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

(3 - 14 September 2001)

CORRELATED BASIS FUNCTIONS THEORY

BEYOND JASTROW-FEENBERG THEORY.....
BEYOND THE GROUND STATE.....
PART I

Eckhard KROTSCHECK
Institut fuer Theoretische Physik
Johannes-Kepler Universitaet Linz
Altenberger Strasse 69
A-4040 Linz
AUSTRIA

Correlated Basis Functions Theory

Beyond Jastrow-Feenberg theory...
Beyond the ground state....

(1) CBF Theory: What, Why, and How ?
(2) Perturbation theory in a non–orthogonal basis
(3) Calculation of effective interactions
(4) Interpretation of effective interactions
(5) Systematics: Coupled clusters with correlations
(6) Dynamics: Linear response in correlated systems
(7) Systematics: Correlated ring diagrams
(8) Conclusions: The view from the top

Correlated Basis Functions: The What, the How, and the Why

Objectives:

⇒ Mostly *fermion* systems

⇒ Expansions, classifications, resummations

⇒ Moving the nodes of the wave function

⇒ Better results, better understanding, dynamics

$$\hat{H} = \hat{T} + \hat{V}, \qquad \hat{T} = -\sum_i \frac{\hbar^2}{2m}\nabla_i^2, \qquad \hat{V} = \sum_{i<j} v(i,j)$$

Early reference material:

P. M. Morse and H. Feshbach, *Methods of Theoretical Physics*, Vol. II.

P.-O. Löwdin, J. Chem. Phys. **18**, 365 (1950).

J. W. Clark and E. Feenberg, Phys. Rev. **113**, 388 (1959).

E. Feenberg *Theory of Quantum Fluids*, Academic, NY (1969),

Beyond Jastrow-Feenberg Theory– –With Jastrow–Feenberg ideas

Jastrow-Feenberg wave function:

$$\Psi_0(1,\ldots,N) = F(\mathbf{r}_1,\ldots,\mathbf{r}_N)\Phi_0(1,\ldots,N)$$

$$F(\mathbf{r}_1,\ldots,\mathbf{r}_N) = \exp\frac{1}{2}\left[\underbrace{\sum_i^N u_1(\mathbf{r}_i)}_{\text{omit}} + \sum_{i<j}^N u_2(\mathbf{r}_i,\mathbf{r}_j) + \ldots\right]$$

Note:

- $\Phi_0(1,\ldots,N)$ is normally a Slater determinant of single–particle orbitals;
- The *correlation operator* $F(1,\ldots,N)$ may be chosen in a more general form, but one needs accurate methods for evaluating matrix elements;
- We will deal with the uniform system only, *i.e.* $u_1(\mathbf{r}) = 0$.

Wanted first: Energy (Polls lectures)

$$E_{\rm var} \equiv H_{oo} = \frac{\langle \Psi_0 | \hat{H} | \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 | \rangle}$$

Optimal choice of the correlations:

$$\frac{\delta H_{oo}}{\delta u_n(\mathbf{r}_1, \ldots, \mathbf{r}_n)} = 0$$

Question: Is the optimal way practical ? (Yes if there is one).

Concern: Even for the most general *local* correlation operator F, $\Psi_0(1, \ldots, N)$ is *normally not* an exact wave function.
Even the optimal F may not be good enough.
(The nodal surface problem !)

Way out: Correlated Basis Functions (CBF).

A correlated basis of the Hilbert space:

Let m be any set of single particle orbitals, and

$$|\Phi_m\rangle = \prod_{\mathbf{k}\in m} a^\dagger_{\mathbf{k}} |0\rangle$$

the corresponding Slater determinant: Define a basis of the Hilbert space by

$$|m\rangle \equiv |\Psi_m\rangle = \frac{1}{\sqrt{I_{mm}}} F_N(1,\ldots,N)\,|\Phi_m\rangle$$

$$I_{mm} \equiv \langle\Psi_m|\, F_N^\dagger(1,\ldots,N) F_N(1,\ldots,N)\,|\Psi_m\rangle \ .$$

The correlated ground state:

$$|o\rangle \equiv |\Psi_o\rangle = \frac{1}{\sqrt{I_{oo}}} F_N(1,\ldots,N)\,|\Phi_o\rangle$$

where $|\Phi_o\rangle$ is the filled Fermi–sea.

Keep $F_N(1,\ldots,N)$ the same for all $|\Phi_m\rangle$ (a matter of practicality.)

Correlated Basis Sets : The generic quantities

- Generating functionals G_{mm}, normalization integrals I_{mm} , and their ratios:

$$G_{mm} - G_{oo} = \ln\left[I_{mm}/I_{oo}\right] ,$$

- Correlated diagonal matrix elements of $\hat{H}$ and their differences

$$H_{mm} - H_{oo} \equiv \langle m|\, \hat{H}\, |m\rangle - \langle o|\, \hat{H}\, |o\rangle \ ,$$

- Correlated off–diagonal matrix elements of $\hat{H}$ and $\hat{1}$:

$$H_{mn} \equiv \langle m|\, \hat{H}\, |n\rangle \ , \qquad (m \neq n), \qquad \mathbf{H} = (H_{mn})$$
$$J_{mn} \equiv \langle m|\, \hat{1}\, |n\rangle \ , \qquad (m \neq n), \qquad \mathbf{J} = (J_{mn})$$

- Auxiliary quantities:

$$H'_{mn} \equiv \langle m| \hat{H} - H_{oo} |n\rangle \ , \qquad (m \neq n)$$

$$W_{mn} \equiv H'_{mn} - \frac{1}{2} \left(H_{mm} + H_{nn} - 2H_{oo}\right) J_{mn}$$

$$= H_{mn} - \frac{1}{2} \left(H_{mm} + H_{nn}\right) J_{mn} \ , \qquad (m \neq n)$$

An second quantized formulation
Shorthand notation

Creation operators ($\alpha_k^\dagger$) and annihilation operators (α_k) for correlated states:

$$\left|\alpha_k^\dagger m\right\rangle = F_{N+1} a_k^\dagger \left|\Phi_m\right\rangle / \left\langle\Phi_m\right| a_k F_{N+1}^\dagger F_{N+1} a_k^\dagger \left|\Phi_m\right\rangle^{\frac{1}{2}} ,$$

$$\left|\alpha_k m\right\rangle = F_{N-1} a_k \left|\Phi_m\right\rangle / \left\langle\Phi_m\right| a_k^\dagger F_{N-1}^\dagger F_{N-1} a_k \left|\Phi_m\right\rangle^{\frac{1}{2}} .$$

The correlated operators obey the same (anti-) commutation rules as their uncorrelated cousins, *but they are not hermitian conjugates.*

Alternative notation: label correlated states by the orbitals in which the corresponding model state, $|\Phi_m\rangle$, differs from the model ground state $|\Phi_o\rangle$:

$$|p\rangle = \frac{1}{\sqrt{I_{p,p}}} F_{N+1} a_p^\dagger \left|\Phi_o\right\rangle , \qquad I_{p,p} = \left\langle\Phi_o\right| a_p F_{N+1}^\dagger F_{N+1} a_p^\dagger \left|\Phi_o\right\rangle ,$$

Single Particle Spectrum
An introductory exercise

Increase/decrease in energy of a Fermi liquid upon adding/removing a particle of momentum p (h):
The $N+1$ (or $N-1$) particle state obtained by inserting a particle of momentum p (removing a particle of momentum h) is

$$|p\rangle = \left|\alpha_p^\dagger o\right\rangle, \qquad e_p \equiv H_{p,p} - H_{o,o} = \langle p|\,\hat{H}\,|p\rangle - \langle o|\,\hat{H}\,|o\rangle$$

$$|h\rangle = |\alpha_h o\rangle, \qquad e_h \equiv H_{oo} - H_{h,h} = \langle o|\,\hat{H}\,|o\rangle - \langle h|\,\hat{H}\,|h\rangle$$

Particle–hole energies: $|ph\rangle = \left|\alpha_p^\dagger \alpha_h o\right\rangle$:

$$e_{ph} \equiv \langle ph|\,\hat{H}\,|ph\rangle - \langle o|\,\hat{H}\,|o\rangle = e_p - e_h + \mathcal{O}(N^{-1})$$

Note: The energy difference is unaffected by a change of correlations:

$$e(p) = H_{p,p} - H_{o,o} + \underbrace{\frac{\delta H_{oo}}{\delta F}}_{=0} \frac{\delta F}{\delta p}$$

Non–orthogonal perturbation expansions
Similar to CIM !

- Expand the exact state in correlated basis states

$$\Psi_0 = \sum_m c_m \, |m\rangle \,, \qquad \mathbf{c} = (c_m)$$

- Write Schrödinger equation as matrix equation

$$[\mathbf{H} - E\,\mathbf{N}]\,\mathbf{c} = 0$$

- Löwdin transformation to an orthogonal metric:

$$\left[\mathbf{N}^{-1/2}\mathbf{H}\mathbf{N}^{-1/2} - E\right]\mathbf{c}' = 0, \qquad \mathbf{c}' = \mathbf{N}^{1/2}\mathbf{c}.$$

- Expand

$$\mathbf{N}^{-1/2} = \left[\hat{1} + \mathbf{J}\right]^{-1/2} = \hat{1} - \frac{1}{2}\mathbf{J} + \ldots$$

- Do orthogonal perturbation theory

Non–orthogonal perturbation expansions
Integral equation methods

- Write down an exponential *ansatz* for the wave function:

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

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

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

- Choose the level of approximation in which one is willing to work, *eg.* $n = 2$
- Determine the $S_{p_1 \ldots p_n; h_1 \ldots h_n}$ by variation

$$\frac{\delta}{\delta S_{p_1 \ldots p_n; h_1 \ldots h_n}} \frac{\langle \Psi_0 |\, \hat{H}\, | \Psi_0 \rangle}{\langle \Psi_0 \,|\Psi_0 \rangle} = 0$$

or by correlated coupled cluster equations.

The big perturbation formula

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

Oops – the last three terms are naively not proportional to the particle number ! $\rightarrow$ Must dig into the structure of matrix elements !

