ATOMISM & QUANTIZATION

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Hepp, Spohn, Erdös,
Schlein; & others.

Introduction

Here is what this lecture will be about:

1. Atomism by deformation-quantization-of cont. field theories of matter
2. Hamiltonian continuum theories of matter as mean-field limits of atomistic theories - a Egorov theorem
3. Newtonian "point particles as "solitons" of continuum theories

Many applications to Physics & Math!

Mathematical themes underlying this lecture

(1) Quantization $\longleftrightarrow$ deformations of assoc. algebras (Poisson br. $\rightarrow$ commutators; Fock space)

(2) Semi-class. analysis for systs. w. ∞ many degs. of freedom (Egorov thm. ...)

(3) NL Hamiltonian evolution equations, soliton dyn.

1. Atomism as quantization

Major developments in 20th Century Physics:

(i) Atomistic constitution of matter $\leftrightarrow$ N_A^{-1}

Three revolutions:

(ii) Quantum Th. $\leftrightarrow$ $\hbar$

(iii) STR $\leftrightarrow$ c^{-1}

(iv) GR $\leftrightarrow$ l_P

deformation parameters

+ combinations of (i)–(iv): Quantum Stat. Mech. & many-body th., RQFT, gauge th.

(i)–(iv) arise by 'deformation' from precursor ths.

<u>To be understood</u>:

$\underline{N_A^{-1}, \hbar}|$

(a) TD $\leftrightarrow$ stat. mech.

(b) Irrev. beh., transport th., quantum Brownian m., …

(c) Deeper meaning of QM

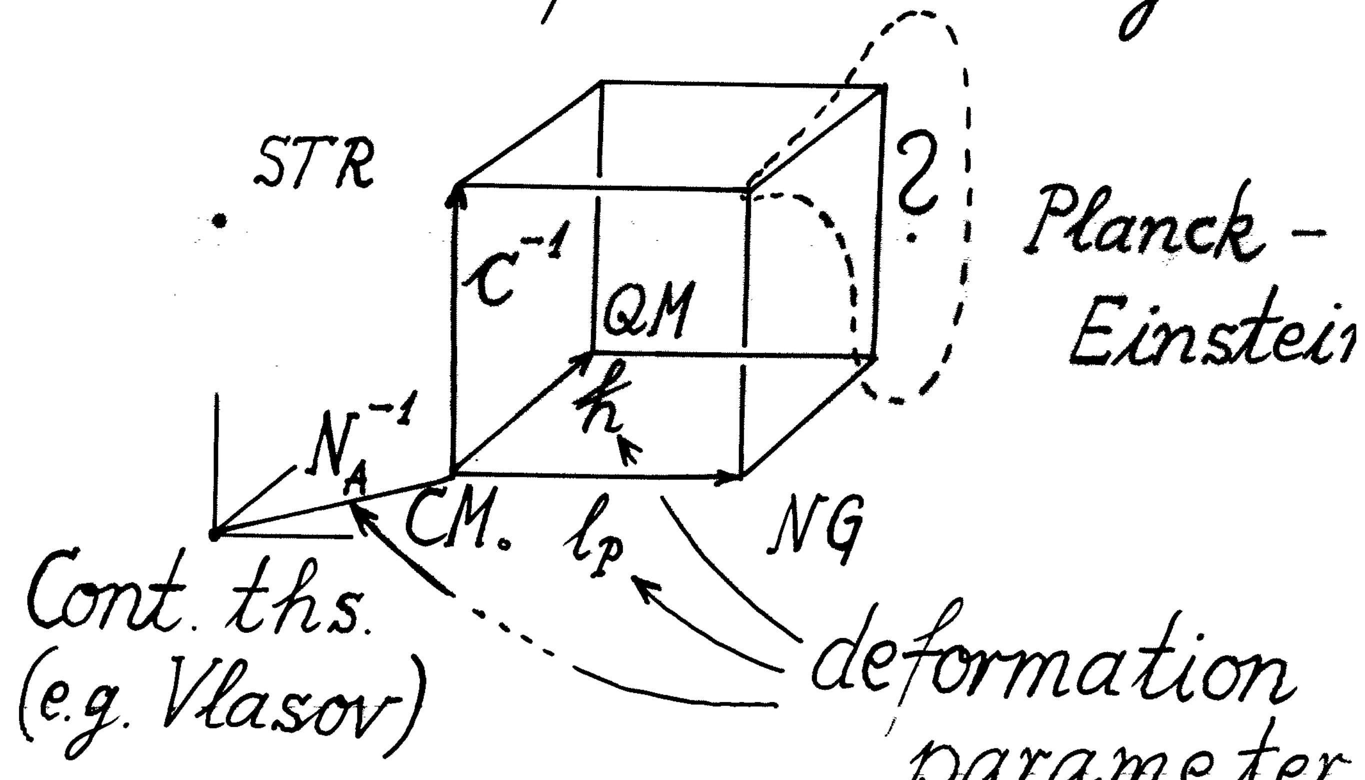
$\underline{\hbar, c^{-1}, l_P}|$

(d) RQFT; emergence of space-time, causal structure, gravitation, …

1st step: <u>Atomism</u>

1. Atomism as quantization

Reflection on main changes in "Weltbild" of 20th Cent. Physics.



(Verification of) old paradigm:

Atomism $\longleftrightarrow$ N_A^{-1}

Three revolutions:

QM $\longleftrightarrow$ $\hbar$

STR $\longleftrightarrow$ c^{-1}

GR $\longleftrightarrow$ l_P

?

21st Cent.: ? $\longleftrightarrow$ α', a_{-}

Atomism

Über das Boltzmann'sche Prinzip und einige unmittelbar aus demselben fliessende Folgerungen.

Die Thermodynamik beruht ~~bekanntlich~~ auf zwei Prinzipien, dem Energieprinzip (auch 1. Hauptsatz genannt) und dem Prinzip von der Nichtumkehrbarkeit des Naturgeschehens (auch 2. Hauptsatz genannt). ~~Letzteres ist Prinzip ... sagt aus,~~ Der Inhalt des letzteren Prinzip lässt sich ~~... Planck'schen~~ nach Planck so aussprechen:

Alle Naturwissenschaft ist auf die Voraussetzung der vollständigen ~~lückenlosen~~ kausalen Verknüpfung jeglichen Geschehens begründet. Nehmen wir an, ~~Wenn~~ Galilei hätte bei seinen ~~Fall- und~~ Pendelversuchen gefunden ~~hätte~~, dass dasselbe Pendel so schwingt, dass die Dauer einer Schwingung in unregelmässiger Weise wechselt, Nehmen wir ferner an, ~~ohne~~ dass dieser Wechsel mit dem Wechsel ~~mit~~ irgend welcher anderer beobachtbarer Verhältnisse nicht hätte in Verbindung gebracht werden können. Dann wäre es Galilei unmöglich gewesen, ~~wohl kaum eingefallen~~ seine Beobachtungen zu einem Gesetze zu vereinigen. Hätten alle uns zugänglichen Erscheinungen einen derart unregelmässigen Charakter, wie wir dies in dem soeben fingierten Falle uns vorgestellt haben, so wären die Menschen gewiss nie auf naturwissenschaftliche Bestrebungen verfallen.

Welchen Charakter mussten die Erscheinungen haben, damit Wissenschaft möglich sei? Darauf möchte man zuerst etwa folgendermassen antworten: Bringen wir ein System in einen bestimmten Zustand, so ist, falls das System von anderen Systemen – etwa durch grosse räumliche Entfernung getrennt ist, so ist ~~der~~ zeitliche Ablauf der Zustände dieses Systems vollkommen bestimmt; d. h. bringen wir beliebig viele ~~zwei~~ gleichbeschaffene isolierte Systeme in genau denselben Zustand und überlassen wir diese Systeme sich selbst, so ist für alle diese Systeme der zeitliche Ablauf der Erscheinungen genau derselbe.

A. Einstein

1911

"Hier (in quantum th.) liegt der Schlüssel der Situation der Schlüssel nicht nur zur Strahlungstheorie, sondern auch zur molekularen (atomistic) Konstitution der Materie ..."

A. Sommerfeld, "Das Plancksche Wirkungsquantum & seine allg. Bedeutung für die Molekularphysik".

Spectroscopy; Brownian motion (Einstein, Perrin, ...)

1.1. Newtonian Mechanics as "quantization" of Vlasov Mech

"Stellar dust" descr. as class continuous medium; states given by mass density

$$M f(x,p)\,dx\,dp$$

on $\mathbb{R}^3_{position} \times \mathbb{R}^3_{velocity}$, with

$$\int f(x,p)\,dx\,dp = \nu$$

(ν : # moles of dust)

Time-dependence of $f(x,p)$ given by Vlasov Equation.

This is a model of matter as a continuous medium!

Vlasov Eq.

$$\partial_t f_t(x,p) = -\frac{1}{M}(p \cdot \nabla_x f_t)(x,p)$$
$$+ (\nabla V_{eff}[f_t] \cdot \nabla_p f_t)(x,p),$$

$$V_{eff}(x) := V(x) + \int dy\, \phi(x-y) \times$$
$$\times \int dp\, f_t(y,p)$$

ϕ : reg. Newtonian pot.

& Neunzert

Braun-Hepp : Vlasov is mean-field limit of $n = \nu N_A$ point particles w. mass $m = \frac{M}{N_A}$, 2-body pot. $\frac{1}{N_A}\phi$, as $N_A \to \infty$.

