THEORETICAL PHYSICS

Swift state-of-the-art calculations of the 2D Electron Liquid in the Hyper-Netted-Chain Theory

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August 23, 2017

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INTRODUCTION AND MOTIVATION

System

- many particle system $\Rightarrow$ no analytic solution

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- consisting of electrons ⇒ Pauli principle

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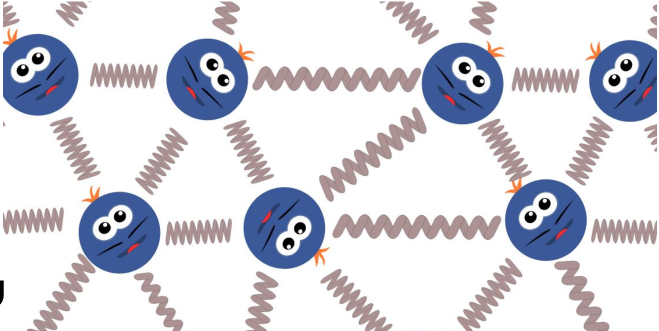
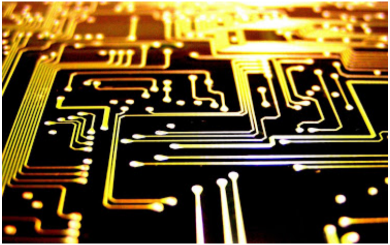
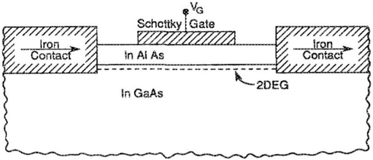


Importance of 2D Electron Systems





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- superconductivity in layered structures (Wang, **Nature** (2015))

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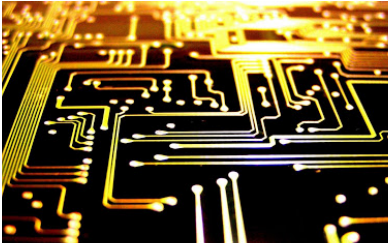

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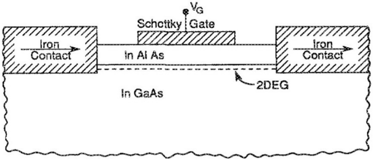

- applications in spintronics
- spin transistor of Datta and Das, **Applied Physics Letters** (1990)

Characterisation

Wigner-Seitz Radius r_s

$r_\mathrm{s} \cdot a_\mathrm{B}$ is the radius of a circle occupied by one electron

- $n \propto 1/r_\mathrm{s}^2$

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excess of electrons with majority spin; $\zeta = \left| n_\uparrow - n_\downarrow \right| / n$

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- **ground state properties of interest:**
  kinetic energy, potential energy, total energy, pressure, compressibility etc.

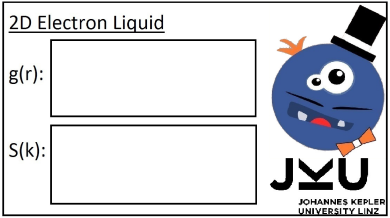
Important Functions

Pair Distribution Function $g(r)$

normalised probability density of finding two particles a distance r apart

Structure Factor $S(k)$

measurable in elastic scattering experiments $\frac{d\sigma}{d\Omega} \propto S(k)$



Fourier-Transform

$$S(k) = 1 + \mathrm{FT}_{2\mathrm{D}}[g - 1](k)$$

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- treat subsystems of spins independently

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$\Rightarrow$ $g(r) = c_1 \, g^{\uparrow\uparrow}(r) \, + c_2 \, g^{\downarrow\downarrow}(r) \, + c_3 \, g^{\uparrow\downarrow}(r)$

- c_i ... constants

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- results in matrix form (intuitive)

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- advantage: further properties accessible

$\Rightarrow$ $g_{\mathrm{M}}(r) = c_1\, g^{\uparrow\uparrow}(r) + c_2\, g^{\downarrow\downarrow}(r) - c_3\, g^{\uparrow\downarrow}(r)$

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- similar for $S(k)$ and $S_{\mathrm{M}}(k)$

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How can $\mathrm{g}(\mathrm{r})$ and $\mathrm{S}(\mathrm{k})$ be calculated?

1. Quantum Monte-Carlo Simulations (QMC)
   - give accurate results
   - take a lot of time
     - **several hours** to calculate $g(r)$ and $S(k)$ for one system at a **single** r_s
   - need powerful computers

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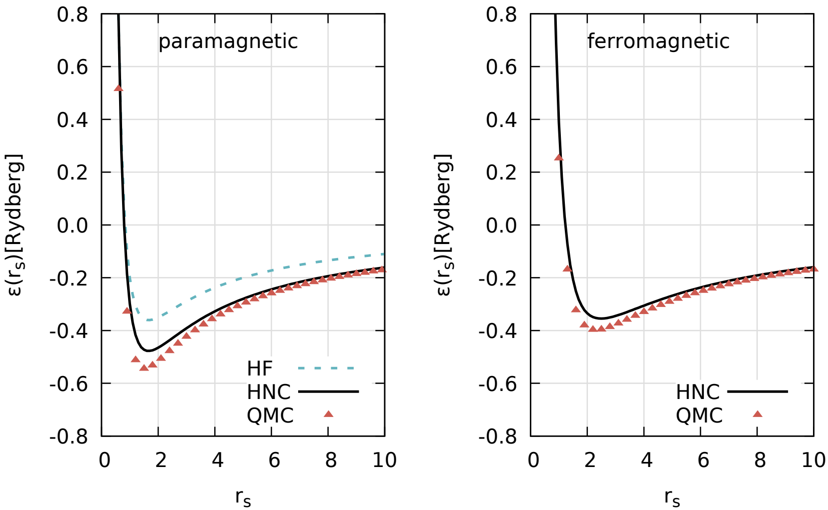
   - need powerful computers
2. Hyper-Netted-Chain Theory (HNC)
   - pair theory which takes correlations into account
   - developed in the 60ies for classical liquids
   - moderate computational effort
     - **59 min** for **100** r_{s}-values ($r_{\mathrm{s}} = 0.1 \ldots 10$, $\Delta r_{\mathrm{s}} = 0.1$) on an average laptop
   - results in agreement with QMC (!)

