Symmetry breaking in the Hartree-Fock jellium

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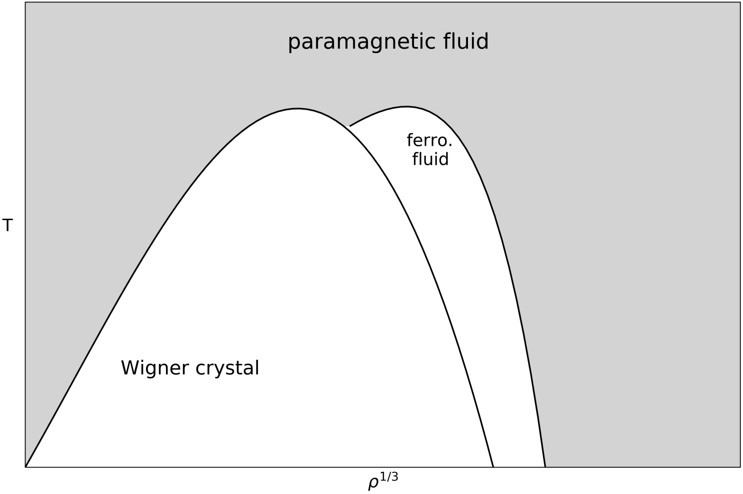
joint work with Mathieu Lewin and Christian Hainzl

Introduction: Expected phase diagram for the 3d jellium

From Jones, Ceperley, PRL 76 (1996) and Zing, Lin, Ceperley, Phys. Rev. E 66 (2002).



Hartree-Fock jellium

= Electrons in uniform positive background, described with Hartree-Fock.

States = one-body density matrices: $\gamma \in \mathcal{S}(L^2(\Omega, \mathbb{C}^2))$, $0 \le \gamma \le 1$. We write $\gamma = \begin{pmatrix} \gamma^{\uparrow\uparrow} & \gamma^{\uparrow\downarrow} \\ \gamma^{\downarrow\uparrow} & \gamma^{\downarrow\downarrow} \end{pmatrix}$.

Energy:
$$\mathcal{E}^{\rm HF}(\gamma, \rho, T) = \frac{1}{2}\mathrm{Tr}\,(-\Delta\gamma) + \frac{1}{2}\iint_{\Omega^2} \frac{(\rho_\gamma(\mathbf{r}) - \rho)(\rho_\gamma(\mathbf{r}') - \rho)}{|\mathbf{r} - \mathbf{r}'|}\mathrm{d}\mathbf{r}\,\mathrm{d}\mathbf{r}' \\ - \frac{1}{2}\iint_{\Omega^2} \frac{\mathrm{tr}_{\mathbb{C}^2}|\gamma(\mathbf{r}, \mathbf{r}')|^2}{|\mathbf{r} - \mathbf{r}'|}\mathrm{d}\mathbf{r}'\,\mathrm{d}\mathbf{r}' - T\,\mathrm{Tr}\,(S(\gamma))$$

where $S(t) := -t\log(t) - (1-t)\log(1-t)$ is the entropy.

Constraint: $\mathrm{Tr}(\gamma) = \rho|\Omega|$.

Thermodynamic limit: $\Omega \to \mathbb{R}^3$, and ρ constant $\to E^{\rm HF}(\rho, T)$.

Goal: Study the phase diagram: features of the minimisers in the (ρ, T) plane.

Spatial symmetry breaking

If $\gamma(\mathbf{r}, \mathbf{r}') = \gamma(\mathbf{r} - \mathbf{r}', \mathbf{0})$, then γ is invariant by translation (fluid phase).
Otherwise, γ breaks spatial symmetry (e.g. Wigner crystallisation).

Spin symmetry breaking

If $\gamma^{\uparrow\uparrow} = \gamma^{\downarrow\downarrow}$ and $\gamma^{\uparrow\downarrow} = \gamma^{\downarrow\uparrow} = 0$, then γ is paramagnetic.
Otherwise, it is (partially) ferromagnetic.

The fluid phase

Perform the minimisation only on translational-invariant states: $\gamma(\mathbf{r},\mathbf{r}') = \gamma(\mathbf{r}-\mathbf{r}')$.
$\implies \rho_\gamma = \rho = \gamma(\mathbf{0})$ is constant $\implies$ the direct term vanishes.

