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SECOND EUROPEAN SUMMER SCHOOL on MICROSCOPIC QUANTUM MANY-BODY THEORIES and their APPLICATIONS

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THEORY OF CORRELATED BASIS FUNCTIONS PART II

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Correlated Coupled Clusters
Third generation CBF theory.

Reference Material:

F. Coester, in *Lectures in Theoretical Physics: Quantum Fluids and Nuclear Matter* (Gordon and Breach, New York, 1969), Vol. XI B.
H. Kümmel, K. H. Lührmann, and J. G. Zabolitzky, Physics Reports **36**, 1 (1978).
R. F. Bishop and K. H. Lührmann, Phys. Rev. B **17**, 3757 (1978).
R. F. Bishop, in *Microscopic Quantum Many–Body Theories and their Applications*, 187-250, Eds. Jesús Navarro and Artur Polls, Lecture Notes in Physics Vol. 510, Springer, Heidelberg (1998).
J. Navarro, these lectures.
E. K., H. Kümmel, and J. G. Zabolitzky, Phys. Rev. A **22**, 1243 (1980).

Goal: Derive CBF perturbative corrections by integral equations.

Conventional CCM: (Navarro lectures)

$$|\Psi_o\rangle = \exp S\,|\Phi_o\rangle\ ,$$

where

$$S = \sum_{n\geq 2} S_n,$$

$$S_n = \frac{1}{n!}\sum_{p_1\ldots h_n} S_{p_1\ldots p_n;h_1\ldots h_n}\, a^\dagger_{p_1}\ldots a^\dagger_{p_n} a_{h_n}\ldots a_{h_1}\ .$$

Write the Schrödinger equation as

$$e^{-S}\,\hat{H}\,e^{S}\,|\Phi_o\rangle = E\,|\Phi_o\rangle\,.$$

Observe that for all n–particle n–hole states $|\Phi_{\mathbf{m}}\rangle$

$$\langle\Phi_{\mathbf{m}}|\,e^{-S}\,\hat{H}\,e^{S}\,|\Phi_o\rangle = 0 \qquad\qquad (m\neq o).$$

A *correlated* coupled cluster wave function
Task–sharing

Let

$$|\Psi_0\rangle = \left|e^S\, o\right\rangle \,,$$

$$S_n = \frac{1}{n!} \sum_{p_1 \ldots h_n} S_{p_1 \ldots p_n ; h_1 \ldots h_n} \alpha^\dagger_{p_1} \ldots \alpha^\dagger_{p_n} \alpha_{h_n} \ldots \alpha_{h_1} \,.$$

Distribution of tasks:

$\Rightarrow$ Jastrow–Feenberg correlations for high-order summations of average geometric correlations;

$\Rightarrow$ Coupled clusters for not–so–high order summations of state–dependent effects.

$\Rightarrow$ Keep the correlation operator F the same for all states.

Schrödinger equation in the correlated basis:

$$\hat{H} \left| e^S o \right\rangle = E \left| e^S o \right\rangle ,$$

Basic C-CCM energy:

$$E = \frac{\left\langle o e^{-S} \right| \hat{H} \left| e^S o \right\rangle}{\left\langle o e^{-S} \right| e^S o \rangle}$$

(Note that $\left\langle o e^{-S} \right| = \langle o |$!)
Project on a correlated basis $\{|m\rangle\}$

Basic C-CCM equations:

$$\frac{\left\langle m e^{-S} \right| \hat{H} \left| e^S o \right\rangle}{\left\langle o e^{-S} \right| e^S o \rangle} = \frac{\left\langle o e^{-S} \right| \hat{H} \left| e^S o \right\rangle}{\left\langle o e^{-S} \right| e^S o \rangle} \frac{\left\langle m e^{-S} \right| e^S o \rangle}{\left\langle o e^{-S} \right| e^S o \rangle}$$

Correlated coupled cluster energy

Take SUB2 approximation of CCM *and* keep only matrix elements that can be written as (unlinked products of) two–body operators ("C-SUB2 approximation")

$$S = S_2 = \frac{1}{2!} \sum_{pp'hh'} S_{pp'hh'} \alpha_p^\dagger \alpha_{p'}^\dagger \alpha_{h'} \alpha_h, \quad \text{define} \quad \hat{S}_2 \equiv \frac{1}{2!} \sum_{pp'hh'} S_{pp'hh'} a_p^\dagger a_{p'}^\dagger a_{h'} a_h \, .$$

$$E = \frac{\langle o | \hat{H} | e^S o \rangle}{\langle o | e^S o \rangle} = H_{\mathbf{oo}} + \frac{\langle o | \hat{H} - H_{oo} | e^S o \rangle}{1 + \langle o | \left(e^S - 1 \right) o \rangle} \equiv H_{\mathbf{oo}} + \frac{\langle o | \hat{H}' | e^S o \rangle}{1 + \langle o | \left(e^S - 1 \right) o \rangle} \, ,$$

(let $\hat{H}' \equiv \hat{H} - H_{oo}$). Expand in powers of S:

$$\begin{aligned} E &= H_{oo} + \langle o | \, \hat{H}' \, | S \, o \rangle + \left[\frac{1}{2!} \langle o | \, \hat{H}' \, | S^2 \, o \rangle - \langle o | \, \hat{H}' \, | S \, o \rangle \, \langle o | \, S \, o \rangle \right] + \ldots \\ &= H_{oo} + (\delta E)_1 + (\delta E)_2 + \ldots \end{aligned}$$

For C-SUB2-approximation:

- First–order Term: Let $S_{mn} \equiv \langle \Phi_m | \, \hat{S} \, | \Phi_n \rangle$

$$\langle o | \, \hat{H}' \, | S \, o \rangle = \sum_m H'_{om} S_{mo} = \frac{1}{(2!)^2} \sum_{pp'hh'} \langle hh' | \, \mathcal{H} \, | pp' \rangle_a \, S_{pp',(hh')_a}$$

- Second–order Term:

(a) $$\frac{1}{2!} \langle o | \, \hat{H}' \, | S^2 \, o \rangle - \langle o | \, \hat{H}' \, | S \, o \rangle \langle o | \, S \, o \rangle$$

$$= \frac{1}{(2!)^2 \, 4!} \sum_{p_i, h_i} \langle h_1 h_2 h_3 h_4 | \, \mathcal{H}_4 \, | p_1 p_2 p_3 p_4 \rangle_a \, S_{p_1 p_2,(h_1 h_2)_a} S_{p_3 p_4,(h_3 h_4)_a}$$

$$- \frac{1}{(2!)^4} \sum_{p_i h_i} \langle h_1 h_2 | \, \mathcal{H} \, | p_1 p_2 \rangle_a \langle h_3 h_4 | \, \mathcal{N} \, | p_3 p_4 \rangle_a \, S_{p_1 p_2,(h_1 h_2)_a} S_{p_3 p_4,(h_3 h_4)_a}$$

(b) Keep the disconnected pieces of the 4-body operator $\mathcal{H}_4$

$$\mathcal{H}_4(1,2,3,4) = \mathcal{H}(1,2)\mathcal{N}(3,4) + \ldots + \mathcal{H}_4^{(c)}(1,2,3,4)$$

(c) cancel unlinked terms against $\langle o|\, H'\, |S\, o\rangle\, \langle o|\, S\, o\rangle$.

- Write energy as

$$E = H_{\mathbf{oo}} + \langle o|\, \hat{H}'\, |\$\, o\rangle$$
$$= H_{\mathbf{oo}} + \frac{1}{4} \sum_{pp'hh'} \langle hh'|\, \mathcal{H}\, |pp'\rangle_a\, \$_{pp',(hh')_a}$$

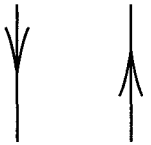
and find rules for the construction of \$.

