$\text{System} \longrightarrow A + B + \ldots = \sum_{C} C$$

fragments

First of all, in the limit of non-interacting fragments, the spin-orbitals of the entire system become the spin-orbitals of subsystems,

$$|p\rangle \Longrightarrow |p_A\rangle, |p_B\rangle, \ldots \quad (|p_C\rangle \text{ in general}),$$

or $|\psi_{p_A}\rangle, |\psi_{p_B}\rangle, \ldots$ (this, of course, depends on how we calculate our spin-orbitals, but with the judicious choice of spin-orbitals, ~~we can guarantee~~ using, say localized ~~unrestricted~~ Hartree-Fock spin-orbitals, we can guarantee that the spin-orbitals of a system of noninteracting fragments are spin-orbitals of subsystems)

Let me illustrate this statement by analyzing the (unrestricted) Hartree-Fock equations. We can easily show that the Hartree-Fock spin-orbitals of noninteracting fragments (let us focus on molecular fragments), satisfying

$$\Big[\underbrace{-\tfrac{1}{2}\Delta_1}_{\text{electronic coordinate}} - \underbrace{\sum_{\gamma\in C}}_{\text{nuclei of } C} \frac{Z_\gamma}{\underbrace{r_{1\gamma}}_{\text{distance between electron 1 and nucleus } \gamma}}\Big] \psi_{i_C}(\underbrace{x_1}_{\text{coordinates of electron 1}})$$

$$+ \sum_{j_C \in \text{occ. in } C} \int \frac{\psi_{j_C}^*(x_2)\,\psi_{j_C}(x_2)}{r_{12}}\,dx_2\;\psi_{i_C}(x_1)$$

$$- \sum_{j_C \in \text{occ. in } C} \int \frac{\psi_{j_C}^*(x_2)\, \psi_{i_C}(x_2)}{r_{12}}\, dx_2\, \psi_{j_C}(x_1)$$

$$= \varepsilon_{i_C}\, \psi_{i_C}(x_1) ,$$

for each subsystem C $(C = A, B, \ldots)$,

satisfy the H-F equations for the whole system,

$$\cancel{\left[-\frac{1}{2}\Delta_1 - \sum_{D} \sum_{\gamma \in C} \frac{Z_\gamma}{r_{1\gamma}}\right] \psi_{i_C}(x_1)}$$

$$\cancel{+ \sum_{C} \sum_{j_C \in \text{occ. in } C} \int \frac{\psi_{j_C}(x_2)^*\, \psi_{j_C}(x_2)}{r_{12}}\, dx_2\, \psi_{i_C}(x_1)}$$

(1) $$\left[-\frac{1}{2}\Delta_1 - \sum_{D} \sum_{\delta \in D} \frac{Z_\delta}{r_{1\delta}}\right] \psi_{i_C}(x_1)$$

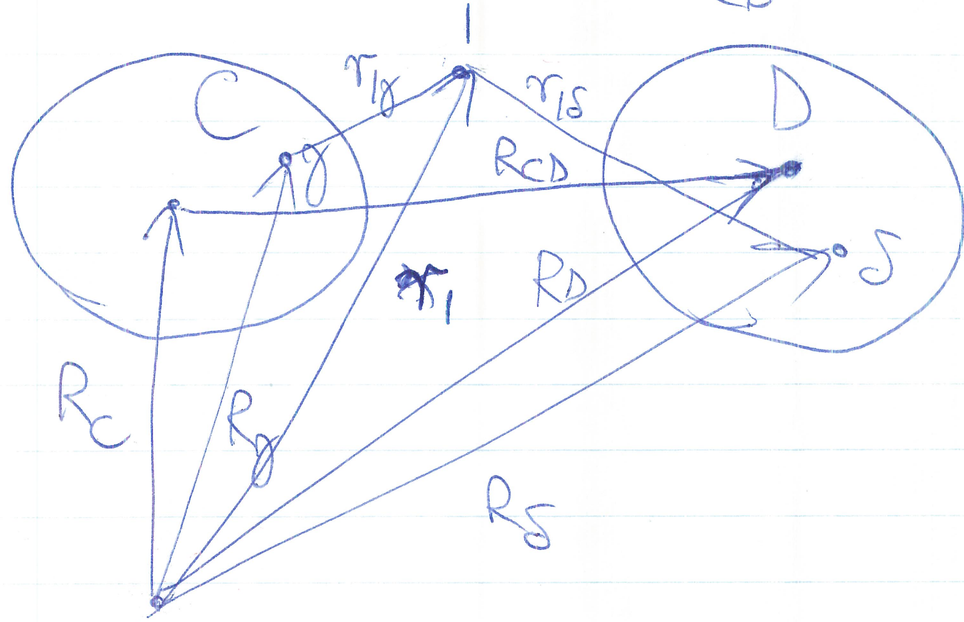
summation over all subsystems

nuclei of subsystem D

(2) $$+ \sum_{D} \sum_{\hat{j}_D \in \text{occ. in } D} \int \frac{\psi_{\hat{j}_D}(x_2)^*\, \psi_{\hat{j}_D}(x_2)}{r_{12}}\, dx_2\, \psi_{i_C}(x_1)$$

(3) $$+ \sum_{D} \sum_{\hat{j}_D \in \text{occ. in } D} \int \frac{\psi_{\hat{j}_D}^*(x_2)\, \psi_{i_C}(x_2)}{r_{12}}\, dx_2\, \psi_{\hat{j}_D}(x_1)$$

$= \varepsilon_{i_C} \psi_{i_C}(x_1)$, when distances between subsystems, $R_{CD} \to \infty$.