Fourier operator, γ is multiplication operator in Fourier by (still denoted by γ)

$$\gamma(\mathbf{k}) = \begin{pmatrix} \gamma^{\uparrow\uparrow}(\mathbf{k}) & \gamma^{\uparrow\downarrow}(\mathbf{k}) \\ \gamma^{\downarrow\uparrow}(\mathbf{k}) & \gamma^{\downarrow\downarrow}(\mathbf{k}) \end{pmatrix}, \quad \gamma(\mathbf{k}) = \gamma(\mathbf{k})^*, \quad 0 \leq \gamma(\mathbf{k}) \leq \mathbb{I}_2.$$

HF energy for fluid states

$$\frac{1}{2(2\pi)^3}\int_{\mathbb{R}^3} k^2 \mathrm{tr}_{\mathbb{C}^2}\gamma(\mathbf{k})\mathrm{d}\mathbf{k} - \frac{1}{(2\pi)^5}\iint_{(\mathbb{R}^3)^2} \frac{\mathrm{tr}_{\mathbb{C}^2}\left[\gamma(\mathbf{k})\gamma(\mathbf{k}')\right]}{|\mathbf{k}-\mathbf{k}'|^2}\mathrm{d}\mathbf{k}\,\mathrm{d}\mathbf{k}' - \frac{T}{(2\pi)^3}\int_{\mathbb{R}^3} S(\gamma(\mathbf{k}))\mathrm{d}\mathbf{k}.$$

Constraints $\quad \dfrac{1}{(2\pi)^3}\displaystyle\int_{\mathbb{R}^3} \mathrm{tr}_{\mathbb{C}^2}\gamma(\mathbf{k})\mathrm{d}\mathbf{k} = \rho.$

No-spin version $\gamma \to g$, that is $g \in L^1(\mathbb{R}^3,\mathbb{R})$, $0 \leq g \leq 1$ and $(2\pi)^{-3}\displaystyle\int_{\mathbb{R}^3} g = \rho$.

$$\frac{1}{2(2\pi)^3}\int_{\mathbb{R}^3} k^2 g(\mathbf{k})\mathrm{d}\mathbf{k} - \frac{1}{(2\pi)^5}\iint_{(\mathbb{R}^3)^2} \frac{g(\mathbf{k})g(\mathbf{k}')}{|\mathbf{k}-\mathbf{k}'|^2}\mathrm{d}\mathbf{k}\,\mathrm{d}\mathbf{k}' - \frac{T}{(2\pi)^3}\int_{\mathbb{R}^3} S(g(\mathbf{k}))\mathrm{d}\mathbf{k}.$$

Lemma

Any minimiser among all fluid states is of the form

$$\gamma(\mathbf{k}) = U \begin{pmatrix} g^{\uparrow}(\mathbf{k}) & 0 \\ 0 & g^{\downarrow}(\mathbf{k}) \end{pmatrix} U^* \quad \textit{with} \quad U \in \mathrm{SU}(2).$$

Proof: $\mathrm{tr}_{\mathbb{C}^2}(UD_1U^*D_2) \leq \mathrm{tr}_{\mathbb{C}^2}(D_1D_2)$ with D_1, D_2 diagonal with ordered entries.

Corollary

$$E^{\mathrm{HF,fluid}}(\rho, T) = \inf_{t \in [0,1/2]} \left\{ E^{\mathrm{HF,fluid}}_{\mathrm{nospin}}(t\rho, T) + E^{\mathrm{HF,fluid}}_{\mathrm{nospin}}((1-t)\rho, T) \right\}.$$

The best $t \in [0, \frac{1}{2}]$ is called the polarisation.

Lemma (Euler-Lagrange)

Any such minimiser γ must satisfy the Euler-Lagrange equation

$$\gamma = \left(1 + \mathrm{e}^{\beta(k^2/2 - \gamma * |\cdot|^{-2} - \mu)}\right)^{-1} \quad \textit{for some Lagrange multiplier} \quad \mu \in \mathbb{R}.$$

In particular, $g^{\uparrow}$ and $g^{\downarrow}$ satisfy $g^{\uparrow/\downarrow}(\mathbf{k}) = \left(1 + \mathrm{e}^{\beta(k^2/2 - g^{\uparrow/\downarrow} * |\cdot|^{-2} - \mu)}\right)^{-1}$ for the same μ.

