THEORETICAL PHYSICS

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

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INTRODUCTION AND MOTIVATION
System

- many particle system ⇒ no analytic solution
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- consisting of electrons $\Rightarrow$ Pauli principle
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Importance of 2D Electron Systems

- electronics and semiconductor heterostructures
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- applications in spintronics
Characterisation

Wigner-Seitz Radius $r_s$

$r_s \cdot a_B$ is the radius of a circle occupied by one electron

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

- $\zeta = 0 \rightarrow$ paramagnetic
- $\zeta = 1 \rightarrow$ ferromagnetic
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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 $\frac{d\sigma}{d\Omega} \propto S(k)$

2D Electron Liquid

<table>
<thead>
<tr>
<th>$g(r)$:</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>$S(k)$:</td>
<td></td>
</tr>
</tbody>
</table>

Fourier-Transform

$$S(k) = 1 + \text{FT}_{2D}[g - 1](k)$$
Spin-Resolved Treatment

- treat subsystems of spins independently
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$$g(r) = c_1 g^{↑↑}(r) + c_2 g^{↓↓}(r) + c_3 g^{↑↓}(r)$$

- $c_i \ldots$ constants
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- \( c_i \ldots \) constants

- results in matrix form (intuitive)
  \[
  g(r) = \begin{pmatrix}
  g^{\uparrow\uparrow}(r) & g^{\uparrow\downarrow}(r) \\
  g^{\downarrow\uparrow}(r) & g^{\downarrow\downarrow}(r)
  \end{pmatrix}
  \]
Spin-Resolved Treatment

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  \[ g(r) = \begin{pmatrix} g^{\uparrow\uparrow}(r) & g^{\uparrow\downarrow}(r) \\ g^{\downarrow\uparrow}(r) & g^{\downarrow\downarrow}(r) \end{pmatrix} \]
- advantage: further properties accessible
  \[ g_M(r) = c_1 g^{\uparrow\uparrow}(r) + c_2 g^{\downarrow\downarrow}(r) - c_3 g^{\uparrow\downarrow}(r) \]
Spin-Resolved Treatment

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\[ g(r) = c_1 \ g^{\uparrow\uparrow}(r) + c_2 \ g^{\uparrow\downarrow}(r) + c_3 \ g^{\uparrow\downarrow}(r) \]

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■ advantage: further properties accessible

⇒ \( g_M(r) = c_1 \ g^{↑↑}(r) + c_2 \ g^{↓↓}(r) - c_3 \ g^{↑↓}(r) \)

■ similar for \( S(k) \) and \( S_M(k) \)
How can $g(r)$ and $S(k)$ 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
How can \( g(r) \) and \( S(k) \) be calculated?

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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 (\( r_s = 0.1 \ldots 10 \), \( \Delta r_s = 0.1 \)) on an average laptop
   - results in agreement with QMC (!)
Energy Comparison with the Literature

HYPER-NETTED-CHAIN THEORY
Ansatz

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

**Jastrow Ansatz**

\[ \psi = \prod_{\sigma, \sigma'} \prod'_{i<j} f(\mathbf{r}_{\sigma, i}, \mathbf{r}_{\sigma', j}) := \exp \frac{1}{4} \left\{ \sum_{\sigma, \sigma'} \sum'_{i, j} u_{2, \sigma', \sigma}(\mathbf{r}_{\sigma, i}, \mathbf{r}_{\sigma', j}) \right\} \]

- includes two-body correlations \( u_{2, \sigma', \sigma} \)
Ansatz

- Ansatz with Bose (!) symmetry

**Jastrow Ansatz**

\[
\psi = \prod_{\sigma, \sigma'} \prod'_{i<j} f(r_{\sigma, i}, r_{\sigma', j}) := \exp \left\{ \frac{1}{4} \sum_{\sigma, \sigma'} \sum'_{i, j} u_{2, \sigma, \sigma'}(r_{\sigma, i}, r_{\sigma', j}) \right\}
\]

