Asymptotic Exactness of Magnetic Thomas-Fermi Theory at Nonzero Temperature

Jakob Yngvason

University of Vienna

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Preamble

I intend to stretch a bit Mathieu's suggestion

"...it might not be appropriate to speak about your very last paper on ArXiV. Do not hesitate to talk about older achievements, or even about open problems or things that you have not been able to solve, if you think they are of general interest..."

and essentially base my talk on a 15 year old paper with a former MS student:

Bergthor Hauksson and Jakob Yngvason, J. Stat. Physics **116**, *pp- 523–546 (2004)*

Preamble (cont.)

The following points may justify my choice

- In the 90's I participated in several astrophysical projects where MTF theory, including the $T > 0$ case, was used for computing the equation of state of surface layers of neutron stars. The resulting papers have been quite well cited in the astrophysics literature.
- Also in the 90's I collaborated with Elliott Lieb and Jan Philip Solovej on rigorous papers on the subject for the $T = 0$ case. These papers have likewise been well cited in the MP and M literature.
- By contrast, the only *rigorous* paper known to me on MTF theory at $T > 0$ has essentially been totally ignored so far!

Preamble (cont.)

- That paper (subject of the present talk) is open to generalizations and refinements which might be suitable for Master or even PhD projects in MP, in particular in view of quite recent work of Mathieu, Peter Madsen and Arnaud Triay, and of Søren Fournais, Mathieu and Jan Philip Solovej on semiclassics for large Fermi systems. Some examples will be mentioned at the end of the talk.

The heuristics behind *all* TF models

Starting point: Relation between **density, pressure and chemical potential** for a homogeneous (electron) gas, valid for all T,

$$\rho = \partial P(\mu)/\partial\mu =: P'(\mu).$$

Next: External potential V, Coulomb interaction between the electrons,

$$V_\rho(\mathbf{x}) := V(\mathbf{x}) + \rho * |\mathbf{x}|^{-1}.$$

Equilibrium condition: The total electrochemical potential

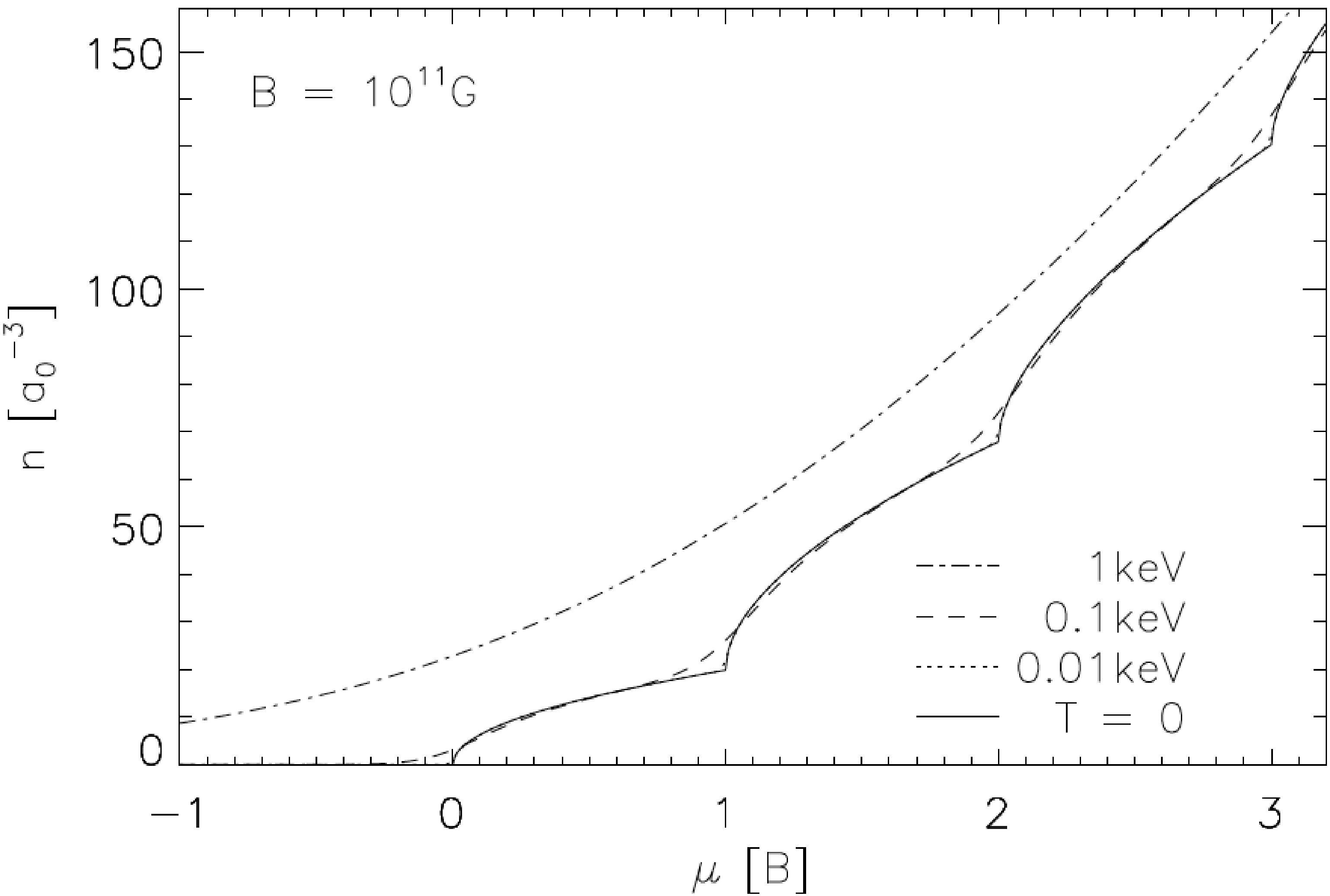
$$\mu_{\mathrm{TF}} := \mu(\mathbf{x}) + V_\rho(\mathbf{x}),$$