Remark: Spin symmetry breaking ($g^{\uparrow} \neq g^{\downarrow}$) can only happen if

- the map $\rho \mapsto \mu(\rho, T)$ is not one-to-one;
- the equation $g \mapsto \left(1 + \mathrm{e}^{\beta(k^2/2 - g * |\cdot|^{-2} - \mu)}\right)^{-1}$ has at least two fixed points.

An important example: the $T = 0$ case.

Lemma

At $T =^0$, for all $\rho > 0$, the no-spin energy $E^{\rm fluid}_{\rm nospin}$ has a unique minimiser, which is $g := \mathbb{1}(k^2 \le c\rho^{3/2})$. Hence

$$E^{\rm fluid}_{\rm nospin}(\rho, T = 0) = C_{\rm TF}\rho^{5/3} - C_D\rho^{4/3},$$

and

$$\mu(\rho, T = 0) = \frac{\partial}{\partial \rho} E^{\rm fluid}_{\rm nospin} = \frac{5}{3} C_{\rm TF}\rho^{2/3} - \frac{4}{3} C_D \rho^{1/3} \quad \textit{(not one-to-one).}$$

Including the spin, we just need to study the map

$$t \mapsto C_{\rm TF}\rho^{5/3}(t^{5/3} + (1-t)^{5/3}) - C_D\rho^{4/3}(t^{4/3} + (1-t)^{4/3}).$$

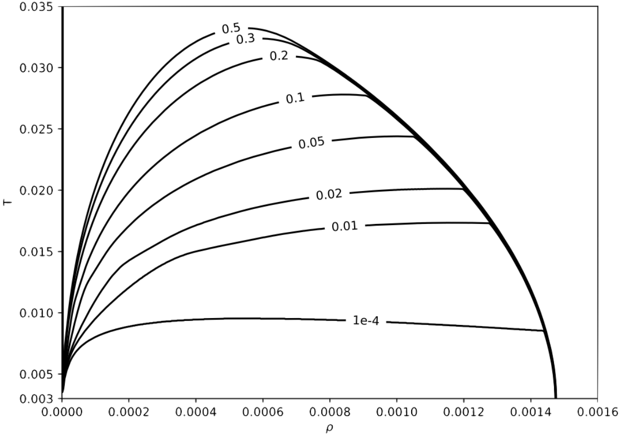
Theorem (G-Lewin 2018)

There is a first order phase transition at $\rho_c = \frac{125}{24\pi^5}\left(\frac{1}{1+2^{1/3}}\right)^3$ ($r_s \approx 5.45$):

- *For $\rho < \rho_c$, the minimiser is unique up to global spin rotation, and it is pure ferromagnetic ($g^\downarrow = 0$);*
- *For $\rho > \rho_c$, the minimiser is unique, and is paramagnetic.*

The energy is continuous, and has a kink at $\rho = \rho_c$.

Fluid phase diagram



Theorem (G-Lewin 2018)

For $T \geq C\rho^{1/3}\mathrm{e}^{-\alpha\rho^{1/6}}$, the minimiser for the spin-fluid energy is unique and paramagnetic.

Spatial symmetry breaking

Theorem (Overhauser, Phys. Rev. Lett. 4, 462 (1960))

At $T = 0$, the fluid minimiser is never a HF minimiser. Actually,

$$E^{\mathrm{HF}}(\rho, T=0) < E^{\mathrm{HF,fluid}}(\rho, T=0) - C\mathrm{e}^{-\alpha\rho^{1/6}}$$ *Delyon, Bernu, Baguet, Holzmann, Phys. Rev. B 92*

Fluid states are **unstable** *with respect to the formation of Spin Density Waves (SDW).*

$\Longrightarrow$ Much more complex phase diagram.

Phase diagram at $T = 0$ (from Baguet, Delyon, Bernu, Holzmann, Phys. Rev. B 90 (2014))