Simple approximations
First and second generation CBF theory

- Choose $\{|m\rangle\} = \{|p_1 p_2 h_1 h_2\rangle\}$ to be correlated *two-particle-two-hole* states:

$$|p_1 p_2 h_1 h_2\rangle = \left|\alpha^\dagger_{p_1} \alpha^\dagger_{p_2} \alpha_{h_2} \alpha_{h_1}\, o\right\rangle$$

Then:

$$H_{mm} - H_{oo} = e_{p_1} + e_{p_2} - e_{h_1} - e_{h_2} + \mathcal{O}(N^{-1})$$

and we can formally write

$$H'_{om} = \langle h_1 h_2|\, \mathcal{H}(1,2)\, |p_1 p_2 - p_2 p_1\rangle \equiv \langle h_1 h_2|\, \mathcal{H}(1,2)\, |p_1, p_2\rangle_a$$

Thus

$$(\Delta E)_2 = -\frac{1}{4} \sum_{p_1 p_2 h_1 h_2} \frac{\left|\langle h_1 h_2|\, \mathcal{H}(1,2)\, |p_1 p_2\rangle_a\right|^2}{e_{p_1} + e_{p_2} - e_{h_1} - e_{h_2}}$$

looks like second–order Rayleigh-Schrödinger perturbation theory.

Calculating matrix elements
Where the work begins

Jackson–Feenberg–Identity:

$$F\nabla^2 F = \frac{1}{2}(\nabla^2 F^2 + F^2\nabla^2) + \frac{1}{2}F^2\left[\nabla,[\nabla,\ln F]\right] - \frac{1}{4}\left[\nabla,\left[\nabla,F^2\right]\right] .$$

For Jastrow correlations $F(1,\ldots,N) = \exp(\frac{1}{2}\sum_{ij} u_2(i,j))$

$$\begin{aligned}
\langle\Phi_m|\, F\hat{T}F\,|\Phi_n\rangle &= -\frac{\hbar^2}{2m}\langle\Phi_m|\, F\sum_i \nabla_i^2 F\,|\Phi_n\rangle \\
&= \frac{1}{2}\left(T_m + T_n\right)\langle\Phi_m|\, F^2\,|\Phi_n\rangle - \frac{\hbar^2}{4m}\langle\Phi_m|\, F^2\sum_{i<j}\nabla^2 u_2(\mathbf{r}_i-\mathbf{r}_j)\,|\Phi_n\rangle \\
&+ \frac{\hbar^2}{8m}\langle\Phi_m|\sum_i\left[\nabla_i,\left[\nabla_i,F^2\right]\right]|\Phi_n\rangle
\end{aligned}$$

$\Rightarrow$ Hamiltonian matrix elements can be done with "prime equation" technique !

Let's look at the terms

$$\frac{\hbar^2}{4m}\langle\Phi_m|\,F^2\sum_{i<j}\nabla^2 u_2(\mathbf{r}_i-\mathbf{r}_j)\,|\Phi_n\rangle \quad \text{and} \quad \langle\Phi_m|\,F^2\sum_{i<j}v(\mathbf{r}_i-\mathbf{r}_j)\,|\Phi_n\rangle$$

Define

$$F(\beta)\equiv\exp\sum_{i\le j}\left[u_2(\mathbf{r}_i-\mathbf{r}_j)+\beta v_{\rm JF}(\mathbf{r}_i-\mathbf{r}_j)\right]$$

and

$$I_{mm}(\beta)\equiv\langle\Phi_m|\,F_N^\dagger(\beta)F_N(\beta)\,|\Phi_m\rangle \qquad J_{mn}(\beta)\equiv\frac{\langle\Phi_m|\,F_N^\dagger(\beta)F_N(\beta)\,|\Phi_n\rangle}{\sqrt{I_{mm}(\beta)I_{nn}(\beta)}}$$

Observe: $I_{mm}(\beta)$and $J_{mn}(\beta)$ can be calculated with the same effort as $I_{mm}=I_{mm}(\beta=0)$and $J_{mn}=J_{mn}(\beta=0)$.

Then

$$\left.\frac{\partial}{\partial\beta}\ln I_{mm}(\beta)\right|_{\beta=0} = \frac{\langle\Phi_m|\, F^2 \sum_{i<j} v_{\rm JF}(\mathbf{r}_i-\mathbf{r}_j)\,|\Phi_m\rangle}{\langle\Phi_m|\, F^2(\mathbf{r}_i-\mathbf{r}_j)\,|\Phi_m\rangle}$$

$\Rightarrow$ local part of the H_{mm} !

Similar:

$$\left.\frac{\partial}{\partial\beta}J_{mn}(\beta)\right|_{\beta=0} = \frac{\langle\Phi_m|\, F^2 \sum_{i<j} v_{\rm JF}(\mathbf{r}_i-\mathbf{r}_j)\,|\Phi_n\rangle}{\sqrt{I_{mm}I_{nn}}} - \frac{1}{2}\left[\left.\frac{\partial}{\partial\beta}\ln I_{mm}(\beta)\right|_{\beta=0} + \left.\frac{\partial}{\partial\beta}\ln I_{nn}(\beta)\right|_{\beta=0}\right] J_{mn}$$

$\Rightarrow$ local part of the W_{mn} !

$\Rightarrow$ Put in kinetic energy corrections "by hand".

$\Rightarrow$ Single particle spectrum and W_{mn} can be calculated without extra effort !

Evaluating matrix elements. I. Diagonal quantities

"Generating functional" (suppress β-dependence)

$$G_{mm} = \ln I_{mm} \,,$$

G_{mm} is the sum of all irreducible diagrams without external points

$\Rightarrow$ $G_{mm} \propto N$ for large N

$\Rightarrow$ G_{mm} differs from the ground state G_{oo} only by the exchange function

$$\ell_m(\mathbf{r}) = \frac{1}{N} \sum_{i \in m} e^{i\mathbf{k}_i \cdot \mathbf{r}}$$

$\Rightarrow$ $G_{mm} - G_{oo} = \mathcal{O}(1)$ for states that deviate from the ground state only by a few orbitals.

$\Rightarrow$ Algorithm: For $|\Phi_m\rangle = a_p^\dagger a_h |\Phi_o\rangle$, get

$$\begin{aligned} G_{mm} - G_{oo} &= \int d^3r \frac{\delta G_{oo}}{\delta \ell(rk_F)} \left[\ell_m(\mathbf{r}) - \ell(rk_F)\right] + \mathcal{O}(1/N) \\ &= \frac{1}{N} \int d^3r \frac{\delta G_{oo}}{\delta \ell(rk_F)} \left[e^{i\mathbf{p}\cdot\mathbf{r}} - e^{i\mathbf{h}\cdot\mathbf{r}}\right] + \mathcal{O}(1/N) \\ &= \delta G(\mathbf{p}) - \delta G(\mathbf{h}) + \mathcal{O}(1/N) \end{aligned}$$

where

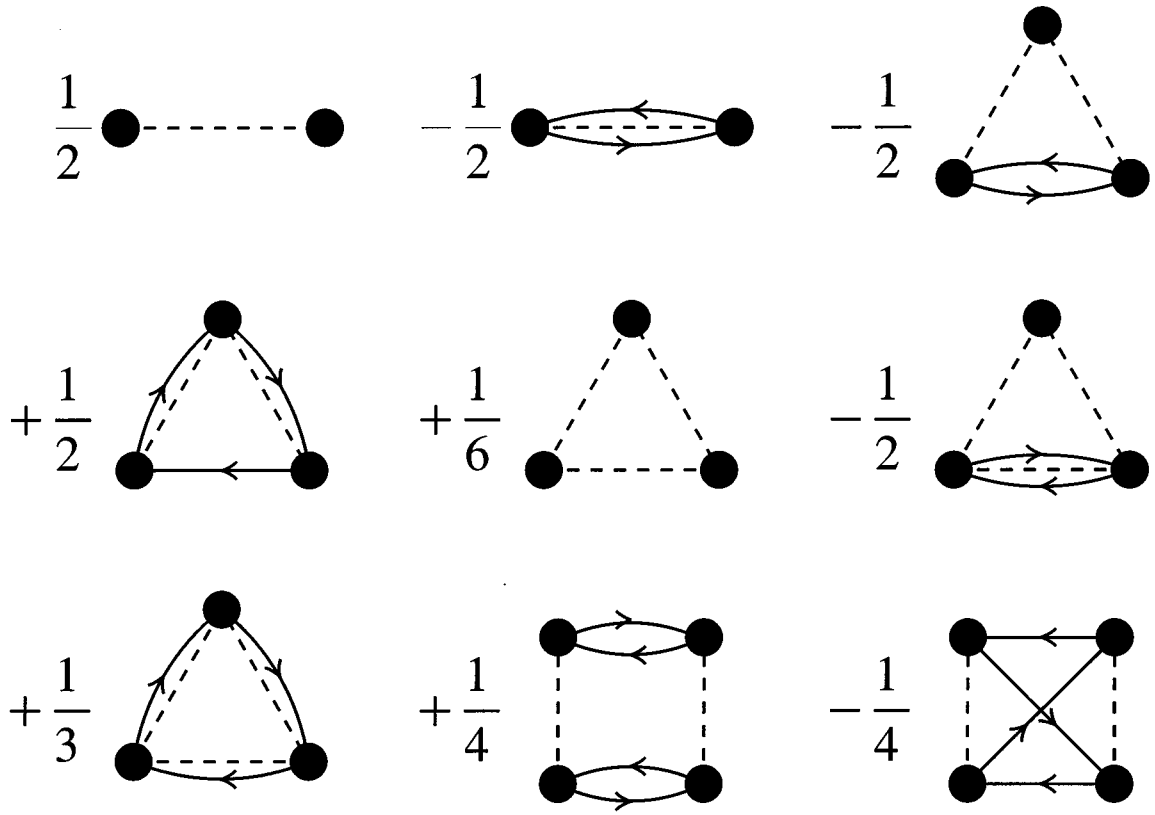
$$\delta G(\mathbf{k}) = \frac{1}{N} \int d^3r \frac{\delta G_{oo}}{\delta \ell(rk_F)} e^{i\mathbf{k}\cdot\mathbf{r}}$$

