Spin symmetry breaking in the Hartree-Fock electron gas

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Joint work with M. Lewin.

Notation and first facts

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What this talk is NOT about: spatial symmetry breaking.

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Translational-invariant states: $\check{\gamma}(\mathbf{x}, \mathbf{y}) = \check{\gamma}(\mathbf{x} - \mathbf{y})$.
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Fourier operator, $\check{\gamma}$ is multiplication operator in Fourier by

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HF energy of this state (at T = 0)

$$\mathcal{E}^{\mathrm{HF}}(\gamma) := \frac{1}{2} \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} k^2 \mathrm{tr}_{\mathbb{C}^2} \gamma(\mathbf{k}) \mathrm{d}\mathbf{k} - \frac{1}{2} \int_{\mathbb{R}^d} w(\mathbf{x}) \mathrm{tr}_{\mathbb{C}^2} \left| \check{\gamma}(\mathbf{x}) \right|^2 \mathrm{d}\mathbf{x}.$$

HF energy of the translation-invariant electron gas

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Remark:

- $\rho = \check{\gamma}(\mathbf{0})$ is the density of the gas. This is the only parameter of the model.
- We assume in the sequel that $\hat{w}$ is positive radial-decreasing (repulsive interaction).

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Remark: If $\gamma = \begin{pmatrix} g^\uparrow & 0 \\ 0 & g^\downarrow \end{pmatrix}$ is diagonal, then

$$\mathcal{E}^{\rm HF}(\gamma) = \mathcal{E}^{\rm HF}_{\rm no.spin}(g^\uparrow) + \mathcal{E}^{\rm HF}_{\rm no.spin}(g^\downarrow).$$

In particular,

$$E^{\rm HF}(\rho) \le \min_{t\in[0,\frac{1}{2}]}\left\{{\rm e}^{\rm HF}_{\rm no.spin}(t\rho) + {\rm e}^{\rm HF}_{\rm no.spin}((1-t)\rho)\right\}.$$

Proposition

Assume $\hat{w} \in L^1(\mathbb{R}^d) + L^\infty(\mathbb{R}^d)$ *is positive radially decreasing. Then the problems are well-posed, and the minimisers of* $\mathcal{E}^{\mathrm{HF}}$ *are all of the form*

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

Hence,

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Proof:

- For all $\mathbf{k}$, $\gamma(\mathbf{k})$ is diagonalisable, of the form $\gamma(\mathbf{k}) = U(\mathbf{k})D(\mathbf{k})U^*(\mathbf{k})$;
- We have $\mathrm{tr}_{\mathbb{C}^2}\gamma = \mathrm{tr}_{\mathbb{C}^2} D \implies$ same density, and same kinetic energy;
- For the Fock term, we use the following lemma:

Lemma

Let $D_1 = \begin{pmatrix} \lambda_1 & 0 \\ 0 & \mu_1 \end{pmatrix}$ *and* $D_2 = \begin{pmatrix} \lambda_2 & 0 \\ 0 & \mu_2 \end{pmatrix}$ *be two diagonal matrices with* $\lambda_1 \geq \mu_1$ *and* $\lambda_2 \geq \mu_2$*.*
Then, for any unitary matrix $U \in \mathrm{SU}(2)$*, we have* $\mathrm{tr}_{\mathbb{C}^2}(D_1 U D_2 U^*) \leq \mathrm{tr}_{\mathbb{C}^2}(D_1 D_2)$*.*

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Let $J = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$. We have $D_i = \mu_i \mathbb{I}_2 + \alpha_i J$ with $\alpha_i := (\lambda_i - \mu_i) \geq 0$. Hence,

$${\rm tr}_{\mathbb{C}^2}(D_1 D_2) - {\rm tr}_{\mathbb{C}^2}(D_1 U D_2 U^*) = \alpha_1 \alpha_2 \left[1 - {\rm tr}_{\mathbb{C}^2}(JUJU^*)\right] = \alpha_1 \alpha_2 \left[1 - |U_{11}|^2\right] \geq 0.$$

It remains to study the no-spin problem.