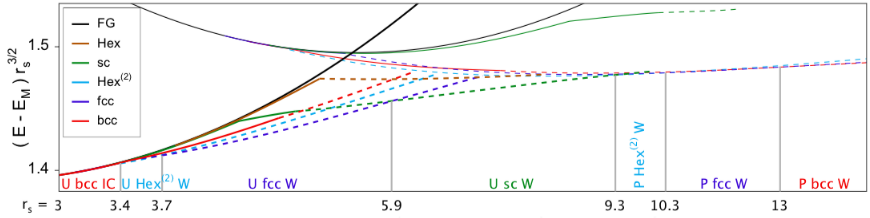


FIG. 2. Hartree-Fock phase diagram of the 3D electron gas. Energies are in Hartree per electron. $E_M = -0.89593/r_s$ is the Madelung energy of a polarized-bcc Wigner crystal. Full lines stand for incommensurate regime ($Q > Q_W$) and dashed lines for the Wigner crystal ($Q = Q_W$). Thin lines stand for the polarized gas (upper curves) and thick lines for the unpolarized gas.[14]

Theorem (G-Hainzl-Lewin 18)

- *At $T = 0$,*
$$\left| E^{\rm HF, fluid}(\rho, T=0) - E^{\rm HF}(\rho, T=0) \right| \le C \mathrm{e}^{-\alpha \rho^{1/6}}.$$
- *If $\rho \gg 1$ and $T > C\mathrm{e}^{-\alpha\rho^{1/6}}$, $E^{\rm HF}(\rho, T)$ has a unique minimiser, which is fluid and paramagnetic. In particular, $E^{\rm HF}(\rho, T) = E^{\rm HF, fluid}(\rho, T)$.*

Idea of the proof: Controlled the difference with the first eigenvalue of the Schrödinger-like operator

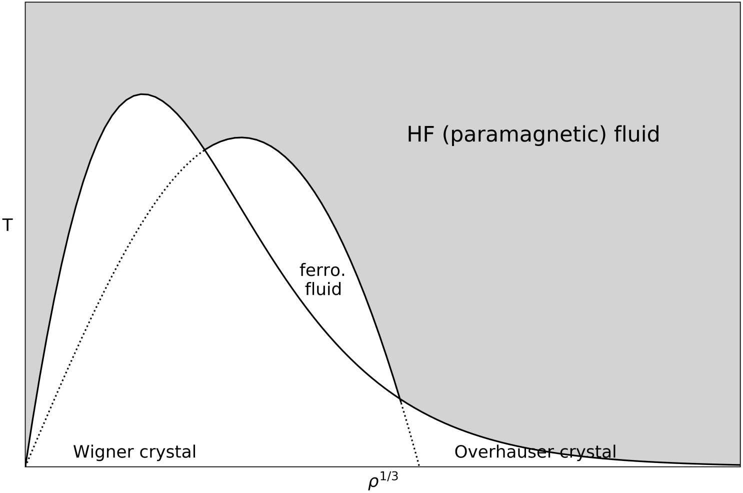
$$H(\varepsilon) := |\Delta + 1| - \frac{\varepsilon}{|\mathbf{r}|}.$$

Lemma (G-Hainzl-Lewin 18)

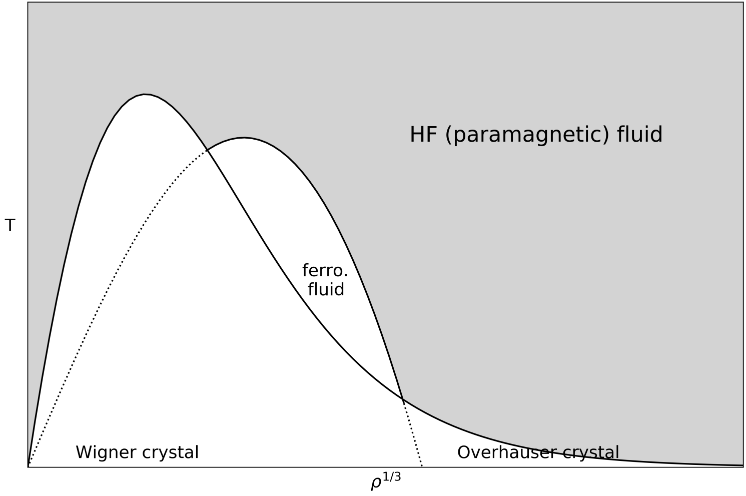
The first eigenvalue $\lambda_1(\varepsilon)$ of $H(\varepsilon)$ satisfies

$$-C\mathrm{e}^{-\alpha/\sqrt{\varepsilon}} \le \lambda_1(\varepsilon) \le -C'\mathrm{e}^{-\alpha'/\sqrt{\varepsilon}}.$$

Expected Phase diagram for the HF jellium



Expected Phase diagram for the HF jellium



Thank you for your attention!