γ, δ - nuclei in C, D

R_C, R_D - vectors of coordinates of centers of C and D

~~(1): ψ_{i_C} is localized on C, so that r_1 ≈ R_C to give a non zero value. For $D \neq C$, $r_{1\delta} \to \infty$~~

(1): ψ_{i_C} is localized on C, so that $r_1 \approx R_C$ to give a non-zero value of $\psi_{i_C}(x_1)$. For $D \neq C$, $r_{1\delta} \to \infty$ if $R_{CD} \to \infty$ and $r_1 \approx R_C$, so that

(1) ~~becomes~~ reduces to

$$\left[-\frac{1}{2}\Delta_1 - \sum_{\gamma \in C} \frac{Z_\gamma}{r_{1\gamma}}\right] \chi_{iC}(x_1)$$

(2): χ_{jD} is localized on D and χ_{iC} is localized on C. Thus, $r_1 \approx R_C$ and $r_2 \approx R_D$ to give nonzero values of χ_{iC} and χ_{jD}. For $C \neq D$, $R_{CD} \to \infty$, $r_{12} \to \infty$, so that (2) ~~becomes~~ reduces to

$$\sum_{jC} \int \frac{\chi_{jC}(x_2)^* \chi_{jC}(x_2)}{r_{12}} dx_2 \, \chi_{iC}(x_1).$$

(3): ~~Again~~ In this case, if $D \neq C$, $\chi_{jD}(x_2)^* \chi_{iC}(x_2) \to 0$ ~~as~~ if $R_{CD} \to \infty$. Thus, (3) ~~becomes~~ reduces to

$$\sum_{jC \in occ.\, in\, C} \int \frac{\chi_{jC}^*(x_2)\, \chi_{iC}(x_2)}{r_{12}} dx_2 \times \chi_{jC}(x_2)$$

In other words, the H-F equations for the entire system reduce to

$$\left[-\frac{1}{2}\Delta_1 - \sum_{\gamma \in C} \frac{Z_\gamma}{r_{1\gamma}}\right] \psi_{i_C}(x_1)$$

$$+ \sum_{j_C} \int \frac{\psi_{j_C}^*(x_2)\,\psi_{j_C}(x_2)}{r_{12}}\, dx_2\, \psi_{i_C}(x_1)$$

$$- \sum_{j_C} \int \frac{\psi_{j_C}^*(x_2)\,\psi_{i_C}(x_2)}{r_{12}}\, dx_2\, \psi_{j_C}(x_1)$$

$$= \varepsilon_{i_C}\, \psi_{i_C}(x_1),$$

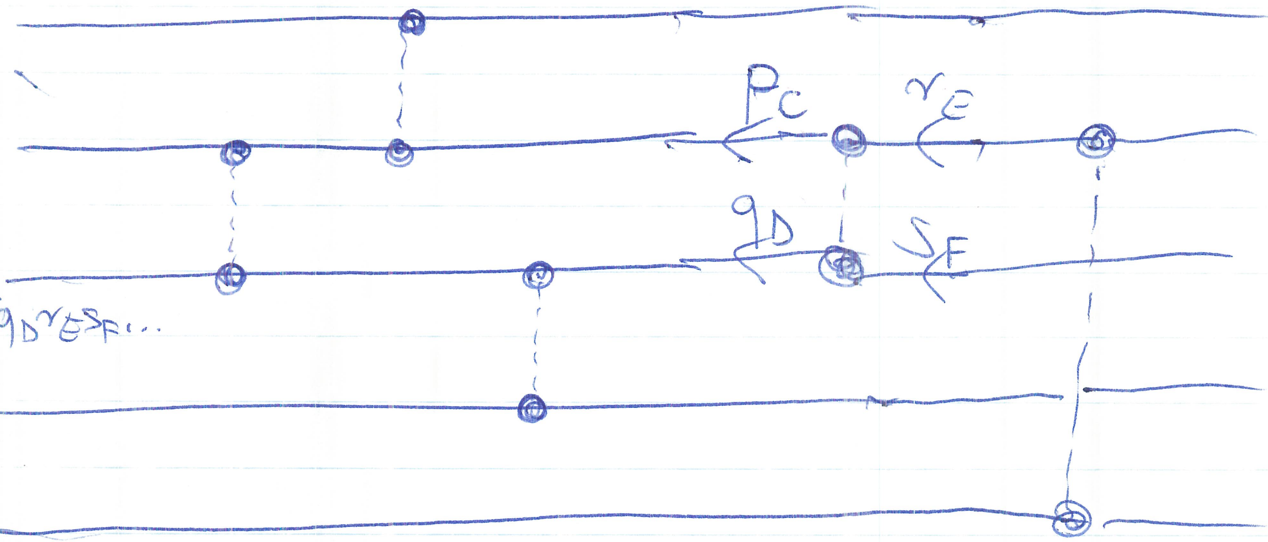
i.e. to the equations for individual subsystems.

Thus, we can indeed assume that the spin-orbitals of a system of noninteracting fragments are spin-orbitals of these fragments.

Now, let us return to quantity Δ.

This quantity consists of the connected diagrams, schematically, the

$$\sum_{\ldots C, D, E, F \ldots} \sum_{\ldots p_C q_D r_E s_F \ldots}$$



(Goldstone representation)

diagrams obtained by connecting some vertices of W vertices. p_C, q_D, r_E, s_F are the spin-orbitals of subsystems C, D, E, F.
Algebraic expressions will contain matrix elements

$$\langle p_C q_D | \hat{v} | r_E s_F \rangle \xrightarrow[v = \frac{1}{r_{12}}]{\text{assume}}$$

$$= \int \frac{\psi_{p_C}(x_1)^* \psi_{q_D}(x_2)^* \psi_{r_E}(x_1) \psi_{s_F}(x_2)}{r_{12}} dx_1 dx_2$$

First of all, in the noninteracting limit,

$$\psi_{p_C}(x_1)^* \psi_{r_E}(x_1) \quad \text{and}$$

$$\psi_{qD}(x_2)^* \psi_{sF}(x_2)$$

vanish if $C \neq E$ and $D \neq F$, (because of a local character of spin orbitals).

Thus, $C = E$, $D = F$, and we are left with terms, such as

$$\int \frac{\psi_{pC}(x_1)^* \psi_{qD}(x_2)^* \psi_{rC}(x_1) \psi_{sD}(x_2)}{r_{12}} \, dx_1 dx_2$$