Vlasov dynamics is Hamiltonian dynamics:

$$f(x,p) = \overline{\alpha(x,p)} \cdot \alpha(x,p),$$

$$\alpha \in \Gamma = H^1(\mathbb{R}^6), \quad \{\alpha^\#, \alpha^\#\} = 0,$$

$$\{\alpha(x,p), \overline{\alpha(x',p')}\} = -i\,\delta(x-x')\,\delta(p-p'),$$

$$\mathcal{H}_V(\bar\alpha,\alpha) = i\iint dx\,dp\;\bar\alpha\left[\frac{1}{M}p\cdot\nabla_x - \nabla V\cdot\nabla_p\right]\alpha$$

$$-\,i\iint dx\,dp\,\bar\alpha\left[\iint dy\,dr\,\nabla\phi(x-y)|\alpha(y,r)|^2\right]\cdot\nabla_p\alpha$$

Hamiltonian Eqs. of motion,

$$(1)\;\; \dot\alpha_t(x,p) = \{\mathcal{H}_V, \alpha_t(x,p)\}, \;\; \dot{\bar\alpha}_t(x,p) = \cdots$$

$$\Rightarrow \text{Vlasov Eqs. for } f_t(x,p)!$$

Wick quantization

$$\alpha(x,p) \to a_N(x,p)\ ,\ \overline{\alpha(x,p)} \to a_N^*(x,p)$$

$$[a_N^\#, a_N^\#] = 0\ , \quad (N \equiv N_A)$$

$$[a_N(x,p), a_N^*(x',p')] = \frac{1}{N}\,\delta(x-x')\,\delta(p-p')$$

$$\sim \frac{i}{N}\{\alpha(x,p), \overline{\alpha(x',p')}\} \ (\text{Dirac})$$

a_N, a_N^* act on Fock space

$$\mathcal{F}_V := \bigoplus_{n=0}^{\infty} \mathcal{F}_V^{(n)},$$

$$\mathcal{F}_V^{(0)} = \mathbb{C}|0\rangle\ ,\ |0\rangle \ \text{vacuum}$$

$$a_N(x,p)|0\rangle = 0,\ \forall x,p.$$

$$\mathcal{F}_V^{(n)} := \left\langle \int \cdots \int \varphi_n(x_1,p_1,\cdots,x_n,p_n) \prod_{i=1}^{n} a_N^*(x_i,p_i)|0\rangle \right\rangle$$

$f_n := |\varphi_n|^2 =$ symm. density on n-point-part. phase space $\Gamma^{(n)}$

Hamilton op. : $\hat{\mathcal{H}}_V := :\mathcal{H}_V(a^*_N, a_N):$

Schrödinger Eq. :

$$iN^{-1}\partial_t \Psi_t = \hat{\mathcal{H}}_V \Psi_t, \quad \Psi_t \in \mathcal{F}_V$$

$\Leftrightarrow$ Liouville's Eq. of motion for symm. n-particle densities, $f_n = \overline{\varphi_n} \cdot \varphi_n$, on $\Gamma^{(n)}$, 2-body potential $\frac{1}{N}\phi$, $n = 0, 1, 2, \cdots$.

Apparently, atomistic Newtonian mech. of point-part.

= quantization of continuum theory given by Vlasov eq.

$\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad \|$

(B-H) "classical limit" of Newtonian mech

Rephrasing Braun-Hepp

$$\psi \equiv \psi^{(n)}(\alpha) := cst. \int \cdots \int \prod_{i=1}^{n} \alpha(x_i, p_i) a_N^*(x_i, p_i) |0\rangle$$

For $n \simeq \nu N$,

$$e^{-itN\hat{\mathcal{H}}_\nu} \psi^{(n)}(\alpha) \simeq \psi^{(n)}(\alpha_t) + O\left(\frac{1}{N}\right),$$

where α_t solves (1), i.e., $f_t = \nu \bar{\alpha}_t \cdot \alpha_t$ solves Vlasov, with $\int f_t = \nu$.

More precise statement in form of a <u>Egorov Theorem</u>.

Alas, description of stars in terms of Vlasov Eq. leads to instabilities

$\longrightarrow$ Quantize ($\hbar$)!

1.2 Quant. gases as "2nd quantization" of Hartree mechanics

Replace $f(x,p) = \overline{\alpha(x,p)} \cdot \alpha(x,p)$

by

(2) $f_\hbar(x,p) := \frac{1}{(2\pi)^3} \int dy\, e^{-iy \cdot p}\, \overline{\psi(x - \frac{\hbar y}{2})} \cdot \psi(x + \frac{\hbar y}{2})$

$f_\hbar$ is Wigner trsf. of ψ

Dynamics of ψ:

(3) $i\hbar \partial_t \psi_t = \left[-\frac{\hbar^2}{2m}\Delta + V\right]\psi_t + \left[|\psi_t|^2 * \phi\right]\psi_t$

Hartree Equation

If solution ψ_t of (3) is plugged into (2) then

$$\lim_{\hbar \searrow 0} f_{\hbar,t}(x,p)$$

solves Vlasov Eq. (1);

($\nearrow$ Narnhofer – Sewell)

Hartree is Hamiltonian Eq. of motion on phase space $\Gamma = H^1(\mathbb{R}^3)$; Poisson brackets

$$\{\psi^\#, \psi^\#\} = 0, \quad \{\psi(x), \overline{\psi(y)}\} = i\delta(x-y)$$

Hamilton functional

$$\mathcal{H}_H(\bar{\psi}, \psi) := \hbar^{-1} \int dx\, \overline{\psi(x)} \left[-\frac{\hbar^2}{2m} \Delta_x + V \right] \psi(x)$$
$$+ \frac{\hbar^{-1}}{2} \int dx \int dy\, |\psi(x)|^2 \phi(x-y) |\psi(y)|^2$$

$$(3') \quad \dot{\psi}_t(x) = \{\mathcal{H}_H, \psi_t(x)\}, \quad \dot{\bar{\psi}}_t(x) = \cdots$$

<u>Continuum</u> (field) theory of a <u>quantum</u> gas

"Second" quantize:

$$\psi(x) \to \hat{\psi}_N(x),\ \overline{\psi(x)} \to \hat{\psi}_N^*(x),\ w.$$

$$[\hat{\psi}_N^\#, \hat{\psi}_N^\#] = 0,\ [\hat{\psi}_N(x), \hat{\psi}_N^*(y)] = \frac{1}{N}\delta(x-y)$$

Fock space

$$\mathcal{F}_H = \bigoplus_{n=0}^{\infty} \mathcal{F}_H^{(n)},\quad \mathcal{F}_H^{(0)} = \mathbb{C}|0\rangle,$$

$$\hat{\psi}_N(x)|0\rangle = 0,\ \forall x$$

$$\mathcal{F}_H^{(n)} := \langle \int \cdots \int \varphi_n(x_1, \dots, x_n) \Pi \hat{\psi}_N^*(x_i)|0\rangle \rangle$$

Many-body Hamiltonian

$$\hat{\mathcal{H}}_N := :\mathcal{H}_H(\hat{\psi}_N^*, \hat{\psi}_N):$$

(4)

$$iN^{-1}\partial_t \Psi_t = \hat{\mathcal{H}}_N \Psi_t$$

is Schrödinger Eq. for Bose gas of $n = 0, 1, 2, 3, \cdots$ quantum point particles, "atoms", with 2-body potential $\frac{1}{N}\phi$.

On n-particle subspace $\mathcal{F}_H^{(n)}$, (4) is equivalent to

$$H^{(n)} = \sum_{j=1}^{n}\left[-\frac{\hbar^2}{2m}\Delta_j + V(x_j)\right] + \frac{1}{N}\sum_{1\leq i<j\leq n}\phi(x_i - x_j)$$

(4')

$$i\hbar\partial_t \varphi_t^{(n)}(x_1,\dots,x_n) = \left[H^{(n)}\varphi_t^{(n)}\right](x_1,\dots,x_n)$$

$$\begin{tikzcd}[column sep=huge, row sep=huge]
\boxed{\text{QM many-body theory}} \arrow[r, shift left, "\hbar"'] \arrow[d, shift right, "\frac{1}{N}"'] & \boxed{\text{Class. mech of pt. part.}} \arrow[l, shift left] \arrow[d, shift right] \\
\boxed{\text{Hartree dynamics}} \arrow[u, shift right] \arrow[r, shift right] & \boxed{\text{Vlasov dynamics}} \arrow[l, shift right, "\hbar"'] \arrow[u, shift right, "\frac{1}{N}"']
\end{tikzcd}$$

Atomism $\longleftrightarrow$ "2^{nd}" Quantization

2. A Egorov Theorem

Continuum theory of quantum gases: "Observables" ~ gauge-inv. functions on Γ

$$A(a^{(p)}) = \int \cdots \int \prod_{1}^{p} \overline{\psi(x_i)}\,dx_i\; a^{(p)}(\underline{x};\underline{y}) \prod_{1}^{p} \psi(y_j)\,dy_j$$

Time evolution given by flow,

$\Phi_t : \overset{(-)}{\psi} \longrightarrow \overset{(-)}{\psi}_t$, where $\overset{(-)}{\psi}_t$ solves Hartree Eq. (3),(3')

$$A(a^{(p)}) \longrightarrow A_t(a^{(p)}) := A(a^{(p)}) \circ \Phi_t$$

Many-body theory of quantum gases: $\psi \mapsto \hat{\psi}_N$, $\overline{\psi} \mapsto \hat{\psi}_N^*$, with CCR; $A(a^{(p)}) \mapsto \hat{A}_N(a^{(p)})$,

$$\hat{A}_N(a^{(p)}) = \int \cdots \int \prod_1^p \hat{\psi}_N^*(x_i)\,dx_i \; a^{(p)}(\underline{x},\underline{y}) \prod_1^p \hat{\psi}_N(y_j)\,dy_j$$

gauge-inv., $\hat{\psi}_N^{\#} \longmapsto e^{\pm i\theta}\,\hat{\psi}_N^{\#}$,

i.e., preserves particle #.

