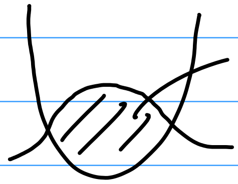
MEAN FIELD EVOLUTION OF FERMIONIC MIXED STATES

22. Sept 2015

Phys. setting: V_{trap} confining:



$\longrightarrow$ $V_{trap} = 0$: Time evolution:

exact: Schrödinger equ. $\xrightarrow{N\to\infty}$ mean field: Hartree-Fock eq.

interact. not too strong

- ground state: gives start point

$T=0$: $i\hbar\partial_t \Psi_{N,t} = \left[-\hbar^2 \sum_{i=1}^{N} -\Delta_i + \lambda \sum_{i<j}^{N} V(x_i - x_j)\right] \Psi_{N,t}$

$\Psi_{N,t} \in L^2_a(\mathbb{R}^{3N})$, $\Psi_{N,0} = \text{Slaterd.} = \frac{1}{\sqrt{N!}} \sum_{\sigma\in S_N} \varphi_{\sigma(1)} \otimes \dots \otimes \varphi_{\sigma(N)}$

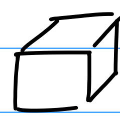
$(\varphi_j \in L^2(\mathbb{R}^3))$

$\hbar = N^{-1/3}$: why?

$i\hbar\partial_t \omega_{N,t} = [-\hbar^2\Delta + V * \varrho_t - X_t, \omega_{N,t}]$

$\omega_{N,t}$: one-particle reduced density trace-class op. on $L^2(\mathbb{R}^3)$, $0 \leq \omega_{N,t} \leq \mathbb{1}$, $\operatorname{tr} \omega_{N,t} = N$.

Consider $i\partial_t \Psi_{N,t} = \left[-\sum_i \Delta_i + \lambda \sum_{i<j} V(x_i - x_j)\right] \Psi_{N,t}$.



Initial data in box side length 1:

$\longrightarrow$ kinetic part $\sim N^{5/3}$ $\Longrightarrow \lambda = N^{-1/3}$.

High velocity: New time scale: $N^{-1/3}$.

$\longrightarrow N^{1/3}$ at $i\partial_t$.

Multiply all by $\hbar^2$ $\longrightarrow$ eq. as stated.

multiplication op. $V * \varrho_t(x) = \int dy \frac{1}{N} V(x-y)\, \omega_{N,t}(y,y)$ direct term

Integral op. with kernel $X_t(x,y) = \frac{1}{N} V(x-y)\, \omega_{N,t}(x,y)$

$[\,,\,]$: commutator

Thm: (B-Porta-Schlein)

Let $\gamma^{(1)}_{N,t} := N \operatorname{tr}_{2,\dots,N} |\Psi_{N,t}\rangle\langle\Psi_{N,t}|$,

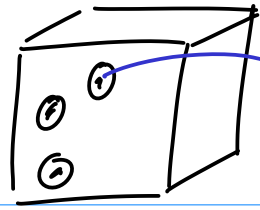
let $\omega_{N,0} = \gamma^{(1)}_{N,0}$ and $\|\overbrace{[x, \omega_{N,0}]}^{\text{position}}\|_{tr} \leq CN\hbar$, $\|\overbrace{[-i\hbar\nabla, \omega_{N,0}]}^{\text{momentum}}\|_{tr} \leq CN\hbar$,

then $\|\gamma^{(1)}_{N,t} - \omega_{N,t}\|_{tr} \leq C \underbrace{N^{1/6}}\, e^{ce^{ct}}$ $(N\to\infty)$.

reads: $\gamma^{(1)}_{N,t} \sim N$, $\omega_{N,t} \sim N$, $\to$ rel. $N^{-5/6}$.

Another word of comment about this commutator assumptions: actually not trivial to prove, but we can construct examples which let us understand that they tell us that we start from a trapped g.s.; stability to translation (if you have a general proof...) $\longrightarrow$ anyway, I will be able to say a bit more for $T>0$.

examples:



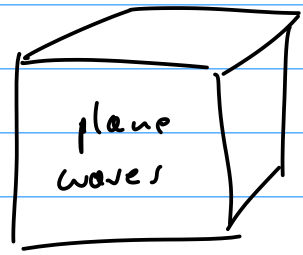
very localized, no overlap

$\Downarrow$

$[-it\partial, \omega_{N,0}]$ large.

no

But of course this initial data is far from being a equilibrium state.