- 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

\[ V^\sigma,\sigma'(r) = \left[ \psi_0^\sigma,\sigma' \right] g^\sigma,\sigma' + \frac{\hbar^2}{m} \left| \nabla \sqrt{g^\sigma,\sigma'} \right|^2 + \left( g^\sigma,\sigma' - 1 \right) w_b^\sigma,\sigma' \]
Fermionic HNC (Kallio (1996), Davoudi)

\[ V^{\sigma,\sigma'}(r) = \left[ v^{\sigma,\sigma'}_C + V_e^{\sigma,\sigma'} \right] g^{\sigma,\sigma'} + \frac{\hbar^2}{m} \left| \nabla \sqrt{g^{\sigma,\sigma'}} \right|^2 + \left( g^{\sigma,\sigma'} - 1 \right) w^{\sigma,\sigma'}_b \]
RESULTS
$g(r)$ & effective interaction (paramagnetic)
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Shift of the Peak in $S_M(k)$ (dilute system)
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Energy Comparison with the Literature\textsuperscript{1}

\begin{figure}
\centering
\begin{minipage}{0.45\textwidth}
\centering
\begin{tikzpicture}
\begin{semilogyaxis}[
    width=\textwidth,
    height=0.8\textwidth,
    xlabel={$r_s$},
    ylabel={$\epsilon(r_s) \text{[Rydberg]}$},
    xmin=0, xmax=10,
    ymin=-0.8, ymax=0.8,
    xtick={0,2,4,6,8,10},
    ytick={-0.8,-0.6,-0.4,-0.2,0.0,0.2,0.4,0.6,0.8},
    legend pos=south west,
]
\addlegendentry{HF}
\addlegendentry{HNC}
\addlegendentry{QMC}
\addplot[blue,mark=triangle] table [x=r_s, y=HF] {data.csv};
\addplot[red] table [x=r_s, y=HNC] {data.csv};
\addplot[black] table [x=r_s, y=QMC] {data.csv};
\end{semilogxaxis}
\end{tikzpicture}
\caption{Paramagnetic Energy Comparison}
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\addlegendentry{HNC}
\addlegendentry{QMC}
\addplot[blue,mark=triangle] table [x=r_s, y=HNC] {data.csv};
\addplot[black] table [x=r_s, y=QMC] {data.csv};
\end{semilogxaxis}
\end{tikzpicture}
\caption{Ferromagnetic Energy Comparison}
\end{minipage}
\end{figure}

Energy Comparison with the Literature\textsuperscript{1}

\begin{figure}
\centering
\includegraphics[width=\textwidth]{energy_comparison.png}
\caption{Comparison of correlation energy $\epsilon(r_s)$ in Rydberg for paramagnetic and ferromagnetic states.}
\end{figure}

\begin{itemize}
\item Paramagnetic state:
- HNC:
- QMC:
\item Ferromagnetic state:
- HNC:
- QMC:
\end{itemize}

Energy Comparison with the Literature

\[ \varepsilon(r_s) \text{[Rydberg]} \]

\( r_s \)

HNC
QMC

\[ \varepsilon(r_s) \text{[Rydberg]} \]

\( r_s \)

HNC
QMC

Phase Transition

\[(\varepsilon - \varepsilon_M) \cdot r_s^{3/2} \text{ [Rydberg]}\]

\[r_s\]

PM

FM

\[24.8 \quad 25.2 \quad 25.6 \quad 26.0\]
Different QMC groups obtain vastly different results!!
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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Influence of Finite Thickness ($\zeta = 0$, $r_s = 10$)

\begin{align*}
g(r) &= r \cdot k_F
\end{align*}

$144.9 \text{ nm}$
Influence of Finite Thickness ($\zeta = 0$, $r_s = 10$)

![Graph showing influence of finite thickness with $g(r)$ vs. $r \cdot k_F$]

- Correlations diminish → peak decreases
- Value of $g(0)$ increases
- GaAs/AlGaAs quantum well
Influence of Finite Thickness ($\zeta = 0$, $r_s = 10$)

- Correlations diminish $\rightarrow$ peak decreases
- Value of $g(0)$ increases
- GaAs/AlGaAs quantum well

$g(r)$ vs. $r \cdot k_F$

362.3 nm
Analogies to Statistical Physics

Statistical Physics

- Canonical Ensemble:
  \[ Z_N = c_N \int d\Gamma \exp(-\beta H) \]

- \[ U = -\frac{\partial}{\partial \beta} \ln Z_N \]

- excellent summaries available at our institute (Bac Hebenstreit, Kobler, Kurunczi-Papp)

- Mayer Cluster Expansion and Diagrammatics

HNC

- Normalisation:
  \[ I = \int dX \exp \left( \sum u_{\sigma,\sigma'}^{\sigma,\sigma'} \right) \]

- \[ g_{\sigma,\sigma'} = \frac{2}{n_{\sigma} n_{\sigma'}} \frac{\delta}{\delta u_{\sigma,\sigma'}^{\sigma,\sigma'}} \ln I \]
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 \( N(r) \)?

