(Simplified) FHNC
Bulk fermions in the ground state

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Problem

Given a system of identical particles, interacting with some potential $v(r)$, how can we calculate bulk properties such as $g(r)$ or $S(k)$?

Jastrow-Slater Wave Function

- Model wave function:

$$\Phi = F\ \Psi \tag{1}$$

  - Ψ is a slater determinant

$$\Psi(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3, ..) = \begin{Vmatrix} \psi_1(\mathbf{r}_1) & \cdots & \psi_1(\mathbf{r}_N) \\ \vdots & & \vdots \\ \psi_N(\mathbf{r}_1) & \cdots & \psi_N(\mathbf{r}_N) \end{Vmatrix}$$

    $\rightarrow$ ψ_i are single particle orbitals – plane waves

  - F is a Jastrow factor

$$F(\mathbf{r}_1, \ldots, \mathbf{r}_N) = \prod_{i<j} f(|\mathbf{r}_i - \mathbf{r}_j|) = \prod_{i<j} e^{u(|\mathbf{r}_i - \mathbf{r}_j|)}$$

    $\rightarrow$ $f(r)$ or $u(r)$ are variaton parameters

Jastrow-Slater: A Simple Example (1)

Two fermions in 1D, with position x_1 and x_2 and spin $\vec{\sigma}_1$ and $\vec{\sigma}_2$

- Slater wave function

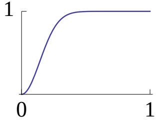
$$\Psi(x_1, x_2) = \psi_1(x_1)\psi_2(x_2) - \psi_1(x_2)\psi_2(x_1)$$

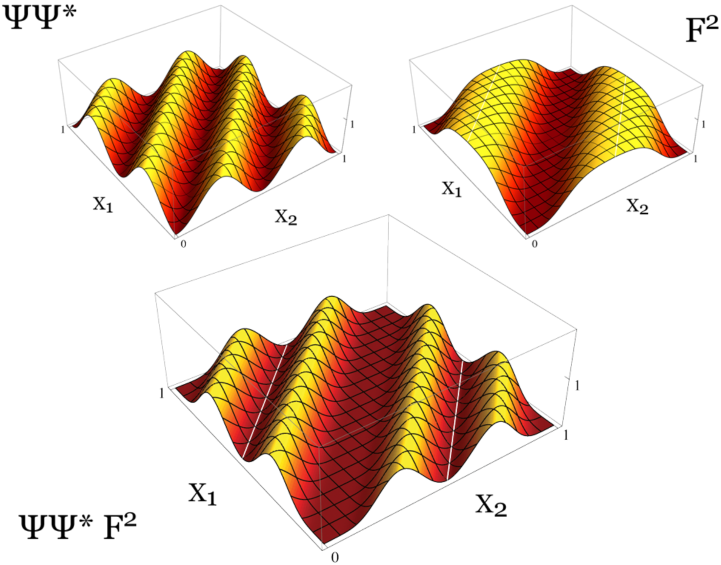
- Single particle orbital

$$\psi_i(x_j) = \vec{\sigma}_j \; e^{ik_i x_j}$$

- Jastrow Factor

$$F(x_1, x_2) = f(|x_1 - x_2|)$$





ΨΨ*
F²
x₁
x₂
ΨΨ* F²

$$\Phi = F\,\Psi$$

- Calculate $g(r)$ from this wavefunction:

$$g(|\mathbf{r}_2 - \mathbf{r}_1|) = \frac{N(N-1)}{\rho^2} \frac{\int d\mathbf{r}_3 \cdots d\mathbf{r}_N F^2 |\Psi|^2}{\int d\mathbf{r}_1 \cdots d\mathbf{r}_N F^2 |\Psi|^2}$$

- Expand the Jastrow Factor

$$\begin{aligned} F^2 = 1 \,&+\, \eta(|r_1 - r_2|) \,+\, \eta(|r_1 - r_3|) \,+\, \ldots \\ &+\, \eta(|r_1 - r_2|)\,\eta(|r_2 - r_3|) \,+\, \ldots \\ &+\, \eta(|r_1 - r_2|)\,\eta(|r_2 - r_3|)\,\eta(|r_3 - r_4|) \,+\, \ldots \end{aligned}$$

