Semiclassical Limit of Large Fermionic Systems

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Interacting fermions in the mean-field regime

Consider N interacting (non-relativistic, quantum mechanical) fermions in $\mathbb{R}^d$. We want to understand the system in the limit where N is large.
Configuration space: $\wedge^N L^2(\mathbb{R}^d)$ (anti-symmetry due to Pauli principle).
Hamiltonian in the mean-field regime:

$$\boxed{H_N := \sum_{j=1}^{N} \left(\left[\frac{-i\nabla_j}{N^{\frac{1}{d}}} + A(x_j)\right]^2 + V(x_j) \right) + \frac{1}{N} \sum_{1 \leq k < \ell \leq N} w(x_k - x_\ell),}$$

Ground state energy

$$\boxed{E(N) = \inf \mathrm{Spec}\, H_N.}$$

$$H_N := \sum_{j=1}^{N} \left[\frac{-i\nabla_j}{N^{\frac{1}{d}}} + A(x_j)\right]^2 + \sum_{j=1}^{N} V(x_j) + \frac{1}{N} \sum_{1\le k<\ell\le N} w(x_k - x_\ell),$$

OBS. The Lieb-Thirring inequality gives for functions localized in a bounded domain Ω,

$$\sum_{j=1}^{N} \int_{\Omega^N} |\nabla_j \Psi|^2 \ge C|\Omega|^{-\frac{2}{d}} N^{1+\frac{2}{d}}.$$

This dictates the semiclassical factor $\hbar = N^{-1/d}$ in front of the gradient in order for all three terms in the Hamiltonian to be morally of the same order (N).

This is the regime where one can reasonably expect a mean-field limit to be correct.

A given physical system can sometimes be described in this form (after scaling). This is famously the case for atoms (Lieb & Simon) and fermion stars (Lieb & Thirring and Lieb & Yau).

The case of atoms (Lieb&Simon)

An atom with N interacting electrons (coordinates $x_j \in \mathbb{R}^3$) and nuclear charge $Z = zN$.

$$
\begin{aligned}
H^{atoms} &= \sum_j (-\Delta_j - zN|x_j|^{-1}) + \sum_{j<k} |x_j - x_k|^{-1} \\
&= N^{4/3}\Big(\sum_j (-\hbar^2 \Delta_{y_j} - z|y_j|^{-1}) + N^{-1} \sum_{j<k} |y_j - y_k|^{-1} \Big)
\end{aligned}
$$

with $y_j = N^{1/3} x_j$, $\hbar = N^{-1/3}$.
Ground state energy is given by (Lieb&Simon)

$$\inf \mathrm{Spec}\, H^{atoms} = N^{7/3} e_{TF}^{atoms} + o(Z^{7/3}).$$

Higher order correction terms have been proved

- Scott-correction $O(Z^2)$ (Siedentop-Weikard, Ivrii-Sigal)
- Dirac-Schwinger term $O(Z^{5/3})$ (Fefferman-Seco).

Vlasov and Thomas-Fermi energies

The Vlasov energy

$$\mathcal{E}_{\mathrm{Vla}}^{V,A}(m) = \frac{1}{(2\pi)^d}\int_{\mathbb{R}^{2d}} |p+A(x)|^2 m(x,p)\,dx\,dp + \int_{\mathbb{R}^d} V(x)\rho_m(x)\,dx$$
$$+\frac{1}{2}\iint_{\mathbb{R}^d\times\mathbb{R}^d} w(x-y)\rho_m(x)\,\rho_m(y)\,dx\,dy.$$

Here $m(x,p)$ is a probability measure on the phase space $\mathbb{R}^d \times \mathbb{R}^d$

$$\rho_m(x) = \frac{1}{(2\pi)^d}\int_{\mathbb{R}^d} m(x,p)\,dp,$$

and

$$\boxed{0 \le m(x,p) \le 1 \quad \text{a.e.}}$$

This condition says that one cannot put more than one particle at x with a momentum p and it is inherited from the Pauli principle.