Time evolution (Heisenberg)

$$\hat{A}_N(a^{(p)}) \longrightarrow$$

$$\hat{A}_{N,t}(a^{(p)}) = e^{itN\hat{\mathcal{H}}_N}\,\hat{A}_N(a^{(p)})\,e^{-itN\hat{\mathcal{H}}_N}$$

Conservation laws:

Gauge-inv. $\longleftrightarrow$ $\mathcal{N}(\bar{\psi},\psi) = \int |\psi|^2\,dx$

$$\downarrow$$

$\hat{\mathcal{N}}$ = part. #

Time-transl.-inv. $\longleftrightarrow$ $\mathcal{H}_H(\bar{\psi},\psi)$

$$\downarrow$$

$$\hat{\mathcal{H}}_N$$

Egorov Theorem (new!)

For $n \lesssim \nu N$, $(\nu < \infty)$,

$$\hat{A}_{N,t}(a^{(p)})\Big|_{\mathcal{J}^{(n)}} \underset{N\to\infty}{=} \left(\widehat{A(a^{(p)})\circ\Phi_t}\right)_N\Big|_{\mathcal{J}^{(n)}} + o(1)$$

Idea of proof:

$\hat{A}_{N,t}(a^{(p)})$ in "interaction pict.";

expand in Lie-Schwinger series; $<$ tree terms / loop terms

Using conservation laws,

$$|\text{loop terms}| \sim O\left(\frac{1}{N}\right);$$

$$\underbrace{\sum \text{tree terms}}_{\text{abs. conv., } |t| \text{ small, unif. in } N.} = \left(\widehat{A(a^{(p)})\circ\Phi_t}\right)_N$$

Related story for Fermions

$\psi \to \hat{\psi}_N$, $\bar{\psi} \to \hat{\psi}^*_N$, with

$$[\hat{\psi}^\#_N, \hat{\psi}^\#_N]_+ = 0, \quad [\hat{\psi}_N(x), \hat{\psi}^*_N(y)]_+ = \frac{1}{N}\delta(x-y),$$

$$[A,B]_+ := AB + BA.$$

$$\mathcal{H}_H \to \hat{\mathcal{H}}^f_N, \quad A(a^{(p)}) \to \hat{A}^f_N(a^{(p)}),$$

$a^{(p)}(x_1,\dots,x_p; y_1,\dots,y_p)$ tot. anti-symm in x's & in y's.

There's again a Egorov-type theorem. But "continuum theory" given by

? Hartree-Fock Eq.

for $n \sim \nu N$ orbitals.

3. Some details on Egorov Thm. for Bosons

$$\mathcal{H}_H = \mathcal{H}_0 + \mathcal{V},$$

$$\mathcal{H}_0(\bar{\psi},\psi) = \hbar^{-1}\int dx\, \bar{\psi}(x)\Big[-\frac{\hbar^2}{2m}\Delta + V(x)\Big]\psi(x)$$

$$\mathcal{V}(\bar{\psi},\psi) = \frac{\hbar^{-1}}{2}\iint dx\,dy\, |\psi(x)|^2\phi(x-y)|\psi(y)|$$

$$= \frac{\hbar^{-1}}{2} A(\phi^{(2)}),$$

$$\phi^{(2)}(x_1,x_2;y_1,y_2) = \phi(x_1-y_1)\delta(x_2-y_1)\delta(y_2-x_1,$$

$$\|\phi^{(2)}\|_{op.} = \|\phi\|_\infty.$$

$$\hat{\mathcal{H}}_N = \hat{\mathcal{H}}_{0,N} + \hat{\mathcal{V}}_N \quad (\text{quant. of } \mathcal{H}_H)$$

<u>Lemma.</u>

$$e^{itN\hat{\mathcal{H}}_{0,N}}\hat{A}_N(a^{(p)})e^{-itN\hat{\mathcal{H}}_{0,N}}$$

$$= \hat{A}_N(\underbrace{e^{itH_0^{(p)}/\hbar}a^{(p)}e^{-itH_0^{(p)}/\hbar}}_{=:\, a_t^{(p)}})$$

$$= \left(A(a^{(p)})\circ\Phi_0^t\right)^\wedge_N$$

$$\|a_t^{(p)}\| = \|a^{(p)}\|$$

Time evol. in interaction pict

$$e^{itN\hat{\mathcal{H}}_N}\hat{A}_N(a^{(p)})e^{-itN\hat{\mathcal{H}}_N}$$

$$= \hat{A}_N(a_t^{(p)}) + \int_0^t ds\, e^{isN\hat{\mathcal{H}}_N}e^{-isN\hat{\mathcal{H}}_{0,N}}$$

$$\times \frac{iN}{2\hbar}\left[\hat{A}_N(\phi_s^{(1)}),\hat{A}_N(a_t^{(p)})\right]$$

$$\times\, e^{isN\hat{\mathcal{H}}_{0,N}}e^{-isN\hat{\mathcal{H}}_N}$$

\#

Iterate $\rightarrow$ Schwinger-Dyson ser

conv. on $\mathcal{F}^{\leq n}$, $\forall n < \infty$, $\forall t$.

Note:

$$\frac{iN}{2\hbar}\left[\hat{A}_N(\phi_s^{(2)}), \hat{A}_N(a_t^{(p)})\right]$$

$$= \sum_{\ell=1}^{2} \binom{p}{\ell}\binom{2}{\ell} \frac{i\ell}{2\hbar N^{\ell-1}} \hat{A}_N([\phi_s^{(2)} \underset{\ell}{\lrcorner} a_t^{(p)}]),$$

$\ell = 1$: tree terms

$\ell = 2$: loop terms, $\propto \frac{1}{N}$!

When a loop term is gen. in iteration of #: stop expanding & estimate it, using unitarity of $e^{\pm isN\mathcal{H}_{(0),N}}$!

This yields:

$$e^{itN\hat{\mathcal{H}}_N}\hat{A}_N(a^{(p)})e^{-itN\hat{\mathcal{H}}_N}$$

$$= \hat{T}_N(a^{(p)},t) + \hat{L}_N(a^{(p)},t),$$

with

$$\hat{T}_N(a^{(p)},t) = \sum_{k=0}^{\infty}\left(\frac{i}{\hbar}\right)^k \binom{p+k-1}{p-1} k! \times$$

$$\times \int_0^t dt_1 \cdots \int_0^{t_{k-1}} dt_k \; \hat{A}_N\Big(\big[\phi^{(2)}_{t_k} \underset{1}{\lrcorner} \big[\phi^{(2)}_{t_{k-1}} \underset{1}{\lrcorner} \cdots \big[\phi^{(2)}_{t_1} \underset{1}{\lrcorner} a^{(p)}_t\big]\cdots\big]\big]\Big) \; *$$

$\hat{L}_N(a^{(p)},t)$: similar sum of terms, but with 1 loop $\propto \frac{1}{N}$

Easy to show: On $\mathcal{F}^{\leq \nu N}$, series for $\hat{T}_N, \hat{L}_N$ converge in norm if

$$|t| \leq \frac{1}{4\nu \|\phi\|_\infty},$$

independently of p!

Now, compare $\hat{T}_N(a^{(p)}, t)$ with

<u>classical</u> time evolution,

in interaction picture:

From $* \Rightarrow$

$$\hat{T}_N(a^{(p)}, t) = \left(A(a^{(p)}) \circ \Phi^t\right)^\wedge_N$$

on $\mathcal{F}^{\leq \nu N}$, $|t| \leq \dfrac{1}{4\nu \|\phi\|_\infty}$.

<u>Arbitary t</u>: Iterate exp., using indep. of p & unit.!

3. Newtonian point particles as "solitons" of cont. theories

Consider, e.g., Hartree Eq. as q.t. model of cont. medium:

$$i\hbar\partial_t\psi_t(x) = \big(T+V(\varepsilon x)\big)\psi_t(x) - g\left(|\psi_t|^2 * \phi\right)(x)\,\psi_t(x) \qquad (5)$$

$$T = -\frac{\hbar^2\Delta}{2m},\ \sqrt{-\hbar^2\Delta+m^2},\ \dots$$

V: e.g., grav. pot. of central "star", $\|V\|_\infty < \infty$.

$$\phi(x) = \frac{1}{|x|},\ \frac{e^{-\mu|x|}}{|x|},\ \dots$$

$$\|\psi_t\|_2^2 =: \nu = O(1),\ g>0.$$

(Model of a "Boson star.")

Hamilton functional:

$$\mathcal{H}(\bar{\psi},\psi;\varepsilon) = \int dx \left\{ \overline{\psi(x)} (T\psi)(x) + \left[V(\varepsilon x) - g \int dy\, |\psi(y)|^2 \phi(y-x) \right] |\psi(x)|^2 \right\}$$

Conservation laws:

- $\mathcal{N}(\bar{\psi},\psi) := \int |\psi(x)|^2 dx \leftrightarrow$ gauge inv.

For $\varepsilon = 0$,

- $\mathcal{P}(\bar{\psi},\psi) := -i\hbar \int (\bar{\psi}\,\nabla\psi)(x)\, dx$

$\leftrightarrow$ translation inv.

Consider "energy funct."

$$\mathcal{E}_v(\psi) := \mathcal{H}(\bar{\psi},\psi;\varepsilon=0) + v \cdot \mathcal{P}(\bar{\psi},\psi)$$

$v \in \mathbb{R}^3$: C-of-M velocity.

(For pseudo-relat. T, $|v| < 1$)

<u>Var. problem</u>: Construct minimizer, $\varphi_{v,\mu}$, for $\mathcal{E}_v$, with $\|\varphi_{v,\mu}\|_2^2 = \nu(\mu)$.

Solves eq.

$$T\varphi_{v,\mu} + iv \cdot \nabla\varphi_{v,\mu} - g(|\varphi_{v,\mu}|^2 * \phi)\varphi_{v,\mu} + \mu\varphi_{v,\mu} = 0$$

(Subaddit. + concentr. - comp.)