should be independent of $\mathbf{x}$. The result is the **Thomas-Fermi equation**:

$$\boxed{\rho(\mathbf{x}) = P'\left(\mu_{\mathrm{TF}} - V_\rho(\mathbf{x})\right)}$$

supplemented by

$\int \rho(\mathbf{x})d\mathbf{x} = N$ (particle number).



B = 10^11 G
150
100
50
0
n [a_0^-3]
−1
0
1
2
3
μ [B]
1keV
0.1keV
0.01keV
T = 0

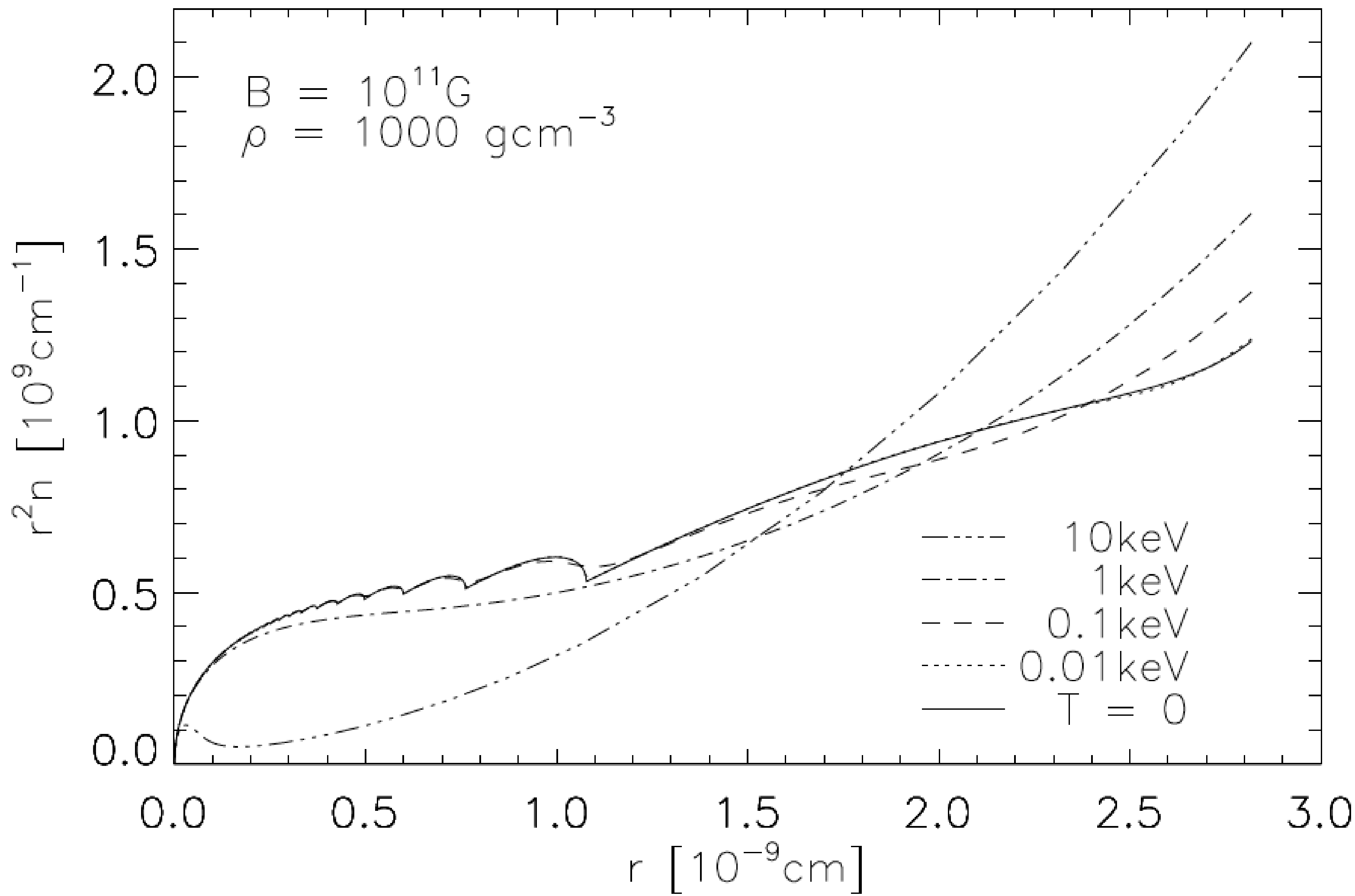
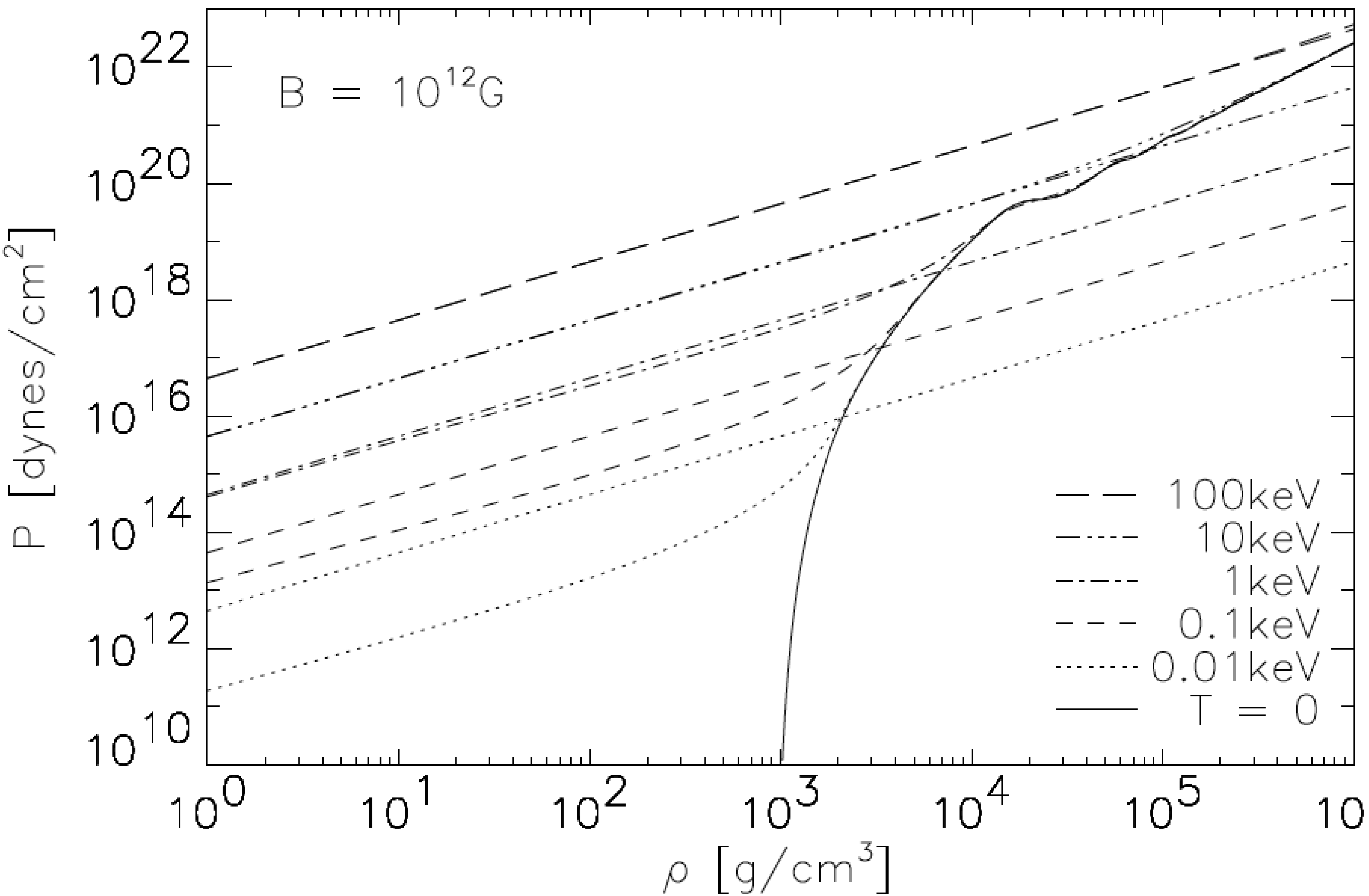


Fig. 3.— The quantity r^2n for a spherical unit cell of iron in the TF approximation. The matter



B = 10^12G
P [dynes/cm^2]
ρ [g/cm^3]
100keV
10keV
1keV
0.1keV
0.01keV
T = 0

The pressure functional and its Legendre transform

The TF equation is associated with minimization of the functional

$$\boxed{\mathcal{P}[\rho] = \int P\left(\mu_{\mathrm{TF}} - V_\rho(\mathbf{x})\right) d\mathbf{x} + D(\rho,\rho),}$$

with

$$D(\rho,\rho) = \tfrac{1}{2}\int\int \tfrac{\rho(\mathbf{x})\rho(\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|} d\mathbf{x}\, d\mathbf{x}'.$$

The minimum over all nonnegative ρ is called the ***TF pressure***.
Alternative form: The derivative $\partial f/\partial\rho =: f'(\rho)$ of free energy density

$$f(\rho) = \sup_\mu\{\mu\rho - P(\mu)\}$$

is the inverse of P'. Hence the TF equation can also be written

$$\boxed{f'(\rho(\mathbf{x})) + V_\rho(\mathbf{x})) = \mu_{\mathrm{TF}}.}$$

It is associated with the minimization of the ***free energy functional***

$$\boxed{\mathcal{F}[\rho] = \int \{f(\rho(\mathbf{x})) + V(\mathbf{x}))\rho(\mathbf{x})\}\, d\mathbf{x} + D(\rho,\rho).}$$