Now, if $C \neq D$ and $R_{CD} \to \infty$,

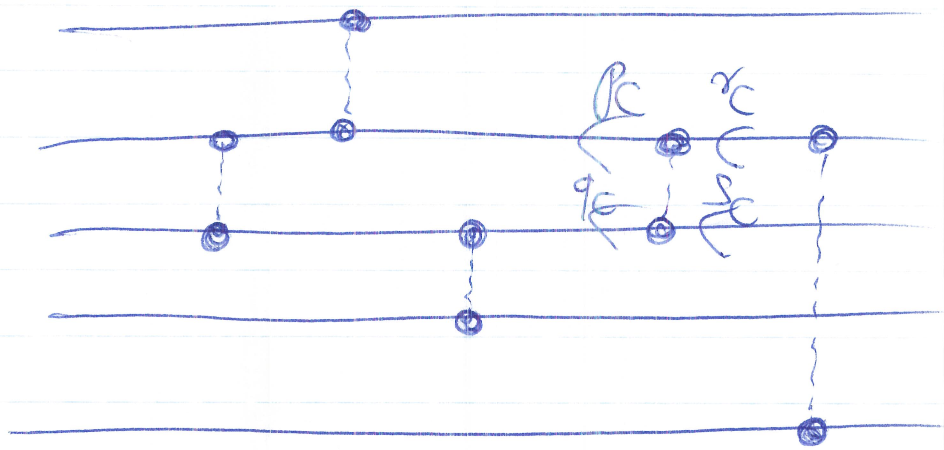
we have: $r_1 \approx R_C$, $r_2 \approx R_D$,

to give nonzero $\psi_{pC}(x_1)$ and $\psi_{qD}(x_2)$ (or $\psi_{rC}(x_1)$ and $\psi_{sD}(x_2)$), in which case $r_{12} \to \infty$ and the integral vanishes. Thus, we can only have integrals with $C = D = E = F$,

$$\langle p_C q_C | \hat{v} | r_C s_C \rangle,$$

and, in diagrams,

$$\sum_{\ldots C \ldots} \; \sum_{p_C q_C r_C s_C}$$



which means that

$$\Lambda = \sum_C \Lambda_C \text{, where } \Lambda_C$$

is a quantity Λ written for fragment C.

For the connected quantities, we have

$$\Lambda = \sum_C \Lambda_C \text{, where}$$

Λ_C ~~is~~ a Λ written (or drawn) for fragment C. Clearly, since spin-orbitals of different fragments satisfy the ZDO condition,

$$\psi_{p_C}(x)^* \psi_{q_D}(x)$$

is zero for $C \neq D$,

They are also orthogonal, $\langle \chi_{pC} | \chi_{qD} \rangle = \delta_{pq} \delta_{CD}$.
and excited configurations
for different fragments are orthogonal, too.
Thus,
$$[A_C, A_D] = 0 \quad \text{for } C \neq D.$$

In particular,
$$k_0^{(n)} = \langle \Phi_0 | \{W (R^{(0)} W)^n\}_C | \Phi_0 \rangle$$
$$= k_0^{(n)}(A) + k_0^{(n)}(B) + \ldots,$$
where
$$k_0^{(n)}(A) = \langle \Phi_0^{(A)} | \{W^{(A)} (R^{(0),A} W^{(A)})^n\}_C | \Phi_0^{(A)} \rangle$$
$$k_0^{(n)}(B) = \langle \Phi_0^{(B)} | \{W^{(B)} (R^{(0),B} W^{(B)})^n\}_C | \Phi_0^{(B)} \rangle$$
etc.,

are energy corrections for the fragments.
FINITE-ORDER (MBPT) CALCULATIONS LEAD TO SIZE EXTENSIVE RESULTS FOR ENERGIES (but not for wave functions!).

N11

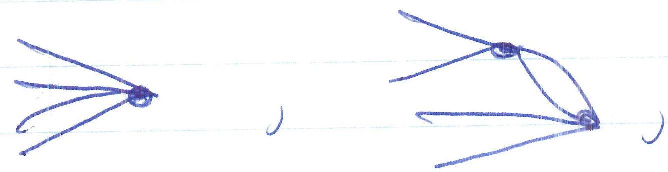
Connected cluster theorem, coupled-cluster ansatz for the wave function

We know that $|\Psi_0^{(n)}\rangle = \{(R^{(0)}W)^n\}_L |\Phi_0\rangle$,

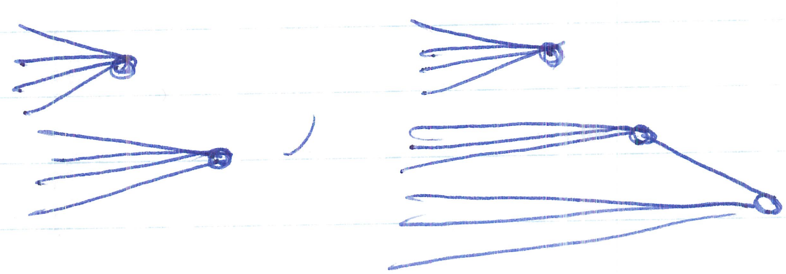
where L designates all linked diagrams, including EPV terms. We can classify all linked terms according to the number of connected components in a diagram:

L_r – all linked diagrams with r connected components.

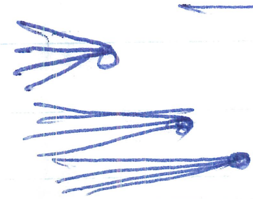
Examples:



, etc. are the $r=1$ diagrams (class L_1)



, etc. are the $r=2$ diagrams (class L_2),



, etc. are the $r=3$ d-ms (class L_3).

Thus, we can write

$$|\Psi_0^{(n)}\rangle = \sum_{r=1}^{n} \underbrace{\{(R^{(0)}W)^n\}_{L_r}}_{\text{linked diagrams with } r \text{ connected components}} |\Phi_0\rangle ,$$

and $$|\Psi_0\rangle = \sum_{n=0}^{\infty} |\Psi_0^{(n)}\rangle$$

$$= |\Phi_0\rangle + \sum_{n=1}^{\infty} \sum_{r=1}^{n} \{(R^{(0)}W)^n\}_{L_r} |\Phi_0\rangle$$

Among classes L_r, we have <u>class L_1 of the connected diagrams</u>. Let us define the CLUSTER OPERATOR $\hat{T}$ as the sum of <u>all</u> connected (L_1) components of $|\Psi_0\rangle$,

$$T|\Phi_0\rangle = \sum_{n=1}^{\infty} \{(R^{(0)}W)^n\}_{L_1} |\Phi_0\rangle$$

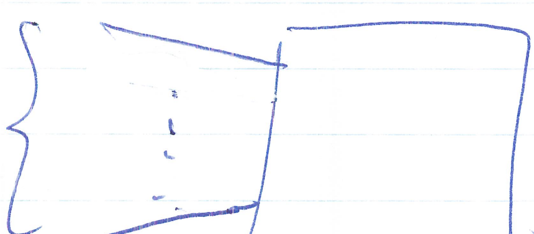
$$= \sum_{n=1}^{\infty} \{(R^{(0)}W)^n\}_{C} |\Phi_0\rangle .$$