Energy Comparison with the Literature[1]



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HYPER-NETTED-CHAIN THEORY

Ansatz

- Ansatz with **Bose (!)** symmetry

Jastrow Ansatz

$$\psi = \prod_{\sigma,\sigma'} {\prod_{i<j}}' f(\mathbf{r}_{\sigma,i}, \mathbf{r}_{\sigma',j}) := \exp \tfrac{1}{4} \left\{ \sum_{\sigma,\sigma'} {\sum_{i,j}}' u_2^{\sigma,\sigma'}(\mathbf{r}_{\sigma,i}, \mathbf{r}_{\sigma',j}) \right\}$$

- includes two-body correlations $u_2^{\sigma,\sigma'}$

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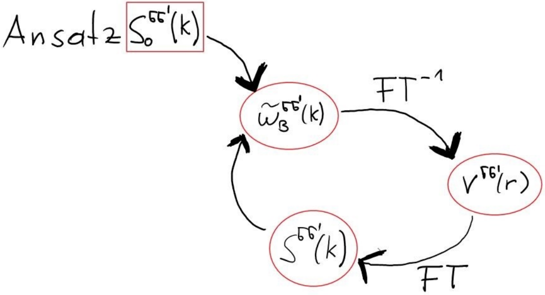
- includes two-body correlations $u_2^{\sigma,\sigma'}$
- $g^{\sigma,\sigma'} \propto \frac{\delta}{\delta u_2^{\sigma,\sigma'}} \ln \langle\psi|\,\psi\rangle$
- Mayer Cluster expansion
- minimise energy

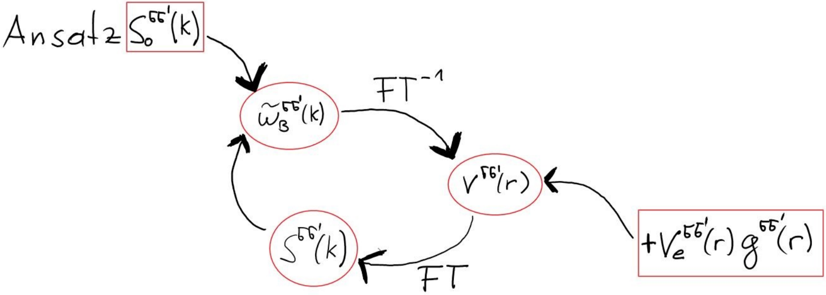
$\Rightarrow$ HNC-EL equations (Euler-Lagrange)

Bosonic HNC



$$V^{\sigma,\sigma'}(r) = \left[v_{\mathrm{C}}^{\sigma,\sigma'} \qquad\qquad \right] g^{\sigma,\sigma'} + \frac{\hbar^2}{m} \left| \nabla \sqrt{g^{\sigma,\sigma'}} \right|^2 + \left(g^{\sigma,\sigma'} - 1 \right) w_{\mathrm{b}}^{\sigma,\sigma'}$$

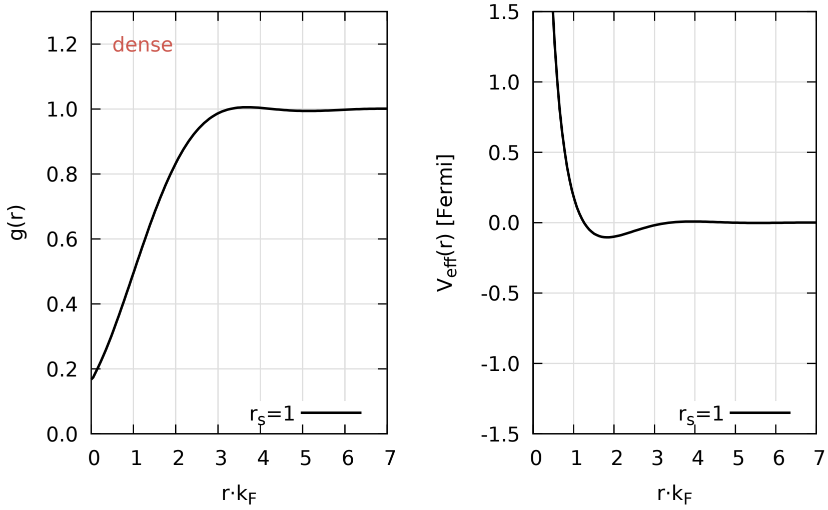
Fermionic HNC (Kallio (1996), Davoudi)



$$V^{\sigma,\sigma'}(r) = \left[v_{\mathrm{C}}^{\sigma,\sigma'} + V_{\mathrm{e}}^{\sigma,\sigma'}\right] g^{\sigma,\sigma'} + \frac{\hbar^2}{m}\left|\nabla\sqrt{g^{\sigma,\sigma'}}\right|^2 + \left(g^{\sigma,\sigma'} - 1\right) w_{\mathrm{b}}^{\sigma,\sigma'}$$

RESULTS

$g(r)$ & effective interaction (paramagnetic)



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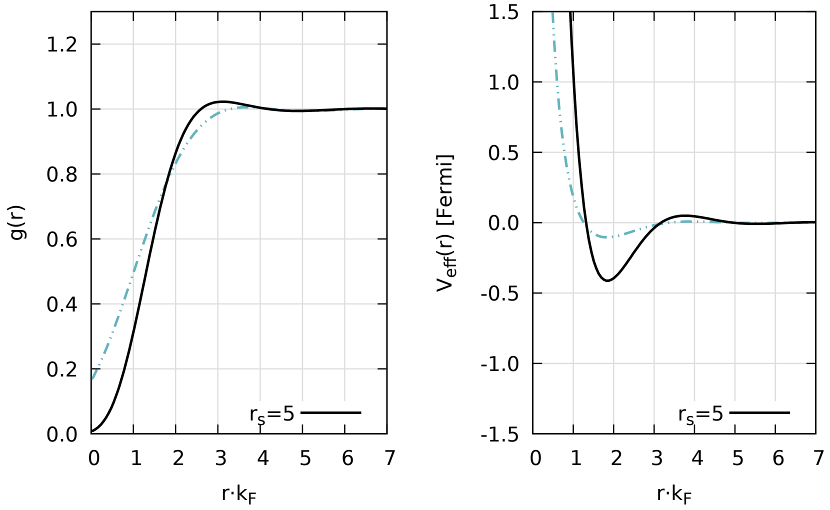