In second order:

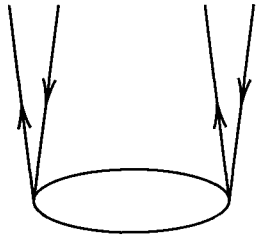
$$\$_{pp',(hh')_a} = S_{pp',(hh')_a} + \frac{1}{8} \sum_{p_1p_2h_1h_2} \langle h_1h_2|\, \mathcal{N}^{(2)}\, |p_1p_2\rangle_a \times$$
$$\times \left[(S^2)_{pp'p_1p_2,(hh'h_2h_2)_a} - S_{pp',(hh')_a} S_{p_1p_2,(h_1h_2)_a}\right] + \ldots$$

Diagrammatic notation (borrowed from CCM):

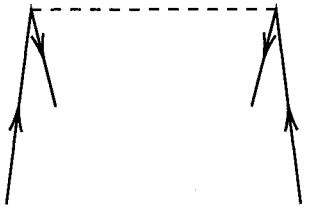
- Up- and down-going directed lines: "particle" or "hole" lines



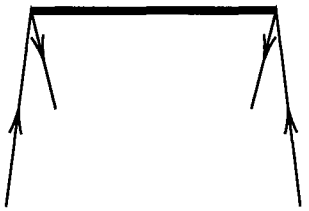
- ellipes: S-operator



- horizontal dashed lines: $\mathcal{N}$-operators



- horizontal heavy solid lines: $\mathcal{H}$ operators

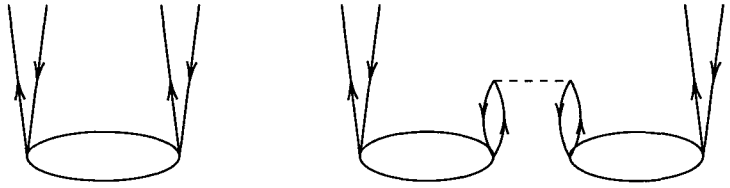


Sum over all internal lines

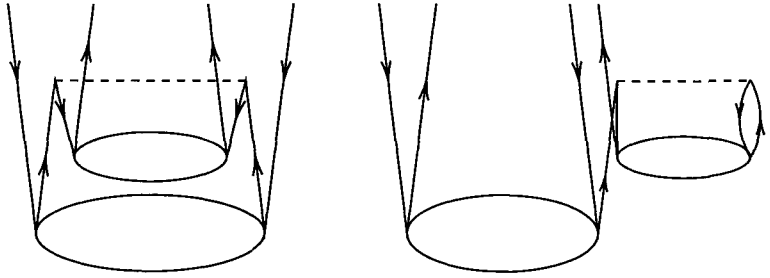
Rules for renormalizing S to \$:

$\$^{(2)}$ is represented by the sum of all diagrams that can be constructed from S_2 and $\mathcal{N}^{(2)}$ such that

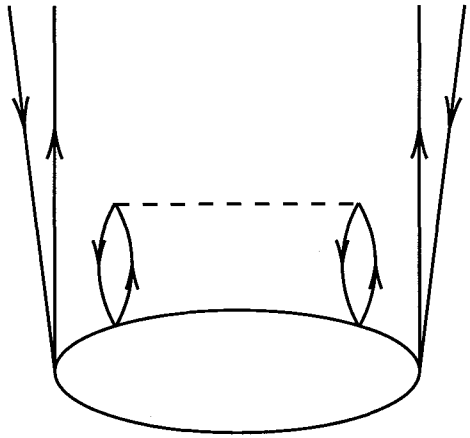
- the external lines enter only $S^{(2)}$;
- only internal lines may enter $\mathcal{N}^{(2)}$.
- no two $\mathcal{N}_2$ operators may be connected directly by a particle or a hole line.



- Verify at higher orders



- Extend to $\$^{(d)}$ if and when needed



Note: The renormalization is useful only if the same procedure simplifies the correlated coupled cluster equations !

C-CCM equations

Choose $|m\rangle$ to be (any) correlated 2p-2h state. Then

$$\left\langle me^{-S}\right| = \delta_{mo}\left\langle o\right| - \left\langle mS\right|$$

Rewrite C-CCM equations

$$\frac{\left\langle me^{-S}\right|\hat{H}\left|e^{S}o\right\rangle}{\left\langle oe^{-S}\right|e^{S}o\rangle} = \frac{\left\langle oe^{-S}\right|\hat{H}\left|e^{S}o\right\rangle}{\left\langle oe^{-S}\right|e^{S}o\rangle}\frac{\left\langle me^{-S}\right|e^{S}o\rangle}{\left\langle oe^{-S}\right|e^{S}o\rangle}$$

in terms of matrix elements of $\hat{H}' = \hat{H} - H_{oo}$

$$\frac{\left\langle m\right|\hat{H}'\left|e^{S}o\right\rangle}{1+\left\langle o\right|(e^{S}-1)o\rangle} = \frac{\left\langle o\right|\hat{H}'\left|e^{S}o\right\rangle}{1+\left\langle o\right|(e^{S}-1)o\rangle}\frac{\left\langle m\right|e^{S}o\rangle}{1+\left\langle o\right|(e^{S}-1)o\rangle}$$

- Expand in powers of S:

$$
\begin{aligned}
0 = & \langle m|\, \hat{H}'\, |o\rangle \\
& + \langle m|\, \hat{H}'\, |So\rangle - \langle m|\, \hat{H}'\, |o\rangle \langle o|\, S\, o\rangle - \langle m|\, o\rangle \langle o|\, \hat{H}'\, |So\rangle \\
& + \frac{1}{2!} \langle m|\, \hat{H}'\, |S^2 o\rangle - \langle m|\, \hat{H}'\, |o\rangle \langle o|\, S^2\, o\rangle - \langle m|\, o\rangle \langle o|\, \hat{H}'\, |S^2 o\rangle \\
& - 2 \langle m|\, \hat{H}'\, |So\rangle \langle o|\, S\, o\rangle - 2 \langle o|\, \hat{H}'\, |So\rangle \langle m|\, S\, o\rangle + \langle m|\, \hat{H}'\, |o\rangle \langle m|\, S\, o\rangle^2 \\
& + \ldots
\end{aligned}
$$

- Separate *diagonal* terms:

$$
\begin{aligned}
0 = & \hat{H}'_{mo} + (H_{mm} - H_{oo}) S_{mo} + \sum_n \left[H'_{mn} - H'_{mo} J_{on} - J_{mo} H'_{on} \right] S_{no} \\
& + \frac{1}{2!} \sum_n \left[H'_{mn} - H'_{mo} J_{on} - J_{mo} H'_{on} \right] (S^2)_{no} \\
& - \sum_{nn'} \left[2\hat{H}'_{mn} J_{on'} + 2\hat{H}'_{on} J_{mn'} - H'_{mo} J_{on} J_{on'} \right] S_{no} S_{n'o} + \ldots
\end{aligned}
$$

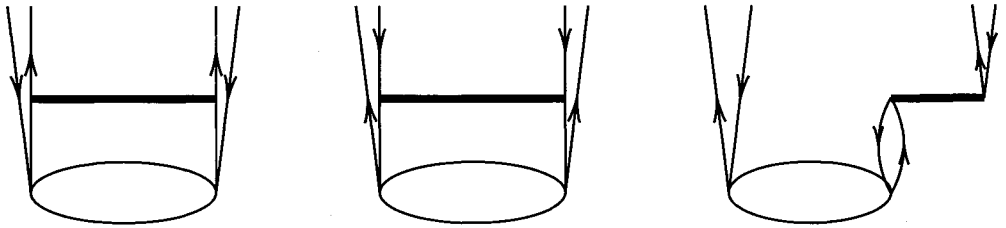
- Second-order CBF is obtained by keeping the first two terms.

- Restrict $|m\rangle$ and $|n\rangle$ to correlared 2p-2h states
- Matrix elements of two-body operators arise when $|\Phi_{\mathbf{m}}\rangle$ and $|\Phi_{\mathbf{n}}\rangle$ differ by two or four orbitals.
- States differing by two orbitals may be generated by coincidence of:

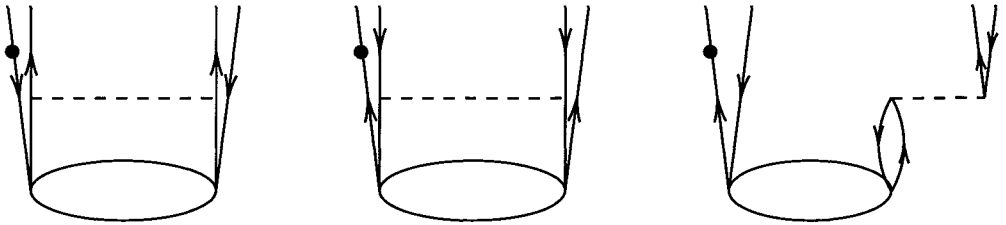
  the particle orbitals in $|\Phi_{\mathbf{m}}\rangle$ with the particle orbitals in $|\Phi_{\mathbf{n}}\rangle$,
  the hole orbitals in $|\Phi_{\mathbf{m}}\rangle$ with the hole orbitals in $|\Phi_{\mathbf{n}}\rangle$, or
  a particle-hole pair in $|\Phi_{\mathbf{m}}\rangle$ with a particle-hole pair in $|\Phi_n\rangle$.
- In the $d = 4$ contribution take all terms that can be written as matrix elements of unlinked products of two-body operators.

Results are best represented diagrammatically:
Some first–order contribution are

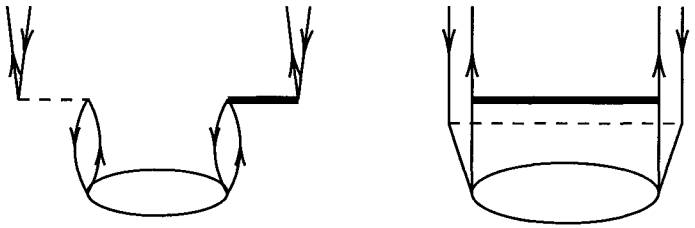
Particle–particle ladders
hole–hole ladders
and ring diagrams
from ordinary CCM



Non-orthogonality corrections
Dot on a line $= e_k$.