Then

$$(6) \qquad \psi_t(x) := e^{i\theta(t)}\varphi_{v,\mu}(x-q-vt)$$

solves Hartree eq. (5): solitary wave sol.

describes giant "molecule"

e.g., a "Boson star", of bound matter travelling inertially w. velocity v.
(For $T = -\frac{\hbar^2 \Delta}{2m}$, φ_v obtained from φ_0 by Galilei boost.)
Solu. (6) of (5) depends on 8 parameters:

$$\xi := (q, v, \mu, \theta) \in S \subset \mathbb{R}^8.$$

ξ: coos. of point in 8-dim. surface in $\Gamma = H^1(\mathbb{R}^3)$:

$$\mathcal{M}_S := \left\{ \varphi_{v,\mu}(\cdot - q) \,\middle|\, \varphi_{v,\mu}(0) = e^{i\theta}, \ \|\varphi_{v,\mu}\|_2^2 = \nu(\mu) \right\}$$

"soliton manifold"

$\omega|_{\mathcal{M}_s}$: non-degenerate

Let ψ_t be solu. of (5) for $\varepsilon > 0$, w. $\text{dist}(\psi_0, \mathcal{M}_s) < O(\varepsilon)$

Let φ_{ξ_t} be "skew-orth." proj. of ψ_t onto $\mathcal{M}_s$

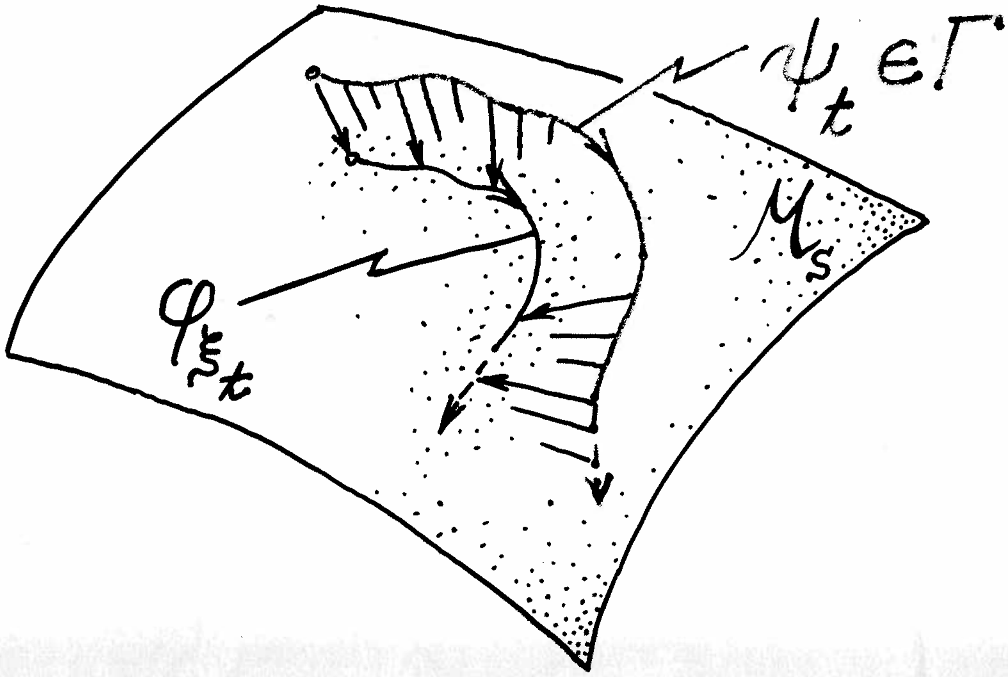
<u>Theorem.</u> For $|t| < O(\varepsilon^{-1 \cdots})$,

$\text{dist}(\psi_t, \mathcal{M}_s) \sim O(\varepsilon) \Rightarrow$

φ_{ξ_t} well def. & unique;

(N) $$\boxed{\begin{aligned} \dot{q}_t &= v_t + O(\varepsilon^2) \\ \gamma \dot{v}_t &= -\varepsilon (\nabla V)(\varepsilon q_t) + O(\varepsilon^2) \end{aligned}}$$

$\dot{\mu} = O(\varepsilon^2)$, $\dot{\theta} = \mu - V(\varepsilon q) + O(\varepsilon^2)$



<u>Interpretation</u>: In an ext. pot. $V(\varepsilon\,\cdot)$, center of mass, q_t, of "molecule" in state ψ_t is solution of Newton's eqs. of motion for point particle in pot. $V(\varepsilon\,\cdot)$ with friction force $\sim O(\varepsilon^2)$

$\downarrow$

structure formation

($\nearrow$ e.g. T. Tao)

Further results.

(1) Motion of several interacting solitons (J.F.; A-S, F, S)

(2) Asy. stability & scattering (R, S, S; G.P.; E.L.)

(3) Ext. to Hartree-Fock & BHF →

dynamical approach to Chandrasekhar limit for white dwarfs;

? BCS pairing of neutrons in groundstate of neutron star; ...

2-body problem: Krieger, Martel, Raphaël

Technicalities

1. Intuition conc. M-F-L

$$H^{(n)} = \sum_{j=1}^{n} \left[-\Delta_j + V(x_j) \right] + \frac{1}{2N} \sum_{i \neq j} \phi(x_i - x_j)$$

on $\mathcal{H}^{(n)} = P_+ L^2(\mathbb{R}^3, d^3x)^{\otimes n}$;

P_+ : symmetrization (bosons!)

Schrödinger Eq.:

$$i \dot{\Psi}_t^{(n)} = H^{(n)} \Psi_t^{(n)}$$

solved by

$$\Psi_t^{(n)} = e^{-itH^{(n)}} \Psi^{(n)},$$

$\Psi^{(n)} \in \mathcal{H}^{(n)}$. If

$$\Psi^{(n)}(x_1, \dots, x_n) = \prod_{j=1}^{n} \psi(x_j) \qquad (1)$$

expect that

$$\Psi_t^{(n)}(x_1, \dots, x_n) = \prod_{j=1}^{n} \psi_t(x_j),$$

where ψ_t solves HE

$$i\dot{\psi}_t(x) = \left(-\Delta + V(x)\right)\psi_t(x) + \nu \int d^3y \, |\psi_t(y)|^2 \phi(y-x) \psi_t(x)$$

$$\text{with } \nu = \frac{n}{N}. \tag{2}$$

"Pot. felt by one part. ≃ average pot. generated by particle density".

Goal: Get rid of special initial condition (1).

2. History

1969 – Egorov (can. trsfs. of pseudodiff. ops., ...)

1974 – Hepp (coherent states, following Schrödinger)

1977 – Braun & Hepp, Neunzert (Vlasov)

1979 – Ginibre & Velo (Hepp for $t \to \infty$)

1981 – Narnhofer & Sewell (Vlasov "for fermions")

1998 – 2009 – J.F. et al. ($\longrightarrow$)
Yau et al.

2009/10 – Pickl

D

Egorov: "Time evolution & quantization commute in semi-classical limit."

$$\Gamma = T^*M,\ \mathcal{A} = C^\infty(\Gamma),\ H,$$

Φ_t: flow on Γ gen. by H.

$$\widehat{(\cdot)}_\hbar : A \in \mathcal{A} \mapsto \hat{A}_\hbar \text{ on } L^2(M)$$

(Weyl quantization)

$$[\hat{A}_\hbar, \hat{B}_\hbar] = \frac{\hbar}{i} \widehat{\{A,B\}}_\hbar + O(\hbar^2)$$

$$\widehat{(A\circ\Phi_t)}_\hbar = e^{it\hat{H}_\hbar} \hat{A}_\hbar e^{-it\hat{H}_\hbar}$$

$$+ o_\hbar(1).$$

Hepp can be cast in this language!

In our model: $\hbar = \frac{1}{N}$,

$\Gamma = \mathcal{H}^1(\mathbb{R}^3)$ (Sobolev).

many-body (bosons) $\xrightarrow[N\to\infty]{}$ Hartree Eq.

3. Notation & framework

$\Gamma = \mathcal{H}^1(\mathbb{R}^3)$ w. complex coos

$\psi, \bar{\psi}$; $\{\psi^{\#}, \psi^{\#}\} = 0$,

$\{\psi(x), \bar{\psi}(y)\} = i\delta(x-y)$

$$\mathcal{H}(\bar{\psi},\psi) = \int d^3x\ \bar{\psi}(x)\underbrace{[-\Delta + V]}_{\equiv h}\psi(x)$$

$$+ \frac{1}{2}\int d^3x \int d^3y\ |\psi(x)|^2\phi(x-y)|\psi(y)|$$

HE becomes

$$\dot{\psi}_t(x) = \{\mathcal{H}, \psi_t(x)\}$$

(e.g., Lenzmann) $\longrightarrow$ can. flow Φ_t.

Conservation laws

- $\mathcal{H}(\bar{\psi}_t, \psi_t) = \mathcal{H}(\bar{\psi}, \psi)$;
- $\mathcal{N}(\bar{\psi}_t, \psi_t) = \mathcal{N}(\bar{\psi}, \psi)$,

where $\mathcal{N}(\bar{\psi}, \psi) = \|\psi\|_2^2$

$\longrightarrow$ Flow Φ_t leaves

$$\Gamma_\nu := \{(\bar{\psi}, \psi) \in \Gamma \mid \mathcal{N}(\bar{\psi}, \psi) = \nu\}$$

invariant.

"Observables"

$$A(a^{(p)}) := \int \prod_1^p \bar{\psi}(x_j)\, d^3x_j \int \prod_1^p \psi(y_j)\, d^3y_j$$
$$\times\, a^{(p)}(x_1, \dots, x_p; y_1, \dots, y_p),$$

$a^{(p)} \in B(\mathcal{H}^{(p)})$.

Time evolution:

$A(a^{(p)}) \circ \Phi_t$ obtained by

$\psi \mapsto \psi_t,\ \bar{\psi} \mapsto \bar{\psi}_t$ in $A(a^{(p)})$.