Clearly, connected diagrams $\{(R^{(0)}W)^n\}_C|\Phi_0\rangle$ have certain number of external lines extending to the left ($2k$ lines, $k=1,2,\ldots,N$ for an N-electron system). Thus, we can write

$$T|\Phi_0\rangle = \sum_{n=1}^{\infty}\sum_{k=1}^{N}\{(R^{(0)}W)^n\}_{C,k}|\Phi_0\rangle,$$

where $2k$ is the number of external lines in diagrams in $\{(R^{(0)}W)^n\}_{C,k}|\Phi_0\rangle$ (it may happen that for some n values, not all k values are possible, in which case $\{(R^{(0)}W)^n\}_{C,k}$ is a zero term). Clearly, k is the excitation number; a diagram

$2k$ lines to the left



is a linear combination of

$$E^{a_1\ldots a_k}_{i_1\ldots i_k} = X^{\dagger}_{a_1}X_{i_1}\ldots X^{\dagger}_{a_k}X_{i_k}$$

or $$|\Phi_{c_1\ldots c_k}^{a_1\ldots a_k}\rangle = C_{c_1\ldots c_k}^{a_1\ldots a_k}|\Phi_0\rangle.$$

Thus,

$$T|\Phi_0\rangle = \sum_{k=1}^{N}\sum_{n=1}^{\infty}\{(R^{(0)}W)^n\}_{C,k}|\Phi_0\rangle$$

$$= \sum_{k=1}^{N} T_k|\Phi_0\rangle,$$

or $$T = \sum_{k=1}^{N} T_k \quad , \text{ where}$$

$$T_k = \sum_{n=1}^{\infty} T_k^{(n)} \quad , \text{ with}$$

$$T_k^{(n)}|\Phi_0\rangle = \underbrace{\{(R^{(0)}W)^n\}_{C,k}|\Phi_0\rangle}_{\substack{\text{all connected diagrams}\\ \text{resulting from } n \text{ vertices with}\\ 2k \text{ external lines}}} .$$

T_k is a k-body cluster component,
$T_k^{(n)}$ is the n-order contribution to T_k.

Clearly,

$$T_k^{(n)} = \frac{1}{k!}\sum_{\substack{a_1\cdots a_k\\ i_1\cdots i_k}} \overbrace{\langle a_1\cdots a_k|t_k^{(n)}|i_1\cdots i_k\rangle}^{\text{some coefficients resulting from } \{(R^{(n)})^m\}}$$

$$\times \underbrace{E^{a_1\cdots a_k}_{i_1\cdots i_k}}_{N[X^\dagger_{a_1}X_{i_1}\cdots X^\dagger_{a_k}X_{i_k}]}$$

$$= \left(\frac{1}{k!}\right)^2 \sum_{\substack{a_1\cdots a_k\\ i_1\cdots i_k}} \langle a_1\cdots a_k|t_k^{(n)}|i_1\cdots i_k\rangle_A \times N[X^\dagger_{a_1}X_{i_1}\cdots X^\dagger_{a_k}X_{i_k}],$$

$$T_k = \frac{1}{k!}\sum_{\substack{a_1\cdots a_k\\ i_1\cdots i_k}} \langle a_1\cdots a_k|t_k|i_1\cdots i_k\rangle \times N[X^\dagger_{a_1}X_{i_1}\cdots X^\dagger_{a_k}X_{i_k}]$$

$$= \left(\frac{1}{k!}\right)^2 \sum_{\substack{a_1\cdots a_k\\ i_1\cdots i_k}} \langle a_1\cdots a_k|t_k|i_1\cdots i_k\rangle_A \times N[X^\dagger_{a_1}X_{i_1}\cdots X^\dagger_{a_k}X_{i_k}]$$

where $\langle a_1\cdots a_k|t_k|i_1\cdots i_k\rangle = \sum_n \langle a_1\cdots a_k|t_k^{(n)}|i_1\cdots i_k\rangle$,

and $\langle a_1\cdots a_k|t_k|i_1\cdots i_k\rangle_A = \sum_{R\in S_k}(-1)^R\langle a_1\cdots a_k|t_k|i_{R_1}\cdots i_{R_k}\rangle$.

For example (pair-cluster operator or the doubly excited cluster component)

$$T_2 = \frac{1}{4} \sum_{ijab} \langle ab|H_2|ij\rangle_A \, N[X_a^\dagger X_i X_b^\dagger X_j]$$

$$= \frac{1}{2} \sum_{ijab} \langle ab|H_2|ij\rangle \, \underbrace{N[X_a^\dagger X_i X_b^\dagger X_j]}_{E_{ij}^{ab}},$$

where

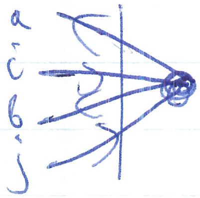
$$\langle ab|H_2|ij\rangle_A = \langle ab|H_2|ij\rangle - \langle ab|H_2|ji\rangle$$

$$T_2 = \sum_{n=1}^{\infty} T_2^{(n)}, \quad \text{where}$$

$$T_2^{(n)}|\Phi_0\rangle = \underbrace{\{(R^{(0)}W)^n\}_{C,2}}_{\text{connected diagrams with 4 external lines.}} |\Phi_0\rangle$$

In the lowest order,

$$T_2^{(1)}|\Phi_0\rangle = \{(R^{(0)}W)\}_{C,2} |\Phi_0\rangle$$

= 

$$= \frac{1}{4} \sum_{ijab} \frac{\langle ab|v|ij\rangle_A}{\varepsilon_i - \varepsilon_a + \varepsilon_j - \varepsilon_b} \times E_{ij}^{ab}|\Phi_0\rangle$$

$$= \sum_{\substack{i<j \\ a<b}} \frac{\langle ab|\hat{v}|ij\rangle_A}{\varepsilon_i - \varepsilon_a + \varepsilon_j - \varepsilon_b} \overbrace{E^{ab}_{ij}|\Phi_0\rangle}^{|\Phi^{ab}_{ij}\rangle}$$

On the other hand

$$T_2^{(1)}|\Phi_0\rangle = \frac{1}{4}\sum_{ijab} \langle ab|t_2^{(1)}|ij\rangle_A E^{ab}_{ij}|\Phi_0\rangle$$

$$= \sum_{\substack{i<j \\ a<b}} \langle ab|t_2^{(1)}|ij\rangle_A |\Phi^{ab}_{ij}\rangle,$$

so that

$$\boxed{\langle ab|t_2^{(1)}|ij\rangle_A = \frac{\langle ab|v|ij\rangle_A}{\varepsilon_i - \varepsilon_a + \varepsilon_j - \varepsilon_b}}$$