More non-orthogonality corrections



Diagrammatic rules for C-CCM equations

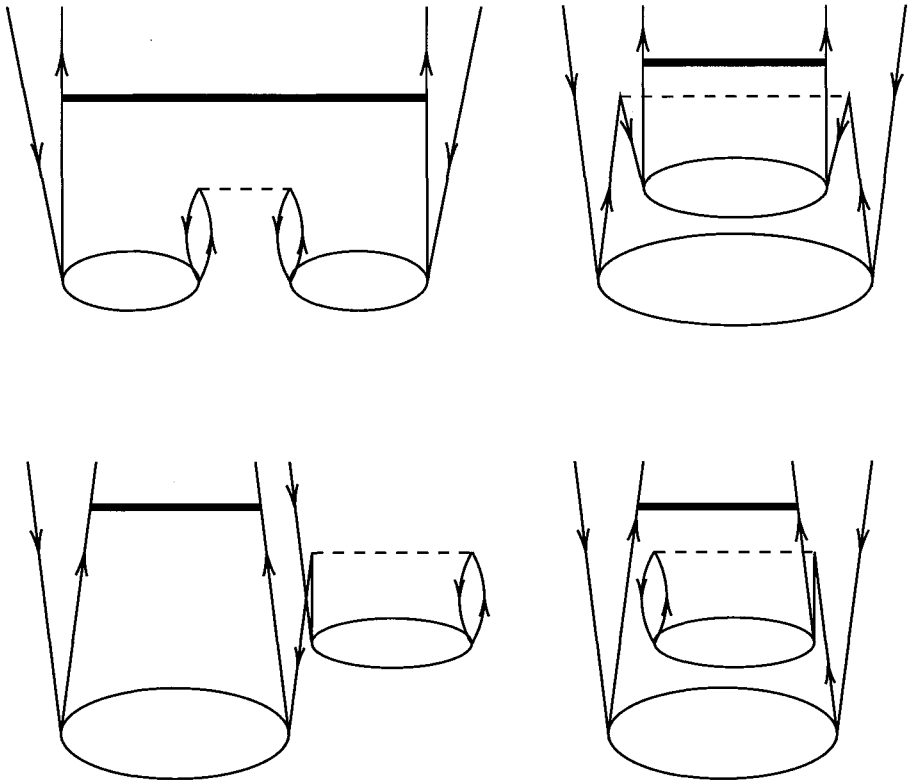
The expansion of the coupled-cluster equations is represented graphically by the sum of all diagrams which have the following properties:

- Two hole lines entering and two particle lines exiting at the top of each diagram,
- an arbitrary number of S elements,
- an arbitrary number of $\mathcal{N}$ elements,
- one effective interaction operator $\mathcal{H}$ or one single-particle (or hole) energy,

They obey the rules

- the S elements have only incoming hole lines and outgoing particle lines,
- no $\mathcal{N}$ line and no $\mathcal{H}$ or e element may be connected directly to another $\mathcal{N}$ element.

Verify at higher orders: Some more diagrams



All these diagrams are included in the first–order term if S is replaced by \$!

- The only subdiagram where all particle–and hole lines enter an S operator is \$

Summary
C-CCM equations

- A set of integral equations to sum systematically CBF perturbative diagrams;
- For the Jastrow–Feenberg–lover: A way to "move the nodes", or to do "single–operator chains";
- For the CCM-lover: A way to solve the hard–core problem.

Review
Effective interactions

$\Rightarrow$ The effective two–body interaction can be written as

$$\langle p,p'|\,\mathcal{H}(1,2)\,|h,h'\rangle_a$$
$$= \langle p,p'|\,\mathcal{W}(1,2)\,|h,h'\rangle_a + \frac{1}{2}\left(e_p + e_{p'} - e_h - e_{h'}\right)\langle p,p'|\,\mathcal{N}(1,2)\,|h,h'\rangle_a$$

It has the "average zero" property

$$\sum_{h\,h'}\sqrt{\frac{I_{mm}}{I_{oo}}}\,\langle \mathbf{h}+\mathbf{q},\mathbf{h}'-\mathbf{q}|\,\mathcal{H}(1,2)\,|\mathbf{h},\mathbf{h}'\rangle_a = 0$$

$\Rightarrow$ In the simplest approximations, we omit exchanges and use

$$\mathcal{N}(1,2) \to \mathcal{N}(r) = \Gamma_{dd}(r)$$
$$\mathcal{W}(1,2) \to \mathcal{W}(r) = \Gamma'_{dd}(r) + \frac{\hbar^2}{4m}\nabla^2\Gamma_{dd}(r)$$
$$e_k \to t(k)$$

Verify the "average zero" property:

$$\sum_{hh'} n(h)\bar{n}(\mathbf{h}+\mathbf{q})n(h')\bar{n}(\mathbf{h}'-\mathbf{q})\Big[\langle \mathbf{h}+\mathbf{q},\mathbf{h}'-\mathbf{q}|\,\mathcal{W}(1,2)\,|\mathbf{h},\mathbf{h}'\rangle$$

$$+\frac{1}{2}\left(t(\mathbf{h}+\mathbf{q})+t(\mathbf{h}'-\mathbf{q})-t(h)-t(h')\right)\langle \mathbf{h}+\mathbf{q},\mathbf{h}'+\mathbf{q}|\,\mathcal{N}_{dd}(1,2)\,|\mathbf{h},\mathbf{h}'\rangle\Big]$$

$$=N\left[S_F^2(q)\left[\tilde{\Gamma}'_{dd}(q)-\frac{t(q)}{2}\tilde{\Gamma}_{dd}(q)\right]+t(q)S_F(q)\tilde{\Gamma}_{dd}(q)\right]=0$$

Use here:

$$\tilde{V}_{\text{p-h}}(q)=\frac{t(q)}{2}\left[\frac{1}{S^2(q)}-\frac{1}{S_F^2(q)}\right]\qquad \tilde{w}_I(q)=-\frac{t(q)}{2}\left[\frac{1}{S_F(q)}-\frac{1}{S(q)}\right]^2\left[2\frac{S(k)}{S_F(k)}+1\right]$$

$$\tilde{\Gamma}'_{dd}(q)-\frac{t(q)}{2}\tilde{\Gamma}_{dd}(q)=\tilde{V}_{\text{p-h}}(q)+w_I(q)=-\frac{t(q)}{S_F(q)}\tilde{\Gamma}_{dd}(q)$$

$$S(q)=S_F(q)(1+S_F(q)\tilde{\Gamma}_{dd}(q))$$

Review: Correlated Coupled Clusters

$\Rightarrow$ We can derive the CBF perturbation series from

$$|\Psi_0\rangle = \left|e^S\, o\right\rangle ,$$

$$S_n = \frac{1}{n!} \sum_{p_1 \ldots h_n} S_{p_1 \ldots p_n; h_1 \ldots h_n} \alpha^\dagger_{p_1} \ldots \alpha^\dagger_{p_n} \alpha_{h_n} \ldots \alpha_{h_1} .$$

$\Rightarrow$ In C-SUB2 approximation, we have

$$\$_2 = \frac{1}{2} \sum_{pp'hh'} \$_{pp';hh'} \alpha^\dagger_p \alpha^\dagger_{p'} \alpha_{h'} \ldots \alpha_h$$

and the leading term is

$$\$_{pp';hh'} \approx S_{pp';hh'} = -\frac{\langle pp'|\, \mathcal{H}(1,2)\, |hh'\rangle_a}{e_p + e_{p'} - e_h - e_{h'}}$$

Interpretation
"Backflow" correlations or what ?

Focus on the direct term:

$$\langle p,p'|\,\mathcal{W}(1,2)\,|h,h'\rangle + \frac{1}{2}\left(e_p + e_{p'} - e_h - e_{h'}\right)\langle p,p'|\,\mathcal{N}(1,2)\,|h,h'\rangle$$

$$= \frac{1}{N}\left[\Gamma'_{dd}(q) - \frac{\hbar^2 q^2}{4m}\tilde{\Gamma}_{dd}(q) + \frac{\hbar^2}{2m}\tilde{\Gamma}_{dd}(q)\mathbf{q}\cdot(\mathbf{h}-\mathbf{h}')\right]$$

where $\mathbf{q} = \mathbf{p} - \mathbf{h}$.

Observe:

⇒ The *Fermi–sea average* of the expression vanishes. CBF corrections do not lead to new local correlations if these have already been optimized.

⇒ The non–local part of the operator can be written, in coordinate space, as

$$\nabla\Gamma_{dd}(r)\cdot\nabla$$

which is exactly the so-called "backflow" form.

