The electron gas in two and three dimensions

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Outline

Motivation

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Setting up the system

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Setting up the system

What could we do?

- The first study of the 2D electron gas with SRG, FCIQMC, and CC
- How well can the methods describe correlations?
- At what densities do SRG and CC break down?
- Theoretical explanation of breakdown?
- Ring and ladder approximations vs. CCD

What could we do?

- What are differences between finite and periodic systems? (QD vs. 2DEG)
- Compare 2D with finite thickness 2D+1D (or 3D?)
- Virial theorem (Jørgen's thesis)?
- More ideas?

Books

- Basics: Fetter and Walecka, Quantum theory of many-particle systems
- E-book: G. Giuliani and G. Vignale, Quantum theory of the electron liquid (library will buy it)

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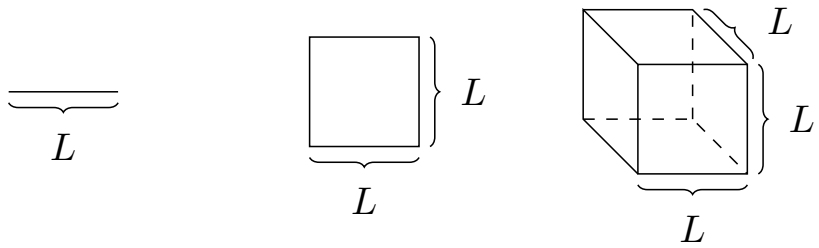
The two-dimensional electron gas



- Interacting electrons in a quadratic box
- Homogeneous system (constant density)
- Constant positive background charge

Single-particle states

One electron in a quadratic box:

$$-\frac{\hbar^2}{2m}\nabla^2\varphi(\mathbf{x}) = \varepsilon\varphi(\mathbf{x}) \tag{1}$$

Solutions:

$$\varphi_{\mathbf{k}}(\mathbf{x}) = \frac{1}{\sqrt{A}}\exp(i\mathbf{k}\cdot\mathbf{x}) \tag{2}$$

Single-particle states

Periodic boundary conditions

$$\varphi_{\mathbf{k}}(x + L, y) = \varphi_{\mathbf{k}}(x, y)$$
$$\varphi_{\mathbf{k}}(x, y + L) = \varphi_{\mathbf{k}}(x, y) \tag{3}$$

gives

$$\mathbf{k} = \frac{2\pi}{L}(n_x, n_y),$$
$$n_x, n_y \in \{0, \pm 1, \pm 2, \dots\}. \tag{4}$$

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Single-particle energies:

$$\varepsilon_{n_x, n_y} = \frac{\hbar^2 k^2}{2m}$$
$$= \frac{\hbar^2}{2m}\left(\frac{2\pi}{L}\right)^2 (n_x^2 + n_y^2) \tag{5}$$

Hamiltonian operator

$$\hat{H} = \hat{H}_0 + \hat{H}_I + \hat{H}_{bb} + \hat{H}_{eb}$$

$$\hat{H}_0 = \sum_{i=1}^{N} -\frac{\hbar^2 \nabla_i^2}{2m}$$

$$\hat{H}_I = \frac{1}{2} e^2 \sum_{i<j}^{N} \frac{e^{-\mu|\mathbf{r}_i - \mathbf{r}_j|}}{|\mathbf{r}_i - \mathbf{r}_j|}$$

$$\hat{H}_{bb} = \frac{1}{2} e^2 \int d\mathbf{r} \int d\mathbf{r}' \rho(\mathbf{r}) \rho(\mathbf{r}') \frac{e^{-\mu|\mathbf{r} - \mathbf{r}'|}}{|\mathbf{r} - \mathbf{r}'|}$$

$$\hat{H}_{eb} = -e^2 \sum_{i=1}^{N} \int d\mathbf{r} \rho(\mathbf{r}) \frac{e^{-\mu|\mathbf{r} - \mathbf{r}_i|}}{|\mathbf{r} - \mathbf{r}_i|}$$

$$\rho(\mathbf{r}) = \text{particle density} = N/A$$

Hamiltonian operator

Can be shown (see Fetter and Walecka for 3D):

$$\hat{H} = \hat{H}_0 + \hat{H}_I - \frac{\pi e^2 N^2}{A\mu} \tag{6}$$

The $\mathbf{q} = 0$ terms in the interaction operator give

$$\frac{\pi e^2}{A\mu}(N^2 - N) \tag{7}$$

Let first $A \to \infty$ and then $\mu \to 0$

Interaction matrix elements

- Fetter and Walecka
- Hamaguchi: Basic Semiconductor Physics (e-book)