Another example:

T_1 (the Hartree-Fock case):

$$T_1 = \sum_{i,a} \langle a|t_1|i\rangle E^a_i ,$$

$$T_1 = \sum_{n=1}^{\infty} T_1^{(n)}, \text{ where}$$

$$T_1^{(n)}|\Phi_0\rangle = \overbrace{\{(R^{(0)}W)^n\}_{C,1}}^{\text{connected d-ms with 2 external lines}} |\Phi_0\rangle$$

In the H-F case, $W = V_N$,

$$T_1^{(n)}|\Phi_0\rangle = \{(R^{(0)}V_N)^n\}_{C,1}|\Phi_0\rangle \,,$$

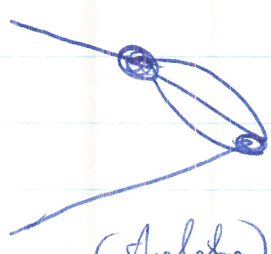
The lowest orders:

$n=1$:

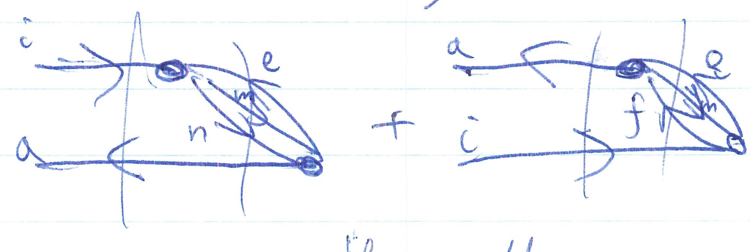
$$T_1^{(1)}|\Phi_0\rangle = \{(R^{(0)}V_N)\}_{C,1}|\Phi_0\rangle$$
$$= 0 \quad (\text{no diagrams})$$

$n=2$:

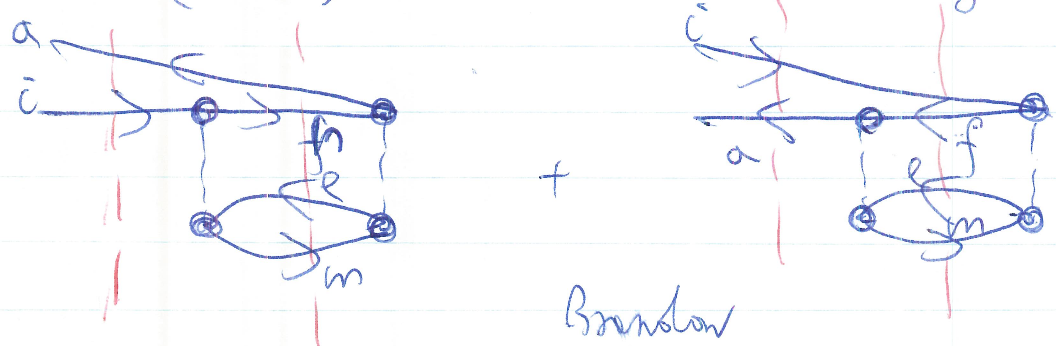
$$T_1^{(2)}|\Phi_0\rangle = \{(R^{(0)}V_N)^2\}_{C,1}|\Phi_0\rangle$$

$=$ 

(skeleton)

$=$ 

Hugenholtz

$=$ 

Brandow

$$= -\frac{1}{2}\sum_{a,i,m,n,e}\frac{\langle ea|\hat{v}|mn\rangle_A\langle mn|\hat{v}|ei\rangle_A}{(\varepsilon_i-\varepsilon_a)(\varepsilon_m+\varepsilon_n-\varepsilon_a-\varepsilon_e)}|\Phi_i^a\rangle$$

$$+\frac{1}{2}\sum_{a,i,m,e,f}\frac{\langle ma|\hat{v}|ef\rangle_A\langle ef|\hat{v}|mi\rangle_A}{(\varepsilon_i-\varepsilon_a)(\varepsilon_m+\varepsilon_i-\varepsilon_e-\varepsilon_f)}|\Phi_i^a\rangle$$

$$= \sum_{a,i}\langle a|t_1^{(2)}|i\rangle|\Phi_i^a\rangle,$$ so that

$$\boxed{\langle a|t_1^{(2)}|i\rangle = \frac{1}{2}\sum_{ef,m}\frac{\langle ma|\hat{v}|ef\rangle_A\langle ef|\hat{v}|mi\rangle_A}{(\varepsilon_i-\varepsilon_a)(\varepsilon_i+\varepsilon_m-\varepsilon_e-\varepsilon_f)} - \frac{1}{2}\sum_{mne}\frac{\langle ea|\hat{v}|mn\rangle_A\langle mn|\hat{v}|ei\rangle_A}{(\varepsilon_i-\varepsilon_a)(\varepsilon_m+\varepsilon_n-\varepsilon_a-\varepsilon_e)}}$$

As we can see, in the H-F case,

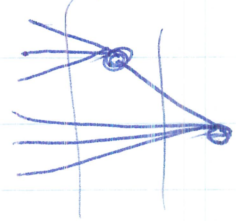
$$T_1 = T_1^{(2)} + \ldots$$

$$T_2 = T_2^{(1)} + \ldots,$$

T_2 is a lot more important than T_1.

We can use similar analysis to show that

$$T_3 = T_3^{(2)} + \ldots$$

( $= T_3^{(2)}$)

$$T_4 = T_4^{(3)} + \ldots .$$

Now, we will prove a CONNECTED CLUSTER THEOREM,

$$|\Psi_0\rangle = e^{T}|\Phi_0\rangle,$$

where

$$T|\Phi_0\rangle = \sum_{n=1}^{\infty}\{(R^{(0)}W)^n\}_C|\Phi_0\rangle .$$

Proof is based on the ~~equation~~ fact that

$$\sum_{n=r}^{\infty}\{(R^{(0)}W)^n\}_{L_r}|\Phi_0\rangle =$$

we must have at least r W vertices to get L_r diagrams

$$= \frac{1}{r!}T^{r}|\Phi_0\rangle . \qquad (A)$$

Let us prove Eq. (A). The $r=1$ case is obvious,

$$\sum_{n=1}^{\infty} \{(R^{(0)}W)^n\}_{L_1} |\Phi_0\rangle =$$

$$= \sum_{n=1}^{\infty} \{(R^{(0)}W)^n\}_{C} |\Phi_0\rangle$$

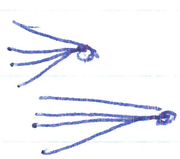
$$\equiv T|\Phi_0\rangle = \frac{1}{1!} T^1 |\Phi_0\rangle .$$