Proposition

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Remark: The minimiser does not depend on w (the exchange term).

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Let $g \in L^1(\mathbb{R}^d)$ with $0 \le g(\mathbf{k}) \le 1$ and $(2\pi)^{-d} \int g = \rho$, consider g^* its symmetric decreasing rearrangement. We have

$$\frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} g^* = \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} g = \rho \quad \text{(trivial)}, \qquad \int_{\mathbb{R}^d} k^2 g^* \le \int_{\mathbb{R}^d} k^2 g \quad \text{(bath tube principle)}$$

$$- \int_{\mathbb{R}} (g^* * \hat{w}) g^* \le - \int_{\mathbb{R}} (g * \hat{w}) g \quad \text{(Riesz inequality)}.$$

Hence $\mathrm{e}^{\mathrm{HF}}_{\mathrm{no.spin}}(g^*) \le \mathrm{e}^{\mathrm{HF}}_{\mathrm{no.spin}}(g)$.

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Hence $\mathrm{e}^{\mathrm{HF}}_{\mathrm{no.spin}}(g^*) \le \mathrm{e}^{\mathrm{HF}}_{\mathrm{no.spin}}(g)$.
$\Longrightarrow$ restrict the minimisation to radially decreasing function between 0 and 1.

The problem is concave[1] in g, hence g saturates the constraints, and $g(\mathbf{k}) \in \{0, 1\}$.

The only radially decreasing function g with value in $\{0, 1\}$ and $(2\pi)^{-d} \int g = \rho$ is $g^*[\rho]$.

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Phase transitions

We proved that

$$\boxed{\mathrm{e}^{\mathrm{HF}}_{\mathrm{no.spin}}(\rho) = \mathcal{E}^{\mathrm{HF}}_{\mathrm{no.spin}}(g^*[\rho]) \quad \text{with} \quad g^*[\rho] := \mathbb{1}(k^2 \leq C_{\mathrm{TF}} \rho^{2/d}).}$$

and that

$$\boxed{E^{\mathrm{HF}}(\rho) = \min_{t \in [0, \frac{1}{2}]} \left\{ \mathrm{e}^{\mathrm{HF}}_{\mathrm{no.spin}}(t\rho) + \mathrm{e}^{\mathrm{HF}}_{\mathrm{no.spin}}((1-t)\rho) \right\}.}$$

Definition

The minimising t is called the polarisation.

- If $t = 0$, the gas is ferromagnetic, and all minimisers are of the form $\gamma = U \begin{pmatrix} g^*(\rho) & 0 \\ 0 & 0 \end{pmatrix} U^*$.
- If $t = \frac{1}{2}$, the gas is paramagnetic, and the unique minimiser is $\gamma = g^*(\frac{1}{2}\rho)\mathbb{I}_2$.

We discuss phase transition as ρ increases.

The case for Riesz interactions.

Proposition

Assume that $w(\mathbf{x}) = \dfrac{1}{|\mathbf{x}|^s}$ *with* $0 < s < d$*, so that* $\hat{w}(\mathbf{k}) := \dfrac{c_{d,s}}{|\mathbf{k}|^{d-s}}$*. Then*

$$\mathrm{e}^{\mathrm{HF}}_{\mathrm{no.spin}}(\rho) = \kappa(d)\rho^{1+\frac{d}{2}} - \lambda(d,s)\rho^{1+\frac{s}{d}}.$$