$\rightarrow$ we introduced $\eta = f^2 - 1$

- Simplify the integrals

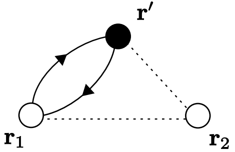
Diagrams

- Sample integral from the expansion:

$$-\frac{\rho}{\nu}\int d\mathbf{r}'\ \ell^2(k_F|\mathbf{r}'-\mathbf{r}_1|)\,\eta(|\mathbf{r}'-\mathbf{r}_2|)\,\eta(|\mathbf{r}_1-\mathbf{r}_2|)$$

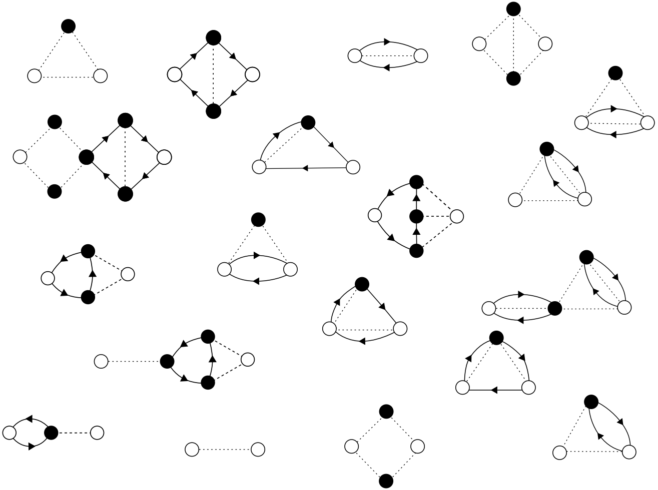
$\rightarrow$ $\ell(k_F r)$ comes from the slater determinant

- express integral as diagram

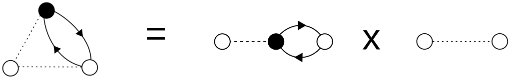


- $g(r)$ and $S(k)$ kan be described as an infinite sum of diagrams.

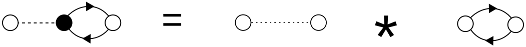
some diagrams in g(r)



Netting and Chaining

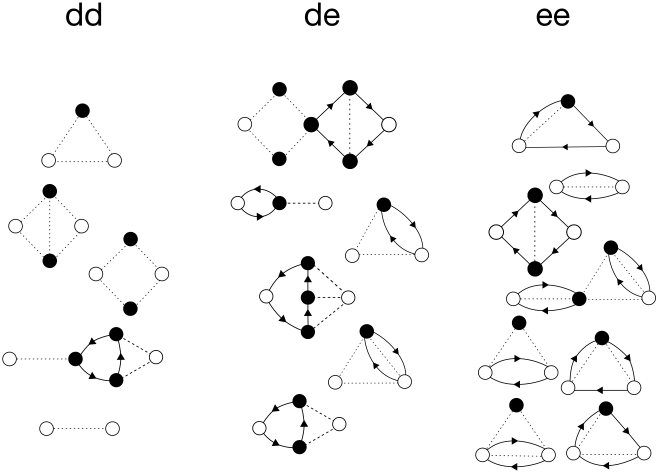


$$\int \mathbf{dr}'\eta(|\mathbf{r}'-\mathbf{r}_1|)\ell^2(|\mathbf{r}_2-\mathbf{r}'|)\eta(|\mathbf{r}_2-\mathbf{r}_1|) = \left[\int \mathbf{dr}'\eta(|\mathbf{r}'-\mathbf{r}_1|)\ell^2(|\mathbf{r}_2-\mathbf{r}'|)\right]\times\left[\eta(|\mathbf{r}_2-\mathbf{r}_1|)\right]$$