Quantization

$$\psi(x) \longmapsto \hat{\psi}_N(x),\ \bar{\psi}(x) \longmapsto \hat{\psi}_N^*(x),$$

with CCR (Heisenberg, Dirac)

$$[\hat{\psi}_N^{\#}(x), \hat{\psi}_N^{\#}(y)] = 0,$$

$$[\hat{\psi}_N(x), \hat{\psi}_N^*(y)] = \frac{1}{N}\, \delta(x-y)$$

Fock space $\mathcal{F} := \bigoplus_{n=0}^{\infty} \mathcal{H}^{(n)}$,

$\mathcal{H}^{(0)} = \mathbb{C}\Omega$, Ω: vacuum,

$$\psi_N(x)\Omega \equiv 0 .$$

$$\mathcal{H}^{(n)} \ni \Phi^{(n)} = \frac{N^{n/2}}{\sqrt{n!}} \int \varphi^{(n)}(x_1, \dots, x_n) \times \prod_1^n \hat{\psi}_N^*(x_j) d^3x_j \; \Omega$$

$$\hat{A}_N(a^{(p)}) := \int \prod_1^p \hat{\psi}_N^*(x_j) d^3x_j \times \int \prod_1^p \psi_N(y_j) d^3y_j \; a^{(p)}(x_1, \dots, x_p; y_1, \dots, y_p)$$

Hamilton operator

$$H_N = N \hat{\mathcal{H}}_N = \underbrace{N(\hat{A}_N(h)}_{H_N^0} + \underbrace{\tfrac{1}{2}\hat{A}_N(\phi))}_{W_N} = \bigoplus_{n=0}^{\infty} H^{(n)} .$$

Quantum time evolution

$$\hat{A}_N(a^{(p)}) \longmapsto e^{itH_N}\hat{A}_N(a^{(p)})e^{-itH_N}$$

4. Goal

If $V, \phi \in L^\infty + L^3_{weak}$,

(e.g. Coulomb pot.), and

for arb. ν, $0 < \nu < \infty$,

arb. $a^{(p)} \in B(\mathcal{H}^{(p)})$, $p = 1, 2, 3, \cdots$,

$$e^{itH_N}\hat{A}_N(a^{(p)})e^{-itH_N}\restriction_{\mathcal{F}^{\leq \nu N}}$$

$$= \left(\widehat{A(a^{(p)})\circ\Phi_t}\right)_N\restriction_{\mathcal{F}^{\leq \nu N}} + o_N(1), \tag{3}$$

where $\mathcal{F}^{\leq \nu N} = \bigoplus_{n=0}^{[\nu N]} \mathcal{H}^{(n)}$.

Moreover, for

$$\Phi^{(n)}(\varphi) := \frac{N^{n/2}}{\sqrt{n!}} \left(\hat{\psi}_N^*(\varphi)\right)^n \Omega,$$

$$\left\langle \Phi^{([\nu N])}(\varphi), e^{itH_N} \hat{A}_N(a^{(p)}) e^{-itH_N} \Phi^{([\nu N])}(\varphi) \right\rangle$$

$$= \left\langle \Phi^{([\nu N])}(\varphi_t), \hat{A}_N(a^{(p)}) \Phi^{([\nu N])}(\varphi_t) \right\rangle + o_N(1)$$

$$= \int \prod_1^p \bar{\psi}_t(x_j)\, dx_j \int \prod_1^p \psi_t(y_j)\, dy_j \; a^{(p)}(x_1, \cdots, x_p ; y_1, \cdots, y_p) + o_N(1) \quad (4)$$

where $\varphi_t = \frac{\psi_t}{\sqrt{\nu}}$ and $\psi_t \in \Gamma_\nu$ is a solution of HE.

Note that $(3) \Rightarrow (4)$.

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5. Key ideas of proof

(i) Schwinger-Dyson exp. of $e^{itH_N}\hat{A}_N(a^{(p)})e^{-itH_N}$.

(ii) "Kato smoothing" plus combinatorial estimates

$\Rightarrow$ S-D exp. conv. on $\mathcal{F}^{\leq \nu N}$ for $|t|$ small enough, indep. of p, unif. in N

ℓ-loop terms $\propto N^{-\ell}$; ($\ell = 0$: "tree terms")

(iii) "Kato smoothing" plus comb. estimates $\Rightarrow$

iterative solu. of HE converges, for small $|t|$

$\rightarrow$ ex. of flow Φ_t on Γ_ν, for small $|t|$, dep. on ν,

$\rightarrow$ for all $|t|$, using cons laws.

(iv) $\left(\widehat{A(a^{(p)}) \circ \Phi_t}\right)_N$

$= \text{Sum tree } (l=0) \text{ terms}$ in (ii), for $|t|$ small

(v) Extend (ii), (iii) to arb. $|t|$, using unitarity, cons. laws, indep. of conv. in (ii), (iii) of p.

6. Algebra of observables

$$\mathcal{A} := \{ A(a^{(p)}) \mid a^{(p)} \in \mathcal{B}(\mathcal{H}^{(p)}), p \in \mathbb{N} \}$$

pointwise mult.

$$\hat{\mathcal{A}} := \{ \hat{A}_N(a^{(p)}) \mid a^{(p)} \in \mathcal{B}(\mathcal{H}^{(p)}), p \in \mathbb{N} \},$$

ops. def. on $\mathcal{F}^{fin.}$, operator mult.

(i) $\hat{A}_N(a^{(p)})^* = \hat{A}_N(a^{(p)*})$

$$= \left(\widehat{A(a^{(p)})}\right)_N$$

(ii) $\hat{A}_N(a^{(p)})\hat{A}_N(b^{(q)})$

$$= \sum_{r=0}^{p \wedge q} \binom{p}{r}\binom{q}{r} \frac{r!}{N^r} \hat{A}_N(a^{(p)} \underset{r}{-} b^{(q)})$$

$$= \underbrace{\left(\widehat{A(a^{(p)})\, A(b^{(q)})}\right)_N}_{\hat{A}_N(a^{(p)} \otimes b^{(q)})} + O\left(\frac{1}{N}\right),$$

where

$$a^{(p)} \underset{r}{\rightharpoondown} b^{(q)} = P_+ \left(a^{(p)} \otimes \mathbb{1}^{(q-r)} \right) \times \left(\mathbb{1}^{(p-r)} \otimes b^{(q)} \right) P_+ \in B(\mathcal{H}^{(p+q-r)}).$$

(iii) $\Gamma(u^{-1}) \hat{A}_N (a^{(p)}) \Gamma(u)$

$$= \hat{A}_N \left((u^{-1})^{\otimes p} a^{(p)} u^{\otimes p} \right),$$

in Segal's notations.

(iv) $\| \hat{A}_N (a^{(p)}) \restriction_{\mathcal{J} \leq n} \| \leq \left(\frac{n}{N} \right)^p \| a^{(p)} \|$

Notation

$$[a^{(p)}, b^{(q)}]_r := a^{(p)} \underset{r}{\rightharpoondown} b^{(q)} - b^{(q)} \underset{r}{\rightharpoondown} a^{(p)}$$

(v) $[\hat{A}_N (a^{(p)}), \hat{A}_N (b^{(q)})]$

$$= \sum_{r=1}^{p \wedge q} \binom{p}{r} \binom{q}{r} \frac{r!}{N^r} \hat{A}_N \left([a^{(p)}, b^{(q)}]_r \right)$$

Note that (iii) $\Rightarrow$

<u>Lemma.</u>

$$e^{itH_N^0}\hat{A}_N(a^{(p)})e^{-itH_N^0} = \hat{A}_N(a_t^{(p)}), \quad \text{where}$$

$$a_t^{(p)} = (e^{ith})^{\otimes p} a^{(p)} (e^{-ith})^{\otimes p}$$

In the following,

$$W_{N,t} := e^{itH_N^0} W_N e^{-itH_N^0}$$

$$\overset{\text{Lemma}}{=} \frac{1}{2} \hat{A}_N\left((e^{ith})^{\otimes 2} \phi (e^{-ith})^{\otimes 2}\right)$$

center-of-mass motion drops out!

"Kato smoothing":

$$\int \|\phi_t \psi\|^2 dt \leq \pi \|\psi\|^2$$

7. Schwinger–Dyson exp.

First assume, V, ϕ boundea

$$e^{itH_N} \hat{A}_N(a^{(p)}) e^{-itH_N}$$

$$= e^{isH_N} e^{-isH_N^0} \hat{A}_N(a_t^{(p)}) e^{isH_N^0} e^{-isH_N} \Big/_{s=}$$

$$= \hat{A}_N(a_t^{(p)}) + \int_0^t dt_1 \, e^{it_1 H_N} e^{-it_1 H_N^0} \times$$

$$iN [W_{N,t_1}, \hat{A}_N(a^{(p)})] e^{it_1 H_N^0} e^{-it_1} \qquad (5)$$

on $\mathcal{F}^{fin.}$. Iterate (5) $\rightarrow$

$$e^{itH_N} \hat{A}_N(a^{(p)}) e^{-itH_N}$$

$$= \sum_{k=0}^{\infty} \int_{\Delta^k(t)} d\underline{t} \, (iN)^k [W_{N,t_k}, \dots,$$