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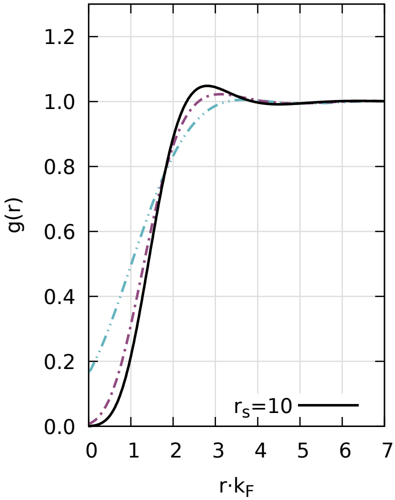

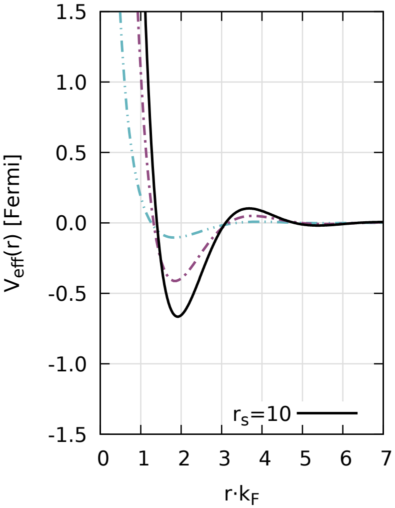

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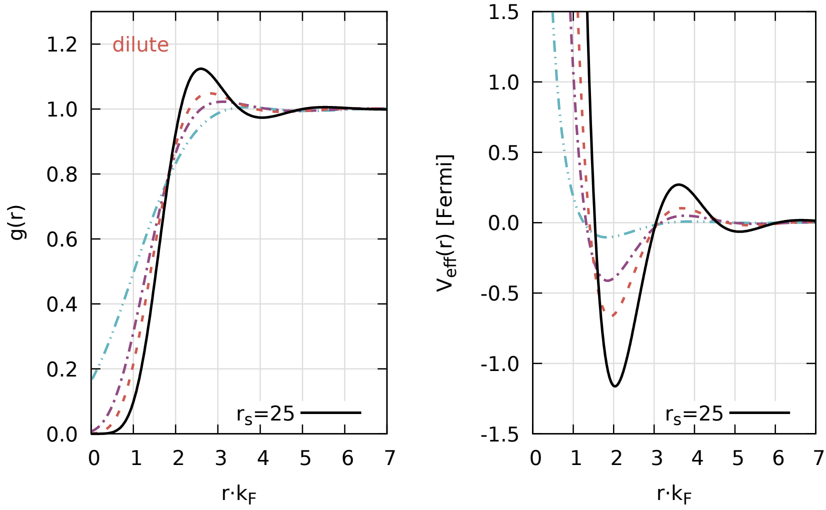
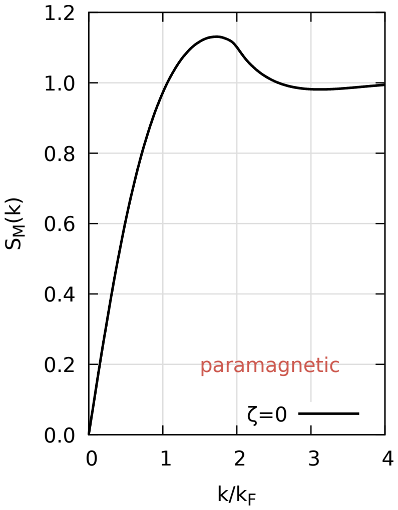
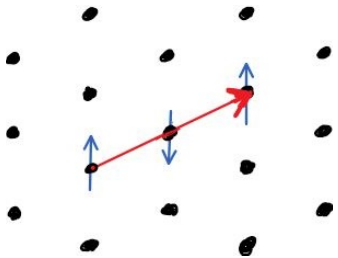


Shift of the Peak in $\mathrm{S_M(k)}$ (dilute system)





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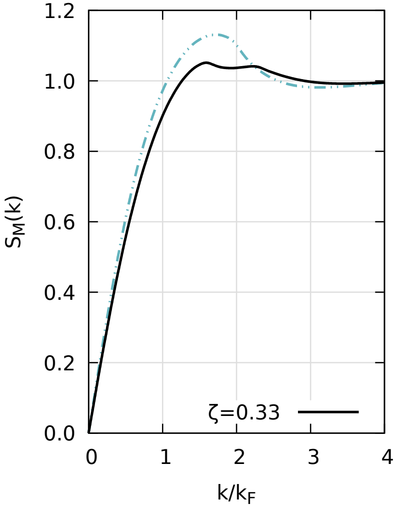

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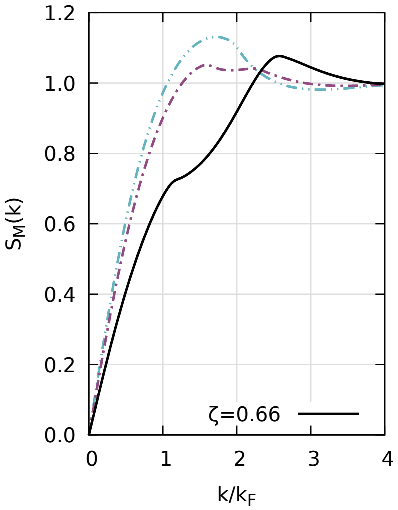

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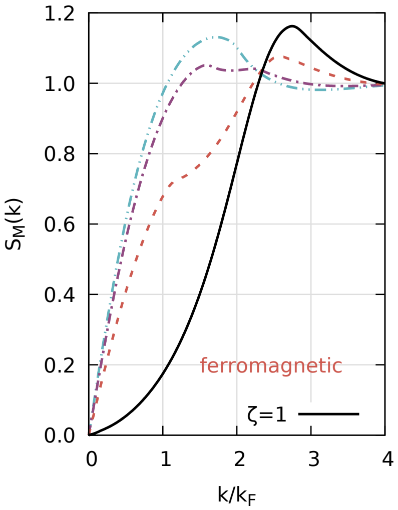