Dynamics in CBF
Rings and Things

Objectives:

$\Rightarrow$ Formulation of a theory of excitations for a strongly interacting system,

$\Rightarrow$ Interpretation of the effective interactions of CBF theory

$\Rightarrow$ Interpretation of FHNC–diagrams

Reference Material:

D. J. Thouless, *The quantum mechanics of many-body systems,* Academic Press, New York (1972).

A. K. Kerman and S. E. Koonin, Ann. Phys. (NY) **100**, 332 (1976).

P. Kramer and M. Saraceno, *Geometry of the time-dependent variational principle in quantum mechanics,* Vol. 140 of *Lecture Notes in Physics* Springer, Berlin, Heidelberg, and New York, (1981).

J. M. C. Chen, J. W. Clark, and D. G. Sandler, Z. Physik A **305**, 223 (1982).

E. K., Phys. Rev. A **26**, 3536 (1982).

Recall Saarela's lectures:

$$|\Psi(t)\rangle = \frac{e^{-iH_{oo}t/\hbar}\, e^{\frac{1}{2}\delta U(t)}\, |\Psi_0\rangle}{\left[\left\langle \Psi_0 \left| e^{\Re e \delta U(t)} \right| \Psi_0 \right\rangle\right]^{1/2}} = e^{-iH_{oo}t/\hbar}\, |\Phi(t)\rangle$$

$$\delta U(t) = \frac{1}{2}\left[\sum_i \delta u_1(\mathbf{r}_i;t) + \sum_{i<j} \delta u_2(\mathbf{r}_i,\mathbf{r}_j;t) + \ldots\right]$$

Action principle: Assume a weak external potential $U_{\rm ext}(\mathbf{r};t)$:

$$\delta \int_{t_0}^{t_1} \left\langle \Psi(t) \left| \hat{H} - i\hbar\frac{\partial}{\partial t} + U_{\rm ext}(t) \right| \Psi(t) \right\rangle dt$$

$$= \delta \int_{t_0}^{t_1} \left\langle \Phi(t) \left| \hat{H} - H_{oo} - i\hbar\frac{\partial}{\partial t} + U_{\rm ext}(t) \right| \Phi(t) \right\rangle dt = 0\,.$$

Fermion generalization: Two–particle–two–hole exctiations still need to be done.

$$\delta U(t) = \sum_{ph} c_{ph}(t)\; a_p^\dagger a_h + \frac{1}{2} \sum_{pp'hh'} d_{pp'hh'}(t)\; a_p^\dagger a_{p'}^\dagger a_{h'} a_h + \ldots$$

Time–Dependent Hartree–Fock
The easy part (compare Bertsch lectures)

Let $\hat{H}$ be a second–quantized Hamiltonian with a weak interaction:

$$\hat{H} = \sum_{\alpha} t(\alpha) a_{\alpha}^{\dagger} a_{\alpha} + \frac{1}{2} \sum_{\alpha\beta\gamma\delta} \langle \alpha\beta | \, V \, | \gamma\delta \rangle \, a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_{\delta} a_{\gamma}$$

(1) Expand the action principle to *second order* in the particle–hole amplitudes $c_{ph}(t)$, ($U_{\rm ext}(\mathbf{r})$ is *first order*),
(2a) Time-derivative term: $I(t)$ is the normalization integral

$$-i\hbar \left\langle \Phi(t) \left| \frac{\partial}{\partial t} \right| \Phi(t) \right\rangle = -i\hbar \sum_{php'h'} \left\langle \Phi_0 a_h^{\dagger} a_p \left| \frac{c_{ph}^*(t)}{I^{1/2}(t)} \frac{\partial}{\partial t} \frac{c_{p'h'}(t)}{I^{1/2}(t)} \right| a_{p'}^{\dagger} a_{h'} \Phi_0 \right\rangle$$

$$= -\frac{i\hbar}{2} \sum_{ph} c_{ph}^*(t) \left[\dot{c}_{ph}(t) - \dot{c}_{ph}^*(t) \right] \; \rightarrow -\frac{i\hbar}{2} \sum_{ph} c_{ph}^*(t) \dot{c}_{ph}(t)$$

(Omit terms that can be written as total time–derivatives)

(2b) Density operator $\hat{\rho}(\mathbf{r}) = \sum_i \delta(\mathbf{r} - \mathbf{r}_i)$ and external field term:

$$\begin{aligned}
\langle \Phi(t) | \hat{\rho}(\mathbf{r}) | \Phi(t) \rangle &= \sum_{ph} \left[c^*_{ph} \left\langle \Phi_0 \left| a^\dagger_h a_p \hat{\rho}(\mathbf{r}) \right| \Phi_0 \right\rangle + \text{c.c.} \right] \\
&= \sum_{ph} \left[c^*_{ph} \varphi^*_p(\mathbf{r}) \varphi_h(\mathbf{r}) + \text{c.c.} \right] \\
\langle \Phi(t) | U_{\text{ext}} | \Phi(t) \rangle &= \int d^3 r U_{\text{ext}}(\mathbf{r}; t) \langle \Phi(t) | \hat{\rho}(\mathbf{r}) | \Phi(t) \rangle \\
&= \sum_{ph} \left[c^*_{ph} \langle p | U_{\text{ext}} | h \rangle + \text{c.c.} \right]
\end{aligned}$$

(2c) Interaction terms:

$$\begin{aligned}
\langle \Phi(t) | H - H_{oo} | \Phi(t) \rangle = \frac{1}{2} \sum_{ph,p'h'} & \left[c^*_{ph} c^*_{p'h'} \left\langle \Phi_0 \left| a^\dagger_h a_p a^\dagger_{h'} a_{p'} H \right| \Phi_0 \right\rangle + \text{c.c.} \right] \\
+ \sum_{ph,p'h'} & c^*_{ph} c_{p'h'} \left\langle \Phi_0 \left| a^\dagger_h a_p H a^\dagger_{p'} a_{h'} \right| \Phi_0 \right\rangle
\end{aligned}$$

Evaluate for second quantized Hamiltonian:

$$A_{ph;p'h'} \equiv \left\langle \Phi_0 \left| a_h^\dagger a_p H a_{p'}^\dagger a_{h'} \right| \Phi_0 \right\rangle = (e_p - e_h)\,\delta_{pp'}\delta_{hh'} + \langle ph'|\, V\, |hp'\rangle_a$$

$$B_{ph;p'h'} \equiv \left\langle \Phi_0 \left| a_h^\dagger a_p a_{h'}^\dagger a_{p'} H \right| \Phi_0 \right\rangle = \langle pp'|\, V\, |hh'\rangle_a$$

with

$$e_k = t(k) + \sum_h \langle k,h|\, V\, |k,h\rangle_a$$

Hartree–Fock single–particle energies.

Let

$$C(t) \equiv \left(c_{ph}(t)\right) , \;\; A = \left(\left\langle \Phi_0 \left| a_h^\dagger a_p H a_{p'}^\dagger a_{h'} \right| \Phi_0 \right\rangle \right) , \;\; B = \left(\left\langle \Phi_0 \left| a_h^\dagger a_p a_{h'}^\dagger a_{p'} H \right| \Phi_0 \right\rangle \right) .$$

(3) Carry out variation *wrt.* c_{ph} and c_{ph}^*:

$$i\hbar \dot{C}(t) = AC(t) + BC^*(t) + U(t)$$

(4) Harmonic decomposition

$$c_{ph}(t) = x_{ph} e^{-i\omega t} + y_{ph}^* e^{i\omega t}$$
$$U_{\text{ext}}(\mathbf{r};t) = U_{\text{ext}}(\mathbf{r};\omega) \left[e^{-i\omega t} + e^{-i\omega t} \right]$$

Then $\rightarrow$ "time-dependent Hartree–Fock" (TDHF) equations:

$$\boxed{\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \begin{pmatrix} X \\ Y \end{pmatrix} = \hbar\omega \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} X \\ Y \end{pmatrix} - \begin{pmatrix} U \\ U^* \end{pmatrix}}$$

Solutions for $U_{\rm ext}(\mathbf{r};t) = 0 \Rightarrow$ excitations !

(5) Response–function: Calculate "transition density"

$$\delta\rho(\mathbf{r};t) = 2\Re e\left[x_{ph}\varphi_p(\mathbf{r})\varphi_h^*(\mathbf{r})e^{-i\omega t} + y_{ph}^*\varphi_p(\mathbf{r})\varphi_h^*(\mathbf{r})e^{i\omega t}\right]$$

(6) To get the familiar RPA:

- (•) approximate $e_k \approx t(k)$
- (•) omit all exchange terms
- (•) Formulate equations in momentum space

Find:

$$\delta\rho(q,\omega) = \chi(q,\omega)U_{\rm ext}(q,\omega)$$

$$\chi(q,\omega) = \frac{\chi_0(q,\omega)}{1-\tilde{V}(q)\chi_0(q,\omega)}$$

$\chi_0(q,\omega)$ Lindhard function.

Time–Dependent CBF
The part that works

Problem with TDHF/RPA: The matrix elements $\langle pp'|\, V\, |hh'\rangle_a$ and $\langle ph'|\, V\, |hp'\rangle_a$ don't exist or are totally unreasonable for strong interactions.