Remark on Firsov's (1957) point of view

Instead of considering $\mathcal{P}$ as a functional of the density ρ it could equivalently be considered as a **functional of the potential** $\check{V} = V_\rho$. This point of view arises naturally of we regard $\mathcal{P}$ as a Legendre transform of $\mathcal{F}$ (and vice versa):

$$\mathcal{P}[\check{V}] = \sup_{\rho} \{ \int \check{V}(\mathbf{x})\rho(\mathbf{x})d^3\mathbf{x} - \mathcal{F}[\rho] \}, \quad \mathcal{F}[\rho] = \sup_{\check{V}} \{ \int \rho(\mathbf{x})\check{V}(\mathbf{x})d^3\mathbf{x} - \mathcal{P}[\check{V}] \}$$

Note that ρ and hence $D(\rho, \rho)$ is determined by V_ρ because

$$4\pi\rho(\mathbf{x}) = -\Delta\rho * |\mathbf{x}|^{-1} = \Delta(V - V_\rho(\mathbf{x})).$$

For the present purpose we find it **more convenient, however, to regard $\mathcal{P}$ as a functional of ρ**. Also, we prefer to study the pressure functional rather than the free energy functional because explicit formulas are available for $P(\mu)$ but not for $f(\rho)$.

The many-body Hamiltonian

The goal is to derive the TF equation for electrons interacting with nuclei and a strong, constant magnetic field from the **many-body Hamiltonian** in a suitable limit.

$$\boxed{H_{N,Z,B} = \sum_{i=1}^{N} \left\{ [\mathbf{p}_i + \mathbf{A}(\mathbf{x}_i)) \cdot \boldsymbol{\sigma}_i]^2 + V_{Z,B}(\mathbf{x}_i) \right\} + \sum_{1 \le i < j \le N} |\mathbf{x}_i - \mathbf{x}_j|^{-1}}$$

Here $\mathbf{p} = -\mathrm{i}\nabla$, $\mathbf{A}(\mathbf{x}) = \frac{1}{2}(-Bx^2, Bx^1, 0)$ and $\boldsymbol{\sigma}$ the vector of Pauli matrices. Units chosen so that $\hbar = 2m = e = 1$, $k_{\mathrm{B}} = 1$. The **external potential** is

$$V_{Z,B}(\mathbf{x}) = -Z \sum_{k=1}^{K} \frac{z_k}{|\mathbf{x} - \ell \mathbf{X}_k|} + Z\ell^{-1} W(\ell^{-1}\mathbf{x})$$

with W a confining potential.

The many-body Hamiltonian (cont.)

The $\mathbf{X}_k$ are fixed positions of nuclei with fixed charges $z_k \leq 1$ which are scaled by an overall parameter Z. The **length scaling factor**

$$\boxed{\ell = \ell_{Z,B} = Z^{-1/3}[1 + (B/Z^{4/3})]^{-2/5}}$$

is the one appropriate for TF atoms in a magnetic field.

The Hamiltonian $H_{N,Z,B}$ operates on the N-electron Hilbert space of antisymmetric wave functions in space and spin variables:

$$\mathcal{H}_N = \wedge^N L^2(\mathbb{R}^3, \mathbb{C}^2).$$

The corresponding Fock space is

$$\widehat{\mathcal{H}} = \bigoplus_{N=0}^{\infty} \mathcal{H}_N$$

with $\mathcal{H}_0 = \mathbb{C}$. If A_N are operators on $\mathcal{H}_N$, $N = 0, 1, \ldots,$ we denote the operator $\oplus_{N=0}^{\infty} A_N$ on $\widehat{\mathcal{H}}$ by $\widehat{A}$.

QM pressure and MTF pressure

Grand canonical QM pressure corresponding to $\hat{H}_{T,B}$:

$$\boxed{P^{\mathrm{QM}}(\mu, B, T, Z) = T\ \ln \mathrm{Tr} \exp[-(\widehat{H}_{Z,B} - \mu\widehat{N})/T].}$$

For the MTF pressure we need first the pressure of a noninteracting electron gas at temperature T in a magnetic field of strength B:

$$P_{T,B}^{\mathrm{free}}(\mu) = T \sum_{\nu=0}^{\infty} d_\nu(B) \int_{-\infty}^{\infty} \ln\left[1 + \exp\{-(\varepsilon_\nu(p) - \mu)/T\}\right] dp$$

with the **Landau spectrum**

$$\varepsilon_\nu(p) = 2B\nu + p^2\,, \quad \nu = 0, 1, \ldots;\ p \in \mathbb{R}$$

and degeneracy per unit area in $\mathbb{R}^2$

$$d_\nu(B) = \begin{cases} B/(2\pi) & \text{if} \quad \nu = 0 \\ B/\pi & \text{if} \quad \nu \geq 1. \end{cases}$$