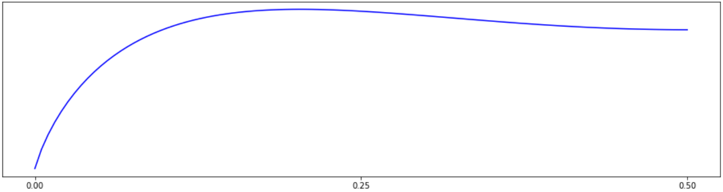
In addition,

- *If* $0 < s < \min(2,d)$*, then there is* $\rho_c > 0$ *such that the system is ferromagnetic for* $\rho < \rho_c$*, and is paramagnetic for* $\rho > \rho_c$ *(sharp transition).*
- *If* $\min(2,d) < s < d$*, then there is* $\rho_{c,p} > \rho_{c,f} > 0$ *such that the system if ferromagnetic for* $\rho < \rho_{c,f}$*, becomes smoothly paramagnetic for* $\rho_{c,f} < \rho < \rho_{c,p}$*, and is paramagnetic for* $\rho > \rho_{c,p}$ *(smooth transition).*

We recover the result for the Coulomb case ($s = 1$ and $d = 3$) found in usual textbooks.

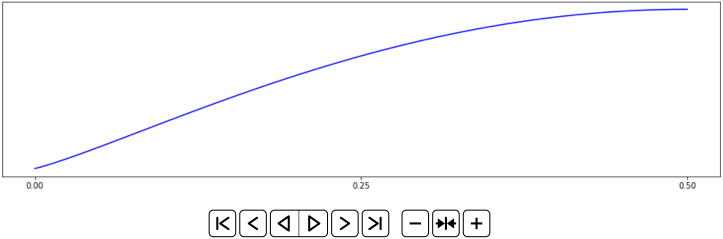
The SHARP transition for Coulomb interaction ($s = 1$ and $d = 3$)

We plot the function $t \mapsto \mathrm{e}^{\mathrm{HF}}_{\mathrm{no.spin}}(t\rho) + \mathrm{e}^{\mathrm{HF}}_{\mathrm{no.spin}}((1-t)\rho)$.



The SMOOTH transition for another Riesz interaction ($s = \frac{5}{2}$ and $d = 3$)

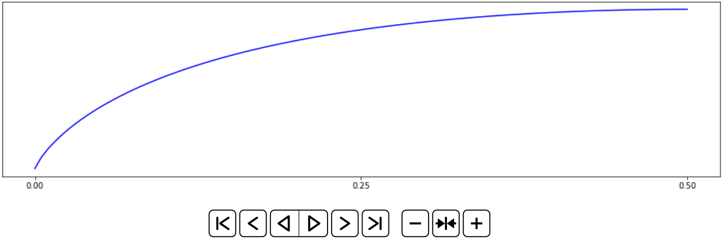
We plot the function $t \mapsto \mathrm{e}^{\mathrm{HF}}_{\mathrm{no.spin}}(t\rho) + \mathrm{e}^{\mathrm{HF}}_{\mathrm{no.spin}}((1-t)\rho)$.



A NON TRIVIAL transition for a sum of Riesz interactions

With $w(\mathbf{x}) = \dfrac{\alpha_1}{|\mathbf{x}|^{s_1}} + \dfrac{\alpha_2}{|\mathbf{x}|^{s_2}}$ (still positive radial decreasing).

We plot the function $t \mapsto \mathrm{e}^{\mathrm{HF}}_{\mathrm{no.spin}}(t\rho) + \mathrm{e}^{\mathrm{HF}}_{\mathrm{no.spin}}((1-t)\rho)$.



Positive temperature

We now add the entropy $S(x) = x \log x + (1-x)\log(1-x)$ (convex).

$$\mathcal{E}^{\mathrm{HF}}(\gamma, T) = \mathcal{E}^{\mathrm{HF}}(\gamma) + \frac{T}{(2\pi)^d}\int_{\mathbb{R}^d} \mathrm{tr}_{\mathbb{C}^2} S(\gamma(\mathbf{k}))\mathrm{d}\mathbf{k}.$$

We set $\mathrm{e}^{\mathrm{HF}}(\rho, T)$, $\mathcal{E}^{\mathrm{HF}}_{\mathrm{no.spin}}(\gamma, T)$ and $\mathrm{e}^{\mathrm{HF}}_{\mathrm{no.spin}}(\rho, T)$ with obvious definition.