$$
\begin{aligned}
&\langle \mathbf{k}_1 m_{s_1} \mathbf{k}_2 m_{s_2} | v | \mathbf{k}_3 m_{s_3} \mathbf{k}_4 m_{s_4} \rangle \\
=&\frac{e^2}{A^2} \int d\mathbf{r}_1 \int d\mathbf{r}_2 e^{-i\mathbf{k}_1 \cdot \mathbf{r}_1} e^{-i\mathbf{k}_2 \cdot \mathbf{r}_2} \frac{e^{-\mu |\mathbf{r}_1 - \mathbf{r}_2|}}{|\mathbf{r}_1 - \mathbf{r}_2|} e^{i\mathbf{k}_3 \cdot \mathbf{r}_1} e^{i\mathbf{k}_4 \cdot \mathbf{r}_2} \\
&\times \langle m_{s_1} | m_{s_3} \rangle \langle m_{s_2} | m_{s_4} \rangle \\
=&\ldots \\
=&\frac{e^2}{A} \delta_{m_{s_1} m_{s_3}} \delta_{m_{s_2} m_{s_4}} \delta_{\mathbf{k}_1 + \mathbf{k}_2, \mathbf{k}_3 + \mathbf{k}_4} \int d\mathbf{r} e^{i(\mathbf{k}_3 - \mathbf{k}_1) \cdot \mathbf{r}} \frac{e^{-\mu r}}{r}
\end{aligned}
$$

Interaction matrix elements

From Abramowitz:

$$\int_0^{2\pi} e^{ipr\cos\phi} = 2\pi J_0(pr) \tag{8}$$

$$J_0(x) = \text{Bessel function of first kind}$$

From Gradshteyn and Ryzhik:

$$\int_0^{\infty} dr e^{-\mu r} J_0(pr) = \frac{1}{\sqrt{\mu^2 + p^2}} \tag{9}$$

Antisymmetrized matrix elements

$$
\begin{aligned}
&\left\langle \mathbf{k}_1 m_{s_1} \mathbf{k}_2 m_{s_2} \middle| v \middle| \mathbf{k}_3 m_{s_3} \mathbf{k}_4 m_{s_4} \right\rangle_{AS} \\
=&\frac{e^2}{A}\delta_{\mathbf{k}_1+\mathbf{k}_2,\mathbf{k}_3+\mathbf{k}_4}\left\{\delta_{m_{s_1}m_{s_3}}\delta_{m_{s_2}m_{s_4}}(1-\delta_{\mathbf{k}_1\mathbf{k}_3})\frac{2\pi}{\sqrt{\mu^2+|\mathbf{k}_3-\mathbf{k}_1|^2}}\right. \\
&\left.-\delta_{m_{s_1}m_{s_4}}\delta_{m_{s_2}m_{s_3}}(1-\delta_{\mathbf{k}_1\mathbf{k}_4})\frac{2\pi}{\sqrt{\mu^2+|\mathbf{k}_4-\mathbf{k}_1|^2}}\right\}
\end{aligned}
$$

- Atomic units: $\hbar = m = e = 1$
- Classical electron radius: $N\pi r_s^2 = A$
- N and r_s input parameters
- Quantum numbers: (n_x, n_y, m_s)

Orbitals

$n_x^2 + n_y^2$	n_x	n_y	$N_{\uparrow\downarrow}$	$N_{\uparrow\uparrow}$
0	0	0	2	1
1	-1	0		
	1	0		
	0	-1		
	0	1	10	5
2	-1	-1		
	-1	1		
	1	-1		
	1	1	18	9
4	-2	0		
	2	0		
	0	-2		
	0	2	26	13
5	-2	-1		
	2	-1		
	-2	1		
	2	1		
	-1	-2		
	-1	2		
	1	-2		
	1	2	42	21

The three-dimensional electron gas

Single-particle energies:

$$\varepsilon_{n_x,n_y,n_z} = \frac{\hbar^2}{2m}\left(\frac{2\pi}{L}\right)^2 (n_x^2 + n_y^2 + n_z^2)$$

Antisymmetrized interaction matrix elements:

$$\begin{aligned}
&\langle \mathbf{k}_1 m_{s_1} \mathbf{k}_2 m_{s_2} | v | \mathbf{k}_3 m_{s_3} \mathbf{k}_4 m_{s_4} \rangle_{AS} \\
=&\frac{e^2}{V}\delta_{\mathbf{k}_1+\mathbf{k}_2,\mathbf{k}_3+\mathbf{k}_4}\left\{\delta_{m_{s_1}m_{s_3}}\delta_{m_{s_2}m_{s_4}}(1-\delta_{\mathbf{k}_1\mathbf{k}_3})\frac{4\pi}{\mu^2+(\mathbf{k}_3-\mathbf{k}_1)^2}\right. \\
&\left.-\delta_{m_{s_1}m_{s_4}}\delta_{m_{s_2}m_{s_3}}(1-\delta_{\mathbf{k}_1\mathbf{k}_4})\frac{4\pi}{\mu^2+(\mathbf{k}_4-\mathbf{k}_1)^2}\right\}
\end{aligned}$$