The ways out:

(1) "medium to large amplitude handwaving" that is, invent effective interactions like
  (1a) "local field corrections" for electrons,
  (1b) "Pseudopotentials" in ^{3}He and ^{4}He,
  (1c) "Time-dependent density functional theory",
  (1d) "Skyrme forces" in nuclear physics.

(2) CBF theory.

Warning: CBF theory does not fix the crimes one made to derive RPA (like omitting exchanges !)

A *correlated* time–dependent wave function:

$$|\Psi(t)\rangle = \frac{e^{-iH_{oo}t/\hbar}\, e^{\frac{1}{2}\delta U(t)}\, |o\rangle}{\left[\left\langle o \left| e^{\Re e \delta U(t)} \right| o \right\rangle\right]^{1/2}} = e^{-iH_{oo}t/\hbar}\, |\Phi(t)\rangle$$

$$\delta U(t) = \sum_{ph} c_{ph}(t)\, \alpha_p^\dagger \alpha_h$$

Recall

$$\alpha_p^\dagger \alpha_h\, |o\rangle \equiv \frac{1}{I_{ph}^{1/2}} F a_p^\dagger a_h\, |\Phi_0\rangle$$

$$I_{ph} = \langle \Phi_0 |\, a_h^\dagger a_p F^\dagger F a_p^\dagger a_h\, |\Phi_0\rangle$$

The same tasks again: Evaluate the action integral and the equations of motion:

(2a) Time-derivative term:

$$-i\hbar \left\langle \Phi(t) \left| \frac{\partial}{\partial t} \right| \Phi(t) \right\rangle = -i\hbar \sum_{php'h'} \left\langle o\, \alpha_h^\dagger \alpha_p \right| \frac{c^*_{ph}(t)}{I^{1/2}(t)} \frac{\partial}{\partial t} \frac{c_{p'h'}(t)}{I^{1/2}(t)} \left| \alpha^\dagger_{p'} \alpha_{h'}\, o \right\rangle$$

$$= -\frac{i\hbar}{2} \sum_{php'h'} c^*_{ph}(t) \left[\dot{c}_{p'h'}(t) - \dot{c}^*_{p'h'}(t) \right] \langle ph|\, p'h' \rangle$$

$$\to -\frac{i\hbar}{2} \sum_{php'h'} c^*_{ph}(t) \dot{c}_{p'h'}(t) \langle ph|\, p'h' \rangle .$$

(Omit terms that can be written as total time–derivatives)

Recall that

$$\langle ph|\, p'h' \rangle = \delta_{pp'}\delta_{hh'} + \langle ph'|\, \mathcal{N}\, |hp' \rangle_a$$

(2c) Interaction terms:

$$\langle \Phi(t) | H - H_{oo} | \Phi(t) \rangle = \frac{1}{2} \sum_{ph,p'h'} \left[c^*_{ph} c^*_{p'h'} \langle o\, \alpha^\dagger_h \alpha_p \alpha^\dagger_{h'} \alpha_{p'} | H - H_{oo} | o \rangle + \text{c.c.} \right]$$
$$+ \sum_{ph,p'h'} c^*_{ph} c_{p'h'} \langle o\, \alpha^\dagger_h \alpha_p | H - H_{oo} | \alpha^\dagger_{p'} \alpha_{h'} o \rangle$$

Evaluate using CBF technology:

$$A_{ph;p'h'} \equiv \langle o\, \alpha^\dagger_h \alpha_p | H - H_{oo} | \alpha^\dagger_{p'} \alpha_{h'}\, o \rangle = (e_p - e_h)\, \delta_{pp'} \delta_{hh'} + \langle ph' |\, \mathcal{H}(1,2)\, | hp' \rangle_a$$
$$B_{ph;p'h'} \equiv \langle o\, \alpha^\dagger_h \alpha_p \alpha^\dagger_{h'} \alpha_{p'} | H | o \rangle = \langle pp' |\, \mathcal{H}(1,2)\, | hh' \rangle_a \ .$$

with

$$e_p - e_h \equiv \langle o\, \alpha^\dagger_h \alpha_p | H - H_{oo} | \alpha^\dagger_p \alpha_h\, o \rangle$$

CBF particle–hole energies.

Let matrices A, B as before, and

$$M = (\langle ph|\, p'h'\rangle)\,,,$$

("Metric matrix").
(3) Carry out variation *wrt.* c_{ph} and c^*_{ph}:

$$i\hbar M\dot{C}(t) = AC(t) + BC^*(t)$$

Normal mode decomposition $\rightarrow$ "Correlated RPA" (CRPA) equations:

$$\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \begin{pmatrix} X \\ Y \end{pmatrix} = \hbar\omega \begin{pmatrix} M & 0 \\ 0 & -M \end{pmatrix} \begin{pmatrix} X \\ Y \end{pmatrix}$$

Observe:

- All matrix elements are well–behaved
- The only evident change is the appearance of the "metric matrix"

Examining the structure of CRPA
Justifying effective interactions

Recall that:

$$\langle pp'|\,\mathcal{H}\,|hh'\rangle_a = \langle pp'|\,\mathcal{W}\,|hh'\rangle_a + \frac{1}{2}\left(e_p + e_{p'} - e_h - e_{h'}\right)\langle pp'|\,\mathcal{N}\,|hh'\rangle_a$$

$$\langle ph'|\,\mathcal{H}\,|hp'\rangle_a = \langle ph'|\,\mathcal{W}\,|hp'\rangle_a + \frac{1}{2}\left(e_p + e_{p'} - e_h - e_{h'}\right)\langle ph'|\,\mathcal{N}\,|hp'\rangle_a$$

- All matrix elements contain "nodal diagrams"
- The "metric matrix" contains "nodal diagrams" as well:

$$\langle ph|\,p'h'\rangle = \delta_{pp'}\delta_{hh'} + \langle ph'|\,\mathcal{N}\,|hp'\rangle_a$$

Reduction of the equations of motion

Define

$$\mathbf{W} = \begin{pmatrix} \langle ph'|\,\mathcal{W}\,|hp'\rangle_a & \langle pp'|\,\mathcal{W}\,|hh'\rangle_a \\ \langle hh'|\,\mathcal{W}\,|pp'\rangle_a & \langle hp'|\,\mathcal{W}\,|ph'\rangle_a \end{pmatrix} \quad \mathbf{N} = \begin{pmatrix} \langle ph'|\,\mathcal{N}\,|hp'\rangle_a & \langle pp'|\,\mathcal{N}\,|hh'\rangle_a \\ \langle hh'|\,\mathcal{N}\,|pp'\rangle_a & \langle hp'|\,\mathcal{N}\,|ph'\rangle_a \end{pmatrix}$$

$$\Omega = \begin{pmatrix} e_p - e_h - \hbar\omega & 0 \\ 0 & e_p - e_h + \hbar\omega \end{pmatrix}$$

Then

$$\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} - \hbar\omega \begin{pmatrix} M & 0 \\ 0 & -M \end{pmatrix} = \Omega + \mathbf{W} + \frac{1}{2}\Omega\mathbf{N} + \frac{1}{2}\mathbf{N}\Omega$$

$$\equiv \left(\hat{1} + \frac{1}{2}\mathbf{N}\right)\left(\Omega + \mathbf{V}_{\text{p-h}}(\omega)\right)\left(\hat{1} + \frac{1}{2}\mathbf{N}\right)$$

$$\mathbf{V}_{\text{p-h}}(\omega) = \left(\hat{1} + \frac{1}{2}\mathbf{N}\right)^{-1} \left(\mathbf{W} - \frac{1}{4}\mathbf{N}\Omega\mathbf{N}\right) \left(\hat{1} + \frac{1}{2}\mathbf{N}\right)^{-1}$$

What have we done ? Let's look at the simple approximation for $\mathcal{W}$ an $\mathcal{N}$, omit exchanges:

$$\langle pp' | \mathcal{N} | hh' \rangle = \frac{1}{N} \delta_{p+p'-h-h'} \tilde{\Gamma}_{dd}(q)$$

Define

$$\left(\hat{1} + \frac{1}{2}\mathbf{N}\right)^{-1} \equiv \left(\hat{1} - \frac{1}{2}\mathbf{X}\right)$$

Prove (by verification) that

$$\mathbf{X} = \begin{pmatrix} \langle ph' | X_{dd} | hp' \rangle & \langle pp' | X_{dd} | hh' \rangle \\ \langle hh' | X_{dd} | pp' \rangle & \langle hp' | X_{dd} | ph' \rangle \end{pmatrix}$$