Vlasov and Thomas-Fermi energies II

With the fermionic constraint, the optimal choice of $m(x,p)$ for a given $\rho(x)$ is

$$\boxed{m_\rho(x,p) = \mathbb{1}_{\{|p+A(x)|^2 \leq c_{\rm TF}\, \rho(x)^{2/d}\}}}$$

This leads to the Thomas-Fermi energy

$$\begin{aligned}\mathcal{E}^V_{\rm TF}(\rho) := \mathcal{E}^{V,A}_{\rm Vla}(m_\rho) = \frac{d}{d+2} c_{\mathsf{TF}} \int_{\mathbb{R}^d} \rho(x)^{1+\frac{2}{d}}\, dx + \int_{\mathbb{R}^d} V(x)\rho(x)\, dx \\ + \frac{1}{2} \iint_{\mathbb{R}^d\times\mathbb{R}^d} w(x-y)\rho(x)\,\rho(y)\, dx\, dy\end{aligned}$$

and where

$$c_{\mathsf{TF}} = 4\pi^2 \Big(\frac{d}{|S^{d-1}|}\Big)^{\frac{2}{d}}.$$

Theorem (Convergence of the ground state energy)

Assume that w is even and that $w, V, |A|^2 \in L^{1+d/2} + L^\infty_\epsilon$ (or V confining). Then we have

$$\boxed{\lim_{N\to\infty} \frac{E(N)}{N} = e^V_{\mathrm{TF}}(1).}$$

Here the Thomas-Fermi energy is,

$$\begin{aligned} e^V_{\mathrm{TF}}(1) &:= \inf\left\{\mathcal{E}^V_{TF}(\rho)\ :\ 0 \le \rho \in L^1 \cap L^{1+2/d}(\mathbb{R}^d),\ \int_{\mathbb{R}^d} \rho = 1\right\} \\ &= \inf_{\substack{0\le m\le 1 \\ (2\pi)^{-d}\int_{\mathbb{R}^{2d}} m=1}} \mathcal{E}^{V,A}_{\mathrm{Vlas}}(m). \end{aligned}$$

Semiclassical measures

Let $f \in L^2(\mathbb{R}^d)$ be real-valued. Define

$$f^{\hbar}_{x,p}(y) = \hbar^{-\frac{d}{4}} f\left(\frac{y-x}{\sqrt{\hbar}}\right) e^{i\frac{p\cdot y}{\hbar}},$$

where we recall that $\hbar = N^{-1/d}$. Then we have the resolution of the identity in $L^2(\mathbb{R}^d)$

$$(2\pi\hbar)^{-d} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} |f^{\hbar}_{x,p}\rangle\langle f^{\hbar}_{x,p}| \, dx \, dp = 1.$$

For any such f and a fermionic N-particle state Ψ_N, we introduce the corresponding k-particle Husimi function

$$\begin{aligned} &m^{(k)}_{f,\Psi_N}(x_1, p_1, ..., x_k, p_k) \\ &\qquad := \left\langle \Psi_N, a^*(f^{\hbar}_{x_1,p_1}) \cdots a^*(f^{\hbar}_{x_k,p_k}) a(f^{\hbar}_{x_k,p_k}) \cdots a(f^{\hbar}_{x_1,p_1}) \Psi_N \right\rangle, \end{aligned}$$

for $k = 1, ..., N$, where a and a^* are the fermionic annihilation and creation operators.

Semiclassical measures

Lemma (Elementary properties of the phase space measures)

For every $1 \leq k \leq N$, the function $m^{(k)}_{f,\Psi_N}$ is symmetric and satisfies

$$0 \leq m^{(k)}_{f,\Psi_N} \leq 1 \quad \textit{a.e. on } \mathbb{R}^{2dk},$$

and

$$\frac{1}{(2\pi)^{dk}} \int_{\mathbb{R}^{2dk}} m^{(k)}_{f,\Psi_N}(x_1, p_1, ..., x_k, p_k)\, dx_1 \cdots dp_k$$
$$= N(N-1)\cdots(N-k+1)\hbar^{dk},$$
$$\frac{1}{(2\pi)^{d}} \int_{\mathbb{R}^{2d}} m^{(k)}_{f,\Psi_N}(x_1, p_1, ..., x_k, p_k)\, dx_k\, dp_k$$
$$= \hbar^d (N-k+1) m^{(k-1)}_{f,\Psi_N}(x_1, p_1, ..., x_{k-1}, p_{k-1}).$$