The **magnetic Thomas-Fermi pressure functional** is now

$$\boxed{\mathcal{P}^{\mathrm{MTF}}[\rho; Z, \mu, T, B] = \int P^{\mathrm{free}}_{T,B}(\mu - V_{Z,B,\rho}(\mathbf{x}))\, d^3\mathbf{x} + D(\rho, \rho)}$$

with

$$V_{Z,B,\rho}(\mathbf{x}) = V_{Z,B}(\mathbf{x}) + \rho * |\mathbf{x}|^{-1}.$$

Domain of definition:

$$\mathcal{M} = \{\rho : \ \rho(\mathbf{x}) \geq 0,\ D(\rho, \rho) < \infty\}.$$

The **pressure according to MTF theory** is

$$\boxed{P^{\mathrm{MTF}}(Z, \mu, T, B) := \inf_{\rho \in \mathcal{M}} \mathcal{P}^{\mathrm{MTF}}[\rho; \mu, T, B, Z].}$$

The Main Result

Theorem (The MTF pressure is a limit of the QM pressure)

If $Z \to \infty$ *and* $B/Z^3 \to 0$ *while the normalized chemical potential and temperature,*

$$\mu/(Z\ell_{B,Z}^{-1}) \quad \text{and} \quad T/(Z\ell_{B,Z}^{-1})$$

with

$$\ell_{B,Z} = Z^{-1/3}[1 + (B/Z^{4/3})]^{-2/5}$$

are kept fixed fixed, then

$$\frac{P^{\mathrm{QM}}(\mu, T, B, Z)}{P^{\mathrm{MTF}}(\mu, T, B, Z)} \to 1$$

Limiting cases:

- $B/Z^{4/3} \ll 1$ corresponding to standard TF theory at positive temperature, studied (albeit not with full mathematical rigor) already in the 1950's. Rigorous results by Thirring and Narnhofer, and Messer in the 1980's.
- $B/Z^{4/3} \gg 1$, **but still** $B/Z^3 \ll 1$. Here only the lowest Landau level is relevant.

The **proof strategy** for the Theorem is in brief:

- Show that MTF can be regarded as a **semiclassical limit** of a mean field model, using magnetic coherent states and a magnetic Lieb-Thirring inequality.
- Compare the mean field model to the full QM theory using **correlation bounds** and the Peierls-Bogoliubov inequality.

Basic properties of the MTF pressure functional

- $\mathcal{P}^{\rm MTF}$ is nonnegative and strictly convex on $\mathcal{M}$, and weakly lower semicontinuous w.r.t. the Hilbert norm $D(\rho,\rho)^{1/2}$ on $\mathcal{M}$.
- There is a ***unique minimizer*** $\rho^{\rm MTF} \in \mathcal{M}$ and it is the unique solution to the **MTF equation**

$$\boxed{\rho(\mathbf{x}) = \partial P^{\rm free}_{T,B}/\partial\mu\,(\mu - V_{Z,B,\rho}(\mathbf{x})).}$$

- **Scaling relations**:

$$\boxed{\mathcal{P}^{\rm MTF}[\rho;\mu,T,B,Z] = Z^2\ell^{-1}\tilde{\mathcal{P}}^{\rm MTF}[\tilde\rho;\tilde\mu,\tilde T,\beta]}$$

where $\tilde\rho(\mathbf{x}) = Z^{-1}\ell^3\rho(\ell\mathbf{x})$ with $\ell = Z^{-1/3}[1+(B/Z^{4/3})]^{-2/5}$ and

$$\beta := B/Z^{4/3}, \quad \tilde\mu =: \mu/(Z\ell^{-1}), \quad \tilde T := T/(Z\ell^{-1}),$$

$$\tilde{\mathcal{P}}^{\rm MTF}[\tilde\rho;\tilde\mu,\tilde T,\beta] = (1+\beta)^{-3/5}\int P_{\tilde T,\beta(1+\beta)^{-2/5}}(\tilde\mu - \tilde V_{\tilde\rho}(\mathbf{x}))d\mathbf{x} + D(\tilde\rho,\tilde\rho),$$

$$\tilde V_{\tilde\rho}(\mathbf{x}) = -\textstyle\sum_k z_k|\mathbf{x}-\mathbf{X}_k|^{-1} + W(\mathbf{x}) + \tilde\rho * |\mathbf{x}|^{-1}.$$

Mean field theory

For $\rho \in \mathcal{M}$ we define a ***mean field (single particle) Hamiltonian*** by

$$H^{(1)}_{Z,B,\rho} = [(\mathbf{p} + \mathbf{A}(\mathbf{x})) \cdot \boldsymbol{\sigma}]^2 + V_{Z,B,\rho}(\mathbf{x})$$

and a ***mean field pressure functional*** by

$$\mathcal{P}^{\mathrm{mf}}[\rho; \mu, T, B, Z] = T\,\mathrm{Tr}\ln\left[1 + \exp\{-(H^{(1)}_{Z,B,\rho} - \mu)/T\}\right] + D(\rho, \rho).$$

Note that the first term is equal to

$$T\ \ln\mathrm{Tr}\exp[-(\widehat{H}_{Z,B,\rho} - \mu\widehat{N})/T]$$

where $\widehat{H}_{Z,B,\rho}$ is the second quantization of $H^{(1)}_{Z,B,\rho}$.