$\rightarrow$ commutator estimates are satisfied. $\longrightarrow$ yes

Good approx. to equilibrium (e.g. given by ~~HF~~ in p.h.c.)

More in a moment for $T > 0$.

$T>0$: Initial data: grand canonical ensemble:

Density matrix $\rho \in \mathcal{F} = \bigoplus_{n\geq 0} L^2_a(\mathbb{R}^{3n})$ different particle numbers

ρ: traceclass op. on $\mathcal{F}$, $\rho \geq 0$, $\operatorname{tr} \rho = 1$. instead of a vector in $L^2(\mathbb{R}^{3N})$

e.g. Gibbs state $\rho = \dfrac{e^{-\beta(H-\mu\mathcal{N})}}{\operatorname{tr} e^{-\beta(H-\mu\mathcal{N})}}$. β = inverse temp

In general very complic. but $\exists$ convenient class. To def. this, let me first def.

One-particle reduced density: $\gamma^{(1)}(x,y) = \operatorname{tr} a_y^* a_x \rho$

2-particle " " : $\gamma^{(2)}(x_1,x_2,y_1,y_2) = \operatorname{tr} a^*_{y_2} a^*_{y_1} a_{x_1} a_{x_2} \rho$.

- Quasifree: If H non-interacting e.g. free Laplacian

$$\gamma^{(2)}(x_1,x_2,y_1,y_2) = \gamma^{(1)}(x_1,y_1)\gamma^{(1)}(x_2,y_2) - \gamma^{(1)}(x_1,y_2)\gamma^{(1)}(x_2,y_1)$$ etc. for k-particle densities

Natural general. of Slater dets from zero temp. to positive temp.; you can easily check that Slater satisfy this;
this prop. is the crucial ingredient to HF - if all states were quasifree there would only be HF.

- Semiclassical commutators: take into account interact. approx. by T.F.:

Weyl quant.: $\gamma^{(1)}(x,y) \simeq \dfrac{1}{(2\pi)^3}\displaystyle\int dp\, M\!\left(\frac{x+y}{2}, p\right) e^{ip\cdot\frac{x-y}{\hbar}}$,

$$M(x,p) = f_{T,\mu}\left(p^2 - c\,\rho_{TF}^{2/3}(x)\right)$$

phase space density

Fermi dist.

$$f_{T,\mu}(E) = \frac{1}{1+e^{(E-\mu)/T}}$$

TF density, minimizing

$$\mathcal{E}_{TF}(\rho) = \frac{3}{5}\hbar^2 \int \rho^{5/3} + \int V_{ext}\,\rho + \iint \rho(x)V(x-y)\rho(y)\,dx\,dy,$$

$\int \rho = N$.

$$[x,\gamma^{(1)}](x,y) \simeq (x-y)\frac{1}{(2\pi)^3}\int dp\, M\left(\frac{x+y}{2},p\right) e^{ip\frac{x-y}{\hbar}}$$

$$= -i\hbar \frac{1}{(2\pi)^3}\int dp\, \nabla_p M\left(\frac{x+y}{2},p\right) e^{ip\frac{x-y}{\hbar}}$$

$$\Rightarrow \|[x,\gamma^{(1)}]\|_{HS} \lesssim \hbar N^{1/2} \int dp\,dx\, |\nabla_p M(x,p)|^2; \quad \|[-i\hbar\nabla,\gamma^{(1)}]\|_{HS} \leq C\hbar N^{1/2}.$$

HS norm: for $T>0$ natural;
for $T=0$ M is step fct., so this
argument here fails & only trace norm
remains possible

$\longrightarrow$ Central assumptions on initial data:
QUASIFREE + SEMICLASS
strictly analogous to $T=0$.