Semiclassical measures

Fermionic annihilation and creation operators:

$$\begin{cases} a^*(f)a(g) + a(g)a^*(f) = \langle g, f\rangle, \\ a^*(f)a^*(g) + a^*(g)a^*(f) = 0. \end{cases}$$

Equivalently,

$$\begin{aligned} &m^{(k)}_{f,\Psi_N}(x_1, p_1, ..., x_k, p_k) \\ &\quad = \frac{N!}{(N-k)!}\Big\langle \Psi_N, \left(P^{\hbar}_{x_1,p_1} \otimes \cdots \otimes P^{\hbar}_{x_k,p_k} \otimes \mathbb{1}_{N-k}\right)\Psi_N \Big\rangle_{L^2(\mathbb{R}^{dN})} \end{aligned}$$

where $P^{\hbar}_{x,p} := |f^{\hbar}_{x,p}\rangle\langle f^{\hbar}_{x,p}|$ is the orthogonal projection onto $f^{\hbar}_{x,p}$.

Theorem (Convergence of states, confined case)

Extra assumption to the energy theorem: $\lim_{|x|\to\infty} V_+(x) = +\infty$. *Let* $\{\Psi_N\} \subset \bigwedge^N L^2(\mathbb{R}^d)$ *be any sequence such that* $\|\Psi_N\| = 1$ *and*

$$\langle \Psi_N, H_N \Psi_N \rangle = E(N) + o(N).$$

Then there exists a subsequence $\{N_j\}$ *and a probability measure* $\mathcal{P}$ *on the set of all the minimizers of the TF functional*

$$\mathcal{M} = \left\{ 0 \leq \rho \in L^1 \cap L^{1+2/d}(\mathbb{R}^d) \ : \ \int_{\mathbb{R}^d} \rho = 1, \ \mathcal{E}^V_{\mathrm{TF}}(\rho) = e^V_{\mathrm{TF}}(1) \right\}$$

such that the following limit holds:

$$\int_{\mathbb{R}^{2dk}} m^{(k)}_{f,\Psi_{N_j}} \phi \to \int_{\mathcal{M}} \left(\int_{\mathbb{R}^{2dk}} (m_\rho)^{\otimes k} \phi \right) d\mathcal{P}(\rho)$$

for every test function $\phi \in L^1(\mathbb{R}^{2dk}) + L^\infty(\mathbb{R}^{2dk})$.

Theorem (Convergence of states, continued)

Furthermore, we have the convergence of the k-particle probability density

$$\int_{\mathbb{R}^d} \cdots \int_{\mathbb{R}^d} |\Psi_{N_j}(x_1, \ldots, x_{N_j})|^2 \, dx_{k+1} \cdots dx_{N_j} \to \int_{\mathcal{M}} \prod_{j=1}^{k} \rho(x_j) \, d\mathcal{P}(\rho)$$

weakly in $L^1(\mathbb{R}^d) \cap L^{1+\frac{2}{d}}(\mathbb{R}^d)$ for $k = 1$, and weakly-$*$ in the sense of measures for $k \geq 2$.

Finally, we have the convergence of the k-particle kinetic energy density

$$\int_{\mathbb{R}^d} \cdots \int_{\mathbb{R}^d} \left| \mathcal{F}_\hbar[\Psi_{N_j}](p_1, \ldots, p_{N_j}) \right|^2 dp_{k+1} \cdots dp_{N_j}$$

$$\to \int_{\mathcal{M}} \prod_{\ell=1}^{k} \left| \left\{ \rho \geq |p_\ell + A|^d c_{\mathrm{TF}}^{-d/2} \right\} \right| \, d\mathcal{P}(\rho),$$

weakly-$*$ in the sense of measures for $k \geq 1$.

In the last statement,

$$\mathcal{F}_\hbar[f](p) := \frac{1}{(2\pi\hbar)^{d/2}} \int_{\mathbb{R}^d} f(x) e^{-i\frac{p\cdot x}{\hbar}}\, dx$$

is the $\hbar$-dependent Fourier transform.