$$[W_{N,t_1}, \hat{A}_N(a_t^{(p)})] \dots]$$

$\uparrow$ simplex

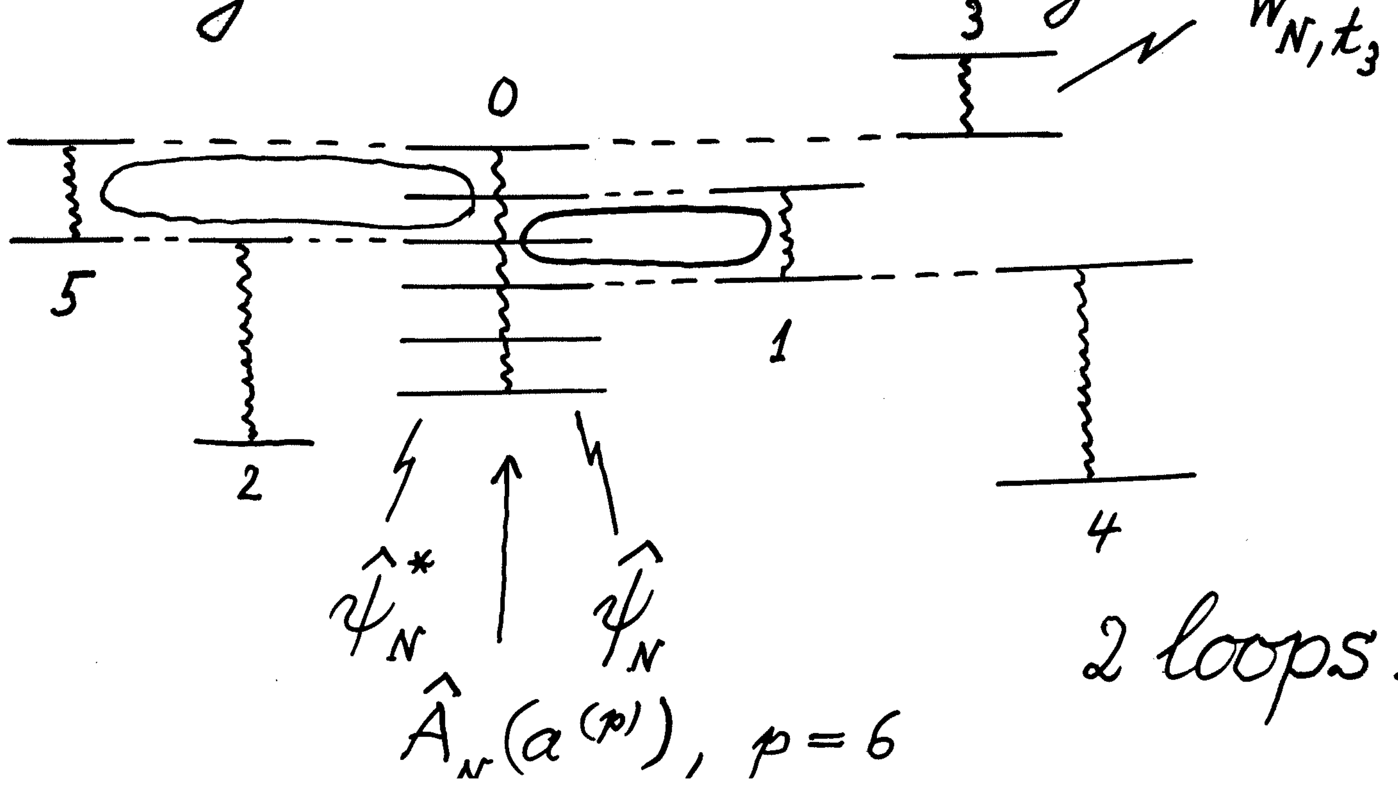
conv. like

$$\sum_k \frac{(|t|n^2\|\phi\|_\infty N^{-1})^k}{k!}\left(\frac{n}{N}\right)^p \|a^{(p)}\|$$

on $\mathcal{H}^{(n)}$ $\longrightarrow$ <u>inadequate</u> to study M-F-L, $n = \nu N$, $N \to \infty$.

Use that multiple commutators only yield "connected terms" (because $[a^{(p)}, b^{(q)}]_{r=0} = 0$).

These terms can be labelled by "admissible" diagr.:



2 loops!

Next

$$(iN)^k \left[W_{N,t_k}, \dots, \left[W_{N,t_1}, \hat{A}_N(a^{(p)}_t)\right] \dots \right] = \sum_{\ell=0}^{k} \frac{1}{N^\ell} \hat{A}_N\left(G^{(k,\ell)}_{t,\underline{t}}(a^{(p)})\right),$$

where

$$G^{(k,\ell)}_{t,\underline{t}}(a^{(p)}) = i(p+k-\ell-1)\left[\phi_{t_k}, G^{(k-1,\ell)}_{t,\underline{t}}(a^{(p)})\right]_1 + i\binom{p+k-\ell}{2}\left[\phi_{t_k}, G^{(k-1,\ell-1)}_{t,\underline{t}}(a^{(p)})\right]_2, \quad (6$$

$\underline{t} := \{t_1, \dots, t_{k(-1)}\}$; $G^{(0,0)}_t(a^{(p)}) := a^{(p)}_t$.

"Adm.", connected diagr., $\mathcal{G}$, $\longleftrightarrow$ "elementary" contributions to $G^{(k,\ell)}_{t,\underline{t}}$; $k, \ell = 0, 1, 2, \dots,$ with $\ell \leq k$, $p+k-\ell \leq$ particl number.

8. Convergence of S-D exp. on $\mathcal{F}^{\leq \nu N}$, unif. in N

$G^{(k,\ell)}_{t,\underline{t}}(a^{(p)})$ is a $(p+k-\ell)$-particle kernel $\leftrightarrow$ op. on $\mathcal{H}^{(p+k-\ell)}$, with (see (6)!)

$$\|G^{(k,\ell)}_{t,\underline{t}}(a^{(p)})\| \leq 2^k \binom{k}{\ell} (p+k-\ell)^\ell \times$$
$$\times (p+k-1)\cdots p \, \|\phi\|^k \, \|a^{(p)}\|$$

(crude combinatorial estimate,

Lemma. $0 < \nu < \infty$, $|t| < (8\nu\|\phi\|)^{-1}$
Then S-D exp. on $\mathcal{F}^{\leq \nu N}$ converges in norm, uniformly in N.

Proof. Recall that $p+k-\ell \overset{!}{\leq} [\nu N]$

$$\Rightarrow \sum_{k=0}^{\infty} \sum_{\ell=0}^{k} \frac{1}{N^\ell} \int_{\Delta^k(t)} d\underline{t} \, \| \hat{A}_N (G^{(k,\ell)}_{t,\underline{t}} (a^{(p)})) \restriction_{\mathcal{F}^{\leq \nu N}} \| \quad (7.$$

$$\leq \sum_{k=0}^{\infty} \sum_{\ell=0}^{k} \underbrace{\frac{(p+k-\ell)^\ell}{N^\ell} \chi_{\{p+k-\ell \leq [\nu N]\}}}_{\leq \nu^\ell \chi_{\{\dots\}}} \frac{1}{k!} \times$$

$$\times \left(2\|\phi\| |t|\right)^k \binom{k}{\ell} \underbrace{(p+k-1)\cdots p}_{= \binom{p+k-1}{k} k!} \nu^{p+k-\ell} \|a^{(p)}\|$$

$$\leq \sum_{k=0}^{\infty} \left(8\nu \|\phi\| |t|\right)^k (2\nu)^p \|a^{(p)}\|,$$

for all $N \geq 1$. ■

Corollary.

$$e^{itH_N} \hat{A}_N (a^{(p)}) e^{-itH_N} \restriction_{\mathcal{F}^{\leq \nu N}}$$

$$= \sum_{\ell=0}^{\infty} \frac{1}{N^\ell} \sum_{k=\ell}^{\infty} \int_{\Delta^k(t)} d\underline{t}\, \hat{A}_N \left(G_{t,\underline{t}}^{(k,\ell)} (a^{(p)}) \right) \Big|_{\mathcal{F}^<}^{U}$$

converges in norm, for $|t| < (8\nu \|\phi\|)^{-1}$ and all suff. large N (dep. on $|t|, p$).

<u>Extension to arbitrary t</u>

Given t, choose $m = 1, 2, 3, \dots$ s.t. $\left|\frac{t}{m}\right| \leq (16\nu \|\phi\|)^{-1}$.

$$e^{itH_N} \hat{A}_N (a^{(p)}) e^{-itH_N}$$

$$= e^{i(t-\frac{t}{m})H_N} \left(e^{i\frac{t}{m}H_N} \hat{A}_N (a^{(p)}) e^{-i\frac{t}{m}H_N} \right) e^{-i(t-\frac{t}{m})H_N}$$

$$= e^{i(t-\frac{t}{m})H_N} \Big(\sum_{k=0}^{K_1} \sum_{\ell=0}^{k} \int_{\Delta_k(\frac{t}{m})} d\underline{t}\, \frac{1}{N^\ell} \times \tag{8}$$

$$\hat{A}_N \left(G_{\frac{t}{m},\underline{t}}^{(k,\ell)} (a^{(p)}) \right) \Big) e^{-i(t-\frac{t}{m})H_N} + \mathcal{E}_N(K)$$

Using unitarity,

$$\| \mathcal{E}_N(K_1)\restriction_{\mathcal{J}\leq \nu N} \| \leq C_p \delta^{K_1}, \quad \delta < 1.$$

Since radius of conv. of S-D exp. is indep. of p, may iterate (8); truncate again, etc.

Corollary

$$e^{itH_N} \hat{A}_N(a^{(p)}) e^{-itH_N} \Big|_{\mathcal{J}\leq \nu N}$$

= (truncated) sum over "tree terms" + $o_N(1)$

$$= \left(A(\widehat{a^{(p)}) \circ \Phi_t} \right)_N \Big|_{\mathcal{J}\leq \nu N} + o_N(1)$$

↑

iterative solu. of Hartree Eq.