because

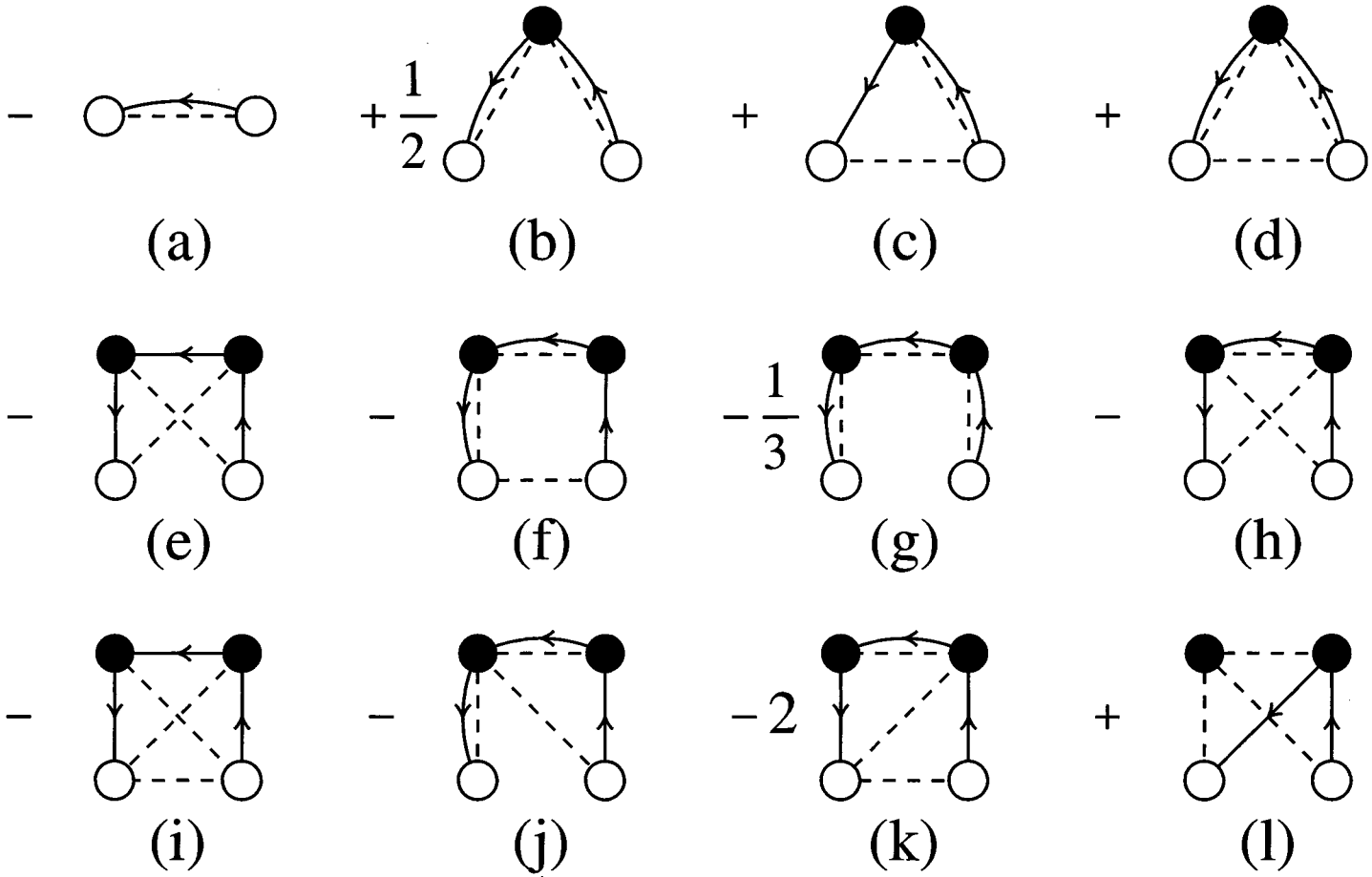
$$\ell_m(\mathbf{r}) - \ell(rk_F) = \frac{1}{N} \left[\sum_{i\in m} e^{i\mathbf{k}_i\cdot\mathbf{r}} - \sum_{i\in o} e^{i\mathbf{k}_i\cdot\mathbf{r}}\right]$$

Algorithm:

- Write down the diagrammatic expansion of G_{oo}:

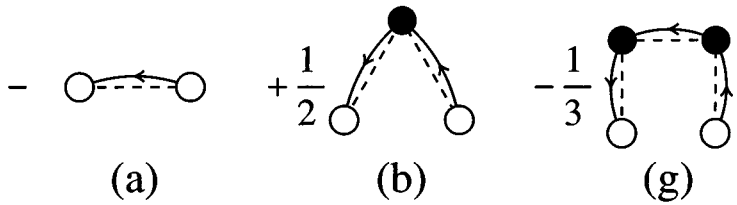


- Calculate $\delta G_{oo}/\delta\ell(rk_F)$ by removing exchange lines:

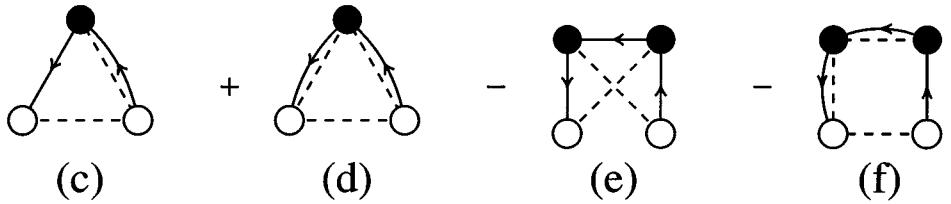


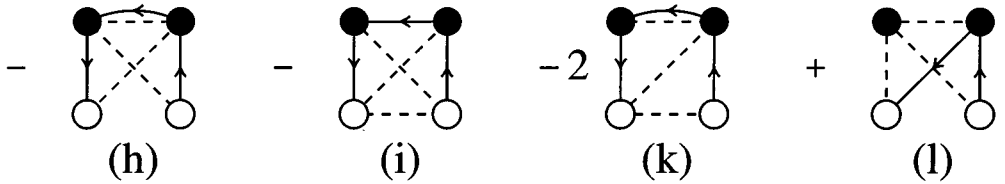
- Identify diagrammatic structures and resum:

"cc"-chain diagrams:

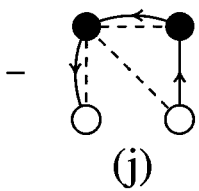


Non-nodal "cc" diagrams:





Combinations:



Result: $$\delta G(\mathbf{k}) = -\ln\left[1 - \tilde{X}_{cc}(k)\right]$$

Single–particle spectrum:

$$e_k = \frac{\hbar^2 k^2}{2m} + \left.\frac{\partial \delta G(\mathbf{k};\beta)}{\partial \beta}\right|_{\beta=0} + \text{const.}$$

$$\equiv t(k) + \frac{\tilde{X}'_{cc}(k)}{1 - \tilde{X}_{cc}(k)} + \text{const.}$$

Note: Some kinetic energy terms are not spelled out !
Note: $t(k) = \frac{\hbar^2 k^2}{2m}$ will be used repeatedly.

Evaluating matrix elements. II. Off-Diagonal quantities

Algorithm as before:

- Specify the orbitals d in which $|\Phi_m\rangle$ and $|\Phi_n\rangle$ differ.

$$|\Phi_m\rangle = a^\dagger_{m_1} \ldots a^\dagger_{m_d} a_{n_d} \ldots a_{n_1} |\Phi_n\rangle$$

- Define non–local $d-$body *operators*

$$\langle n_1 \ldots n_d| \mathcal{N}(1,\ldots,d;n) |m_1 \ldots m_n\rangle_a \equiv \frac{\langle\Phi_m| F^2 |\Phi_n\rangle}{\sqrt{I_{mm} I_{nn}}}$$

- $\mathcal{N}(1,\ldots,d;n) = \mathcal{N}(1,\ldots,d;o) + \mathcal{O}(1/N)$ for $d \ll N$.
- Derive expansions for the operators $\mathcal{N}(1,\ldots,d) = \sum_{s,t} (\Delta\mathcal{N})^{(t)}_s (1,\ldots,d)$.
- Obtain Hamiltonian matrix elements by "diagrammatic differentiation":

$$W_{mn} = H_{mn} - \frac{1}{2}(H_{mm} + H_{nn}) J_{mn} = \left.\frac{\partial N_{mn}(\beta)}{\partial\beta}\right|_{\beta=0}$$

$$= \langle n_1 \ldots n_d| \mathcal{W}(1,\ldots,d;n) |m_1 \ldots m_d\rangle_a$$

Consider especially $d = 2$:

$$|m\rangle = \alpha^\dagger_{m_1}\alpha^\dagger_{m_2}\alpha_{n_2}\alpha_{n_1}\,|n\rangle$$

Any p-body contribution to J_{mn} has the form

$$\sum_{h_1\ldots h_{p-2}} \langle n_1 n_2 h_1 \ldots h_{p-2}|\, D(\mathbf{r}_1,\ldots\mathbf{r}_p)\,|P(m_1 m_2 h_1 \ldots h_{p-2})\rangle$$

where $D(\mathbf{r}_1,\ldots\mathbf{r}_p)$ is *some* combination of $h(r_{ij}) = \exp(u(r_{ij})) - 1$ bonds with $1 \le i,j \le p$, and the h_i the occupied ground state orbitals ("hole states").
Depending on the exchange structure, we can have three types:

$$d^{(p)}_{dd} = \sum_{j_1\ldots j_{p-2}} \langle n_1 \ldots j_{p-2}|\, D(\mathbf{r}_1\ldots\mathbf{r}_p)\,|(m_1 m_2)P(j_1\ldots j_{p-2})\rangle\,,$$

$$d^{(p)}_{dc} = \sum_{j_1\ldots j_{p-2}} \langle n_1 \ldots j_{p-2}|\, D(\mathbf{r}_1\ldots\mathbf{r}_p)\,|j(m_2 m_1)P(j_1\ldots(j)\ldots j_{p-2})\rangle\,,$$

$$d^{(p)}_{cc} = \sum_{j_1\ldots j_{p-2}} \langle n_1 \ldots j_{p-2}|\, D(\mathbf{r}_1\ldots\mathbf{r}_p)\,|jk(m_1 m_2)P(j_1\ldots(j)(k)\ldots j_{p-2})\rangle\,.$$