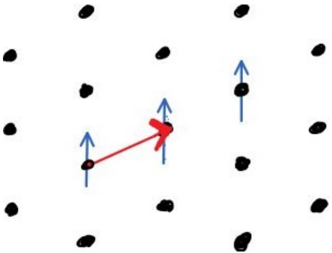

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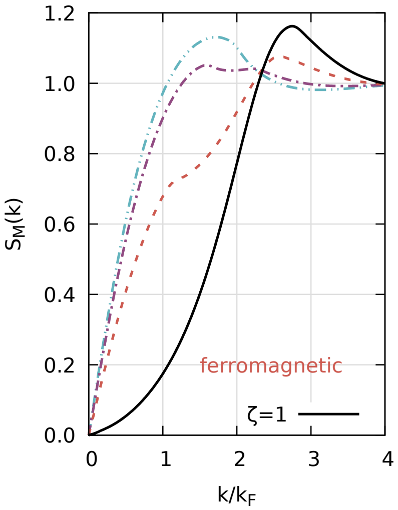

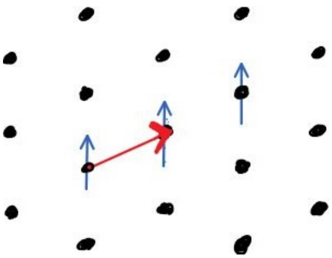

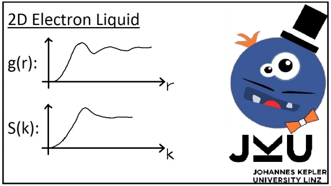

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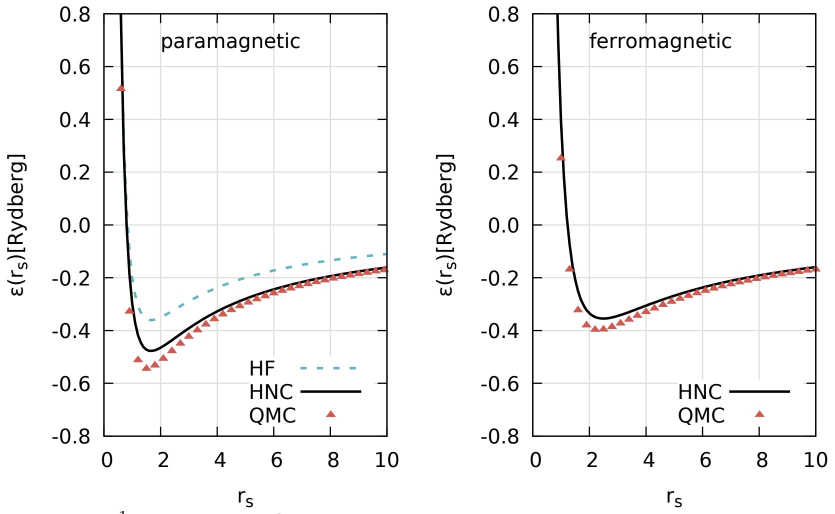

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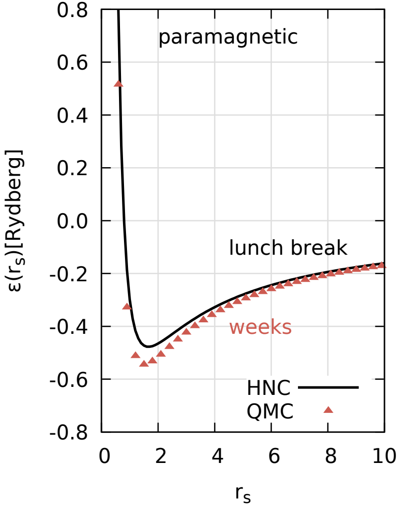

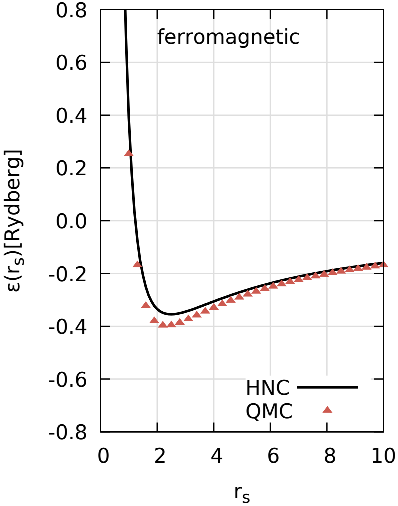

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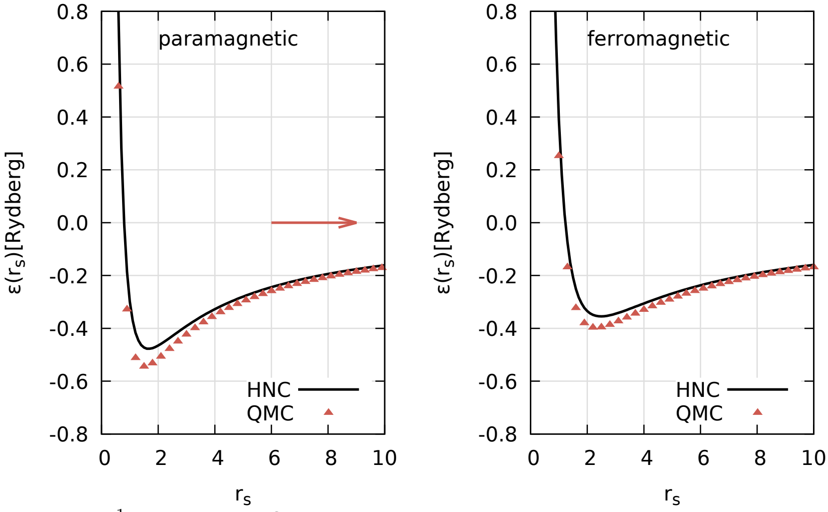