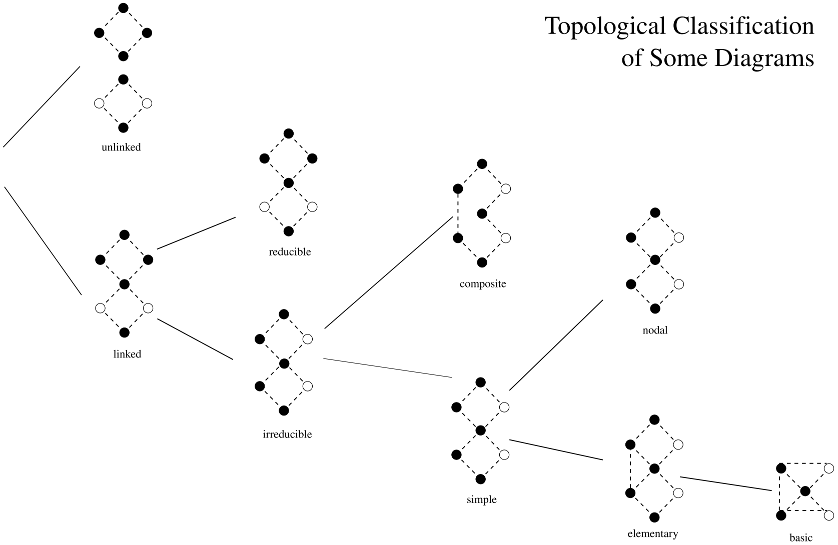


$$\left\{\int \mathbf{dr}'\eta(|\mathbf{r}'-\mathbf{r}_1|)\ell^2(|\mathbf{r}_2-\mathbf{r}'|)\right\}^{\mathcal{F}} = \left\{\eta(|\mathbf{r}_2-\mathbf{r}_1|)\right\}^{\mathcal{F}} \times \left\{\ell^2(|\mathbf{r}_2-\mathbf{r}_1|)\right\}^{\mathcal{F}}$$

some diagrams in g(r)



Topological Classification of Some Diagrams



- Examine topological properties of the expansion:
  - The expansion contains only irreducible diagrams.
  - Internal points come with a coefficient ρ.
  - For n exchange lines, there is a factor $(-\nu)^{n-1}$.
- Define several subsets of diagrams in the expansion:
  - N_{dd} the sum of all nodal diagrams with no exchange lines at the external points
  - N_{de} the sum of all nodal diagrams with two exchange lines at one external point
  - N_{ee} the sum of all nodal diagrams with two exchange lines at both external points
  - X_{dd} the sum of all non-nodal diagrams with no exchange lines at the external points
  - X_{de} the sum of all non-nodal diagrams with two exchange lines at one external point
  - X_{ee} the sum of all non-nodal diagrams with two exchange lines at both external points
  - Γ_{xy} $= N_{\mathrm{xy}} + X_{\mathrm{xy}}$ (the sum of all diagrams with corresponding exchange structure)
  - E_{xy} the sum of all elementary diagrams with corresponding exchange structure
  - ...
- Derive algebraic relations between these quantities

The FHNC equations

Coordinate space:

$$
\begin{aligned}
X_{\mathrm{dd}} &= \exp\left(u_2 + N_{\mathrm{dd}} + E_{\mathrm{dd}}\right) - 1 - N_{\mathrm{dd}} \\
\Gamma_{\mathrm{dd}} &= X_{\mathrm{dd}} + N_{\mathrm{dd}} \\
X_{\mathrm{de}} &= (1 + \Gamma_{\mathrm{dd}})(N_{\mathrm{de}} + E_{\mathrm{de}}) - N_{\mathrm{de}} \\
X_{\mathrm{ee}} &= (1 + \Gamma_{\mathrm{dd}})\left(-\frac{1}{\nu}L^2 + N_{\mathrm{ee}} + E_{\mathrm{ee}}\right) - N_{\mathrm{ee}} \\
&\qquad + (1 + \Gamma_{\mathrm{dd}})(N_{\mathrm{de}} + E_{\mathrm{de}})^2 \\
L &= \ell - \nu\left(N_{\mathrm{cc}} + E_{\mathrm{cc}}\right)
\end{aligned}
$$