Therefore

$$\mathcal{N}(1,2) = \mathcal{N}_{dd}(12,1'2') + \mathcal{N}_{dc}(12,1'2') + \mathcal{N}_{dc}(21,2'1') + \mathcal{N}_{cc}(12,1'2')$$

$$\mathcal{N}_{dd}(12,1'2') = \mathcal{N}_{dd}(r_{12})\delta(\mathbf{r}_1 - \mathbf{r'}_1)\delta(\mathbf{r}_2 - \mathbf{r'}_2)$$

$$\mathcal{N}_{dc}(12,1'2') = \mathcal{N}_{d,cc}(\mathbf{r}_1,\mathbf{r}_2;\mathbf{r'}_1,\mathbf{r'}_2)\delta(\mathbf{r}_1 - \mathbf{r'}_1)$$

$$\mathcal{N}_{cc}(12,1'2') = \mathcal{N}_{cc,cc}(\mathbf{r}_1,\mathbf{r}_2;\mathbf{r'}_1,\mathbf{r'}_2)$$

Symmetry:

$$\mathcal{N}(12,1'2') = \mathcal{N}(21,2'1') = \mathcal{N}(1'2',12).$$

Simplest case: Two–body approximation

$$\frac{\langle n_1 n_2 h_3 \ldots h_N | \prod_{i<j} f^2(r_{ij}) \, | m_1 m_2 h_3 \ldots h_N \rangle_a}{\sqrt{I_{mm} I_{nn}}}$$

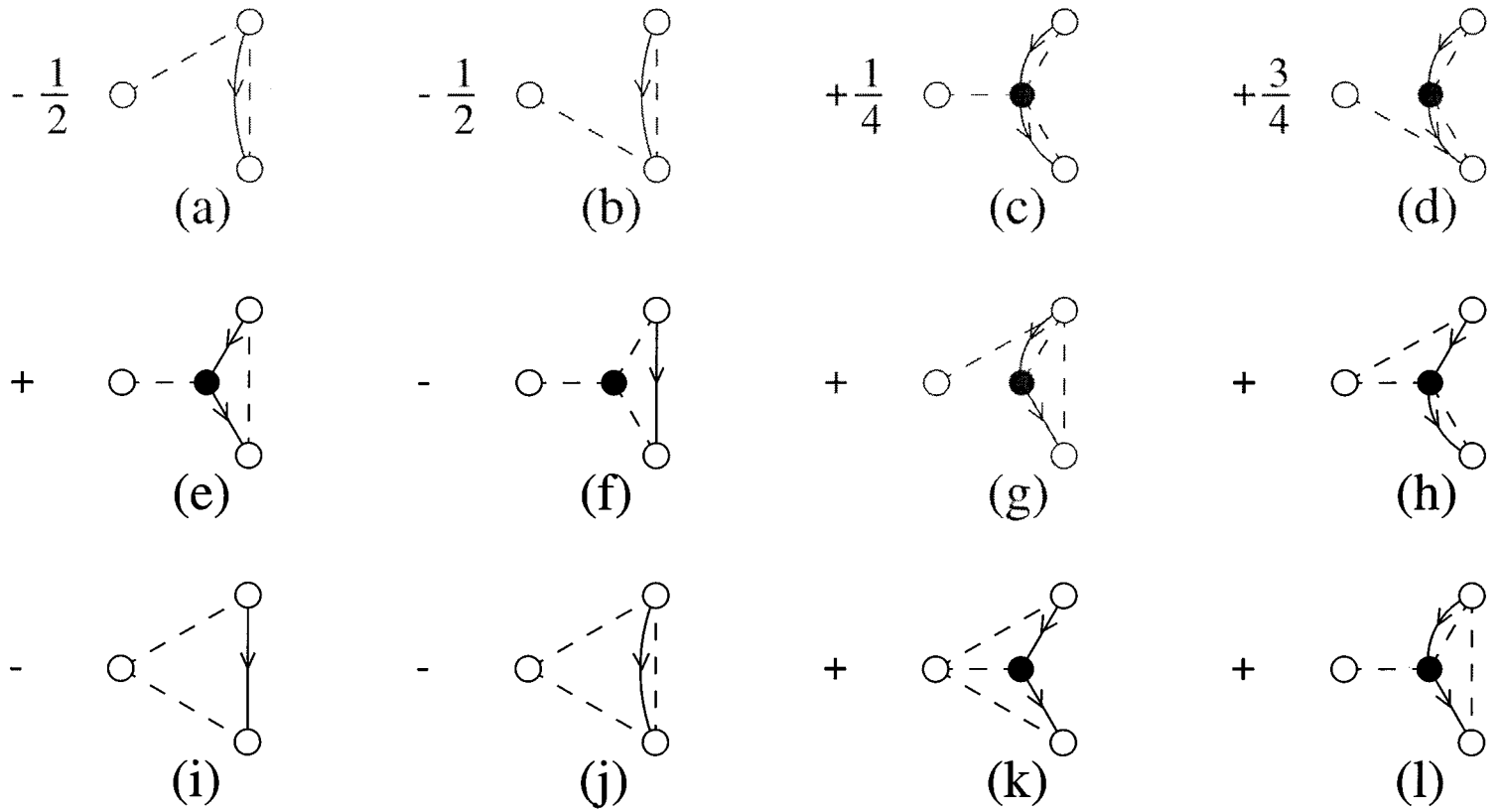
$$= \langle n_1 n_2 h_3 \ldots h_N | \, 1 + \sum_{i<j} (f^2(r_{ij}) - 1) \, | m_1 m_2 h_3 \ldots h_N \rangle_a + \ldots$$

$$= \langle n_1 n_2 | \, f^2(r_{12}) - 1 \, | m_1 m_2 \rangle_a + \ldots$$

Generalize to

$$\mathcal{N}_{dd}(1,2) = \Gamma_{dd}(r_{12})$$

Expansion of $\mathcal{N}_{dc}(12, 1'2')$ in dressed bonds $\Gamma_{dd}(r_{ij})$



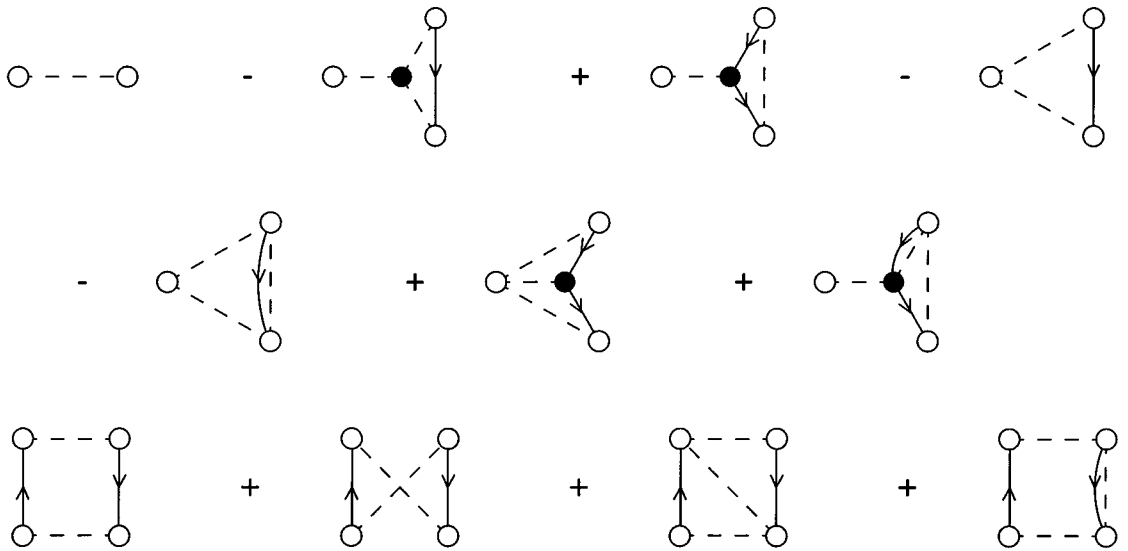
Factorizable diagrams have only a nodal path from point 1 to point 1'

Factorization theorem for $\mathcal{N}(12, 1'2')$:

$$\langle m_1 m_2 | \mathcal{N}(1,2) | n_1 n_2 \rangle_a = z(m_1) z(m_2) z(n_1) z(n_2) \langle m_1 m_2 | \mathcal{N}^B(1,2) | n_1 n_2 \rangle_a$$

$$z(m) = \frac{1}{\sqrt{1 - \tilde{X}_{cc}(k_m)}}$$

"Basic" part of $\mathcal{N}(12, 1'2')$



Local part of $\mathcal{W}(12, 1'2')$:

(a) Replace $\Gamma_{dd}(r)$ by $\Gamma'_{dd}(r)$ obtained from fermion Euler equation

(b) Add kinetic energy acting on coordinates 1 and 2 (All others are included in $\Gamma'_{dd}(r)$)

$$\frac{\hbar^2}{8m} \langle n_1 n_2 h_3 \dots h_N | \sum_{i=1,2} \left[\nabla_i, \left[\nabla_i, F^2\right]\right] | (m_1 m_2)_1 (h_3 \dots h_N)_a \rangle$$

$$= \frac{\hbar^2}{8m} \langle n_1 n_2 | \left[\nabla_1^2 \Gamma_{dd}(r_{12}) + \nabla_2^2 \Gamma_{dd}(r_{12})\right] | m_1 m_2 \rangle_a$$

$$= \langle n_1 n_2 | \frac{\hbar^2}{4m} \nabla^2 \Gamma_{dd}(r_{12}) | m_1 m_2 \rangle_a$$

Hence

$$\mathcal{W}^B_{dd}(1,2) = \Gamma'_{dd}(r_{12}) + \frac{\hbar^2}{4m} \nabla^2 \Gamma_{dd}(r_{12})$$

CBF effective interactions
Physical interpretation and properties

Objectives:

$\Rightarrow$ Interpretation I: Landau's quasiparticle interaction
$\Rightarrow$ Interpretation II: BCS interaction
$\Rightarrow$ Optimization
$\Rightarrow$ Static screening, kinetic energy, and phonon exchange

Landau Fermi–Liquid Theory
A crash-course

Reference Material:

L. D. Landau, Sov. Phys. JETP **3**, 920 (1957).
L. D. Landau, Sov. Phys. JETP **5**, 101 (1957).
D. Pines and P. Nozieres, *The Theory of Quantum Liquids* Vol. I. (Benjamin, New York, 1966).
G. E. Brown, *Many Body Problems* (North Holland, Amsterdam, 1972).
G. Baym and C. Pethick, *Landau Fermi Liquid Theory* (Wiley, New York, 1991).