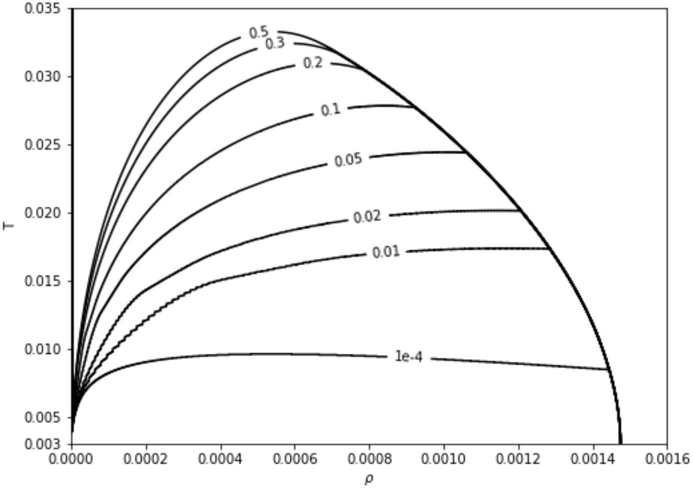
As before (same proof),

$$\boxed{\mathrm{e}^{\mathrm{HF}}(\rho, T) = \inf_{t\in[0,\frac{1}{2}]}\left\{\mathrm{e}^{\mathrm{HF}}_{\mathrm{no.spin}}(t\rho, T) + \mathrm{e}^{\mathrm{HF}}_{\mathrm{no.spin}}((1-t)\rho, T)\right\}.}$$

Question: Does $\mathrm{e}^{\mathrm{HF}}_{\mathrm{no.spin}}(\rho, T)$ have a unique minimiser?

Numerical results

Phase diagram of the polarisation for the 3d Coulomb gas ($d = 3$ and $s = 1$).



Uniqueness of the minimiser?

Euler-Lagrange equations: All minimisers g of $\mathrm{e}^{\mathrm{HF}}_{\mathrm{no.spin}}(\rho, T)$ satisfy

$$\frac{1}{2}k^2 - g * \hat{w}(\mathbf{k}) + TS'(g(\mathbf{k})) = \mu \quad \text{for some} \quad \mu \in \mathbb{R}.$$

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Fixed point equation

$$g = \mathcal{G}_{\mu,T}(g) \quad \text{with} \quad \mathcal{G}_{\mu,T}(g) : \mathbf{k} \mapsto \frac{1}{1 + \mathrm{e}^{\frac{1}{T}\left(\frac{1}{2}k^2 - g*\hat{w}(\mathbf{k}) - \mu\right)}}.$$

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Proposition (High temperature regime)

There is $T_c > 0$ such that, for all $T > T_c$, the map $\mathcal{G}_{\mu,T}$ has a unique fixed point $g_{\mu,T}$ for all $\mu \in \mathbb{R}$, and the map $\mu \mapsto \rho[\mu, T] := (2\pi)^{-d} \int g_{\mu,T}$ is increasing.

In particular, $\mathrm{e}^{\mathrm{HF}}_{\mathrm{no.spin}}(\rho, T)$ has a unique minimiser for all $\rho > 0$, the map $\rho \mapsto \mathrm{e}^{\mathrm{HF}}_{\mathrm{no.spin}}(\rho, T)$ is convex, and the system with spin is always paramagnetic.

Remark: This result cannot be true for all $T > 0$. Otherwise, the system would always be paramagnetic.