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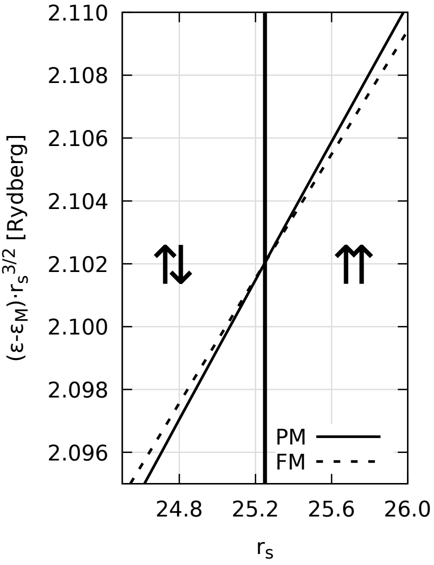
Phase Transition



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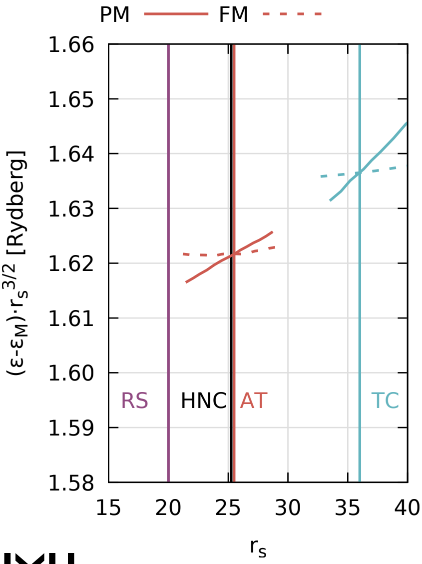

Year	Group	Transition
1978	Ceperley	$r_\mathrm{s} = 13$
1989	Tanatar	$r_\mathrm{s} = 37$
1996	Senatore	$r_\mathrm{s} = 20$
2002	**Attaccalite**	$r_\mathrm{s} = 26$
2009	Drummond	$r_\mathrm{s} = 31$

- Different QMC groups obtain vastly different results!!

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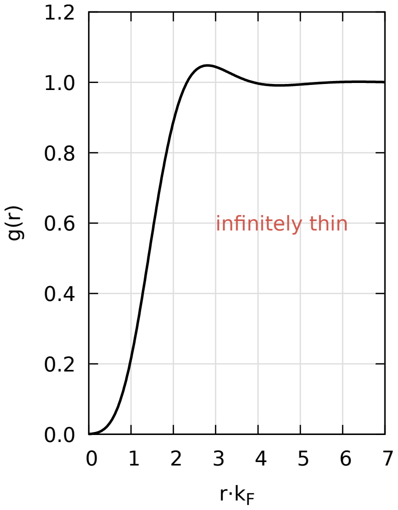
Outlook

- algorithm also applicable to other Fermi systems
- systems with more than two components
- spin-resolved extension to 2D systems with finite thickness
- input for dynamic theories

Thank you!

- **Helga Böhm**
- **Raphael Hobbiger**
- Dominik Kreil
- Jürgen Drachta
- Michaela Haslhofer
- Robert Zillich
- Arthur Ernst
- all members of the ITP

Influence of Finite Thickness ($\zeta = 0$, $r_s = 10$)



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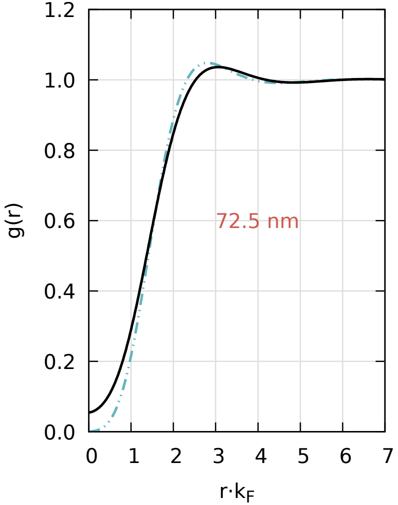

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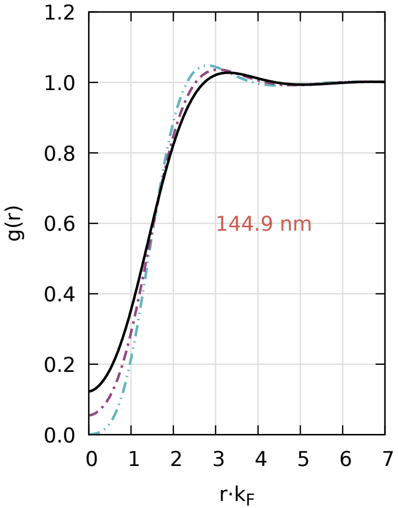

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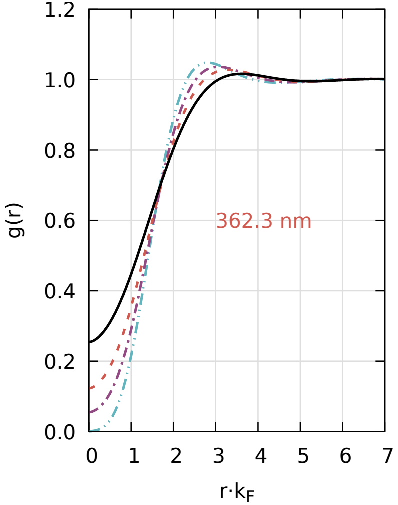

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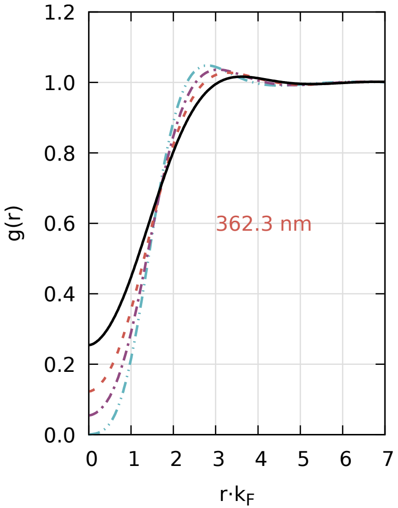

- correlations diminish → peak decreases
- value of $g(0)$ increases
- GaAs/AlGaAs quantum well

Analogies to Statistical Physics

Statistical Physics

- Canonical Ensemble:
  $Z_{\mathrm{N}} = c_{\mathrm{N}} \int d\Gamma \exp(-\beta H)$
- $U = -\frac{\partial}{\partial \beta} \ln Z_{\mathrm{N}}$