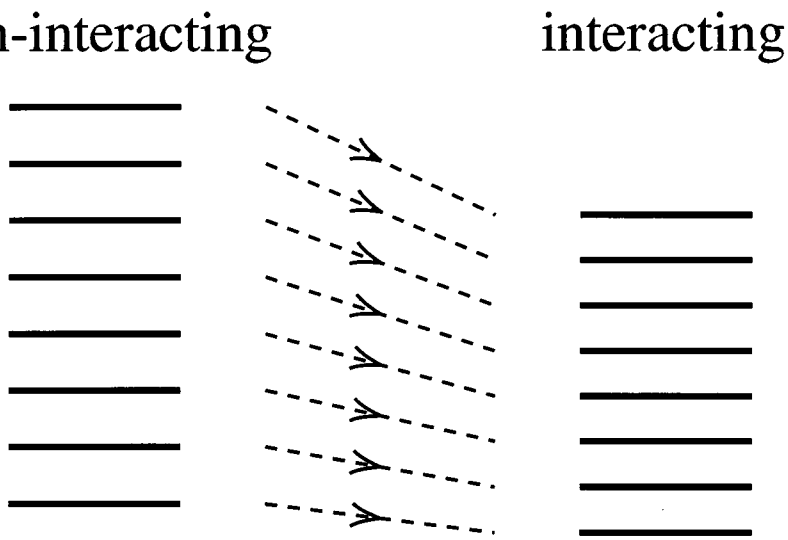
and many more....

Landau's quasiparticle concept:

- There is a one–to–one relationship between the (low-lying) states of a non–interacting Fermi–system, and the states of the interacting system

$\Rightarrow$ no level crossings

$\Rightarrow$ no gaps in the spectrum



- The states of the *non–interacting* system are characterized by quantum numbers $\mathbf{k}$, σ and corresponding *particle occupation numbers* $n_{\mathbf{k},\sigma}$.
- The states of the *interacting* system are characterized by quantum numbers $\mathbf{k}$, σ and corresponding *quasiparticle occupation numbers* $n_{\mathbf{k},\sigma}$.

- The energy is a functional of the *quasiparticle occupation number* $n_{\mathbf{k},\sigma}$:

$$E\left[n_{\mathbf{k},\sigma}\right] .$$

- Changes in the system are due to changes of $n_{\mathbf{k},\sigma}$:

$$n_{\mathbf{k},\sigma} = n^{(0)}_{\mathbf{k},\sigma} + \delta n_{\mathbf{k},\sigma} .$$

- The *quasiparticle spectrum* is the first variation

$$e^{(0)}_{\mathbf{k},\sigma} = \left.\frac{\delta E\left[n_{\mathbf{k},\sigma}\right]}{\delta n_{\mathbf{k},\sigma}}\right|_{n^{(0)}_{\mathbf{k},\sigma}} .$$

- The *quasiparticle interaction* is

$$f_{\mathbf{k}\sigma,\mathbf{k}'\sigma'} = \left.\frac{\delta^2 E\left[n_{\mathbf{k},\sigma}\right]}{\delta n_{\mathbf{k}\sigma}\delta n_{\mathbf{k}',\sigma'}}\right|_{n^{(0)}_{\mathbf{k},\sigma}} .$$

- Excitation spectrum:

$$e_{\mathbf{k},\sigma} = e^{(0)}_{\mathbf{k},\sigma} + \sum_{\mathbf{k}',\sigma'} f_{\mathbf{k}\sigma,\mathbf{k}'\sigma'}\delta n_{\mathbf{k}',\sigma'}$$

- "Effective mass"

$$\frac{\hbar k_F}{m^*} \equiv \left. \frac{de^{(0)}_{\mathbf{k},\sigma}}{dk} \right|_{k=k_F}$$

- Spin–dependence: Let (recall that $k = k' = k_F$)

$$f_{\mathbf{k}\uparrow,\mathbf{k}'\uparrow} = f^s_{\mathbf{k},\mathbf{k}'} + f^a_{\mathbf{k},\mathbf{k}'} = \sum_{\ell=0}^{\infty} (f^s_\ell + f^a_\ell)\, P_\ell(\cos\xi) \equiv \frac{\pi^2\hbar^2}{\Omega m^* k_F} \sum_{\ell=0}^{\infty} (F^s_\ell + F^a_\ell)\, P_\ell(\cos\xi)$$

$$f_{\mathbf{k}\uparrow,\mathbf{k}'\downarrow} = f^s_{\mathbf{k},\mathbf{k}'} - f^a_{\mathbf{k},\mathbf{k}'} = \sum_{\ell=0}^{\infty} (f^s_\ell - f^a_\ell)\, P_\ell(\cos\xi) \equiv \frac{\pi^2\hbar^2}{\Omega m^* k_F} \sum_{\ell=0}^{\infty} (F^s_\ell - F^a_\ell)\, P_\ell(\cos\xi)$$

Physical observables:

Specific heat:	$c_V = \frac{1}{3} m^* k_F T$
Sound velocity:	$c^2 = \frac{\hbar^2 k_F^2}{3mm^*} (1 + F^s_0)$
Magnetic susceptibility:	$\frac{\chi^0_M}{\chi_M} = 1 + F^a_0$
Effective mass:	$\frac{m^*}{m} = 1 + \frac{1}{3} F^s_1$

Interpretation I: Landau's quasiparticle interaction

Microscopic theory: The mapping is produced by the correlation operator F which may in principle depend on the occupation numbers

$$H_{\mathbf{m},\mathbf{m}} = H_{oo}\left[F(n_{\mathbf{k},\sigma}); \ell(n_{\mathbf{k},\sigma})\right] = H_{oo}\left[F(n_{\mathbf{k},\sigma}); n_{\mathbf{k},\sigma}\right]$$

In practice, F cannot depend on the occupation number. How bad is this ? Assume, for all quasiparticle occupation numbers $n_{\mathbf{k},\sigma}$.

$$\forall_{n_{\mathbf{k},\sigma}} \quad \frac{\delta H_{oo}\left[n_{\mathbf{k},\sigma}\right]}{\delta F} = 0 \qquad \Rightarrow \qquad \frac{\delta}{\delta n_{\mathbf{k},\sigma}} \frac{\delta H_{oo}\left[n_{\mathbf{k},\sigma}\right]}{\delta F} = 0\,.$$

Then

$$f^{var}_{\mathbf{k}\sigma,\mathbf{k}'\sigma'} = \left\{ \frac{\delta^2 H_{oo}\left[n_{\mathbf{k},\sigma}\right]}{\delta n_{\mathbf{k},\sigma} \delta n_{\mathbf{k}',\sigma'}} \right\}$$

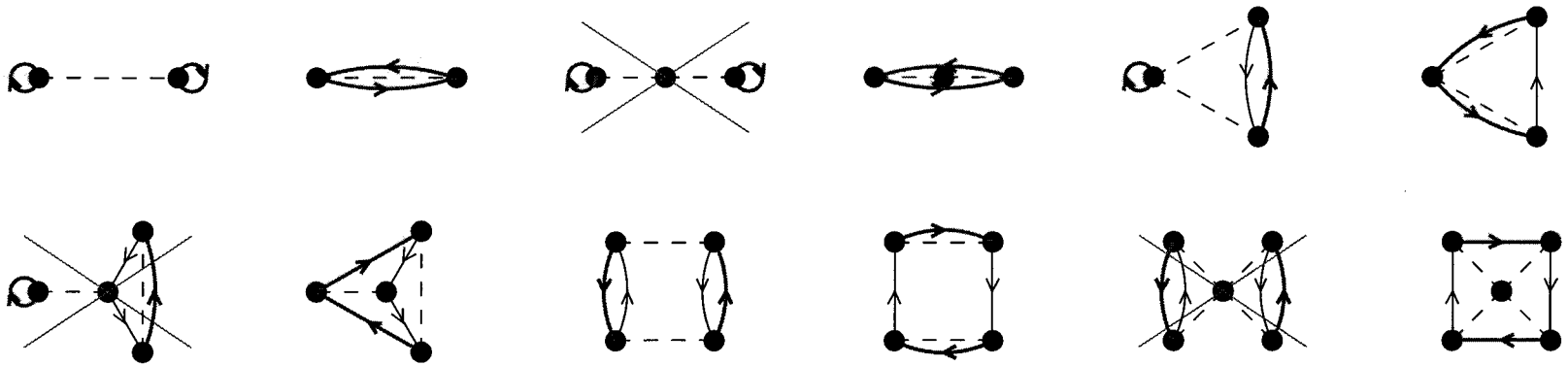
$$= \left\{ \frac{\partial^2 H_{oo}}{\partial n_{\mathbf{k},\sigma} \partial n_{\mathbf{k}',\sigma'}} \right\} - \left\{ \frac{\delta^2 H_{oo}\left[n_{\mathbf{k},\sigma}\right]}{\delta F^2} \frac{\delta F}{\delta n_{\mathbf{k},\sigma}} \frac{\delta F}{\delta n_{\mathbf{k}',\sigma'}} \right\} \geq \left\{ \frac{\partial^2 H_{oo}}{\partial n_{\mathbf{k},\sigma} \partial n_{\mathbf{k}',\sigma'}} \right\}$$

Explicit construction:

- For the variation, interpret the density factor as "1-point" exchange loop $\ell(r_{ii}k_F)$.

$$f^{var}_{\mathbf{k}\sigma;\mathbf{k}'\sigma'} = \frac{1}{N^2}\int d^3r_i d^3r_j d^3r_k d^3r_l \left(\frac{\delta^2 H_{oo}}{\delta l(r_{ij}k_F)\delta l(r_{kl}k_F)}\right) e^{i(\mathbf{k}\cdot\mathbf{r}_{ij}+\mathbf{k}'\cdot\mathbf{r}_{kl})}$$