Momentum space:

$$
\begin{aligned}
\widetilde{N}_{\mathrm{dd}} &= \frac{\widetilde{X}_{\mathrm{dd}}}{(1 - \widetilde{X}_{\mathrm{de}})^2 - (1 + \widetilde{X}_{\mathrm{ee}})\widetilde{X}_{\mathrm{dd}}} - \widetilde{X}_{\mathrm{dd}} \\
\widetilde{N}_{\mathrm{de}} &= \frac{1 - \widetilde{X}_{\mathrm{de}} - \widetilde{X}_{\mathrm{dd}}}{(1 - \widetilde{X}_{\mathrm{de}})^2 - (1 + \widetilde{X}_{\mathrm{ee}})\widetilde{X}_{\mathrm{dd}}} - 1 - \widetilde{X}_{\mathrm{de}} \\
\widetilde{N}_{\mathrm{ee}} &= \frac{\widetilde{X}_{\mathrm{dd}} + 2\widetilde{X}_{\mathrm{de}} + \widetilde{X}_{\mathrm{ee}} - 1}{(1 - \widetilde{X}_{\mathrm{de}})^2 - (1 + \widetilde{X}_{\mathrm{ee}})\widetilde{X}_{\mathrm{dd}}} + 1 - \widetilde{X}_{\mathrm{ee}} \\
\widetilde{N}_{\mathrm{cc}} &= -\widetilde{X}_{\mathrm{cc}}\,\frac{\nu^{-1}\widetilde{\ell} - \widetilde{X}_{\mathrm{cc}}}{1 - \widetilde{X}_{\mathrm{cc}}}
\end{aligned}
$$

Energy Calculation

Jackson Feenberg Energy functional:

$$\frac{E}{N} = \frac{T_F}{N} + \int d^2r \; g(r)\, v_{JF}(r) + \frac{T^2_{JF}}{N} + \frac{T^3_{JF}}{N} \tag{2}$$

where

$$\begin{aligned}
v_{JF}(r) &= v(r) - \frac{\hbar^2}{4m}\nabla^2 u_2(r) \\
\frac{T^2_{JF}}{N} &= -\frac{\hbar^2\rho}{8m\nu}\int d^2r \; \Gamma_{dd}(r)\nabla^2\ell^2(rk_F) \\
\frac{T^3_{JF}}{N} &= \frac{\hbar^2\rho^2}{8m\nu^2}\int d^2r_{12}d^2r_{13} \; \Gamma_{dcc}(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)\nabla^2_1\ell(r_{12}k_F)\ell(r_{13}k_F)
\end{aligned}$$

Euler equation

Condition for minimal energy

$$\frac{\delta E}{\delta u(r)} = 0 \tag{3}$$

Euler equation in real space

$$\frac{\hbar^2}{4m}\nabla^2 g(r) = \underbrace{\int d^2r' v_{JF}(r') \frac{\delta g(r')}{\delta u(r)} + \frac{2}{\rho}\frac{\delta T_{JF}/N}{\delta u(r)}}_{\equiv g'(r)} \tag{4}$$

Euler equation in momentum space

$$-\frac{\hbar^2 k^2}{4m}\left(S(k) - 1\right) = S'(k) \tag{5}$$

Primed FHNC equations

- Every diagrammatic sum has a primed counterpart
- This leads to the FHNC' equations
- Use FHNC and FHNC' equations to eliminate $u(r)$

To determine $g(r)$ from $v(r)$:

- Find a self-consistent solution for 8 FHNC equations and 8 FHNC' equations
- Many different iteration paths possible

Effective potentials

We introduce effective potentials

$$V_{\rm dd} = X'_{\rm dd}(k) - \frac{\hbar^2 k^2}{4m} X_{\rm dd}(k) \tag{6}$$

$$V_{\rm de} = X'_{\rm de}(k) \tag{7}$$

$$V_{\rm ee} = X'_{\rm ee}(k) - \frac{\hbar^2 k^2}{4m} X_{\rm ee}(k) \tag{8}$$

Write Euler Equation in terms of these potentials:

$$\frac{\hbar^2 k^2}{2m} \left[\frac{1 - S_d(k)^2}{S(k)^2}\right] = \widetilde{V}_{\rm dd}(k) + 2 \left[\frac{S_d(k)}{S(k)}\right] \widetilde{V}_{\rm de}(k) + \left[\frac{S_d(k)}{S(k)}\right]^2 \widetilde{V}_{\rm ee}(k) \tag{9}$$