HNC

- Normalisation:
  $I = \int dX \exp\left(\sum u_2^{\sigma,\sigma'}\right)$
- $g^{\sigma,\sigma'} = \frac{2}{n_\sigma n_{\sigma'}} \frac{\delta}{\delta u_2^{\sigma,\sigma'}} \ln I$

- excellent summaries available at our institute (Bac Hebenstreit, Kobler, Kurunczi-Papp)
- Mayer Cluster Expansion and Diagrammatics

HNC-Equations

$$g(r) = \exp\left[u_2(r) + N(r) + E(r)\right]$$

$$S(k) = 1 + FT\left[g(r) - 1\right](k)$$

$$\tilde{N}(k) = S(k)\left(1 - \frac{1}{S(k)}\right)^2$$

- What are $u_2(r)$, $E(r)$ and $N(r)$??
- $E(r) := 0 \rightarrow$ HNC/0

Euler-Equation

$$\frac{\delta\left\langle \hat{H} \right\rangle}{\delta u_2(r)} \stackrel{!}{=} 0$$

Euler-Equation

$$\left(\frac{\hbar^2}{m}\right)\Delta\sqrt{g^{\sigma,\sigma'}} = \underbrace{\left(v_{\mathrm{C}} + w_{\mathrm{b}}^{\sigma,\sigma'}\right)}_{\equiv V_{\mathrm{eff}}^{\sigma,\sigma'}}\sqrt{g^{\sigma,\sigma'}}$$

$$\left(\frac{\hbar^2}{m}\right)\Delta\sqrt{g^{\sigma,\sigma'}} = \left[v_{\mathrm{p}}^{\sigma,\sigma'} + \underbrace{\left(v_{\mathrm{C}} + w_{\mathrm{b}}^{\sigma,\sigma'} + w_{\mathrm{e}}^{\sigma,\sigma'}\right)}_{\equiv V_{\mathrm{eff}}^{\sigma,\sigma'}}\right]\sqrt{g^{\sigma,\sigma'}}$$

$$\tilde{w}_{\mathrm{e}}^{\sigma,\sigma'}(k) = -\lim_{r_{\mathrm{s}}\to 0}\tilde{w}_{\mathrm{b}}^{\sigma,\sigma'}(k) = \frac{\hbar^2 k^2}{2m}\left(1 + 2S_{\mathrm{F}}^{\sigma,\sigma'}(k)\right)\left(\frac{S_{\mathrm{F}}^{\sigma,\sigma'}(k) - 1}{S_{\mathrm{F}}^{\sigma,\sigma'}(k)}\right)^2$$

$$v_{\mathrm{p}}^{\sigma,\sigma'}(r) = \frac{\hbar^2}{m}\frac{\Delta\sqrt{g_{\mathrm{F}}^{\sigma,\sigma'}(r)}}{\sqrt{g_{\mathrm{F}}^{\sigma,\sigma'}(r)}}$$

HNC-EL Equations for Bosons

- (bosonic) induced potential

$$\underline{\underline{\tilde{w}}}_{\mathrm{b}}(k) = -\frac{1}{2}\left(\underline{\underline{S}}.\underline{\underline{T}} + \underline{\underline{T}}.\underline{\underline{S}} - 3\underline{\underline{T}} + \underline{\underline{S}}^{-1}.\underline{\underline{T}}.\underline{\underline{S}}^{-1}\right)$$

- particle-hole potential

$$V^{\sigma,\sigma'}(r) = v_{\mathrm{C}}^{\sigma,\sigma'} g^{\sigma,\sigma'} + \frac{\hbar^2}{m}\left|\nabla\sqrt{g^{\sigma,\sigma'}}\right|^2 + \left(g^{\sigma,\sigma'} - 1\right) w_{\mathrm{b}}^{\sigma,\sigma'}$$

- structure factor

$$\underline{\underline{S}}(k) = \sqrt{\underline{\underline{T}}}.\left(2\sqrt{\underline{\underline{T}}}.\underline{\underline{\tilde{V}}}.\sqrt{\underline{\underline{T}}} + \underline{\underline{T}}^2\right)^{-\frac{1}{2}}.\sqrt{\underline{\underline{T}}}$$

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Turning Bosons into Fermions

- include fermionic properties
- solution: alter interaction appropriately!

$$V^{\sigma,\sigma'}(r) = \left[v_{\mathrm{C}}^{\sigma,\sigma'} + v_{\mathrm{p}}^{\sigma,\sigma'} + w_{\mathrm{e}}^{\sigma,\sigma'}\right] g^{\sigma,\sigma'} + \frac{\hbar^2}{m}\left|\nabla\sqrt{g^{\sigma,\sigma'}}\right|^2 + \left(g^{\sigma,\sigma'} - 1\right) w_{\mathrm{b}}^{\sigma,\sigma'}$$

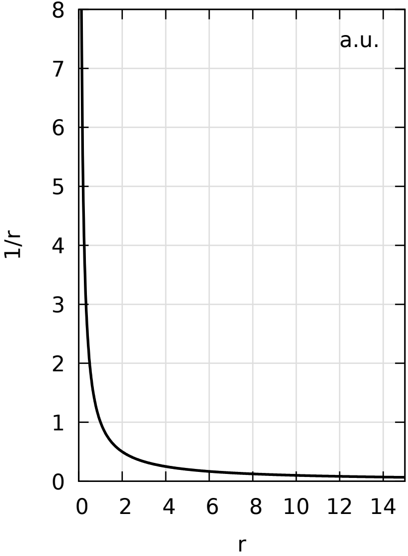
- $v_{\mathrm{p}}^{\sigma,\sigma'}(r)$ and $w_{\mathrm{e}}^{\sigma,\sigma'}(r)$ contain the quantities of the free system ($S_{\mathrm{F}}^{\sigma,\sigma'}(k)$ and $g_{\mathrm{F}}^{\sigma,\sigma'}(r)$) in a way that in the limit of $r_{\mathrm{s}} \to 0$ the solution of the equations is $S_{\mathrm{F}}^{\sigma,\sigma'}(k)$ and $g_{\mathrm{F}}^{\sigma,\sigma'}(r)$
- **feasible solution from a physical point of view**
- Solve the equations!