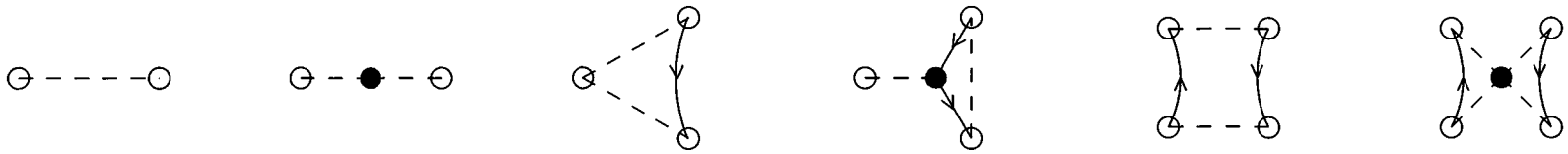
$$= \frac{1}{N^2}\int d^3r_i d^3r_j d^3r_k d^3r_l \mathcal{V}_{QP}(\mathbf{r}_i,\mathbf{r}_j;\mathbf{r}_k,\mathbf{r}_l) e^{i(\mathbf{k}\cdot\mathbf{r}_{ij}+\mathbf{k}'\cdot\mathbf{r}_{kl})}$$



- blue oriented lines represent $\exp(i\mathbf{k}\cdot(\mathbf{r}_i - \mathbf{r}_j))$
- crossed–out diagrams do not occur

If the crossed–out diagrams were present, we could write $f^{var}_{\mathbf{k}\sigma,\mathbf{k}'\sigma'}$ as anti-symmetrized matrix elements of $\mathcal{W}(1,2)$

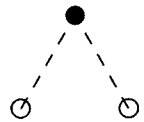
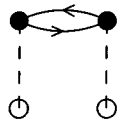
$$f^{var}_{\mathbf{k}\sigma,\mathbf{k}'\sigma'} = \langle \mathbf{k}\sigma, \mathbf{k}'\sigma' | \, \mathcal{W}(1,2) \, | \mathbf{k}\sigma\mathbf{k}'\sigma' \rangle_a$$



Consider the *diagonal limit*

$$\lim_{q\to 0} \langle \mathbf{k}+\mathbf{q}\sigma, \mathbf{k}'\sigma' | \, \mathcal{W}(r_{12}) \, | \mathbf{k}\sigma, \mathbf{k}'+\mathbf{q}\sigma' \rangle_a \ .$$

Sample diagrams

$$\lim_{q\to 0} \langle \mathbf{k}+\mathbf{q}, \mathbf{k}' |$$   $$| \mathbf{k}, \mathbf{k}'+\mathbf{q} \rangle$$

$$= \lim_{q\to 0} \frac{1}{N} \left[\tilde{h}^2(q) + \tilde{h}^2(q)(S_F(q)-1) \right]$$

$$= \lim_{q\to 0} \frac{1}{N} \tilde{h}^2(q) S_F(q) = 0$$

for *short–ranged correlations*.

Rule: The variational quasiparticle interaction is the sum of all those contributions to $\mathcal{W}(1,2)$ that survive in the diagonal limit.

or

Rule: The variational quasiparticle interaction is the sum of all those contributions to $\langle \mathbf{k}\sigma, \mathbf{k}'\sigma' | \, \mathcal{W}(r_{12}) \, | \mathbf{k}\sigma, \mathbf{k}'\sigma' \rangle_a$ where the path between the plane–wave orbitals is non–nodal.

Interpretation II: Superfluidity with strong interactions

Historical reference material:

J. Bardeen, L. N. Cooper, and J. R. Schrieffer, Phys. Rev. **108**, 1175 (1957).

N. N. Bogoljubov, V. V. Tolmachov, and D. V. Shirkov, *A New Method in the Theory of Superconductivity,* Consultants Bureau, New York, 1959.

S. T. Beliaev, *Lecture notes of the 1957 Les Houches Summer School.*

Many newer books on superconductivity and superfluidity.

Pairing theory with correlations:

S. Fantoni, Nucl. Phys. A **363**, 381 (1976)

E. K. and J. W. Clark, Nucl. Phys. A **328**, 73 (1979); Nucl. Phys. **A333**, 77 (1980).

E. K., R. A. Smith and A. D. Jackson, Phys. Rev. B **24**, 6404, 1981

Wave function for s-wave superfluidity in a *weakly interacting* system:

$$|\mathrm{BCS}\rangle = \prod_{\mathbf{k}} (u_{\mathbf{k}} + v_{\mathbf{k}} a^{\dagger}_{\mathbf{k},\uparrow} a^{\dagger}_{-\mathbf{k},\downarrow}) \, |0\rangle \ ,$$

Normalization for the "Bogoljubov amplitudes" $u_{\mathbf{k}}$, $v_{\mathbf{k}}$:

$$u_{\mathbf{k}}^2 + v_{\mathbf{k}}^2 = 1 \qquad u_{\mathbf{k}} = \cos\eta_{\mathbf{k}}, \quad v_{\mathbf{k}} = \sin\eta_{\mathbf{k}} \, .$$

Normal state $v_{\mathbf{k}}^{(0)} = \Theta(k_F - k)$.

Energy of the BCS state (spin sums implied)

$$\langle \mathrm{BCS}|\, \hat{H} - \mu \hat{N} \,|\mathrm{BCS}\rangle = 2 \sum_{\mathbf{k}} \left[t(k) - \mu + \sum_{\mathbf{k}'} \langle \mathbf{k}, \mathbf{k}'|\, V \,|\mathbf{k}, \mathbf{k}'\rangle_a \, v_{\mathbf{k}'}^2 \right] v_{\mathbf{k}}^2 + \sum_{\mathbf{k},\mathbf{k}'} \langle \mathbf{k}\uparrow, -\mathbf{k}\downarrow|\, V \,|\mathbf{k}'\uparrow, -\mathbf{k}'\downarrow\rangle_a \, u_{\mathbf{k}} v_{\mathbf{k}} u_{\mathbf{k}'} v_{\mathbf{k}'}$$

Variational determination of the Bogoljubov amplitudes:

$$\frac{\delta}{\delta \eta_{\mathbf{k}}} \langle \mathrm{BCS}|\, \hat{H} - \mu \hat{N} \,|\mathrm{BCS}\rangle = 0\,,$$

subject to the constraint

$$\langle \hat{N} \rangle = \sum_{\mathbf{k}} v_{\mathbf{k}}^2\,.$$

Resulting "gap equations":

$$\Delta(\mathbf{k}) \equiv -\frac{1}{2}\sum_{\mathbf{k}'} \mathcal{P}_{\mathbf{k},\mathbf{k}'} u_{\mathbf{k}'} v_{\mathbf{k}'} = -\frac{1}{2}\sum_{\mathbf{k}'} \mathcal{P}_{\mathbf{k},\mathbf{k}'} \frac{\Delta(\mathbf{k}')}{\sqrt{\xi^2(\mathbf{k}') + \Delta^2(\mathbf{k}')}}$$

$$\xi(\mathbf{k}) = t(k) - \mu + \sum_{\mathbf{k}'} \langle \mathbf{k}, \mathbf{k}' | \, V \, | \mathbf{k}, \mathbf{k}' \rangle_a \, v^2_{\mathbf{k}'}$$

$$\mathcal{P}_{\mathbf{k},\mathbf{k}'} = \langle \mathbf{k}\uparrow, -\mathbf{k}\downarrow | \, V \, | \mathbf{k}'\uparrow, -\mathbf{k}'\downarrow \rangle_a$$

$$v^2_{\mathbf{k}'} = \frac{1}{2}\left[1 - \frac{\xi(\mathbf{k})}{\sqrt{\xi^2(\mathbf{k}') + \Delta^2(\mathbf{k}')}}\right]$$

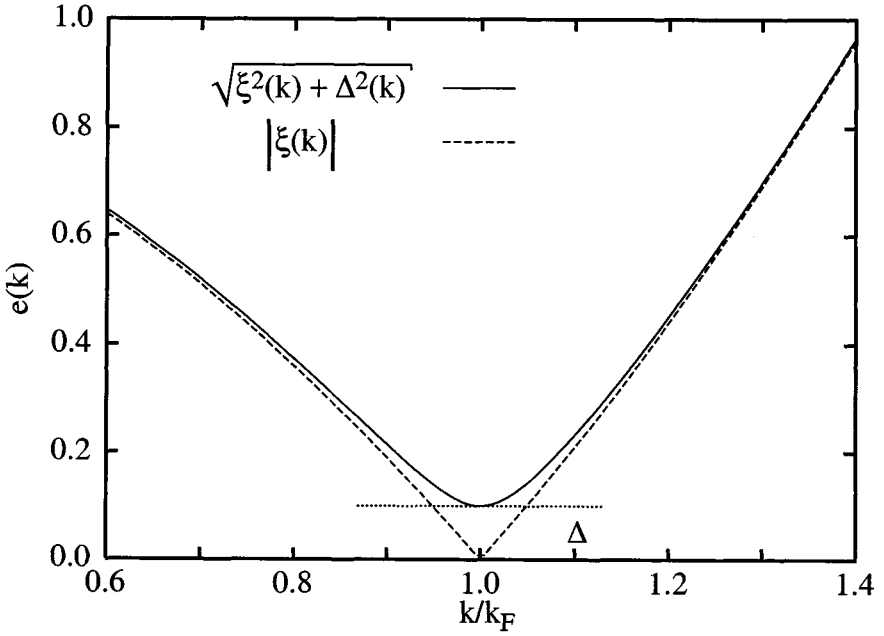
$\Rightarrow$ *"Decoupling approximation"* $v^2_{\mathbf{k}} = n(k)$ is accurate to 10^{-3} in the definition of $\xi(k)$.