W

9. Convergence for Coulomb potentials.

Idea: Use "Kato smoothing",

$$\int \| |x|_\varepsilon^{-1} e^{it\Delta} \psi \|^2 dt \le \pi \|\psi\|^2,$$

$\forall \varepsilon$, where $|x|_\varepsilon^{-1} = \begin{cases} |x|^{-1}, & |x| \ge \varepsilon \\ \varepsilon^{-1}, & \text{elsew.} \end{cases}$

We set $\phi_\varepsilon(x) := \kappa |x|_\varepsilon^{-1}$ (2-body pot.) Then

$$\int \| \phi_\varepsilon(x_k - x_\ell) e^{it(\sum_j \Delta_j)} \Phi^{(n)} \|^2 dt$$

$$\le \frac{\pi \kappa^2}{2} \|\Phi^{(n)}\|^2, \ \forall \varepsilon.$$

Pf. W.l.o.g., set $k=1, \ell=2$, & use c-o-m coos., $X = \frac{x_1 + x_2}{2}$, $\xi = x_1 - x_2$. Then

$$\Delta_1 + \Delta_2 = \frac{1}{2}\Delta_X + 2\Delta_\xi \,, \quad [\Delta_X, \phi_\varepsilon(\xi)] = 0 .$$

Using unitarity, we find that

$$\int dt \, \| \phi_\varepsilon(\xi) e^{it(\sum_j \Delta_j)} \Phi^{(n)} \|^2$$

$$\overset{\text{Fub.}}{=} \int d^3X \prod_3^n d^3x_j \int dt\, d^3\xi \, \Big| \phi_\varepsilon(\xi) e^{2it\Delta_{\xi_X}} \times \Phi^{(n)}\big(X + \tfrac{\xi}{2}, X - \tfrac{\xi}{2}, \cdots\big) \Big|^2$$

$$\overset{\text{Ksm.}}{\leqslant} \frac{\pi \varkappa^2}{2} \| \Phi^{(n)} \|^2 .$$

Cauchy-Schwarz $\Longrightarrow$

$$\int_0^t ds \, \| \phi_\varepsilon(\xi) e^{-is(\sum_j \Delta_j)} \Phi^{(n)} \| \leqslant \left(\frac{\pi \varkappa^2 t}{2} \right)^{1/2} \| \Phi^{(n)} \| \qquad (9)$$

Apply this iteratively to

bound terms in (7), using unitarity, and:

(i) $G^{(k,l)}_{t,\underline{t}}(a^{(p)}) = \sum_{adm.\,\mathcal{G}_{k,l}} G^{\mathcal{G}_{k,l}}_{t,\underline{t}}(a^{(p)})$

(ii) For $\pi \in \mathcal{S}_k$, $\mathcal{G}_{k,l}$ a diagr. (as above) of order k w. l loops, $\mathcal{G}^{\pi}_{k,l}$ obtained from $\mathcal{G}_{k,l}$ by applying π to time-ordering of vertices.

(iii) $\mathcal{G}_{k,l}$ admissible $\not\Rightarrow$ $\mathcal{G}^{\pi}_{k,l}$ admissible; but true, e.g., for $l = 0$

(and, dep. on l, for π in "large" subgroups of γ_k).

(iv) $\mathcal{G}_1 \sim \mathcal{G}_2$ iff $\mathcal{G}_1 = \mathcal{G}_2^{\pi}$, for some permutation π; (equiv classes denoted by $[\mathcal{G}]$).

Then we find that

$$\int_{\Delta_k(t)} d\underline{t} \, \| G_{t,\underline{t}}^{(k,l)} (a^{(p)}) \Phi^{(n)} \|$$

$$\leq \sum_{\text{adm.}\, \mathcal{G}_{k,l}} \int_{\Delta_k(t)} d\underline{t} \, \| G_{t,\underline{t}}^{\mathcal{G}_{k,l}} (a^{(p)}) \Phi^{(n)} \|$$

$$\leq \sum_{\pi \in \gamma_k} \sum_{\substack{[\mathcal{G}_{k,l}] \\ \mathcal{G}_{k,l}\, \text{adm.}}} \int_{\Delta_k(t)} d\underline{t} \, \| G_{t,\underline{t}}^{\mathcal{G}_{k,l}^{\pi}} (a^{(p)}) \Phi^{(n)} \|$$

$$= \sum_{\substack{[\mathcal{G}_{k,\ell}] \\ \mathcal{G}_{k,\ell}\ adm.}} \int_0^t dt_1 \cdots \int_0^t dt_k \left\| G_{t,\underline{t}}^{\mathcal{G}_{k,\ell}} (a^{(p)}) \Phi^{(n)} \right\|$$

(9)
$$\leq \left| \{ [\mathcal{G}_{k,\ell}] \,|\, \mathcal{G}_{k,\ell}\ adm. \} \right| \left(\frac{\pi \kappa^2 |t|}{2} \right)^{k/2}$$

$$\times \|a^{(p)}\| \, \|\Phi^{(n)}\| \quad (10)$$

A fairly well known combi. estimate is

$$\left| \{ [\mathcal{G}_{k,\ell}] \,|\, \mathcal{G}_{k,\ell}\ adm. \} \right| \leq 2^k \binom{k}{\ell} \binom{2p+3k}{k}$$

$$\times (\underbrace{p+k-\ell}_{\leq n_{max.} = [\nu N]})^{\ell}$$

(11)

(10) & (11) yield

<u>Theorem.</u> For $\phi_\varepsilon(x) = x|x|_\varepsilon^{-1}$, $\varepsilon \geq 0$, and $|t|$ small enough, [indep. of ε & p!],

$$e^{itH_N}\hat{A}_N(a^{(p)})e^{-itH_N}\restriction_{\mathcal{F}^{\leq \nu N}}$$

$$= \sum_{k=0}^{\infty}\sum_{\ell=0}^{k}\frac{1}{N^\ell}\int_{\Delta_k(t)} d\underline{t}\,\hat{A}_N\left(G_{t,\underline{t}}^{(k,\ell)}(a^{(p)})\right)\restriction_{\mathcal{F}^{\leq \nu N}}$$

converges in norm, unif. in $N \geq 1$.

Extension to arb. $|t|$, & convergence of pert. solu. of HE on Γ_ν ($|t|$ small enough) as before, using K sm. (9).

10. Sketch of Pickl's method

Instead of the Heisenberg-
employ the Schrödinger
picture.

$$i\dot{\Psi}_t^{(N)} = H_N \Psi_t^{(N)}$$

$$H_N = \sum_1^N \left(-\Delta_j + V_t(x_j)\right) + \sum_{i<j} \underbrace{\phi_N(x_i - x_j)}_{O(N^{-1})}$$

$$\Psi_0^{(N)} \simeq \prod_{j=1}^N \varphi(x_j)$$

Consider evolution of φ
according to HE:

$$i\dot{\varphi}_t = \left(-\Delta + V_t + \phi_{\varphi_t}\right)\varphi_t,$$

$$\phi_{\varphi_t}(x) := \int d^3y \, |\varphi_t(y)|^2 \phi(y-x)$$

$$\bar{H}_N^{\varphi_t} := \sum_j \left(-\Delta_j + V_t(x_j) + \phi_{\varphi_t}(x_j) \right)$$

One-particle reduced density matrix:

$$\mu^{\Psi^{(N)}}(x,y) := \int \prod_{j=2}^{N} d^3 x_j \times$$

$$\times\, \overline{\Psi^{(N)}(x, x_2, \dots, x_N)}\, \Psi^{(N)}(y, x_2, \dots, x_N)$$

For $\varphi \in L^2(\mathbb{R}^3)$, define $p^\varphi := |\varphi\rangle\langle\varphi|$

$q^\varphi := 1 - p^\varphi$,

$$p_j^\varphi := \mathbb{1} \otimes \cdots \otimes \underset{\substack{\uparrow \\ j}}{p^\varphi} \otimes \cdots \otimes \mathbb{1},$$

$$q_j^\varphi := \mathbb{1}_N - p_j^\varphi$$

$$P_{N,k}^\varphi := \sum_{\substack{\underline{a}, \\ \sum_j a_j = k}} \prod_{\ell=1}^{N} (p_\ell^\varphi)^{1-a_\ell} (q_\ell^\varphi)^{a_\ell}$$

Then $\sum_k P^{\varphi}_{N,k} = \mathbb{1}_N$, and

$P^{\varphi}_{N,0}$ projects onto $\prod_{j=1}^{N} \varphi(x_j)$;

$P^{\varphi}_{N,k}$ —"— —"— states,

where k particles are in orbitals $\perp \varphi$.

Pick fu. $n(\cdot) > 0$ on $\{1, \cdots, N\}$, $\left(0 < n(k) < 1\text{, e.g., } n(k) = \frac{k}{N}\right)$, and define

$$\alpha^{n}_{N}(\Psi^{(N)}, \varphi) := \left\langle \Psi^{(N)}, P^{\varphi}_{N}(n) \Psi^{(N)} \right\rangle,$$

where

$$P^{\varphi}_{N}(n) := \sum_{k=0}^{N} n(k) P^{\varphi}_{N,k}.$$

If $n_0(k) = \frac{k}{N}$ then

$$P_N^{\varphi}(n_0) = N^{-1} \sum_{j=1}^{N} q_j^{\varphi} .$$

Next

(i) $\lim_{N \to \infty} \langle \Psi^{(N)}, P_N^{\varphi}(n_0) \Psi^{(N)} \rangle = 0$

$$\Leftrightarrow \; n\text{-}\lim_{N \to \infty} \mu^{\Psi^{(N)}} = p^{\varphi}$$

(ii) $\lim_{N \to \infty} \langle \Psi^{(N)}, P_N^{\varphi}(n_0) \Psi^{(N)} \rangle = 0$

$$\Leftrightarrow \lim_{N \to \infty} \langle \Psi^{(N)}, P_N^{\varphi}(n_0)^j \Psi^{(N)} \rangle = 0,$$

$$j = 1, 2, 3, \cdots .$$

<u>Key idea</u>

Control $\dot{\alpha}_N(t) \equiv \dot{\alpha}_N(\Psi_t^{(N)}, \varphi_t) =$

$$= i \langle \Psi_t^{(N)}, [H_N - \bar{H}_N^{\varphi_t}, P_N^{\varphi_t}(n_0)] \Psi_t^{(N)} \rangle$$

by estimating R.S., with
$\Psi_0^{(N)} = \prod_{j=1}^{N} \varphi(x_j)$, hence
$\alpha_N(0) \equiv \alpha_N(\Psi_0^{(N)}, \varphi) = 0$.