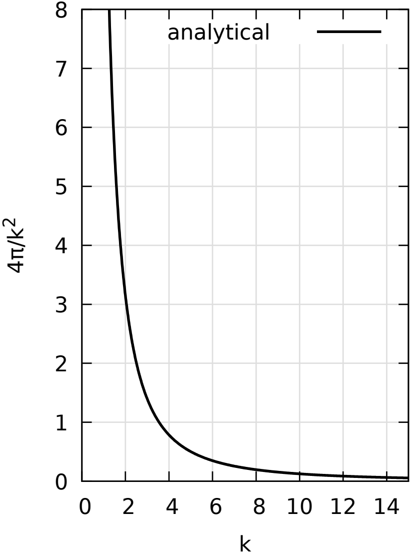
Pair Distribution Function (Full Form)

$$g(r) = \left(\frac{1+\zeta}{2}\right)^2 g^{\uparrow\uparrow}(r) + \left(\frac{1-\zeta}{2}\right)^2 g^{\downarrow\downarrow}(r) + \frac{1-\zeta^2}{2} g^{\uparrow\downarrow}(r)$$

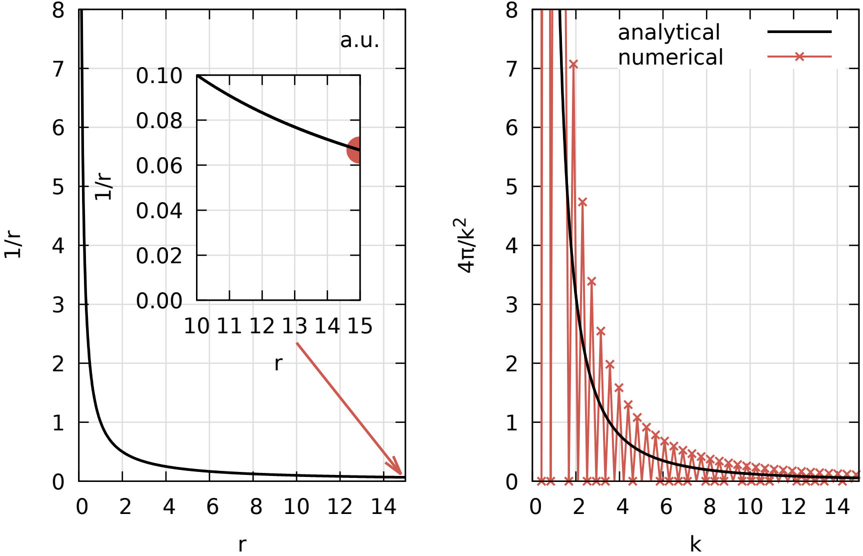
$$g_{\mathrm{M}}(r) = \left(\frac{1+\zeta}{2}\right)^2 g^{\uparrow\uparrow}(r) + \left(\frac{1-\zeta}{2}\right)^2 g^{\downarrow\downarrow}(r) - \frac{1-\zeta^2}{2} g^{\uparrow\downarrow}(r)$$

Analytical FT





Numerical FT



Calculating Thermodynamic Observables

$$\varepsilon(r_\mathrm{s},\zeta) = \varepsilon_0(r_\mathrm{s},\zeta) + \frac{1}{r_\mathrm{s}^2}\int\limits_0^{r_\mathrm{s}} dr'_\mathrm{s}\; r'_\mathrm{s} u(r'_\mathrm{s})$$

$$\left\langle \frac{V}{N} \right\rangle \equiv u(r_\mathrm{s}) = \frac{1}{2N}\sum_{\mathbf{k}\neq 0} \tilde{v}_\mathrm{C}(k;r_\mathrm{s})\left[S(k;r_\mathrm{s})-1\right]$$

$$p = -\left.\frac{\partial E}{\partial V}\right|_{T,N} = n^2 \left.\frac{\partial \varepsilon}{\partial n}\right|_{T,N}, \qquad \varepsilon = E/N$$

$$\frac{1}{\kappa} = -V\left.\frac{\partial p}{\partial V}\right|_{T,N} = -\frac{r_\mathrm{s}}{4}\frac{\partial \varepsilon}{\partial r_\mathrm{s}} + \frac{r_\mathrm{s}^2}{4}\frac{\partial^2 \varepsilon}{\partial r_\mathrm{s}^2}$$

Contributions to the Energy

$$\varepsilon(r_\mathrm{s},\zeta) = \varepsilon_0(r_\mathrm{s},\zeta) + \varepsilon_\mathrm{x}(r_\mathrm{s},\zeta) + \varepsilon_\mathrm{c}(r_\mathrm{s},\zeta)$$

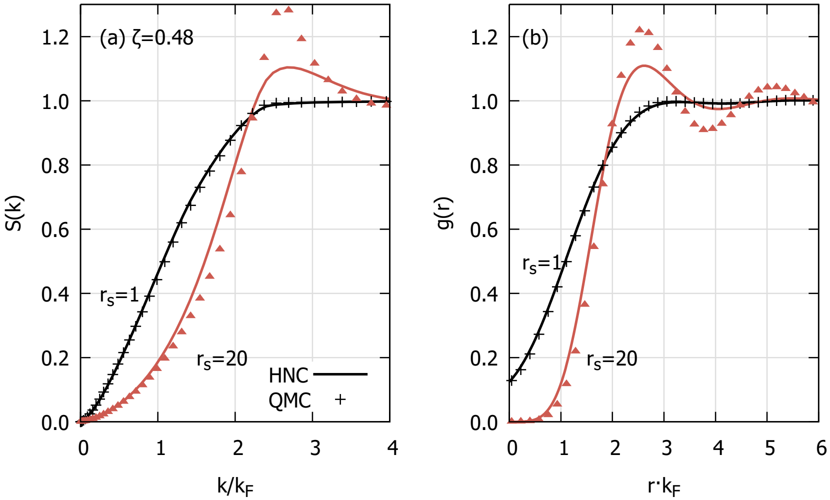
$$\varepsilon_0(r_\mathrm{s},\zeta) = \varepsilon_0(r_\mathrm{s})\,\frac{(1+\zeta)^{\frac{D+2}{D}} + (1-\zeta)^{\frac{D+2}{D}}}{2}\,, \quad \varepsilon_0(r_\mathrm{s}) = D\varepsilon_\mathrm{F}/(D{+}2)$$