Let's see for the 1-1 element how this works:

$$\left[\left(\hat{1}+\frac{1}{2}\mathbf{N}\right)\left(\hat{1}-\frac{1}{2}\mathbf{X}\right)\right]_{11}$$

$$= \sum_{p''h''}\left[\left(\delta_{pp''}\delta_{hh''}+\frac{1}{2}\langle ph''|\,\Gamma_{dd}\,|hp''\rangle\right)\left(\delta_{p''p'}\delta_{h''h'}-\frac{1}{2}\langle p''h'|\,X_{dd}\,|h''p'\rangle\right)\right.$$

$$\left.-\frac{1}{4}\langle ph''|\,\Gamma_{dd}\,|hp''\rangle\langle p''h'|\,X_{dd}\,|h''p'\rangle+\langle pp''|\,\Gamma_{dd}\,|hh''\rangle\langle h''h'|\,X_{dd}\,|p''p'\rangle\right]$$

$$= \delta_{pp'}\delta_{hh'}+\frac{1}{2}\langle ph'|\,\Gamma_{dd}\,|hp'\rangle-\frac{1}{2}\langle ph'|\,X_{dd}\,|hp'\rangle$$

$$-\frac{1}{4}\sum_{p''h''}\left[\langle ph''|\,\Gamma_{dd}\,|hp''\rangle\langle p''h'|\,X_{dd}\,|h''p'\rangle+\langle pp''|\,\Gamma_{dd}\,|hh''\rangle\langle h''h'|\,X_{dd}\,|p''p'\rangle\right]$$

$$= \delta_{pp'}\delta_{hh'}+\frac{1}{2}\langle ph'|\,N_{dd}\,|hp'\rangle-\frac{1}{2N^2}\tilde{\Gamma}_{dd}(q)\tilde{X}_{dd}(q)\delta_{p+p'-h-h'}\underbrace{\sum_{p''h''}\delta_{p+p''-h-h''}}_{=NS_F(q)}$$

$$= \delta_{pp'}\delta_{hh'}$$

Prove further (by verification) that

$$\mathbf{V}_{\text{p-h}}(\omega) = \begin{pmatrix} \langle ph'|\, V_{\text{p-h}}\, |hp'\rangle & \langle pp'|\, V_{\text{p-h}}\, |hh'\rangle \\ \langle hh'|\, V_{\text{p-h}}\, |pp'\rangle & \langle hp'|\, V_{\text{p-h}}\, |ph'\rangle \end{pmatrix}$$

$$\tilde{V}_{\text{p-h}}(q) = \tilde{X}'_{dd}(q) - \frac{\hbar^2 q^2}{4m}\tilde{X}_{dd}(q)$$

This means that we have reduced our problem of finding the excitations in the correlated basis onto an ordinary RPA equation with a local, energy independent effective interaction $\tilde{V}_{\text{p-h}}(q)$.
The rest is as in ordinary RPA: Get a response function

$$\chi(q,\omega) = \frac{\chi_0(q,\omega)}{1 - \tilde{V}_{\text{p-h}}(q)\chi_0(q,\omega)}$$

Including exchanges and more complicated FHNC diagrams is messy. It leads to similar eliminations of "nodal" diagrams, but no great new insight.

Closing the loop
Back to FHNC-EL:

We now have two ways to get $S(k)$:

- We have the FHNC-EL result

$$S(q) = \frac{S_F(q)}{\sqrt{1 + 2\frac{S_F^2(q)}{t(q)}\tilde{V}_{\text{p-h}}(q)}}$$

- On the other hand, RPA tells us that

$$S(q) = -\int_0^\infty \frac{d(\hbar\omega)}{\pi} \Im m\, \chi(q,\omega)$$

$$\chi(q,\omega) = \frac{\chi_0(q,\omega)}{1 - \tilde{V}_{\text{p-h}}(q)\chi_0(q,\omega)}$$

- Connection:

  (a) Define a "collective" or "mean spherical" approximation for $\chi_0(q,\omega)$

$$\chi_0^{\mathrm{MSA}}(q,\omega) \equiv \frac{2t(q)}{(\omega+i\eta)^2 - \left(\frac{t(q)}{S_F(q)}\right)^2}\,.$$

  (b) Observe that

$$\Im m \int d\omega\, \chi_0^{\mathrm{MSA}}(q,\omega) = \Im m \int d\omega\, \chi_0(q,\omega)$$

$$\Im m \int d\omega\, \omega\chi_0^{\mathrm{MSA}}(q,\omega) = \Im m \int d\omega\, \omega\chi_0(q,\omega),$$

  (c) Then

$$S^{\text{FHNC-EL}}(q) = \frac{S_F(q)}{\sqrt{1+2\frac{S_F^2(q)}{t(q)}\tilde{V}_{\text{p-h}}(q)}} = -\int_0^\infty \frac{d(\hbar\omega)}{\pi} \Im m \frac{\chi_0^{\mathrm{MSA}}(q,\omega)}{1-\tilde{V}_{\text{p-h}}(q)\chi_0^{\mathrm{MSA}}(q,\omega)}$$

Conclusion: FHNC-EL replaces the particle–hole continuum by an effective collective mode.

More questions: Ring diagrams in CBF

Issue:

- Knowing $S(k)$ lets us in principle calculate the energy by coupling–constant integration.
- FHNC-EL and RPA lead to slightly different $S(k)$'s.
- The difference must be due to CBF ring diagrams, so let's sum them.

In MSA, the sum of ring diagrams is easily obtained by coupling constant integration:

$$E_{\text{rings}} = \frac{1}{2}\int \frac{d^3k}{(2\pi)^3\rho}\tilde{V}_{\text{p-h}}(k)\int_0^1 d\lambda\,(S_\lambda(k) - S_F(k))$$

$$S_\lambda(k) = \frac{S_F(k)}{\sqrt{1 + 2\frac{S_F^2(k)}{t(k)}\lambda\tilde{V}_{\text{p-h}}(k)}}$$

$$E_{\text{rings}}^{\text{MSA}} = \frac{1}{4}\int \frac{d^3k}{(2\pi)^3\rho}t(k)\tilde{X}_{dd}^2(k)S_F(k)$$

Let's to back to the big perturbation formula

$$
\begin{aligned}
E = H_{oo} &- {\sum_{m}}' \frac{H'_{om}H'_{mo}}{H_{mm}-H_{oo}} + {\sum_{mn}}' \frac{H'_{om}H'_{mn}H'_{no}}{(H_{mm}-H_{oo})(H_{nn}-H_{oo})} \\
&+ {\sum_{mnp}}' \frac{H'_{om}H'_{mn}H'_{np}H'_{po}}{(H_{mm}-H_{oo})(H_{nn}-H_{oo})(H_{pp}-H_{oo})} \\
&+ {\sum_{mn}}' \left[\frac{H'_{om}H'_{mo}H'_{on}H'_{no}}{(H_{mm}-H_{oo})^2(H_{nn}-H_{oo})} \right. \\
&\left. - \frac{J_{om}H'_{mo}H'_{on}H'_{no}}{(H_{mm}-H_{oo})(H_{nn}-H_{oo})} + \frac{H'_{om}J_{mo}H'_{on}H'_{no}}{(H_{mm}-H_{oo})(H_{nn}-H_{oo})} \right] \\
&+ \ldots
\end{aligned}
$$

To make contact with RPA:

- Keep only CBF diagrams that can be written as "ring–diagrams":
- Keep only FHNC diagrams with topology of rings:

$$\tilde{\mathcal{W}}(q) = \tilde{\Gamma}'_{dd}(q) - \frac{t(q)}{2}\tilde{\Gamma}_{dd}(q)\,, \qquad \tilde{\mathcal{N}}(q) = \tilde{\Gamma}_{dd}(q)$$

- Take only free kinetic energies $e_k \approx t(k)$, $e_{ph} \equiv t(p) - t(h)$
  Let $d = 2$, recall

$$(\Delta E)_2 = -\frac{1}{4}\sum_{pp'hh'} \frac{\left|\langle hh'|\,\mathcal{H}(1,2)\,|pp'\rangle_a\right|^2}{e_{ph} + e_{p'h'}} \approx -\frac{1}{2}\sum_{pp'hh'} \frac{\left|\langle hh'|\,\mathcal{H}(1,2)\,|pp'\rangle\right|^2}{e_{ph} + e_{p'h'}}$$

and

$$\langle hh'|\,\mathcal{H}(1,2)\,|pp'\rangle = \langle hh'|\,\mathcal{W}(1,2)\,|pp'\rangle + \frac{1}{2}\left(e_{ph} + e_{p'h'}\right)\langle hh'|\,\mathcal{N}(1,2)\,|pp'\rangle$$

Now expand

$$
\begin{aligned}
(\Delta E)_2 &= (\Delta E)_2^{(1)} + (\Delta E)_2^{(0)} \,, \\
(\Delta E)_2^{(1)} &= -\frac{1}{2} \sum \frac{|\langle pp'| \mathcal{W} |hh'\rangle|^2}{e_{ph} + e_{p'h'}} \,, \\
(\Delta E)_2^{(0)} &= -\frac{1}{4} \sum \Big[\langle pp'| \mathcal{N} |hh'\rangle \langle hh'| \mathcal{W} |pp'\rangle + \langle pp'| \mathcal{W} |hh'\rangle \langle hh'| \mathcal{N} |pp'\rangle \\
&\qquad + e_{ph} \langle pp'| \mathcal{N} |hh'\rangle \langle hh'| \mathcal{N} |pp'\rangle \Big] \,.
\end{aligned}
$$