The result says that, in the limit $N \to \infty$, the many-body approximate minimizers Ψ_N become purely semi-classical to leading order and that the corresponding semi-classical measures are a convex combination of factorized states involving the Vlasov minimizers m_ρ with $\rho \in \mathcal{M}$. Note that if the Thomas-Fermi energy has a unique minimizer ρ_0, then there is no need to extract subsequences and the probability measure $\mathcal{P}$ has to be a delta measure at ρ_0.

The unconfined case

In the unconfined case we have a similar result, except that the limits are *a priori* local. Since some of the particles can escape to infinity, our result will involve the minimizers of the problems $e^V_{\rm TF}(\lambda)$ for a mass $0 \leq \lambda \leq 1$.

Recall:

$$e^V_{\rm TF}(\lambda) := \inf \left\{ \mathcal{E}^V_{TF}(\rho) \ : \ 0 \leq \rho \in L^1(\mathbb{R}^d) \cap L^{1+2/d}(\mathbb{R}^d), \ \int_{\mathbb{R}^d} \rho = \lambda \right\},$$

$$\begin{aligned} \mathcal{E}^V_{\rm TF}(\rho) = \frac{d}{d+2} c_{\mathsf{TF}} \int_{\mathbb{R}^d} \rho(x)^{1+\frac{2}{d}}\, dx + \int_{\mathbb{R}^d} V(x) \rho(x)\, dx \\ + \frac{1}{2} \iint_{\mathbb{R}^d \times \mathbb{R}^d} w(x-y) \rho(x)\, \rho(y)\, dx\, dy \end{aligned}$$

Theorem (Convergence of states, unconfined case)

Assumptions as for energy convergence, plus

$$V_+ \in L^{1+d/2}(\mathbb{R}^d) + L^\infty_\epsilon(\mathbb{R}^d).$$

Let $\{\Psi_N\} \subset \bigwedge^N L^2(\mathbb{R}^d)$ *be any sequence such that* $\|\Psi_N\| = 1$ *and*

$$\langle \Psi_N, H_N \Psi_N \rangle = E(N) + o(N).$$

Then there exists a subsequence $\{N_j\}$ *and a probability measure* $\mathcal{P}$ *on the set*

$$\mathcal{M} = \Big\{ 0 \le \rho \in L^1(\mathbb{R}^d) \cap L^{1+2/d}(\mathbb{R}^d) \ : \ \int_{\mathbb{R}^d} \rho \le 1, \\ \mathcal{E}^V_{\mathrm{TF}}(\rho) = e^V_{\mathrm{TF}}\Big(\int_{\mathbb{R}^d} \rho\Big) = e^V_{\mathrm{TF}}(1) - e^0_{\mathrm{TF}}\Big(1 - \int_{\mathbb{R}^d} \rho\Big) \Big\}$$

To be continued...

Theorem (Continued)

such that

$$\int_{\mathbb{R}^{2dk}} m^{(k)}_{f,\Psi_{N_j}} \phi \to \int_{\mathcal{M}} \left(\int_{\mathbb{R}^{2dk}} (m_\rho)^{\otimes k} \phi \right) \, d\mathcal{P}(\rho)$$

for every test function $\phi \in L^1(\mathbb{R}^{2dk}) + L^\infty_\epsilon(\mathbb{R}^{2dk})$.

- A similar convergence result holds for the k-particle density but is not known for the k-particle kinetic energy density.
- Notice that $\mathcal{M}$ is the set of all the possible weak limits of minimizing sequences for the Thomas-Fermi problem.

In the unconfined case some particles may be lost at infinity (if not all), and the limiting minimizing densities ρ might not be probability measures. Nevertheless, the result says that the remaining particles must solve the minimization problem $e^{V}_{\rm TF}(\int \rho)$, corresponding to the fraction $\int_{\mathbb{R}^d} \rho$ of the N particles which have not escaped to infinity. Furthermore, if no particle is lost ($\int_{\mathbb{R}^d} \rho = 1$ on $\mathcal{M}$), then the convergence is the same as in the confined case.