$$\varepsilon_\mathrm{x}(r_\mathrm{s},\zeta) = \varepsilon_\mathrm{x}(r_\mathrm{s})\,\frac{(1+\zeta)^{\frac{D+1}{D}} + (1-\zeta)^{\frac{D+1}{D}}}{2}$$

$$\varepsilon_\mathrm{x}(r_\mathrm{s}) = -\frac{4}{3}\frac{e^2k_\mathrm{F}}{\pi} = -\frac{8\sqrt{2}}{3\pi r_\mathrm{s}}\varepsilon_\mathrm{R} \quad \text{in 2D}$$

$$\varepsilon_\mathrm{x}(r_\mathrm{s}) = -\frac{3}{4}\frac{e^2k_\mathrm{F}}{\pi} = -\frac{3}{2\pi\alpha r_\mathrm{s}}\varepsilon_\mathrm{R} \quad \text{in 3D}$$

Comparison with QMC[1]



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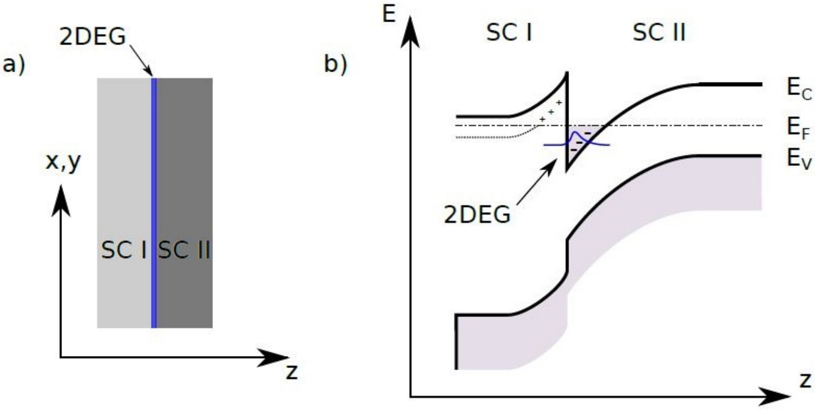
2D Electron System in a Semiconductor[1]



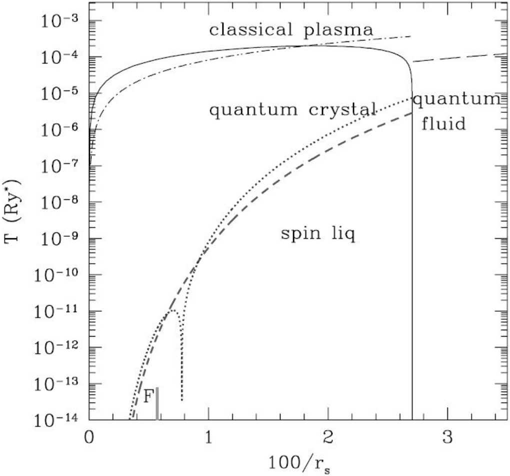
[1] J. T. Drachta Plasmon Properties in dilute, two dimensional Electron Liquids

Real Units[1]

	r_S	r_S	GaAs/AlGaAs 1	10	20
$n[\mathrm{cm}^{-2}]$	$\frac{1.14\times10^{16}}{r_S{}^2}\left(\frac{\bar{m}_b}{\varepsilon_b}\right)^2$	$\frac{3.02\times10^{11}}{r_S^2}$	3.02×10^{11}	3.02×10^{9}	7.55×10^{8}
$k_F[10^5\,\mathrm{cm}^{-1}]$	$\frac{2673}{r_S}\frac{\bar{m}_b}{\varepsilon_b}$	$\frac{13.78}{r_S}$	13.78	1.38	0.69
$E_F[\mathrm{meV}]$	$\frac{27230}{r_S^2}\frac{\bar{m}_b}{\varepsilon_b^2}$	$\frac{10.80}{r_S^2}$	10.80	0.11	2.7×10^{-2}

[1] J. T. Drachta Plasmon Properties in dilute, two dimensional Electron Liquids

Phase Diagram[1]



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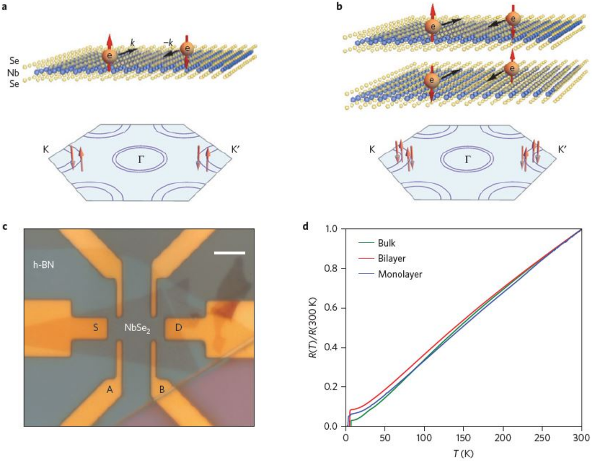
Superconductivity[1]



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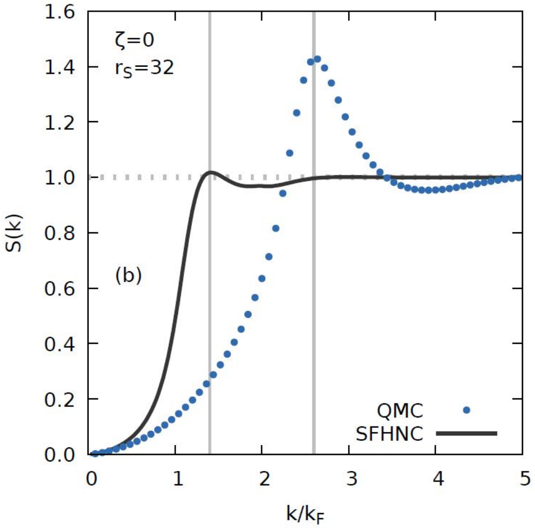
SFHNC vs. QMC[1]



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