$(\Delta E)_2^{(0)}$ has no energy denominators. Use $\bar{n}(k) = 1 - n(k) = \theta(k - k_F)$:

$$
\begin{aligned}
\sum_h n(h)\bar{n}(\mathbf{h} + \mathbf{q}) &= N S_F(q) \\
\sum_h n(h)\bar{n}(\mathbf{h} + \mathbf{q}) e_{ph} &= N t(q)
\end{aligned}
$$

Hence: Evaluate

$$(\Delta E)_2^{(0)} = -\frac{1}{4}\sum_q S_F(q)\tilde{\Gamma}_{dd}(q)\left[2\,S_F(q)(\Gamma'_{dd}(q) - \frac{t(q)}{2}\tilde{\Gamma}_{dd}(q)) + t(q)\tilde{\Gamma}_{dd}(q)\right]$$

$$= -\frac{1}{2}\sum_q S_F(q)\tilde{\Gamma}_{dd}(q)\underbrace{\left[S_F(q)(\Gamma'_{dd}(q) - \frac{t(q)}{2}\tilde{\Gamma}_{dd}(q)) + t(q)\tilde{\Gamma}_{dd}(q)\right]}_{=0 \text{ for optimized correlations}}$$

$$+\frac{1}{4}\sum_q t(q)\tilde{\Gamma}^2_{dd}(q)S_F(q)$$

To derive the generic rules, rewrite the series

$$E = \sum_n (\Delta E)_n$$

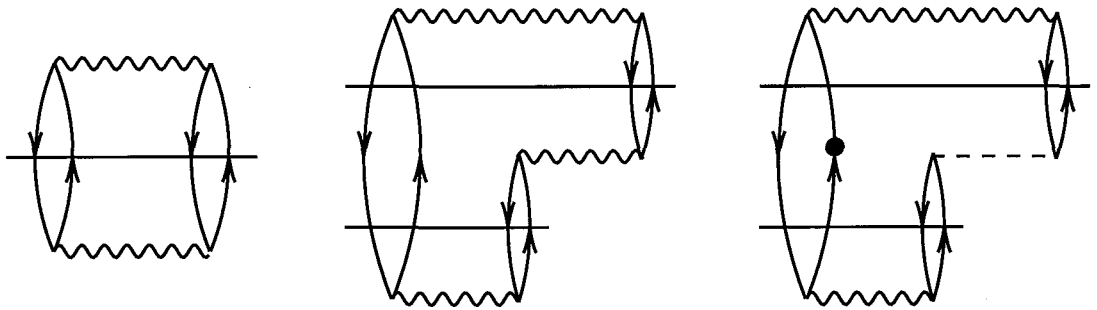
of all CBF ring–diagrams in terms of the interaction H'_{mn} and J_{mn} as

$$E = \sum_n (\delta E)_n$$

by canceling all energy numerator terms and rearranging according to the number of remaining energy denominators.

> Warning: Keep all terms.
> *"Thou shalt not split small quantities into large pieces"*
> (Coester's commandment)

Three–body order:



$|m\rangle$ and $|n\rangle$ are two–particle, two–hole states, and may differ only by one particle–hole pair, *i.e.*

$$|m\rangle = \alpha_p^\dagger \alpha_{p''}^\dagger \alpha_{h''} \alpha_h \, |o\rangle \qquad |n\rangle = \alpha_p^\dagger \alpha_{p'}^\dagger \alpha_{h'} \alpha_h \, |o\rangle \; .$$

For this pair of states, we have therefore

$$\begin{aligned} H'_{mn} &= W_{mn} + \frac{1}{2} \left(H_{mm} + H_{nn} - H_{oo} \right) J_{mn} \\ &= \langle h'p'' | \, \mathcal{W} \, | p'h'' \rangle + \frac{1}{2} \left(2e_{ph} + e_{p'h'} + e_{p''h''} \right) \langle h'p'' | \, \mathcal{N} \, | p'h'' \rangle \\ &= \langle h'p'' | \, \mathcal{H} \, | p'h'' \rangle + e_{ph} \, \langle h'p'' | \, \mathcal{N} \, | p'h'' \rangle \end{aligned}$$

(Second and third diagram above)

Expand $(\Delta E)_3$

$$(\Delta E)_3 = (\Delta E)_3^{(2)} + (\Delta E)_3^{(1)} + (\Delta E)_3^{(0)} ,$$

$$(\Delta E)_3^{(2)} = \sum \frac{\langle pp'|\,\mathcal{W}\,|hh'\rangle\,\langle h'p''|\,\mathcal{W}\,|p'h''\rangle\,\langle hh''|\,\mathcal{W}\,|pp''\rangle}{(e_{ph}+e_{p'h'})(e_{ph}+e_{p''h''})}$$

$$(\Delta E)_3^{(1)} = \frac{1}{2}\sum \frac{\langle pp'|\,\mathcal{W}\,|hh'\rangle}{e_{ph}+e_{p'h'}} \left[\frac{1}{2} e_{p''h''}\,\langle h'p''|\,\mathcal{N}\,|p'h''\rangle\,\langle hh''|\,\mathcal{N}\,|pp''\rangle \right.$$

$$\left. + \langle h'p''|\,\mathcal{W}\,|p'h''\rangle\,\langle hh''|\,\mathcal{N}\,|pp''\rangle + \langle h'p''|\,\mathcal{N}\,|p'h''\rangle\,\langle hh''|\,\mathcal{W}\,|pp''\rangle \right]$$

$$+ \frac{1}{2}\sum \frac{\langle hh''|\,\mathcal{W}\,|pp''\rangle}{e_{ph}+e_{p''h''}} \left[\frac{1}{2} e_{p'h'}\,\langle pp'|\,\mathcal{N}\,|hh'\rangle\,\langle h'p''|\,\mathcal{N}\,|p'h''\rangle \right.$$

$$\left. + \langle pp'|\,\mathcal{W}\,|hh'\rangle\,\langle h'p''|\,\mathcal{N}\,|p'h''\rangle + \langle pp'|\,\mathcal{N}\,|hh'\rangle\,\langle h'p''|\,\mathcal{W}\,|p'h''\rangle \right]$$

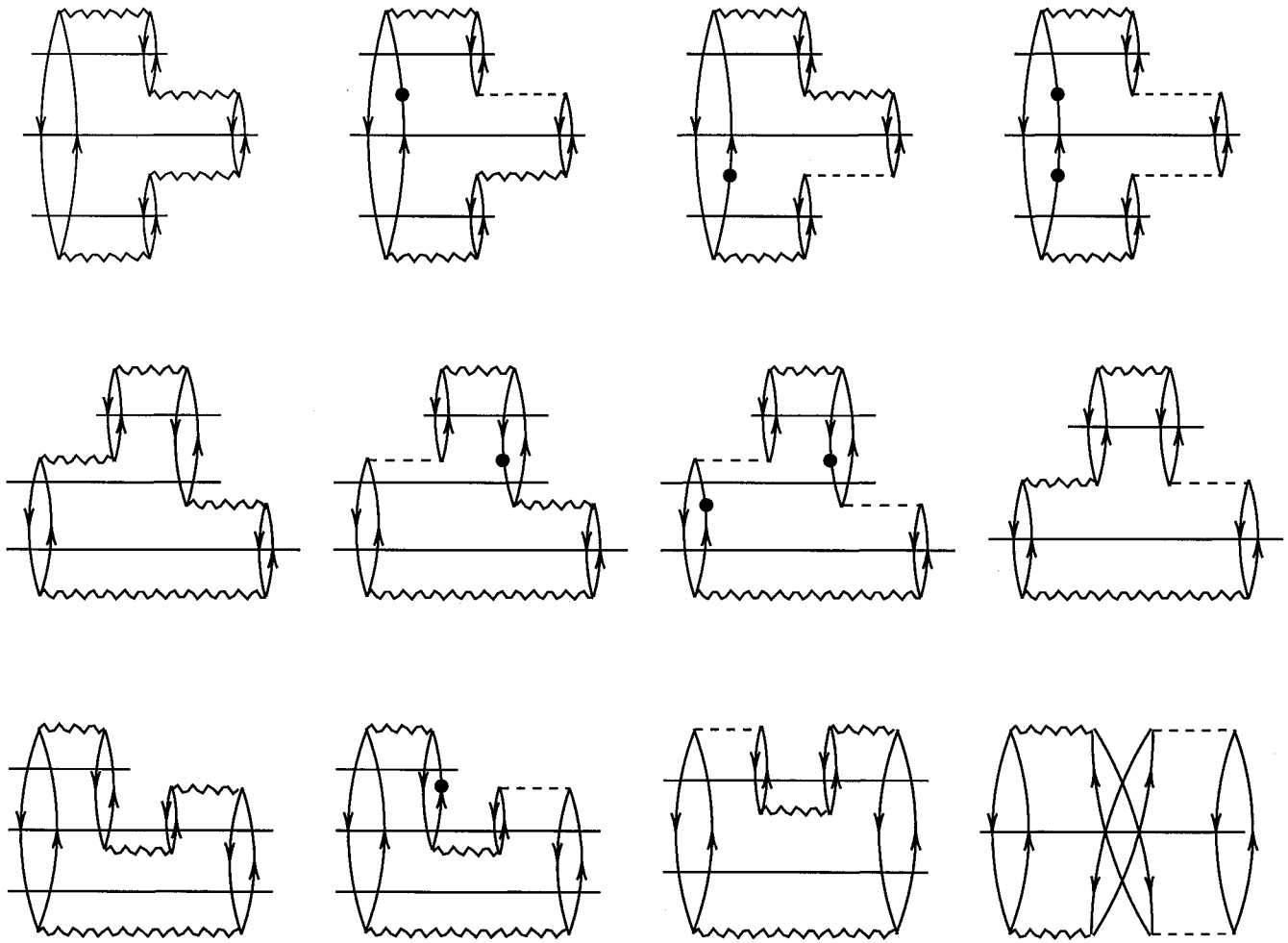
$$(\Delta E)_3^{(0)} = \frac{1}{8}\sum\Big[3\,\langle pp'|\,\mathcal{W}\,|hh'\rangle\,\langle h'p''|\,\mathcal{N}\,|p'h''\rangle\,\langle hh''|\,\mathcal{N}\,|pp''\rangle$$
$$+\,\langle pp'|\,\mathcal{N}\,|hh'\rangle\,\langle hh''|\,\mathcal{W}\,|pp''\rangle)$$
$$+\,2\,\langle pp'|\,\mathcal{N}\,|hh'\rangle\,\langle h'p''|\,\mathcal{W}\,|p'h''\rangle\,\langle hh''|\,\mathcal{N}\,|pp''\rangle$$
$$+\,(2e_{ph}+e_{p'h'}+e_{p''h''})\,\langle pp'|\,\mathcal{N}\,|hh'\rangle\,\langle h'p''|\,\mathcal{N}\,|p'h''\rangle\,\langle hh''|\,\mathcal{N}\,|pp''\rangle\Big].$$