The $r=2$ case:

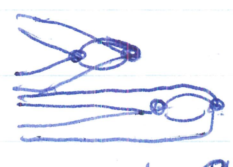
$$\sum_{n=2}^{\infty} \{(R^{(0)}W)^n\}_{L_2} |\Phi_0\rangle$$

$$= \sum_{n=2}^{\infty} \sum_{[A]} \sum_{t_1<t_2} \{(R^{(0)}W)^n\}_{[A]_{t_1},[A]_{t_2}} |\Phi_0\rangle$$

[diagrams with equivalent connected components $\boxed{A}$ $\boxed{A}$ + all time versions leading to nonequivalent diagrams (not all time versions, since we can get a given diagram as two time versions; cf. the



case, where there are 2 time versions, but only 1 is needed, or the

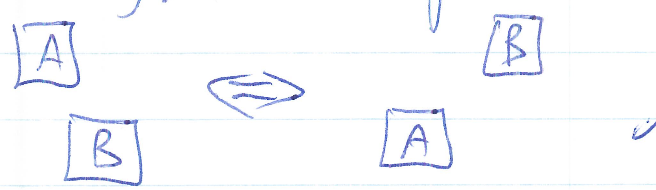


case, where there are 6 time versions, but only 3 are nonequivalent; the nonequivalent time versions are produced by having a symbolic ordering of $[A]_{t_1} [A]_{t_2}$ diagrams, $t_1 < t_2$, to avoid repetitions]

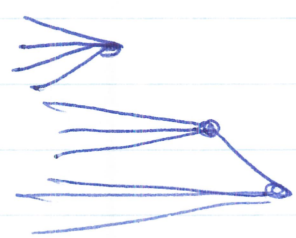
$$+ \sum_{n=2}^{\infty} \sum_{[A]<[B]} \sum_{t_1,t_2} \{(R^{\infty}W)^n\}_{[A]_{t_1}[B]_{t_2}} |\Phi_0\rangle$$

[diagrams with different connected components, $\boxed{A}$ $\boxed{B}$ + all time versions. (in this case, $\boxed{A}$ and $\boxed{B}$ are different, so that we need all time versions to get all diagrams of a given type)

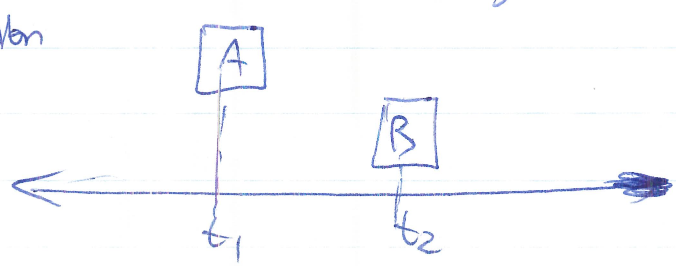
To eliminate repetitions, we "order" the connected components in some way; this is important since



examples:

the  case]

In the above notation, $[A]_{t_1}[B]_{t_2}$ is a time version



of a given diagram $\mathcal{Z}$ consisting of components [A] and [B].

We assume that components [A] and [B] are connected (the $\angle_2$ case). Clearly, both components have some external lines (otherwise, we would get an unlinked contribution).

We obtain,

$$\sum_{n=2}^{\infty} \left\{ \left(R^{(0)} W \right)^n \right\}_{\angle_2} |\Phi_0\rangle$$

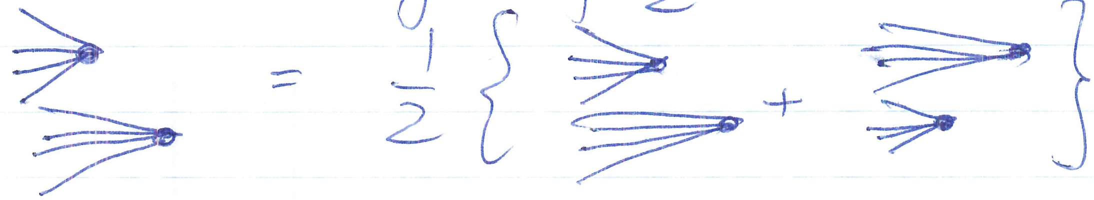
$$= \sum_{n=2}^{\infty} \sum_{[A]} \sum_{t_1 < t_2} \left\{ \left(R^{(0)} W \right)^n \right\}_{[A]_{t_1}, [A]_{t_2}} |\Phi_0\rangle$$

$$+ \sum_{n=2}^{\infty} \sum_{[A] < [B]} \sum_{t_1, t_2} \left\{ \left(R^{(0)} W \right)^n \right\}_{[A]_{t_1}, [B]_{t_2}} |\Phi_0\rangle$$

$$= \frac{1}{2} \sum_{n=2}^{\infty} \sum_{[A]} \sum_{t_1, t_2} \left\{ \left(R^{(0)} W \right)^n \right\}_{[A]_{t_1}, [A]_{t_2}} |\Phi_0\rangle$$

(t_1 cannot be t_2 anyway)

(we include ALL time versions; to avoid repetitions we must include a factor of $\frac{1}{2}$, as in)



$$+ \frac{1}{2} \sum_{n=2}^{\infty} \sum_{[A]\neq[B]} \sum_{t_1,t_2} \left\{ \left(R^{(0)} W\right)^n \right\}_{[A]_{t_1}[B]_{t_2}} |\Phi_0\rangle$$

$$= \frac{1}{2} \underbrace{\sum_{n=2}^{\infty} \sum_{[A],[B]} \sum_{t_1,t_2} \left\{ \left(R^{(0)} W\right)^n \right\}_{[A]_{t_1},[B]_{t_2}} |\Phi_0\rangle}_{\text{All time versions of the } L_2 \text{ diagrams consisting of pieces } [A] \text{ and } [B]}$$

$$= \frac{1}{2} \sum_{k=1}^{\infty} \sum_{l=1}^{\infty} \sum_{\substack{[A],[B] \\ \uparrow \quad \uparrow \\ k \text{ vertices } W \quad l \text{ vertices } W}} \sum_{t_1,t_2} \left\{ \left(R^{(0)} W\right)^k \left(R^{(0)} W\right)^l \right\}_{[A]_{t_1}[B]_{t_2}} |\Phi_0\rangle$$