Iteration (1)

$$V_{\mathrm{dd}} \to S(k) \to \Gamma_{\mathrm{dd}} \to w_i \to V_{\mathrm{dd}}$$

(and, between these steps, also approximate $\widetilde{X}_{\mathrm{de}}(k)$, $\widetilde{X}_{\mathrm{ee}}(k)$, $\widetilde{\Gamma}'_{\mathrm{dd}}(k)$, ...)

Iteration (2)

$$S(k) = \frac{1}{\sqrt{\left[\frac{1-\widetilde{X}_{\rm de}(k)}{1+\widetilde{X}_{\rm ee}(k)}\right]^2 + \frac{4m}{\hbar^2 k^2}\left[\widetilde{V}_{\rm dd}(k) + 2\left[\frac{1-\widetilde{X}_{\rm de}(k)}{1+\widetilde{X}_{\rm ee}(k)}\right]\widetilde{V}_{\rm de}(k) + \left[\frac{1-\widetilde{X}_{\rm de}(k)}{1+\widetilde{X}_{\rm ee}(k)}\right]^2 \widetilde{V}_{\rm ee}(k)\right]}} \tag{10}$$

$$\widetilde{\Gamma}_{\rm dd}(k) = S(k)\left[\frac{1-\widetilde{X}_{\rm de}(k)}{1+\widetilde{X}_{\rm ee}(k)}\right]^2 - \frac{1}{1+\widetilde{X}_{\rm ee}(k)} \tag{11}$$

$$\Gamma_{\rm dd}(r) = \left\{\widetilde{\Gamma}_{\rm dd}(k)\right\}^{\mathcal{F}}(r) \tag{12}$$

Now calculate $\widetilde{\Gamma}'_{\rm dd}(k)$, $\widetilde{X}_{\rm de}(k)$, $\widetilde{X}_{\rm ee}(k)$, $\widetilde{V}_{\rm de}(k)$, $\widetilde{V}_{\rm ee}(k)$. (Not shown)

$$\begin{aligned} w_i(k) = &- \frac{\hbar^2 k^2}{4m}\left[\frac{1}{S(k)^2} - \left[\frac{1-\widetilde{X}_{\rm de}(k)}{1+\widetilde{X}_{\rm ee}(k)}\right]^2\right] \\ &+ \left[\left[\frac{1-\widetilde{X}_{\rm de}(k)}{1+\widetilde{X}_{\rm ee}(k)}\right]^2\left[1 - S(k)^2\left[\frac{1-\widetilde{X}_{\rm de}(k)}{1+\widetilde{X}_{\rm ee}(k)}\right]^2\right] + \widetilde{\Gamma}_{\rm dd}(k)\right]\left[\frac{\hbar^2 k^2}{4m} + \widetilde{V}_{\rm ee}(k)\right] \\ &+ 2\,\frac{1-\widetilde{X}_{\rm de}(k)}{1+\widetilde{X}_{\rm ee}(k)}\left[1 - S(k)^2\left[\frac{1-\widetilde{X}_{\rm de}(k)}{1+\widetilde{X}_{\rm ee}(k)}\right]^2 + \widetilde{\Gamma}_{\rm dd}(k)S(k)\right]\widetilde{V}_{\rm de}(k) \end{aligned} \tag{13}$$

$$w_i(r) = \left\{w_i(k)\right\}^{\mathcal{F}}(r) \tag{14}$$

$$V_{\rm dd}(r) = 2\left[\frac{d}{dr}\sqrt{\Gamma_{\rm dd}(r) - 1}\right]^2 + w_i(r)\Gamma_{\rm dd}(r) + v(r)\left[\Gamma_{\rm dd}(r) + 1\right] \tag{15}$$

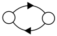
$$\widetilde{V}_{\rm dd}(k) = \left\{V_{\rm dd}(r)\right\}^{\mathcal{F}}(k) \tag{16}$$

Simplified FHNC?