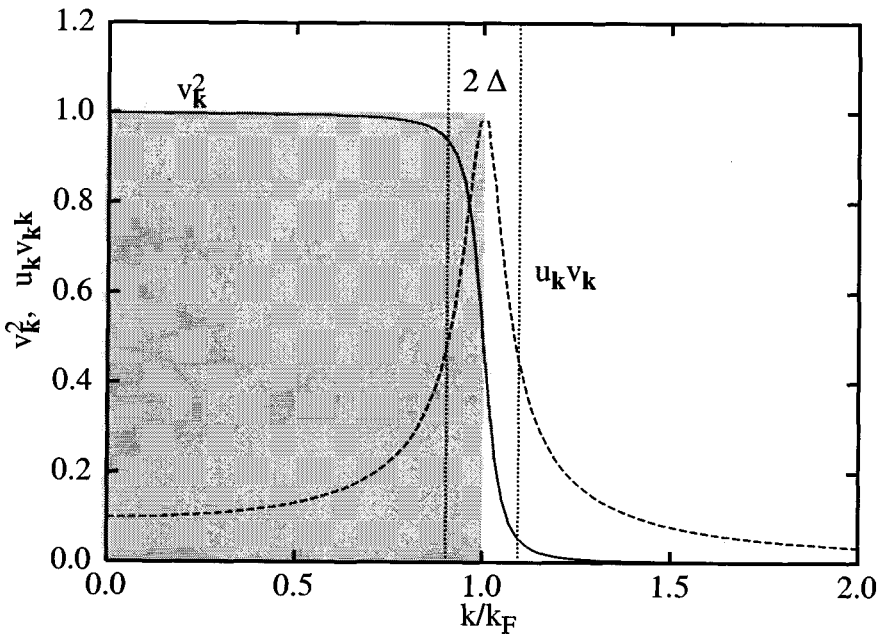
Features of the superfluid state:

- $|\mathrm{BCS}\rangle$ is not an eigenstate of $\hat{N}$.
- Excitation spectrum has a gap $\Delta(k_F)$

$$\epsilon(k) = \sqrt{\xi^2(k) + \Delta^2(k)}$$

- Energy shift is $\propto \Delta(k_F)/\mu^2$
- Deviations from normal behavior in ares $|\Delta(k_F)/\mu|$ around Fermi surface
- $|\Delta(k_F)/\mu| \approx 0.05$ in nuclear matter, 10^{-3} in ^{3}He





Stability of the normal state
Another way to look at pairing

Stability condition:

$$\frac{\delta^2}{\delta v_{\mathbf{k}} \delta v_{\mathbf{k}'}} \langle \mathrm{BCS} | \, \hat{H} - \mu \hat{N} \, | \mathrm{BCS} \rangle \, \Big|_{v_{\mathbf{k}}^2 = n(k)} > 0$$

Equivalent to

$$\left(2 \left| \xi_{\mathbf{k}}^{(0)} \right| \delta_{\mathbf{k}\mathbf{k}'} + \mathcal{P}_{\mathbf{k}\mathbf{k}'} \right)_{\mathbf{k}\mathbf{k}'}$$

be positive definite, where

$$\xi_{\mathbf{k}}^{(0)} = t(k) - \mu + \sum_{\mathbf{k}} \langle \mathbf{k}, \mathbf{k}' | \, V \, | \mathbf{k}, \mathbf{k}' \rangle_a \, \Theta(k_F - k).$$

Sufficient condition for pairing:

$$\mathcal{P}_{k_F, k_F} < 0$$

BCS theory with correlations
Strongly interacting systems:

Procedure:

- Write down BCS many–body state,
- Project on complete sets of states $\left|\Phi_m^{(N)}\right\rangle$ with particle numbers N,
- Correlate with N-body operators $F_N(1,\ldots,N)$ and normalize,
- Add all states:

$$|\mathrm{CBCS}\rangle = \prod_{\mathbf{k}} (u_{\mathbf{k}} + v_{\mathbf{k}} \alpha^\dagger_{\mathbf{k},\uparrow} \alpha^\dagger_{-\mathbf{k},\downarrow}) \, |0\rangle = \sum_{m,N} \left|m^{(N)}\right\rangle \left\langle \Phi_m^{(N)} \middle| \, \mathrm{BCS} \right\rangle ,$$

- Calculate *correlated* expectation value

$$\frac{\langle \mathrm{CBCS}| \, \hat{H} - \mu \hat{N} \, |\mathrm{CBCS}\rangle}{\langle \mathrm{CBCS} \, | \mathrm{CBCS}\rangle} ,$$

- Simplify by keeping terms of leading order in Δ/e_F only ("decoupling approximation").

Consider any operator $\hat{O}$ (specifically $\hat{H}$ or $\hat{N}$), calculate

$$\left\langle \hat{O} \right\rangle_s = \frac{\langle \mathrm{CBCS}| \hat{O} |\mathrm{CBCS}\rangle}{\langle \mathrm{CBCS} |\mathrm{CBCS}\rangle} ,$$

$$|\mathrm{CBCS}\rangle = \sum_{m,N} \left| m^{(N)} \right\rangle \left\langle \Phi_m^{(N)} \right| P_N \prod_{\mathbf{k}} (u_{\mathbf{k}} + v_{\mathbf{k}} a^\dagger_{\mathbf{k},\uparrow} a^\dagger_{-\mathbf{k},\downarrow}) |0\rangle$$

Expand the expectation value in the deviation of the Bogoljubov-amplitudes $u_{\mathbf{k}}$, $v_{\mathbf{k}}$ from their normal-state values $v_{\mathbf{k}}^{(0)} = n(\mathbf{k}) = \Theta(k_F - k)$ (First order terms are zero because of momentum conservation). Keep all terms that give a non–zero contribution to

$$\frac{\delta^2}{\delta v_{\mathbf{k}} \delta v_{\mathbf{k}'}} \frac{\langle \mathrm{CBCS}| \hat{H} - \mu \hat{N} |\mathrm{CBCS}\rangle}{\langle \mathrm{CBCS} |\mathrm{CBCS}\rangle} \Big|_{v_{\mathbf{k}}^2 = \Theta(k_F - k)}$$

Define

$$\beta^\dagger_{\mathbf{k}} = \alpha^\dagger_{\mathbf{k}\uparrow} \alpha^\dagger_{-\mathbf{k}\downarrow}$$

$$\beta_{\mathbf{k}} = \alpha_{-\mathbf{k}\downarrow} \alpha_{\mathbf{k}\uparrow} .$$

$$
\begin{aligned}
\langle \hat{O} \rangle_s = & \left\langle o \middle| O^{(N)} \middle| o \right\rangle \\
& + \sum_{k>k_F} v_{\mathbf{k}}^2 \left\langle o\, \beta_{\mathbf{k}} \middle| \left[O^{(N+2)} - O_{oo}^{(N)} \right] \middle| \beta_{\mathbf{k}}^\dagger\, o \right\rangle \\
& + \sum_{k<k_F} u_{\mathbf{k}}^2 \left\langle o\, \beta_k^\dagger \middle| \left[O^{(N-2)} - O_{oo}^{(N)} \right] \middle| \beta_{\mathbf{k}}\, o \right\rangle \\
& + \sum_{k>k_F, k'<k_F} u_{\mathbf{k}} v_{\mathbf{k}} u_{\mathbf{k}'} v_{\mathbf{k}'} \left\langle o \middle| \left[O^{(N)} - O_{oo}^{(N)} \right] \middle| \beta_{\mathbf{k}}^\dagger \beta_{\mathbf{k}'}\, o \right\rangle \\
& + \sum_{k>k_F, k'>k_F} u_{\mathbf{k}} v_{\mathbf{k}} u_{\mathbf{k}'} v_{\mathbf{k}'} \left\langle o\, \beta_{\mathbf{k}} \middle| \left[O^{(N+2)} - O_{oo}^{(N)} \right] \middle| \beta_{\mathbf{k}'}^\dagger\, o \right\rangle \\
& + \sum_{k<k_F, k'<k_F} u_{\mathbf{k}} v_{\mathbf{k}} u_{\mathbf{k}'} v_{\mathbf{k}'} \left\langle o\, \beta_{\mathbf{k}}^\dagger \middle| \left[O^{(N-2)} - O_{oo}^{(N)} \right] \middle| \beta_{\mathbf{k}'}\, o \right\rangle \\
& + \sum_{k<k_F, k'>k_F} u_{\mathbf{k}} v_{\mathbf{k}} u_{\mathbf{k}'} v_{\mathbf{k}'} \left\langle o\, \beta_{\mathbf{k}}^\dagger \beta_{\mathbf{k}'} \middle| \left[O^{(N)} - O_{oo}^{(N)} \right] \middle| o \right\rangle
\end{aligned}
$$

Let $\hat{O} = \hat{H} - \mu\hat{N}$, evaluate the terms:
Diagonal terms:

$$k > k_F : \quad \left\langle o\,\beta_{\mathbf{k}}\right| \left[H^{(N+2)} - \mu(N+2) - H_{oo}^{(N)} + \mu N\right] \left|\beta_{\mathbf{k}}^{\dagger}\, o\right\rangle$$
$$= \left\langle o\,\beta_{\mathbf{k}}\right| \left[H^{(N+2)} - H_{oo}^{(N+2)}\right] \left|\beta_{\mathbf{k}}^{\dagger}\, o\right\rangle = 2[e_k - \mu],$$

Off–diagonal terms:

$k > k_F\, k' < k_F$:

$$\left\langle o\right| \left[H^{(N)} - H_{oo}^{(N)}\right] \left|\beta_{\mathbf{k}}^{\dagger}\beta_{\mathbf{k}'}\, o\right\rangle = \langle k', -k'|\, \mathcal{H}(1,2)\, |k, -k\,\rangle$$
$$= \langle k', -k'|\, \mathcal{W}(1,2)\, |k, -k\,\rangle + (e_k - e_{k'})\, \langle k', -k'|\, \mathcal{N}(1,2)\, |k, -k\,\rangle$$
$$= \langle k', -k'|\, \mathcal{W}(1,2)\, |k, -k\,\rangle + (|e_k - \mu| + |e_{k'} - \mu|)\, \langle k', -k'|\, \mathcal{N}(1,2)\, |k, -k\,\rangle$$
$$\equiv \mathcal{P}_{\mathbf{k},\mathbf{k}'}$$

Hence

$$\left\langle \hat{H} - \mu\hat{N}\right\rangle_s = \text{const.} + 2\sum_k [e_k - \mu] v_{\mathbf{k}}^2 + \sum_{\mathbf{k},\mathbf{k}'} \mathcal{P}_{\mathbf{k},\mathbf{k}'} u_{\mathbf{k}} v_{\mathbf{k}} u_{\mathbf{k}'} v_{\mathbf{k}'}$$

Summary of "Correlated BCS theory

$\Rightarrow$ Correlations have mapped the strongly interacting system to a weakly interacting system with the BCS energy functional

$\Rightarrow$ "effective pairing interaction" is

$$\mathcal{P}_{\mathbf{k},\mathbf{k}'} = \langle k' \uparrow, -k' \downarrow | \, \mathcal{W}(1,2) \, | k \uparrow, -k \downarrow \rangle + (|e_k - \mu| + |e_{k'} - \mu|) \, \langle k' \uparrow, -k' \downarrow | \, \mathcal{N}(1,2) \, | k \uparrow, -k \downarrow \rangle$$

$\Rightarrow$ Since $\Delta(k)/\sqrt{\xi^2(k) + \Delta^2(k)}$ is peaked around k_F, the second term is unimportant.