$$\underset{\text{Lemma}}{\overset{\text{Factorization}}{=\!=}} \frac{1}{2} \sum_{k=1}^{\infty} \sum_{l=1}^{\infty} \sum_{[A]} \sum_{[B]} \left\{ \left(R^{(0)} W\right)^k \right\}_{\underset{\text{connected d-ms } [A]}{[A]}} \times$$

$$\times \left\{ \left(R^{(0)} W\right)^l \right\}_{\underset{\text{connected d-ms } [B]}{[B]}} |\Phi_0\rangle$$

$$= \frac{1}{2} \underbrace{\sum_{k=1}^{\infty} \sum_{[A]} \left\{ \left(R^{(0)} W\right)^k \right\}_{[A]}}_{T} \underbrace{\sum_{l=1}^{\infty} \left\{ \left(R^{(0)} W\right)^l \right\}_{[B]}}_{T} |\Phi_0\rangle$$

$$= \frac{1}{2} T^2 |\Phi_0\rangle.$$

Thus, $\sum_{n=2}^{\infty} \{(R^{(0)}H)^n\}_{L_2} |\Phi_0\rangle = \frac{1}{2!} T^2 |\Phi_0\rangle.$

For a general r case, we just recognize that

$$\sum_{n=r}^{\infty} \{(R^{(0)}H)^n\}_{L_r} |\Phi_0\rangle =$$

$$= \frac{1}{r!} \sum_{n=r}^{\infty} \sum_{[A_1],\ldots,[A_r]} \underbrace{\sum_{t_1,\ldots,t_r}}_{\text{all time versions}} \underbrace{\{(R^{(0)}H)^n\}_{[A_1]_{t_1}\ldots[A_r]_{t_r}}}_{\text{diagrams composed of } [A_1],\ldots,[A_r]} |\Phi_0\rangle$$

to eliminate repetitions, as in the $r=2$ case

connected pieces $[A_1],\ldots,[A_r]$

$$= \frac{1}{r!} \sum_{k_1=1}^{\infty} \cdots \sum_{k_r=1}^{\infty} \sum_{[A_1],\ldots,[A_r]} \sum_{t_1,\ldots,t_r}$$

k_1 vertices k_r vertices

$$\{(R^{(0)}H)^{k_1} \cdots (R^{(0)}H)^{k_r}\}_{[A_1]_{t_1}\cdots[A_r]_{t_r}} |\Phi_0\rangle$$

Factorization lemma

$$\frac{1}{r!} \overbrace{\sum_{k_1=1}^{\infty} \{(R^{(0)}W)^{k_1}\}_{[A_1]}}^{T} \times$$

connected with ext. lines

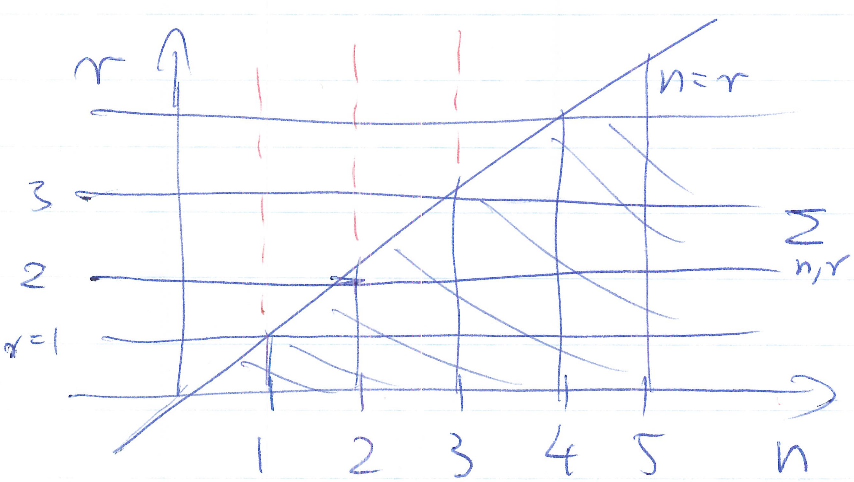
$$\times \dots \times \underbrace{\sum_{k_r=1}^{\infty} \{(R^{(0)}W)^{k_r}\}_{[A_r]}}_{T} |\Phi_0\rangle$$

$$= \frac{1}{r!} T^r |\Phi_0\rangle.$$

Now,

$$|\Psi_0\rangle = |\Phi_0\rangle + \sum_{n=1}^{\infty} \sum_{r=1}^{n} \{(R^{(0)}W)^n\}_{L_r} |\Phi_0\rangle$$

$$= |\Phi_0\rangle + \sum_{r=1}^{\infty} \sum_{n=r}^{\infty} \{(R^{(0)}W)^n\}_{L_r} |\Phi_0\rangle$$



$$= |\Phi_0\rangle + \sum_{r=1}^{\infty} \frac{1}{r!} T^r |\Phi_0\rangle = e^T |\Phi_0\rangle,$$

which completes the proof.

Other arguments in favor of

$$|\Psi_0\rangle = e^T |\Phi_0\rangle.$$

We know that the exact wave function

$$|\Psi_0\rangle = c_0 |\Phi_0\rangle + \sum_{i,a} c_a^i |\Phi_i^a\rangle$$

$$+ \sum_{\substack{i<j \\ a<b}} c_{ab}^{ij} |\Phi_{ij}^{ab}\rangle + \ldots$$

$$= c_0 |\Phi_0\rangle + \sum_{r=1}^{N} \hat{C}_r |\Phi_0\rangle,$$

where $\hat{C}_r |\Phi_0\rangle = \sum_{\substack{i_1 < \ldots < i_r \\ a_1 < \ldots < a_r}} c_{a_1 \ldots a_r}^{i_1 \ldots i_r} |\Phi_{i_1 \ldots i_r}^{a_1 \ldots a_r}\rangle$

are the r-body excitation operators.