<u>Thm:</u> (B–Jakšić–Porta–Saffirio–Seiler)

Let
- interaction V with $\int dp\,(1+|p|^2)\,\hat{V}(p) < \infty$.
- ω_N a family of fermionic 1-pdms s.th.

$$\left.\begin{aligned} &\|[x,\sqrt{\omega_N}]\|_{HS},\ \|[-i\hbar\nabla,\sqrt{\omega_N}]\|_{HS} \\ &\|[x,\sqrt{1-\omega_N}]\|_{HS},\ \|[-i\hbar\nabla,\sqrt{1-\omega_N}]\|_{HS}\end{aligned}\right\} \leq C\hbar N^{1/2}.$$

- ρ_N (approximately) a quasifree possibly mixed state with $\gamma_N^{(1)} = \omega_N$.
- $\gamma_{N,t}^{(1)}$ the 1-pdm. of $e^{-iH_N t/\hbar}\rho_N e^{iH_N t/\hbar}$.

Then:
$$\|\gamma_{N,t}^{(1)} - \omega_{N,t}\|_{HS} \leq C e^{ce^{ct}},$$

where $\omega_{N,t}$ solves $i\hbar\partial_t\omega_{N,t} = [-\hbar^2\Delta + V*\rho_t - X_t, \omega_{N,t}]$,
$$\omega_{N,0} = \omega_N.$$

<u>Proof:</u> 1) "Purify": mixed state on $\mathcal{F}(L^2(\mathbb{R}^3)) \longmapsto$ pure state in $\mathcal{F}(L^2(\mathbb{R}^3)\oplus L^2(\mathbb{R}^3))$.
2) represent through a Bog. trafo: $R_N\Omega$.
3) compare SE and HF through
bound "# excitations" w.r.t. HF evolved $R_{N,t}\Omega$
through Gronwall. Follows quite closely "coherent states method"
from bosonic m.f. theory.

1) <u>Purification</u> (Araki - Wyss):

- spectral decomposition: $\varrho = \sum_n \lambda_n |\psi_n\rangle\langle\psi_n|$ trace class
- square root: $\tilde{\kappa} = \sum_n \sqrt{\lambda_n}\, |\psi_n\rangle\langle\phi_n|$ HS

orthonormal set, free to choose

- $\mathcal{L}^2(\mathcal{F}) \simeq \mathcal{F} \otimes \overline{\mathcal{F}}$: lin. ext. $\kappa = \sum_n \sqrt{\lambda_n}\, \psi_n \otimes \overline{\phi_n}$.

HS op.

- $\mathcal{F}(L^2(\mathbb{R}^3)) \otimes \mathcal{F}(L^2(\mathbb{R}^3)) \simeq \mathcal{F}(L^2(\mathbb{R}^3) \oplus L^2(\mathbb{R}^3))$: "exponential law"

$$\begin{aligned} U: \quad \Omega &\mapsto \Omega \\ a(f) \otimes 1 &\mapsto a(f \oplus 0) =: a_\ell(f) \\ (-1)^{\mathcal{N}} \otimes a(f) &\mapsto a(0 \oplus f) =: a_r(f). \end{aligned}$$

guarantees that a_ℓ and a_r anticommute

acting from left; i.e. on left tensor (fixed by choice of square root)

$$\boxed{\begin{aligned} \operatorname{tr} B \varrho &= \operatorname{tr} B \tilde{\kappa}\tilde{\kappa}^* = \langle \kappa, (B \otimes 1)\kappa \rangle_{\mathcal{F}(L^2)\otimes \mathcal{F}(L^2)} \\ &= \langle U\kappa, B_\ell U\kappa \rangle_{\mathcal{F}(L^2 \oplus L^2)} = \operatorname{tr}_{L^2(\mathbb{R}^3)} b\, \gamma^{(1)}_{U\kappa}. \end{aligned}}$$

operator on $\mathcal{F}$; observable

write out

$B = \int b(x,y)\, a_x^* a_y$

1-part operator

$\operatorname{tr} b\, \gamma^{(1)}_{SW}$ //

$$\gamma^{(1)}_{U\kappa}(x,y) = \langle U\kappa, a^*_{y,\ell}\, a_{x,\ell}\, U\kappa \rangle$$

So what we do is:
- ϱ is given
- determine corresponding $U\kappa$
- translate the time-evol. of ϱ into time evol. $U\kappa$ through the chain of isomorphisms
- compare 1-pdm. of $U\kappa$ to 1-pdm. from HF.