Mean field theory (cont.)

The mean field pressure functional is strictly convex and weakly lower semicontuous on $\mathcal{M}$. The minimizer, $\rho^{\rm mf}$, is the unique solution of the **Hartree equation**

$$\rho(\mathbf{x}) = 2\left\langle \mathbf{x} \left| \left(\exp\{(H^{(1)}_{Z,B,\rho} - \mu)/T\} + 1\right)^{-1} \right| \mathbf{x} \right\rangle .$$

By the unitary transformation $U_\ell(\psi)(\mathbf{x}) = \ell^{-3/2}\psi(\ell^{-1})$ the mean field Hamiltonian is unitarily equivalent to

$$\tilde{H}^{(1)}_{h,b,\tilde{\rho}} = [(h\mathbf{p} + b\mathbf{a}(\mathbf{x}))\cdot\boldsymbol{\sigma}]^2 + \tilde{V}_{\tilde{\rho}}(\mathbf{x}).$$

Here $\mathbf{a}(\mathbf{x}) = \frac{1}{2}(-x^2, x^1, 0)$, and

$$\begin{aligned} h &:= \ell^{-1/2}Z^{-1/2} = Z^{-1/3}(1+\beta)^{1/5}, \\ b &:= B\ell^{3/2}Z^{-1/2} = Z^{1/3}\beta(1+\beta)^{-3/5}, \\ \tilde{V}_{\tilde{\rho}}(\mathbf{x}) &= -\textstyle\sum_k z_k|\mathbf{x}-\mathbf{X}_k|^{-1} + W(\mathbf{x}) + \tilde{\rho} * |\mathbf{x}|^{-1} \end{aligned}$$

Semiclassics

We consider now generally the operator

$$\boxed{H^{(1)}_{h,b,v} = [(h\mathbf{p} + b\mathbf{a}(\mathbf{x}))\cdot\boldsymbol{\sigma}]^2 + v(\mathbf{x})}$$

with $h > 0$, $b \in \mathbb{R}$, $\mathbf{a}(\mathbf{x}) = \frac{1}{2}(-x_2, x_1, 0)$, and

$$v(\mathbf{x}) = v_1(\mathbf{x}) + v_2(\mathbf{x})$$

where $v_1 \in L^{5/2}_{\mathrm{loc}}$, and v_2 is confining and sufficiently regular.

For the present application

$$v_1(\mathbf{x}) = -\sum_k z_k |\mathbf{x} - \mathbf{X}_k|^{-1} + \tilde{\rho} * |\mathbf{x}|^{-1}$$

and

$$v_2(\mathbf{x}) = W(\mathbf{x}) - \tilde{\mu}.$$

Semiclassical limit theorem for the mean field pressure

The pressure (without the $D(\rho, \rho)$ term) corresponding to the the mean field Hamiltonian $H^{(1)}_{h,b,v}$ is

$$P^{\mathrm{Q}}(h, b, v, \tau) = \tau \,\mathrm{Tr} \ln \left(1 + \exp\left(-H^{(1)}_{h,b,v}/\tau\right)\right).$$

Its **semiclassical approximation** is

$$P^{\mathsf{scl}}(h, b, v, \tau) = h^{-3} \int P^{\mathrm{free}}_{\tau,hb}(-v(\mathbf{x}))\, d\mathbf{x}.$$

Theorem (Semiclassical limit theorem)

For fixed τ and v

$$\lim_{h\to 0} \frac{P^{\mathsf{Q}}(h, b, v, \tau)}{P^{\mathsf{scl}}(h, b, v, \tau)} = 1$$

uniformly in b.

Tools

A basic tool for the proof of the semiclassical limit theorem is a partition of unity by means of **magnetic coherent states** (operators) $\Pi_{\nu,\mathbf{u},p}$ with $\nu = 0, 1, 2, \ldots$, $\mathbf{u} \in \mathbb{R}^3$ and $p \in \mathbb{R}$. They are defined by their integral kernels

$$\boxed{\Pi_{\nu,\mathbf{u},p}(\mathbf{x}, s; \mathbf{x}', s') = g_r(\mathbf{x} - \mathbf{u})\Pi_\nu^\perp(\mathbf{x}^\perp, s; \mathbf{x}'^\perp, s')e^{ip(z-z')}g_r(\mathbf{x}' - \mathbf{u})}$$

where $\Pi_\nu^\perp$ is the projector on the ν-th Landau level and g_r a smooth localization function.

Another tool is the **magnetic Lieb-Thirring inequality** that implies an upper bound on P^{Q} in terms of P^{scl}:

$$\boxed{P^{\mathrm{Q}}(h, b, v, \tau) \leq (\text{const.})P^{\mathrm{scl}}(h, b, v, \tau).}$$

Consequences for MTF

After replacing h, β, τ by Z, B, T, and adding the $D(\rho,\rho)$ term, the semiclassical pressure is just the MTF pressure. Likewise P^{Q} is, after taking $D(\rho,\rho)$ into account, the mean field pressure P^{mf}.