\[ E(r) := 0 \rightarrow \text{HNC/0} \]

**Euler-Equation**

\[ \frac{\delta \langle \hat{H} \rangle}{\delta u_2(r)} = 0 \]
Euler-Equation

\[
\left( \frac{\hbar^2}{m} \right) \Delta \sqrt{g^{\sigma,\sigma'}} = \left( v_C + w_b^{\sigma,\sigma'} \right) \sqrt{g^{\sigma,\sigma'}} \\
\equiv V_{\text{eff}}^{\sigma,\sigma'}
\]

\[
\left( \frac{\hbar^2}{m} \right) \Delta \sqrt{g^{\sigma,\sigma'}} = \left[ v_p^{\sigma,\sigma'} + \left( v_C + w_b^{\sigma,\sigma'} + w_e^{\sigma,\sigma'} \right) \right] \sqrt{g^{\sigma,\sigma'}} \\
\equiv V_{\text{eff}}^{\sigma,\sigma'}
\]

\[
\tilde{w}_e^{\sigma,\sigma'}(k) = - \lim_{r_s \to 0} \tilde{w}_b^{\sigma,\sigma'}(k) = \frac{\hbar^2 k^2}{2m} \left( 1 + 2 S_F^{\sigma,\sigma'}(k) \right) \left( \frac{S_F^{\sigma,\sigma'}(k) - 1}{S_F^{\sigma,\sigma'}(k)} \right)^2
\]

\[
v_p^{\sigma,\sigma'}(r) = \frac{\hbar^2}{m} \frac{\Delta \sqrt{g_F^{\sigma,\sigma'}(r)}}{\sqrt{g_F^{\sigma,\sigma'}(r)}}
\]
HNC-EL Equations for Bosons

■ (bosonic) induced potential

\[ \tilde{w}_b(k) = -\frac{1}{2} \left( S \cdot T + T \cdot S - 3T + S^{-1} \cdot T \cdot S^{-1} \right) \]

■ particle-hole potential

\[ V^{\sigma,\sigma'}(r) = v_C^{\sigma,\sigma'} g^{\sigma,\sigma'} + \frac{\hbar^2}{m} \left| \nabla \sqrt{g^{\sigma,\sigma'}} \right|^2 + \left( g^{\sigma,\sigma'} - 1 \right) w_b^{\sigma,\sigma'} \]

■ structure factor

\[ S(k) = \sqrt{T} \cdot \left( 2 \sqrt{T} \cdot \tilde{V} \cdot \sqrt{T} + T^2 \right)^{-\frac{1}{2}} \cdot \sqrt{T} \]
Turning Bosons into Fermions

- include fermionic properties
- solution: alter interaction appropriately!

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

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

\[ g(r) = \left( \frac{1 + \zeta}{2} \right)^2 g_{↑↑}(r) + \left( \frac{1 - \zeta}{2} \right)^2 g_{↓↓}(r) + \frac{1 - \zeta^2}{2} g_{↑↓}(r) \]

\[ g_M(r) = \left( \frac{1 + \zeta}{2} \right)^2 g_{↑↑}(r) + \left( \frac{1 - \zeta}{2} \right)^2 g_{↓↓}(r) - \frac{1 - \zeta^2}{2} g_{↑↓}(r) \]
Analytical FT

1/r vs. r

4π/k² vs. k

a.u.
Numerical FT

![Graph showing numerical and analytical FT comparison]

- **Graph Description:**
  - The graph compares numerical and analytical Fourier transforms (FTs).
  - The x-axis represents the variable $r$, ranging from 0 to 15.
  - The y-axis represents $1/r$, ranging from 0 to 8.
  - The inset graph shows $4\pi/k^2$ on the y-axis and $k$ on the x-axis, ranging from 0 to 15.
  - The numerical results are indicated by red crosses, while the analytical results are shown as a black line.