<u>$U\kappa$ is pure</u> $\rightsquigarrow$ machinery of Bog. trafos applys.

<u>Time evolution:</u>

write out with op. valued dist.

$$\varrho_t = e^{-iHt/\hbar} \varrho\, e^{iHt/\hbar} \mapsto \tilde{\kappa}_t = e^{-iHt/\hbar} \tilde{\kappa}\, e^{iHt/\hbar} \mapsto \kappa_t = (e^{-iHt/\hbar} \otimes e^{iHt/\hbar})\kappa$$

$$= e^{-i(H\otimes 1 - 1 \otimes H)t/\hbar} \kappa \longmapsto e^{-i(H_\ell - H_r)t/\hbar}\, U\kappa =: e^{-i\mathcal{L}t/\hbar}\, U\kappa.$$

2) Representing $U\mathcal{K} \in \mathcal{F}(L^2 \oplus L^2)$ through a Bogoliubov trafo:

Let $A(f,g) := a(f) + a^*(\bar{g})$, $f,g \in L^2 \oplus L^2$. $(f,g) \in (L^2\oplus L^2)\oplus(L^2\oplus L^2)$

Then: i) $A^*(f,g) = A\left(\begin{pmatrix} 0 & \mathcal{J} \\ \mathcal{J} & 0 \end{pmatrix}\begin{pmatrix} f \\ g \end{pmatrix}\right)$, $\mathcal{J} =$ c.c.

ii) $\{A(f_1,g_1), A^*(f_2,g_2)\} = \langle (f_1,g_1),(f_2,g_2)\rangle_{(L^2\oplus L^2)\oplus(L^2\oplus L^2)}$.

A Bogoliubov trafo is a linear $\nu : (L^2\oplus L^2)\oplus(L^2\oplus L^2) \circlearrowleft$ on itself s.th. $B(f,g) := A(\nu(f,g))$ satisfies i), ii) as well.

$$\Rightarrow \quad \nu = \begin{pmatrix} U & \bar{V} \\ V & \bar{U} \end{pmatrix}, \quad \begin{matrix} U^*U + V^*V = \mathbb{1}_{L^2\oplus L^2} \\ U^*\bar{V} + V^*\bar{U} = 0. \end{matrix} \qquad U,V : L^2\oplus L^2 \circlearrowleft$$

$\mathcal{J}U\mathcal{J} = \bar{U}$

conjugate with c.c. integral kernel just c.c.

Central for our construction:

Thm. (Shale-Stinespring): $\exists R : \mathcal{F}(L^2\oplus L^2) \circlearrowleft$ unitary s.th. $R^* A(f,g) R = A(\nu(f,g))$ iff V is H.S.

Choose $U = \begin{pmatrix} u_N & 0 \\ 0 & u_N \end{pmatrix}$, $V = \begin{pmatrix} 0 & \bar{v}_N \\ -v_N & 0 \end{pmatrix}$, $u_N = \sqrt{1-\omega_N}$, $v_N = \sqrt{\omega_N}$.

V is HS. Let $\underline{\psi := R\Omega}$. candidate for representing initial data.

Let us verify that this is right repres. of initial data:

$$R^* a_\ell(f) R = R^* a(f\oplus 0) R = R^* A(f\oplus 0, 0) R$$
$$= A\left(\begin{pmatrix} U & \bar{V} \\ V & \bar{U} \end{pmatrix}\begin{pmatrix} f\oplus 0 \\ 0 \end{pmatrix}\right) = A\left(\begin{pmatrix} u_N & 0 \\ 0 & u_N \end{pmatrix}\begin{pmatrix} f \\ 0 \end{pmatrix}, \begin{pmatrix} 0 & \bar{v}_N \\ -v_N & 0 \end{pmatrix}\begin{pmatrix} f \\ 0 \end{pmatrix}\right)$$
$$= A(u_N f \oplus 0, 0 \oplus -v_N f) = a_\ell(u_N f) - a_r^*(v_N f).$$