Structure of measures for large N

Theorem (Convergence to factorized measures on phase space)

Let Ψ_N be a seq. of normalized fermionic functions, $\hbar = N^{-1/d}$. Then, there exists a subseq. N_j and a probability measure P on

$$\mathcal{B} = \left\{ \mu \in L^1(\mathbb{R}^{2d}) \ : \ 0 \leq \mu \leq 1, \ (2\pi)^{-d} \int_{\mathbb{R}^{2d}} \mu \leq 1 \right\}$$

such that, for every $k \geq 1$,

$$\int_{\mathbb{R}^{2dk}} m^{(k)}_{f,\Psi_{N_j}} \phi \to \int_{\mathcal{B}} \left(\int_{\mathbb{R}^{2dk}} \mu^{\otimes k} \phi \right) \, d\mathrm{P}(\mu),$$

for every normalized, real-valued function $f \in L^2(\mathbb{R}^d)$ and every $\phi \in L^1(\mathbb{R}^{2dk}) + L^\infty_\epsilon(\mathbb{R}^{2dk})$.

The confined case

For an arbitrary sequence (Ψ_N), the functions $(m^{(k)}_{f,\Psi_N})_{N\geq k}$ are bounded in $L^1(\mathbb{R}^{2dk}) \cap L^\infty(\mathbb{R}^{2dk})$, for every fixed k.

Clearly up to a subsequence (and a diagonal sequence argument)

$$\int_{\mathbb{R}^{2dk}} m^{(k)}_{f,\Psi_N}\phi \to \int_{\mathbb{R}^{2dk}} m^{(k)}_f \phi$$

for every $\phi \in L^1(\mathbb{R}^{2dk}) + L^\infty_\epsilon(\mathbb{R}^{2dk})$.

In the limit we obtain a family of symmetric functions $(m^{(k)}_f)_{k\geq 1}$.

Some mass can be lost at infinity, so $\int m^{(k)}_f \leq 1$.

However, if the sequence $(m^{(1)}_{f,\Psi_N})$ is tight, that is,

$$\lim_{R\to\infty} \limsup_{N\to\infty} \int_{|x|+|p|\geq R} m^{(1)}_{f,\Psi_N}(x,p)\,dx\,dp = 0,$$

then the $m^{(k)}_{f,\Psi_N}$ are also tight for $k \geq 2$ and the limiting $m^{(k)}_f$ are all probability measures.

Using the tightness, we get the consistency condition, for all $k \geq 1$:

$$\frac{1}{(2\pi)^d} \int_{\mathbb{R}^{2d}} m^{(k)}(x_1, ..., x_k, p_k)\, dx_k\, dp_k = m^{(k-1)}(x_1, ..., x_{k-1}, p_{k-1})$$

The famous de Finetti-Hewitt-Savage theorem deals with the structure of such infinite sequences of symmetric probability measures. In our situation, the result can be stated as follows.

Theorem (Fermionic semi-classical measures on phase space)

Let $m^{(k)}$ be a consistent family of symmetric positive densities in $L^1(M^k)$, with $M \subset \mathbb{R}^D$, with $m^{(0)} = 1$ and $0 \leq m^{(k)} \leq 1$. Then there exists a Borel probability measure P on the set

$$\mathcal{S} := \left\{ \mu \in L^1(M) \ : \ 0 \leq \mu \leq 1,\ (2\pi)^{-d} \int_M \mu = 1 \right\}$$

such that, for all $k \geq 1$,

$$m^{(k)} = \int_{\mathcal{S}} \mu^{\otimes k}\, d\mathrm{P}(\mu),$$

Proof.

The usual theorem furnishes a probability measure P on the set $\mathcal{P}(M)$ of all the Borel probability measures on M such that the conclusion holds with $\mathcal{S}$ replaced by $\mathcal{P}(M)$.

We therefore only have to prove that this measure P has its support on $\mathcal{S}$, which can be identified as a subset of $\mathcal{P}(M)$. The assumption that $0 \leq m^{(k)} \leq 1$ implies $m^{(k)}(A^k) \leq |A|^k$ for any Borel set $A \subset M$, and this gives (for all k)

$$\int_{\mathcal{P}(M)} \left(\frac{\mu(A)}{|A|} \right)^k \, d\mathrm{P}(\mu) \leq 1.$$

Taking $k \to \infty$ proves that P is supported on the subset of $\mathcal{P}(M)$ containing all the probability measures μ such that $\mu(A) \leq |A|$ for all Borel sets A.

These measures are absolutely continuous with respect to Lebesgue measure and the corresponding density is between 0 and 1. $\square$