![Inset Graph showing $4\pi/k^2$ vs $k$]

- **Inset Graph Details:**
  - The inset graph illustrates the behavior of $4\pi/k^2$ as $k$ varies.
  - The graph is scaled to show the relationship between $4\pi/k^2$ and $k$ over the specified range.
Calculating Thermodynamic Observables

\[ \varepsilon(r_s, \zeta) = \varepsilon_0(r_s, \zeta) + \frac{1}{r_s^2} \int_0^{r_s} dr'_s \ r'_s u(r'_s) \]

\[ \left\langle \frac{V}{N} \right\rangle \equiv u(r_s) = \frac{1}{2N} \sum_{k \neq 0} \tilde{v}_C(k; r_s) [S(k; r_s) - 1] \]

\[ p = - \left. \frac{\partial E}{\partial V} \right|_{T,N} = n^2 \left. \frac{\partial \varepsilon}{\partial n} \right|_{T,N}, \quad \varepsilon = \frac{E}{N} \]

\[ \frac{1}{\kappa} = -V \left. \frac{\partial p}{\partial V} \right|_{T,N} = -\frac{r_s}{4} \left. \frac{\partial \varepsilon}{\partial r_s} \right| + \frac{r_s^2}{4} \left. \frac{\partial^2 \varepsilon}{\partial r_s^2} \right| \]
Contributions to the Energy

\[ \varepsilon(r_s, \zeta) = \varepsilon_0(r_s, \zeta) + \varepsilon_x(r_s, \zeta) + \varepsilon_c(r_s, \zeta) \]

\[ \varepsilon_0(r_s, \zeta) = \varepsilon_0(r_s) \left( \frac{1 + \zeta}{D} \right) \frac{D+2}{2} + \frac{(1 - \zeta) D+2}{D} , \quad \varepsilon_0(r_s) = D \varepsilon_F/(D+2) \]

\[ \varepsilon_x(r_s, \zeta) = \varepsilon_x(r_s) \left( \frac{1 + \zeta}{D} \right) \frac{D+1}{2} + \frac{(1 - \zeta) D+1}{D} \]

\[ \varepsilon_x(r_s) = -\frac{4}{3} \frac{e^2 k_F}{\pi} = -\frac{8\sqrt{2}}{3\pi r_s} \varepsilon_R \quad \text{in 2D} \]

\[ \varepsilon_x(r_s) = -\frac{3}{4} \frac{e^2 k_F}{\pi} = -\frac{3}{2\pi \alpha r_s} \varepsilon_R \quad \text{in 3D} \]
Comparison with QMC

(a) $\zeta=0.48$

$S(k)$

$b$ $g(r)$

$0.0$ $0.2$ $0.4$ $0.6$ $0.8$ $1.0$ $1.2$

$0$ $1$ $2$ $3$ $4$

$\frac{k}{k_F}$

$HNC$ $QMC$

$b$ $r_s=20$

$g(r)$

$b$ $r_s=20$

$0.0$ $0.2$ $0.4$ $0.6$ $0.8$ $1.0$ $1.2$

$0$ $1$ $2$ $3$ $4$ $5$ $6$

$\frac{r}{k_F}$

$1$ $C. P. Gori-Giorgi, S. Moroni and G. B. Bachelet.

2D Electron System in a Semiconductor

1 J. T. Drachta Plasmon Properties in dilute, two dimensional Electron Liquids
Real Units

<table>
<thead>
<tr>
<th></th>
<th>$\tilde{\gamma}$</th>
<th>$\gamma$</th>
<th>GaAs/AlGaAs</th>
</tr>
</thead>
<tbody>
<tr>
<td>$n$ [cm$^{-2}$]</td>
<td>$\frac{1.14 \times 10^{16}}{\gamma^2} \left( \frac{\tilde{m}_b}{\varepsilon_b} \right)^2$</td>
<td>$\frac{3.02 \times 10^{11}}{\gamma^2}$</td>
<td>$3.02 \times 10^{11}$</td>
</tr>
<tr>
<td>$k_F$ [10$^5$ cm$^{-1}$]</td>
<td>$\frac{2673 \tilde{m}_b}{\gamma \varepsilon_b}$</td>
<td>$13.78 \gamma$</td>
<td>13.78</td>
</tr>
<tr>
<td>$E_F$ [meV]</td>
<td>$\frac{27230 \tilde{m}_b}{\gamma^2 \varepsilon_b^2}$</td>
<td>$\frac{10.80}{\gamma^2}$</td>
<td>10.80</td>
</tr>
</tbody>
</table>

$^1$J. T. Drachta Plasmon Properties in dilute, two dimensional Electron Liquids
Phase Diagram\textsuperscript{1}

Superconductivity \(^1\)

SFHNC vs. QMC$^1$

$\zeta=0$
$r_s=32$

$S(k)$

$k/k_F$

$QMC$
$SFHNC$

$^1$R. A. Hobbiger, Ground state and excitations of two-dimensional electron liquids, PHD Thesis