$\Rightarrow$ The "sufficient condition" for pairing needs only the first term

$\Rightarrow$ We can identify $\mathcal{W}(1,2)$ with an effective pairing interaction.

$\Rightarrow$ Full FHNC analysis for $|\mathrm{CBCS}\rangle$ is also feasible and necessary if $\Delta \ll e_F$ is violated.

More on effective interactions: FHNC diagrammatic structures and operations:

Non–nodal	Nodal	Sum
$X_{dd}(r)$	$N_{dd}(r)$	$\Gamma_{dd}(r)$
$X_{de}(r)$	$N_{de}(r)$	$\Gamma_{de}(r)$
$X_{ee}(r)$	$N_{ee}(r)$	$\Gamma_{ee}(r)$
$X_{cc}(r)$	$N_{cc}(r)$	$\Gamma_{cc}(r)$

Momentum space FHNC for the static structure function

$$S(k) = \frac{\left[1 + \tilde{X}_{ee}(k)\right]\left[1 + \left[1 + \tilde{X}_{ee}(k)\right]\tilde{\Gamma}_{dd}(k)\right]}{\left[1 - \tilde{X}_{de}(k)\right]^2}$$

Exact properties (important for optimization !)

$$1 + \tilde{X}_{ee}(k) \sim S_F(k) + \mathcal{O}(k^2) \qquad \text{as} \qquad k \to 0.$$
$$\tilde{X}_{de}(k) \sim k \qquad \text{as} \qquad k \to 0.$$

Free static structure function

$$S_F(k) = \begin{cases} \frac{3k}{4k_F} - \frac{k^3}{16k_F^3}, & \text{if } k < k_F; \\ 1 & \text{if } k \geq k_F. \end{cases}$$

Reason for long–wavelength behavior: Projector property of the fermion exchange function, recall

$$\frac{\rho}{\nu} \int d^3 r_i \ell(r_{ij} k_F) \ell(r_{ik} k_F) = \ell(r_{jk} k_F)$$

ν is the degeneracy of the single–particle states.

CBF and the optimization problem

$$
\begin{aligned}
0 = \delta_u H_{oo} &= \frac{1}{2}\left[\langle \mathbf{o}| \left(\hat{H} - H_{oo}\right) \sum_{i<j} \delta u_2(\mathbf{r}_i, \mathbf{r}_j) \left|\mathbf{o}\right\rangle + c.c.\right] \\
&= \frac{1}{4}\int d^3r d^3r' \delta u_2(\mathbf{r}, \mathbf{r}') \left[\langle \mathbf{o}| \left(\hat{H} - H_{oo}\right)(\hat{\rho}(\mathbf{r})\hat{\rho}(\mathbf{r}') - \delta(\mathbf{r} - \mathbf{r}')\hat{\rho}(\mathbf{r})) \left|\mathbf{o}\right\rangle + c.c.\right] \\
&= \frac{1}{4I_{oo}}\int \frac{d^3q d^3q'}{(2\pi)^6} \delta u_2(\mathbf{q}, \mathbf{q}') \times \\
&\times \sum_{h\,h'} \left[\langle \Phi_0| F^\dagger (\hat{H} - H_{oo}) F a^\dagger_{\mathbf{h}+\mathbf{q}} a^\dagger_{\mathbf{h}'+\mathbf{q}'} a_{\mathbf{h}} a_{\mathbf{h}'} \left|\Phi_0\right\rangle + c.c.\right] \\
&= \frac{1}{4}\int \frac{d^3q d^3q'}{(2\pi)^6} \delta u_2(\mathbf{q}, \mathbf{q}') \underbrace{\sum_{hh'} \sqrt{\frac{I_{mm}}{I_{oo}}} \langle \mathbf{h}, \mathbf{h}'| \mathcal{H}(1,2) \left|\mathbf{h}+\mathbf{q}, \mathbf{h}'+\mathbf{q}'\right\rangle_a}_{= 0 \qquad \text{because } \delta u_2(\mathbf{q}, \mathbf{q}') \text{ is arbitrary}}
\end{aligned}
$$

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

The Fermi-sea average of the effective CBF interaction vanishes for optimal correlations. "The strength of CBF theory is the weakness of its effective interactions".

Note: Since there is no "Fermi-sea" for bosons, there is no CBF perturbation expansion for an optimized bosonic Jastrow–Feenberg ground state.

Observe: Optimizing correlations means that (a) the effective interactions come for free, and (b) they are as small as possible.

Watch out: "Average–zero" does not mean "everywhere small" !

Optimization
FHNC' - equations

Formal Euler equation:

$$\frac{\hbar^2 k^2}{4m}(S(k)-1)+S'(k)=0$$

The "priming operation"

$\Rightarrow$ Replace, in turn, each line
$f^2(r_{ij})-1 \quad \longrightarrow \quad f^2(r_{ij})\left[v(r_{ij})-\frac{\hbar^2}{4m}\nabla^2 u(r_{ij})\right]$

$\Rightarrow$ Replace, in turn, each pair
$\ell(r_{ij}k_F)\ell(r_{ik}k_F) \quad \longrightarrow \quad (\hbar^2/8m)\nabla_i^2\ell(r_{ij}k_F)\ell(r_{ik}k_F).$

$\Rightarrow$ For off-diagonal matrix elements, replace, in turn, each pair
$\exp(i\mathbf{p}\cdot\mathbf{r}_{ij})\exp(i\mathbf{q}\cdot\mathbf{r}_{ik}) \quad \longrightarrow \quad (\hbar^2/8m)\nabla_i^2\exp(i\mathbf{p}\cdot\mathbf{r}_{ij})\exp(i\mathbf{q}\cdot\mathbf{r}_{ik})$

Simplest version FHNC consistent with optimization:

$$\tilde{X}_{ee}(k) = S_F(k) - 1\,, \qquad \tilde{X}_{de}(k) = 0$$

$$\Gamma_{dd}(r) = e^{[u_2(r)+N_{dd}(r)]} - 1$$

$$\tilde{X}_{dd}(k) = \frac{\tilde{\Gamma}_{dd}(k)}{1+\tilde{\Gamma}_{dd}(k)S_F(k)}\,, \qquad \tilde{N}_{dd}(k) = \tilde{\Gamma}_{dd}(k) - \tilde{X}_{dd}(k)$$

$$S(k) \;\; = \frac{S_F(k)}{1-\tilde{X}_{dd}(k)S_F(k)} = S_F(k)\left[1+\tilde{\Gamma}_{dd}(k)S_F(k)\right]$$

Algorithm to generate fermion $S'(k)$:

- $S'_F(k) = -\frac{1}{2}t(k)(S_F(k)-1)$ (Single–loop approximation).
- $\Gamma'_{dd}(r) = (1+\Gamma_{dd}(r))\left[v(r) - \frac{\hbar^2}{4m}\nabla^2 u_2(r) + N'_{dd}(r)\right]$
- Choose $\Gamma_{dd}(r)$ as independent variable.
- Use $u_2(r) = \ln\left[1+\Gamma_{dd}(r)\right] - N_{dd}(r)$ to eliminate $u_2(r)$.
- Solve for $S(k)$

Define "particle–hole interaction"

$$\tilde{V}_{\text{p-h}}(k) \equiv \tilde{X}'_{dd}(k) - \frac{1}{2}t(k)\tilde{X}_{dd}(k)$$

Then "optimized fermion $S(k)$":

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

$$V_{\text{p-h}}(r) = \left[1 + \Gamma_{dd}(r)\right] v(r) + \Gamma_{dd}(r) w_I(r) + \frac{\hbar^2}{m}\left|\nabla\sqrt{1 + \Gamma_{dd}(r)}\right|^2$$

$$\tilde{w}_I(k) = \frac{t(k)}{2}\left[\frac{1}{S_F(k)} - \frac{1}{S(k)}\right]^2\left[2\frac{S(k)}{S_F(k)} + 1\right]$$

What do these equations mean ? (Later....)

Simplified effective interactions
Not necessarily the best !

$$\mathcal{N}(1,2) \to \mathcal{N}(r) = \Gamma_{dd}(r)$$

$$\mathcal{W}(1,2) \to \mathcal{W}(r) = \Gamma'_{dd}(r) + \frac{\hbar^2}{4m}\nabla^2\Gamma_{dd}(r)$$

$$e_k \to t(k)$$

Look at the pieces of $\mathcal{W}(r)$:

$$\mathcal{W}(r) = [1+\Gamma_{dd}(r)]\left[v(r) - \frac{\hbar^2}{4m}\nabla^2 u_2(r) + N'_{dd}(r)\right] + \frac{\hbar^2}{4m}\nabla^2\Gamma_{dd}(r)$$

$$= [1+\Gamma_{dd}(r)]\,v(r) + \frac{\hbar^2}{m}\left|\nabla\sqrt{1+\Gamma_{dd}(r)}\right|^2$$

$$+ [1+\Gamma_{dd}(r)]\underbrace{\left[\frac{\hbar^2}{4m}\nabla^2 N_{dd}(r) + N'_{dd}(r)\right]}_{= w_I(r)} = V_{\text{p-h}}(r) + w_I(r)$$

Interpretation: (^{3}He at saturation)

$\mathcal{W}(r)$ effective potential

$[1 + \Gamma_{dd}(r)]\, v(r)$ screened potential

$\frac{\hbar^2}{m} \left| \nabla \sqrt{1 + \Gamma_{dd}(r)} \right|^2$ kinetic energy

$[1 + \Gamma_{dd}(r)]\, w_I(r)$ phonon exchange

$v(r)$ bare potential