As a Corollary of the semiclassical limit theorem and various bounds on the error terms, which depend on the potentials v_1 and v_2 and the parameters, one now obtains

Corollary (MTF as a limit of mean field theory)

If $Z \to \infty$ while $B/Z^3 \to 0$ and $\tilde{\mu} = \mu/(Z\ell^{-1})$ and $\tilde{T} = T/(Z\ell^{-1})$ are fixed,

$$\lim \frac{P^{\mathrm{MTF}}(\mu, T, B, Z)}{P^{\mathrm{mf}}(\mu, T, B, Z)} = 1.$$

Final step: QM vs mf

To link P^{MTF} and P^{QM} the remaining step is to show that

$$P^{\mathrm{QM}}/P^{\mathrm{mf}} \to 1$$

in the limit considered.

For the upper bound $P^{\mathrm{QM}} \leq P^{\mathrm{mf}}(1+o(1))$ we need to **bound the two-body Coulomb interaction by a one-body operator**. This can be done by the **Lieb-Oxford inequality**, or alternatively by the easier inequality

$$\sum_{i<j}^{N} \frac{1}{|\mathbf{x}_i - \mathbf{x}_j|} \geq \sum_{i=1}^{N} \int_{\mathbb{R}^3} \frac{\rho(\mathbf{x})}{|\mathbf{x}-\mathbf{x}_i|} d\mathbf{x} - D(\rho,\rho) - 3,68\gamma N - \frac{3}{5\gamma}\int_{\mathbb{R}^3} \rho^{5/3}(\mathbf{x})\, d\mathbf{x}$$

that holds for all $\gamma > 0$ and all $\rho \in \mathcal{M} \cap L^1(\mathbb{R}^3) \cap L^{5/3}(\mathbb{R}^3)$. It is a corollary of the classical Lieb-Thirring proof of stabilty of matter.

For the lower bound we use the Peierls-Bogoliubov inequality: If A_1, A_2 and $A_1 + A_2$ are self-adjoint operators and $F(A) = \ln \mathrm{Tr}\, e^{-A/T}$, then

$$F(A_1 + A_2) \geq F(A_1) - \langle A_2 \rangle_{A_1}$$

where

$$\langle A_2 \rangle_{A_1} := \frac{\mathrm{Tr}\ \left(A_2 e^{-A_1/T}\right)}{\mathrm{Tr}\ e^{-A_1/T}}.$$

We use this inequality with $A_1 + A_2 = \widehat{H}_{Z,B} - \mu \widehat{N}$ and $A_1 = \widehat{H}_{Z,B,\rho} - \mu \widehat{N} - D(\rho, \rho)$. Then A_2 is, apart from the constant $D(\rho, \rho)$, the second quantization of

$$\sum_{i<j}^{N} |\mathbf{x}_i - \mathbf{x}_j|^{-1} - \sum_{i=1}^{N} \rho * |\mathbf{x}_i|^{-1}.$$

QM vs mf (cont.)

Choosing $\rho = \rho^{\mathrm{mf}}$, the minimizer of the mean field pressure functional, this leads to the bound $P^{\mathrm{QM}} \geq P^{\mathrm{mf}}$.

In combination with the semiclassical limit theorem for P^{mf} and the relation between P^{scl} and P^{MTF}, the upper and lower bounds on P^{QM} lead to the desired final result:

If $Z \to \infty$ and $B/Z^3 \to 0$ while

$$\mu/(Z\ell_{B,Z}^{-1}) \quad \text{and} \quad T/(Z\ell_{B,Z}^{-1})$$

with

$$\ell_{B,Z} = Z^{-1/3}[1 + (B/Z^{4/3})]^{-2/5}$$

are kept fixed fixed, then

$$\boxed{\frac{P^{\mathrm{QM}}(\mu, T, B, Z)}{P^{\mathrm{MTF}}(\mu, T, B, Z)} \to 1}$$

Some open problems

- Prove a limit theorem for the free energy functional rather than the grand canonical pressure functional (perhaps via a Vlasov functional).
- Relax the conditions on the confining potential W, allowing e.g. hard walls.
- Study the thermodynamic limit of the MTF model.
- Study MTF theory for 2D systems (quantum dots) with 3D Coulomb interaction at $T > 0$.
- Investigate the case $B \gtrsim Z^3$ at $T > 0$.
- Allow other interactions that Coulomb, in the spirit of the recent work by Lewin, Madsen, Triay, and Fournais, Lewin, Solovej .