Clearly,

$$C^{i_1 \ldots i_\nu}_{a_1 \ldots a_\nu} = \langle \Phi^{a_1 \ldots a_\nu}_{i_1 \ldots i_\nu} | \Psi_0 \rangle .$$

Since $|\Phi^{a_1 \ldots a_\nu}_{i_1 \ldots i_\nu}\rangle$ are antisymmetric with respect to permutations of $i_1, \ldots, i_\nu$ or $a_1, \ldots, a_\nu$, the same property applies to $C^{i_1 \ldots i_\nu}_{a_1 \ldots a_\nu}$ (in particular, if two i's or two a's are identical, $C^{i_1 \ldots i_\nu}_{a_1 \ldots a_\nu} = 0$), so that

$$\hat{C}_\nu |\Phi_0\rangle = \left(\frac{1}{\nu!}\right)^2 \sum_{\substack{i_1 \ldots i_\nu \\ a_1 \ldots a_\nu}} C^{i_1 \ldots i_\nu}_{a_1 \ldots a_\nu} |\Phi^{a_1 \ldots a_\nu}_{i_1 \ldots i_\nu}\rangle$$

or

$$\hat{C}_\nu = \left(\frac{1}{\nu!}\right)^2 \sum_{\substack{i_1 \ldots i_\nu \\ a_1 \ldots a_\nu}} \underbrace{C^{i_1 \ldots i_\nu}_{a_1 \ldots a_\nu}}_{= \langle a_1 \ldots a_\nu | \hat{C}_\nu | i_1 \ldots i_\nu \rangle_A} E^{a_1 \ldots a_\nu}_{i_1 \ldots i_\nu} .$$

We can always renormalize $|\Psi_0\rangle$ to satisfy

$$\langle \Phi_0 | \Psi_0 \rangle = 1 .$$ In this case, $C_0 = 1$.

Thus,

$$|\Psi_0\rangle = |\Phi_0\rangle + \sum_{r=1}^{N} \hat{C}_r |\Phi_0\rangle$$

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

where

$$\hat{C} = \sum_{r=1}^{N} \hat{C}_r = \hat{C}_1 + \hat{C}_2 + \dots + \hat{C}_N \text{ is}$$

the excitation operator.

Let us define

$$\hat{T} = \ln(1 + \hat{C}) =$$

$$= \sum_{m=1}^{\infty} (-1)^{m+1} \frac{\hat{C}^m}{m}.$$

In general, operator $\hat{T}$ may not exist.

However, in our case,

$$\hat{C}^m = 0 \text{ for } m > N.$$

($\hat{C}$ is nilpotent)

Thus,

$$T = \sum_{m=1}^{\infty} (-1)^{m+1} \frac{\hat{C}^m}{m}$$

$$= \sum_{m=1}^{N} (-1)^{m+1} \frac{\hat{C}^m}{m}$$

is a well-defined operator, represented by a finite expression.

Clearly, T is an excitation operator,

$$T = C - \frac{C^2}{2} + \frac{C^3}{3} - \ldots$$

$$= C_1 + C_2 + C_3 + \ldots - \frac{(C_1 + C_2 + \ldots)^2}{2} + \ldots$$

$$\Rightarrow \quad T_1 = C_1$$

$$T_2 = C_2 - \frac{C_1^2}{2}, \text{ etc.}$$

Since $T = \ln(1 + C) \Rightarrow$

$$1 + C = e^T \Rightarrow |\Psi_0\rangle = e^T|\Phi_0\rangle.$$

This does not tell us what is T from the MBPT point of view, but certainly T exists.

The advantage of the connected cluster theorem is that T is defined by a well-defined class of diagrams (connected ones) which gives us a deep insight into the structure of a many-~~electron~~ fermion wave function.

The

$$e^T |\Phi_0\rangle \text{ ansatz for } |\Psi_0\rangle$$

is the basis of the COUPLED-CLUSTER theory, which is based ~~on~~ solving the Schrödinger eqn. for T, treating T as an unknown. In practice, we truncate T at a given excitation level, say $T = T_1 + T_2$, and we are solving for $\langle a|t_1|i\rangle \equiv t_a^i$, $\langle ab|t_2|ij\rangle_A \equiv$ $\equiv t_{ab}^{ij}$, etc. - <u>cluster amplitudes</u> defining T_1, T_2, etc.

This has an advantage, since CC ansatz guarantees the correct description of separability of a system into subsystems:

$$AB \longrightarrow A + B$$

$$H_{AB} = H_A + H_B$$

$$|\Phi_0^{(AB)}\rangle = |\Phi_0^{(A)}\rangle |\Phi_0^{(B)}\rangle$$ (we are assuming that reference separates OK).

$$|\Psi_0^{(AB)}\rangle = e^{T^{(AB)}} |\Phi_0^{(AB)}\rangle.$$

$T^{(AB)}$ is connected, so that (cf. earlier discussion)

$$T^{(AB)} = T^{(A)} + T^{(B)},$$

$$[T^{(A)}, T^{(B)}] = 0.$$

In math, $e^{X+Y} = e^X e^Y$ if $[X,Y]=0$.

Thus,

$$|\Psi_0^{(AB)}\rangle = e^{T^{(A)}+T^{(B)}}|\Phi_0^{(A)}\rangle|\Phi_0^{(B)}\rangle$$

$$= e^{T^{(A)}}|\Phi_0^{(A)}\rangle\, e^{T^{(B)}}|\Phi_0^{(B)}\rangle$$

$$= |\Psi_0^{(A)}\rangle\,|\Psi_0^{(B)}\rangle,$$ which is

a desirable behavior.

The energy,

$$E^{(AB)} = \langle\Phi_0^{(AB)}|H_{AB}\underbrace{e^{T^{(AB)}}|\Phi_0^{(AB)}\rangle}_{|\Psi_0^{(AB)}\rangle}$$

$$= \langle\Phi_0^{(A)}|\langle\Phi_0^{(B)}|(H_A+H_B)\underbrace{e^{T^{(A)}}|\Phi_0^{(A)}\rangle}_{|\Psi_0^{(A)}\rangle}\underbrace{e^{T^{(B)}}|\Phi_0^{(B)}\rangle}_{|\Psi_0^{(B)}\rangle}$$

$$= \langle\Phi_0^{(A)}|H_A|\Psi_0^{(A)}\rangle\underbrace{\langle\Phi_0^{(B)}|\Psi_0^{(B)}\rangle}_{1} + \langle\Phi_0^{(B)}|H_B|\Psi_0^{(B)}\rangle$$

$$\times \underbrace{\langle\Phi_0^{(A)}|\Psi_0^{(A)}\rangle}_{1} = E^{(A)} + E^{(B)},$$ which is perfect.

The CC ansatz guarantees the correct separability and size extensivity of the results.