(*)
$$\gamma^{(1)}(x,y) = \langle R\Omega, a^*_{y,\ell}\, a_{x,\ell} R\Omega\rangle$$
$$= \langle \Omega, (a^*_\ell(u_N(\cdot,y)) - \underline{a_r(v_N(\cdot,y))})(a_\ell(u_N(\cdot,x)) - \underline{a^*_r(\bar{v}_N(\cdot,x))})\Omega\rangle$$
$$= \{a_r(v_N(\cdot,y)), a^*_r(\bar{v}_N(\cdot,x))\} = (v_N^* v_N)(x,y) = \sqrt{\omega_N}\sqrt{\omega_N}(x,y) = \omega_N(x,y).$$

Convince yourself that $R\Omega$ is quasifree $\rightarrow$ since $\gamma^{(1)}$ is correct, it gives <u>all</u> reduced densities correctly. (and $\alpha(x,y) = 0$)

$$\boxed{\begin{array}{l} \Rightarrow \text{Instead of } \varrho_N \text{ with 1-pdm. } \omega_N \text{ and evolution } e^{-iHt/\varepsilon}\varrho_N e^{iHt/\varepsilon}, \\ \text{we can look directly at } R\Omega \text{ with evolution } e^{-i\mathcal{L}t/\varepsilon} R\Omega. \end{array}}$$

3) Comparing $e^{-iLt/\hbar} R\Omega$ with $R_t \Omega$:

(where R_t is defined as the BT s.th. it's reduced density is $\omega_{N,t}$, the HF solution — notice that there is no direct way of calculating $e^{-iLt/\hbar} R\Omega$, again: this is just another way of writing the full, interacting Schrödinger evolution!)

Same calc. as (*) $\Rightarrow$ $\| \gamma^{(1)}_{N,t} - \omega_{N,t} \|_{HS} \leq \langle R_t^* e^{-iLt/\hbar} R\Omega, (\mathcal{N}_e + \mathcal{N}_r) \times R_t^* e^{-iLt/\hbar} R\Omega \rangle$

from $e^{-iLt/\hbar} R\Omega$ from $R_t\Omega$

in the spirit of bosonic theory

$=: \langle \mathcal{U}(t)\Omega, (\mathcal{N}_e + \mathcal{N}_r)\mathcal{U}(t)\Omega \rangle$

Calc. $\hbar \frac{d}{dt} \langle \mathcal{U}(t)\Omega, (\mathcal{N}_e + \mathcal{N}_r)\mathcal{U}(t)\Omega \rangle$:

- HF eqn. shows up as cancellation of all terms $(a^\#)^2$
- remaining: $(a^\#)^4$; to be bounded with $(\mathcal{N}_e + \mathcal{N}_r)$ (Grönwall!)

$\times$ factor $\hbar$ to compensate the $\hbar$'s going with all the time derivatives

$\longrightarrow$ use $\| [x, \nu_N] \| \leq C N^{1/2} \hbar$ etc.

(propagated to time t, $\nu_{N,t} = \sqrt{\omega_{N,t}}$)

Vlasov equation: HF eqn. dep. on $\hbar = N^{-1/3}$:

$$i\hbar \partial_t \omega_{N,t} = [-\hbar^2 \Delta + V * \varrho_t - X_t, \omega_{N,t}].$$

What do we get for $\hbar \longrightarrow 0$?

Wigner transform: (inverse Weyl quantization)

easy heuristic calculation

$$W_{N,t}(x,p) = \frac{1}{(2\pi)^3 N} \int dy \, \omega_{N,t}\left(x + \frac{\hbar y}{2}, x - \frac{\hbar y}{2}\right) e^{iy\cdot p} \qquad (x,p) \in \mathbb{R}^3 \times \mathbb{R}^3$$

$$\Rightarrow \partial_t W_{N,t} + 2p \cdot \nabla_x W_{N,t} = -\nabla(V * \varrho_t) \cdot \nabla_p W_{N,t} + \mathcal{O}(\hbar)$$

Easy if you have very regular $W_{N,0}$.

Not natural; we can't expect much more than

$\nabla_p W_{N,0} \sim [x, \omega_{N,t}]$ and $\nabla_x W_{N,0} \sim [-i\hbar\nabla, \omega_{N,t}]$.

Most recent of our papers in this line: ok for "semiclass. observables".

with Porta - Saffirio - Schlein.