Renormalize

$$\langle pp'|\,\mathcal{W}\,|hh'\rangle - \sum_{p''h''}\Big[\langle ph''|\,\mathcal{W}\,|hp''\rangle\,\langle p''p'|\,\mathcal{N}\,|h''h'\rangle$$
$$+\,\langle ph''|\,\mathcal{N}\,|hp''\rangle\,\langle p''p'|\,\mathcal{W}\,|h''h'\rangle$$
$$+\frac{1}{4}\,[2e_{p'h'}+e_{ph}-e_{p''h''}]\,\langle ph''|\,\mathcal{N}\,|hp''\rangle\,\langle p''p'|\,\mathcal{N}\,|h''h'\rangle\Big]$$

Sum all terms for $(\Delta E)_0$

4^{th} order verification: (slightly lengthier)



Last two diagrams come from third and secoond order CBF !

The short lesson from the long story:

$$(\Delta E)_0 = \frac{1}{4}\sum e_{ph} X_{ph,h'p'} X_{hp,p'h'}$$

$$\sum_{i>0} (\Delta E)_i = \text{Sum of all ordinary ring diagrams in terms of } \tilde{V}_{\text{p-h}}(q)$$

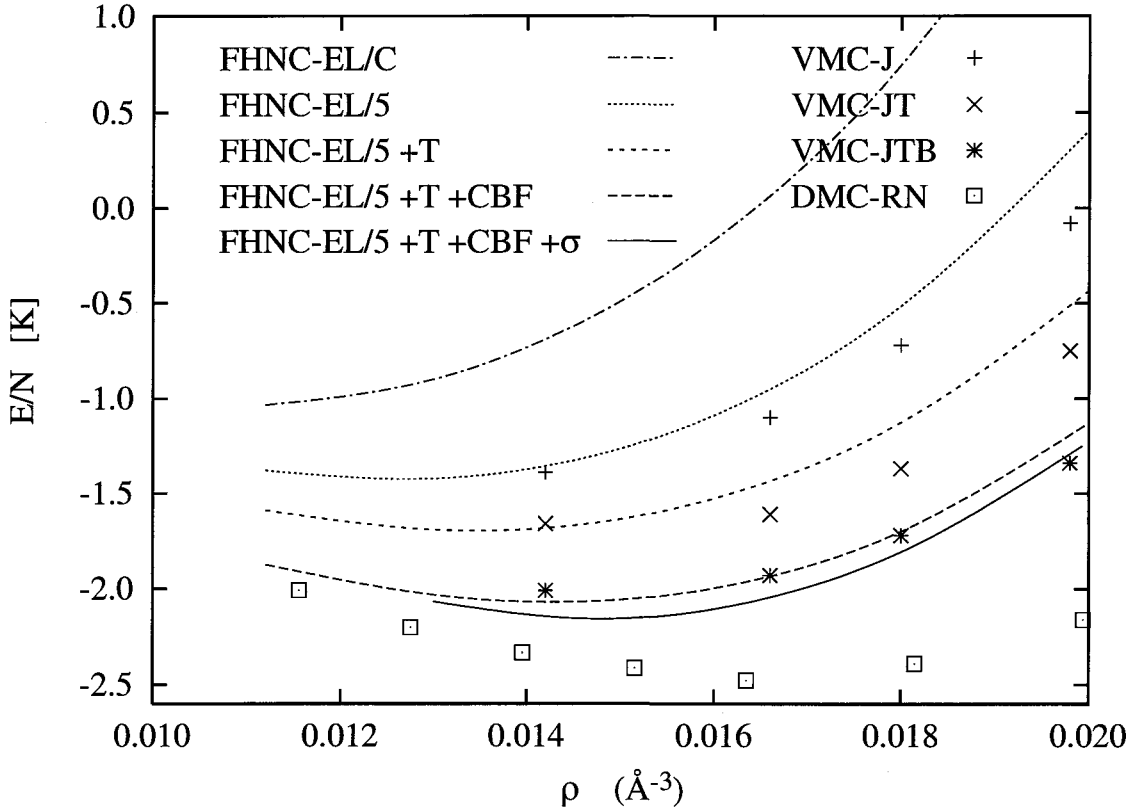
Conclusion

FHNC + CRPA = FHN + RPA

As a formula:

$$
\begin{aligned}
E_{\text{CRPA-Rings}} &= E_{\text{rings}} - E_{\text{rings}}^{\text{MSA}} \\
&= \frac{1}{2} \int \frac{d^3k}{(2\pi)^3 \rho} \tilde{V}_{\text{p-h}}(k) \int_0^1 d\lambda \left(S_\lambda(k) - S_F(k) \right) \\
&= \frac{1}{2} \int \frac{d^3k}{(2\pi)^3 \rho} \tilde{V}_{\text{p-h}}(k) \int_0^1 d\lambda \left(S_\lambda^{\text{MSA}}(k) - S_F(k) \right)
\end{aligned}
$$

Equation of state of ^{3}He
FHNC-EL with all the works



Fermi Jastrow–Feenberg and CBF
The "do"s and "don't"s

(a) The Jastrow-Feenberg wave function replaces the Lindhard function by a collective mode.

(a.1) More "complete" versions of FHNC-EL will not change this.

(a.2) We can interpret the diagrams of FHNC-EL as approximate Feynman diagrams. Identify by momentum flux.

(a.3) The power of (F)HNC-EL lies in the fact that it sums vast classes of Feynman diagrams approximately, that cannot be summed exactly.

(a.4) There is no point in calculating a quantity with JF wave functions unless this advantage is exploited !

(b) Observe (by numerical integration): The approximation is accurate at the percent level for $S(k)$.

(b.1) **Do** expect that FHNC-EL works for other integrated quantities (e.g. the energy),

(b.2) **Do NOT** expect that the same approximation works for quantities specific to Fermi statistics (e.g. Fermi–Liquid parameters),

(b.3) **Do NOT** expect that the naïve extension to finite temperatures works.

(c) CBF perturbation theory: A way to do better

(c.1) CBF moves the nodes,

(c.2) CBF must be consistent between evaluation of the energy and CBF matrix elements,

(c.3) The Lindhard function has nothing to do with Feynman–Cohen backflow.

(c.4) "Chain diagrams" are just approximations for ring diagrams.

(d) Time–dependent "Correlated Hartree–Fock" (= Correlated RPA, CRPA) provides justification to use $\tilde{V}_{\text{p-h}}(k)$ as effective interaction in an ordinary RPA

(d.1) A technically complicated proof,

(d.2) A plausible result after all we have seen !

(e) **Do** expect that all of these statements are true in an inhomogeneous geometry.