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The map $\mu \mapsto \mathcal{G}_{\mu,T}$ is increasing. Hence, if $\mu_1 < \mu_2$,

$$\mathcal{G}^{(n)}_{\mu_1,T}(\mathbf{0}) < \mathcal{G}^{(n)}_{\mu_2,T}(\mathbf{0}), \quad \text{hence} \quad g_1 \leq g_2 \quad \text{and} \quad \rho[\mu_1] \leq \rho[\mu_2].$$

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Convexity. We can define $\rho \mapsto \mu[\rho, T]$, and we have

$$\frac{\partial}{\partial\rho} \mathrm{e}^{\mathrm{HF}}_{\mathrm{no.spin}}(\rho, T) = \mu[\rho, T] \quad \text{hence} \quad \frac{\partial^2}{\partial\rho^2} \mathrm{e}^{\mathrm{HF}}_{\mathrm{no.spin}} \geq 0.$$

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Convexity. We can define $\rho \mapsto \mu[\rho, T]$, and we have

$$\frac{\partial}{\partial\rho} \mathrm{e}^{\mathrm{HF}}_{\mathrm{no.spin}}(\rho, T) = \mu[\rho, T] \quad \text{hence} \quad \frac{\partial^2}{\partial\rho^2} \mathrm{e}^{\mathrm{HF}}_{\mathrm{no.spin}} \ge 0.$$

Paramagnetism. Finally, since $\mathrm{e}^{\mathrm{HF}}_{\mathrm{no.spin}}$ is convex in ρ, for all $0 \le t \le 1$,

$$\frac{1}{2}\mathrm{e}^{\mathrm{HF}}_{\mathrm{no.spin}}(t\rho, T) + \frac{1}{2}\mathrm{e}^{\mathrm{HF}}_{\mathrm{no.spin}}((1-t)\rho, T) \ge \mathrm{e}^{\mathrm{HF}}_{\mathrm{no.spin}}\left(\frac{1}{2}t\rho + \frac{1}{2}(1-t)\rho, T\right) = \mathrm{e}^{\mathrm{HF}}_{\mathrm{no.spin}}\left(\frac{1}{2}\rho, T\right).$$

In other words, the minimum is attained for $t = \frac{1}{2}$ ($\implies$ paramagnetism).

Conjecture

For all $w \in L^1 + L^\infty$, all $T > 0$ and all $\rho > 0$, there is always a unique pair (μ, g) solution to

$$g = \mathcal{G}_{\mu,T}(g) \quad \textit{and} \quad \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} g = \rho.$$

The map $g \mapsto \mathcal{G}_{\mu,T}(g)$ is increasing, and $0 \le g \le 1$. We can define

$$g_{\min}[\mu, T] := \lim_{n\to\infty} \mathcal{G}^{(n)}_{\mu,T}(\mathbf{0}) \quad \text{and} \quad g_{\max}[\mu, T] := \lim_{n\to\infty} \mathcal{G}^{(n)}_{\mu,T}(\mathbf{1}).$$

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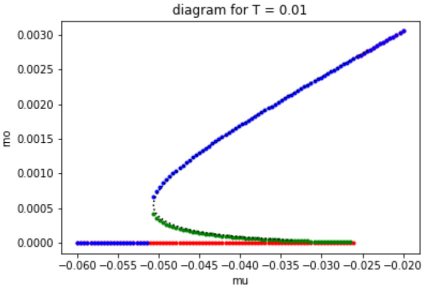

Remark: The middle g (green) is not so simple to find. Here, we use a *string method*, and compute

$$\mathcal{C} := (g_t)_{t\in[0,1]}, \quad g_0 = g_{\min},\ g_1 = g_{\max}, \quad \mathcal{G}_{\mu,T}(\mathcal{C}) = \mathcal{C}.$$

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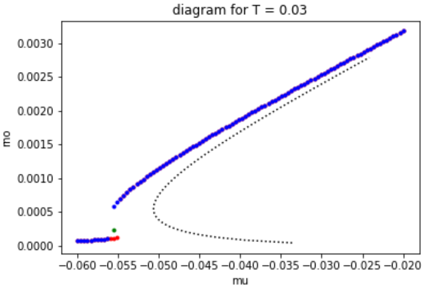

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Conclusions

- Nice and simple problem to study phase transitions.
- Not so trivial: already shows complex phase transitions.
- It remains to prove uniqueness for all ρ and all T.

Thank you for your attention.