The full FHNC (and FHNC') equations are difficult to evaluate. For long wavelengths (small k), some terms become considerably simpler. We use the following approximations to the full FHNC equations:

$$X_{\mathrm{de}} = 0 \tag{17}$$

$$X_{\mathrm{ee}} = S_F(k) - 1 = \tag{18}$$



and therefore:

$$V_{\mathrm{de}} = 0 \tag{19}$$

$$V_{\mathrm{ee}} = 0 \tag{20}$$

This approximation is called FHNC//0

Iteration (3)

FHNC//0:

$$S(k) = \frac{1}{\sqrt{\frac{1}{S_F(k)^2} + \frac{4m}{\hbar^2 k^2} \widetilde{V}_{\mathrm{dd}}(k)}} \tag{21}$$

$$\widetilde{\Gamma}_{\mathrm{dd}}(k) = \frac{S(k)}{S_F(k)^2} - \frac{1}{S_F(k)} \tag{22}$$

$$\Gamma_{\mathrm{dd}}(r) = \left\{ \widetilde{\Gamma}_{\mathrm{dd}}(k) \right\}^{\mathcal{F}}(r) \tag{23}$$

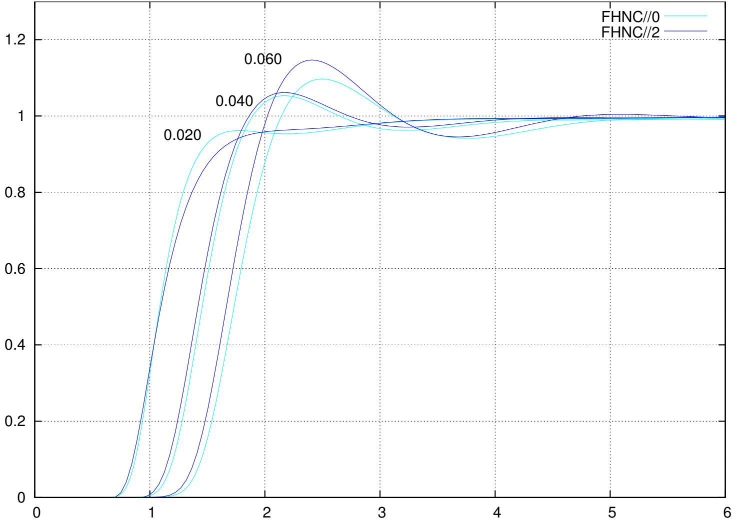
$$w_i(k) = \frac{\hbar^2 k^2}{4m} \left[\frac{1}{S_F(k)} - \frac{1}{S(k)} \right]^2 \left[2 \frac{S(k)}{S_F(k)} + 1 \right] \tag{24}$$

$$w_i(r) = \left\{ w_i(k) \right\}^{\mathcal{F}}(r) \tag{25}$$

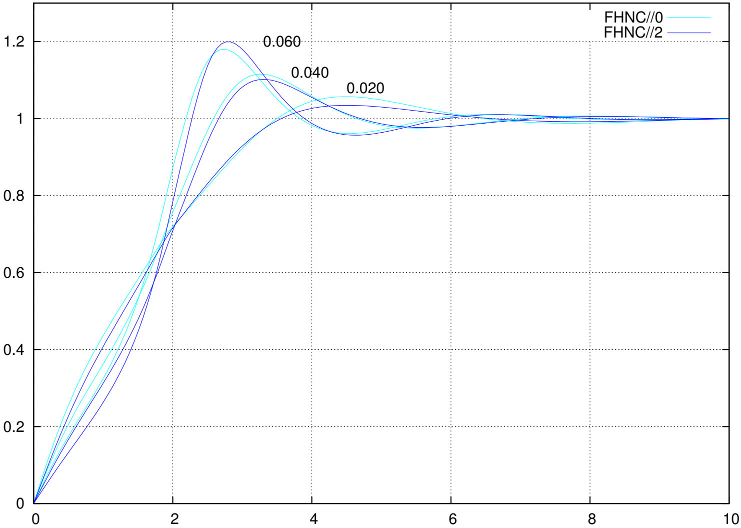
$$V_{\mathrm{dd}}(r) = 2 \left[\frac{d}{dr} \sqrt{\Gamma_{\mathrm{dd}}(r) - 1} \right]^2 + w_i(r) \Gamma_{\mathrm{dd}}(r) + v(r) \left[\Gamma_{\mathrm{dd}}(r) + 1 \right] \tag{26}$$