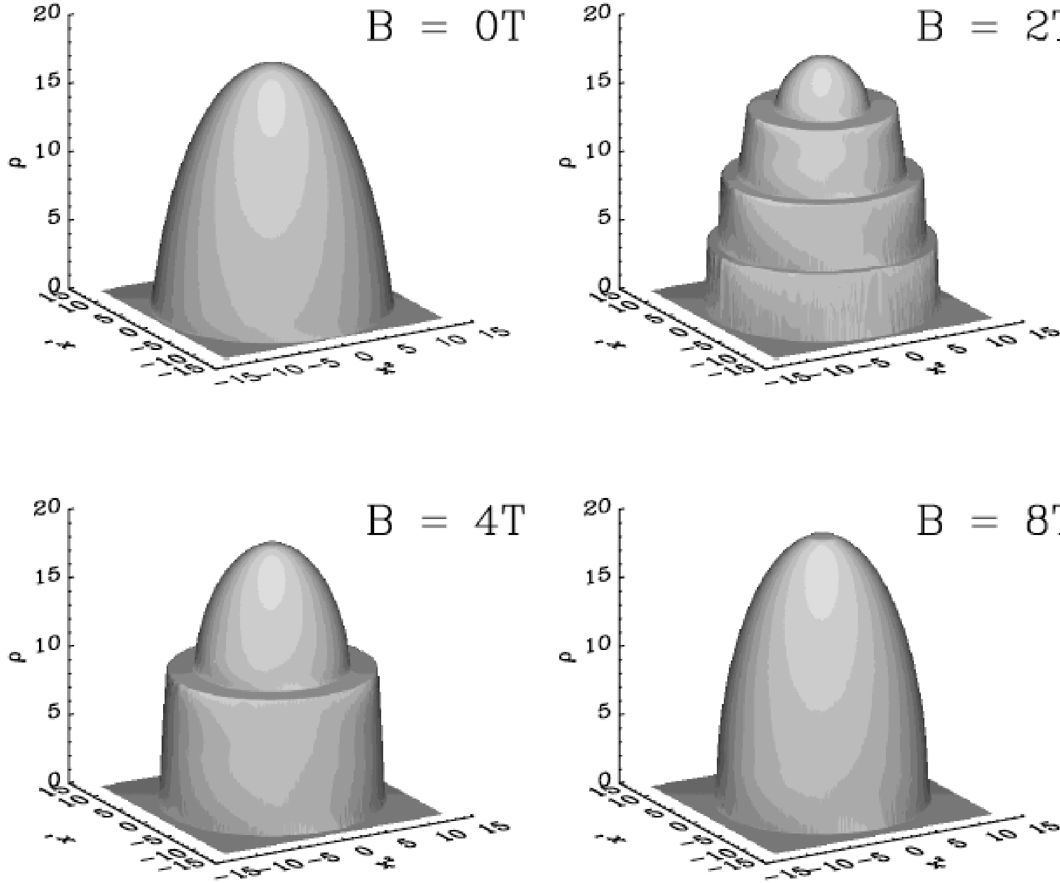


Figure 3: Quantum dots at various magnetic field strengths. The potential is

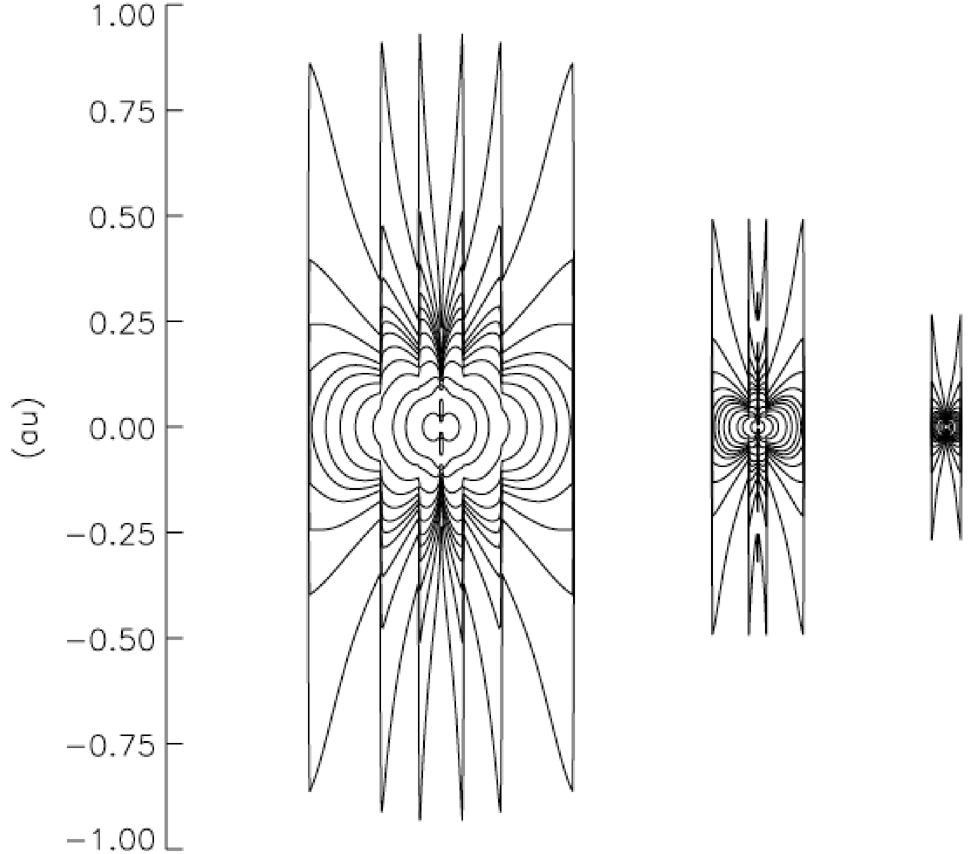


Figure 2: Contour plots of iron atoms in DM theory in magnetic fields $B = 10^8$, 10^9 and 10^{10} T