$$\widetilde{V}_{\mathrm{dd}}(k) = \left\{ V_{\mathrm{dd}}(r) \right\}^{\mathcal{F}}(k) \tag{27}$$

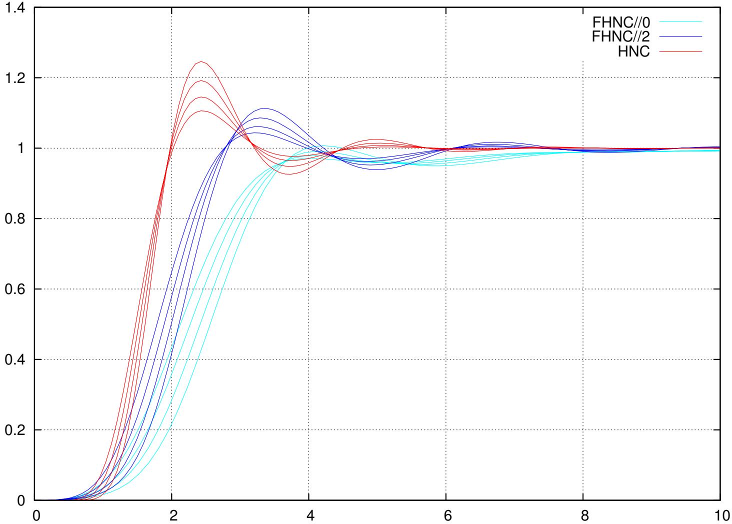
Pair distribution function g(r) for 2D $_3$He



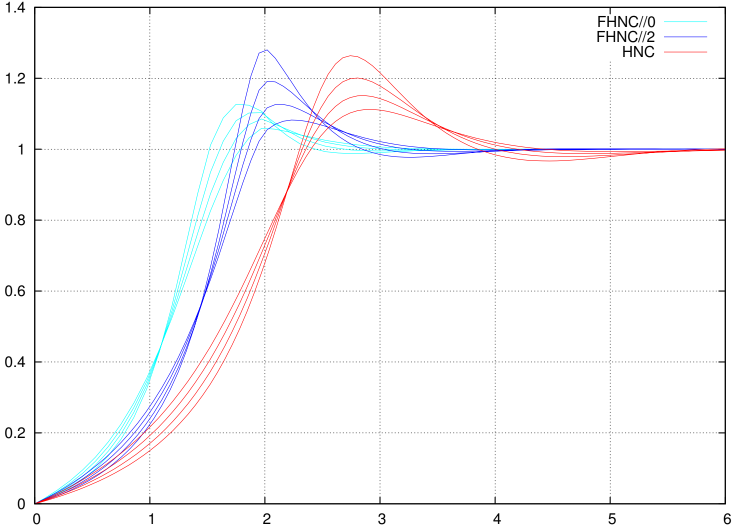
Static structure function S(k) for 2D $_3$He



Pair distribution function g(r) for 2D dipoles



Static structure function S(k) for 2D dipoles



Summary

- FHNC allows to calculate $g(r)$ and $S(k)$ from the interaction potential $v(r)$
- FHNC is a variational approach - fast but with some limits
- we have implemented a form of FHNC for 2D Systems
    - works well for $_3He$
    - problems with long range potentials such as $\frac{1}{r^3}$, $\frac{1}{r}$

Outlook

Possibilities:

- improve precision by considering more classes of diagrams
    - solve the dipole problem?
- extend the algorithm to spin-dependent potentials

Thank you for coming!

Questions?