<u>Lemma.</u>

$$|\dot{\alpha}_N(t)| \leq C_t \alpha_N(t) + O\left(\tfrac{1}{N}\right),$$

$C_t \sim \text{const.}\, \|\phi\|_{2r} \cdot \|\varphi_t\|_{2s}$,

$r \geq 1, \quad s = \frac{r}{r-1}$.

<u>Corollary.</u>

$$\alpha_N(t) \leq e^{\int_0^t d\tau C_\tau} \alpha_N(0) + O\left(\tfrac{1}{N}\right)$$

$$\Rightarrow \quad n\text{-}\lim_{N\to\infty} \mu^{\Psi_t^{(N)}} = p^{\varphi_t}.$$

Note: C_t controlled by

properties of Hartree flow.

Can be used to discuss Gross-Pitaevskii limit!

2 Die Entdeckung der Quantenmechanik – Heisenbergs Matrizenmechanik

In den Jahren 1923-1925 zeichnete sich immer mehr ab, dass eine Änderung der bisherigen Methoden in der Behandlung der Atomstruktur und der Spektrallinien unabdingbar war. Vor allem in den beiden Zentren Göttingen (Born) und Kopenhagen (Bohr) machte sich langsam Unbehagen über die fehlerhafte Beschreibung von Mehrkörpersystemen innerhalb der alten Quantentheorie breit.

Der Ausweg aus dieser misslichen Lage wurde von Werner Heisenberg, in seiner Arbeit *Über quantentheoretische Umdeutung kinematischer und mechanischer Beziehungen* [Hei25] gefunden. Heisenberg war 23 Jahre alt, als er die Arbeit schrieb.

2.1 Heisenbergs Umdeutung

In der Einleitung seiner Arbeit drückt Heisenberg die konzeptuellen Probleme der alten Quantentheorie folgendermassen aus:

> Bekanntlich läßt sich gegen die formalen Regeln, die allgemein in der Quantentheorie zur Berechnung beobachtbarer Größen (z.B. der Energie im Wasserstoffatom) benutzt werden, der schwerwiegende Einwand erheben, daß jene Rechenregeln als wesentlichen Bestandteil Beziehungen enthalten zwischen Größen, die scheinbar prinzipiell nicht beobachtet werden können (wie z.B. Ort, Umlaufszeit des Elektrons), daß also jenen Regeln offenbar jedes anschauliche physikalische Fundament mangelt, wenn man nicht immer noch an der Hoffnung festhalten will, daß jene bis jetzt unbeobachtbare Größen später vielleicht experimentell zugänglich gemacht werden könnten.

Weiter spricht er die Bereiche an, in denen die alte Quantentheorie versagt (anomaler Zeeman-Effekt, Unmöglichkeit der Behandlung von Atomen mit mehreren Elektronen). Die Notwendigkeit einer neuen Quantentheorie – der Quantenmechanik – welche nicht mehr auf der alten Idee der quantenmechanisch erlaubten klassischen Bahnen basiert, wird deutlich:

> [Es scheint] geratener, jene Hoffnung auf eine Beobachtung der bisher unbeobachtbaren Größen (wie Lage, Umlaufszeit des Elektrons) ganz aufzugeben, gleichzeitig also einzuräumen, daß die teilweise Übereinstimmung der genannten Quantenregeln mit der Erfahrung mehr oder weniger zufällig sei, und zu versuchen, eine der klassischen Mechanik analoge quantentheoretische Mechanik auszubilden, in welcher nur Beziehungen zwischen beobachtbaren Größen vorkommen.

Heisenberg liess sich in der Entwicklung seiner Theorie von folgenden Prinzipien leiten:

1. Es muss eine quantentheoretische Mechanik gefunden werden, in welcher nur Beziehungen zwischen beobachtbaren Grössen vorkommen. Dies wurde schon von Born in [Bor24] in ähnlicher Weise verlangt.

Puzzling features of quantum mechanics originate in its combination with atomism

Quantum spins

$\mathbb{Z}^d \ni x \mapsto \vec{S}_x$, quantum spin of spin s

$$\hat{\vec{S}}_x := \frac{1}{s}\vec{S}_x$$

Hamiltonian (Heisenberg)

$$H = \vec{h}\cdot\sum_x \hat{\vec{S}}_x - \sum_{x,y} J(x-y)\hat{\vec{S}}_x\cdot\hat{\vec{S}}_y + \dots$$

$$\hat{\vec{S}}_x(t) := e^{istH}\hat{\vec{S}}_x e^{-istH}$$

Class. limit $\sim$ large-s limit

$$\text{“}\hat{\vec{S}}_x \xrightarrow[s\to\infty]{} \vec{M}_x\text{”}, \quad \hbar \leftrightarrow \frac{1}{s}$$

$\vec{M}_x \in S^2$ classical spin

$\vec{M}_x \xmapsto[s]{} \hat{\vec{S}}_x$: geom. quant.

ordering prescription!

$$\{M_x^i, M_y^j\} = \delta_{xy}\,\varepsilon^{ijk} M_x^k$$

$$\longleftrightarrow \quad [\hat{S}_x^i, \hat{S}_y^j] = \frac{i}{S}\,\delta_{xy}\,\varepsilon^{ijk}\hat{S}_x^k$$

Result: If ^ denotes quant.

$$\hat{\vec{S}}_x(t) = \left(\vec{M}_x(t)\right)^\wedge + \underbrace{\varepsilon_s}_{\to 0,\ \text{as } S\to\infty},$$

where

$$\dot{\vec{M}}_x(t) = \vec{h}\wedge\vec{M}_x(t) - \Big(\sum_y J(x-y)\vec{M}_y(t)\Big)\wedge\vec{M}_x(t)$$

Landau-Lifschitz Eq.

Is Hamiltonian Eq. of motion,

$$\mathcal{H} = \vec{h}\cdot\sum_x \vec{M}_x - \sum_{x,y} J(x-y)\,\vec{M}_x\cdot\vec{M}_y$$

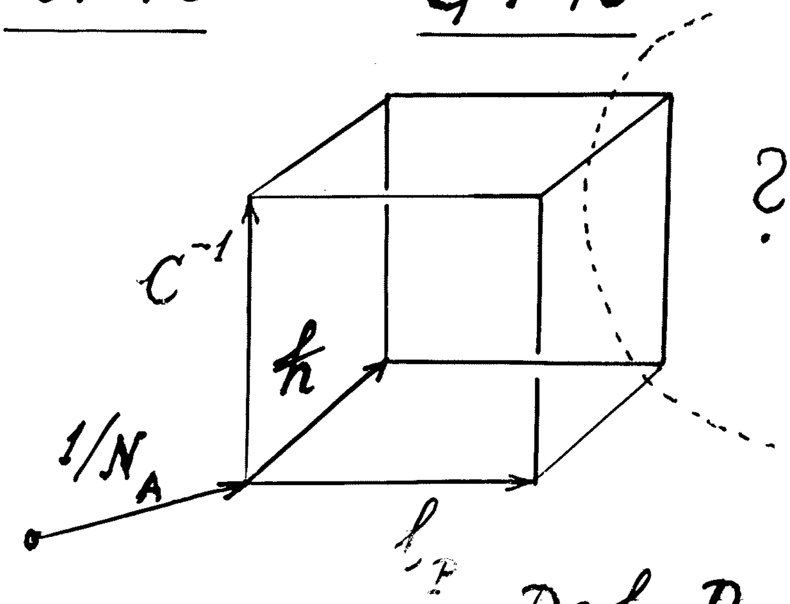
INTRODUCTION

3 stories – only 1.5 will be told

- Atomism as a deformation of cont. (field) theories of matter ⟷ mean-field limits
- Physics Bose/Fermi gases stellar dynamics & collapse, mean-field & Vlasov limit; th. of friction
- Mathematics non linear Hamiltonian evolution eqs.; semi-classical analysis.

(1) 3 Revolutions of 20^{th} Century Physics + pd.

- Atomism $\leftrightarrow$ Quantum Th.,
- STR $\rightarrow$ GTR



Planck-
Einstei

Def. Param

Pd.	Atomism	$\leftrightarrow$	$1/N_A$
Rev.	QT	$\leftrightarrow$	$\hbar$
	STR	$\leftrightarrow$	c^{-1}
	GTR	$\leftrightarrow$	l_P
21^{st} Ct.	?	$\leftrightarrow$	α', g_{string}

?

② Physics

(i) Newtonian lim of quantum theory: Explain why point-particle mech. is viable

(ii) Dissipative transport; origin of friction forces

(iii) Th. of Bose gases (in traps); atom-beam lasers;

(iv) Stellar dynamics & -collapse; neutron stars

(v) radiation damping

3 Mathematics

Mean-field limit of (quantum[illegible]
many-body theory →
NL Hamiltonian evolution Eq[illegible]

Ex.: $$i\hbar\partial_t \vec{\psi}_t = \mathring{H}\vec{\psi}_t - g\left(|\vec{\psi}_t|^2 * |x|^{-1}\right)\vec{\psi}_t + g\sum_j \left(\vec{\psi}_t \overline{\psi}_t^{\,j} * |x|^{-1}\right)\psi_t^j$$

HF Eq.

$$\vec{\psi} = \begin{pmatrix} \psi^1 \\ \vdots \\ \psi^N \end{pmatrix}, \quad \langle \psi^i, \psi^j \rangle = \delta^{ij},$$

$$\mathring{H} \overset{e.g.}{=} \sqrt{-\Delta + m^2} + V(x)$$

Bosons: $N = 1$ …

Fermions: $N = \#$ particles

Focussing NL $(g>0)$ → solitary waves (→ Newtonian lim)

"Hier[1] liegt der Schlüssel der Situation, der Schlüssel nicht nur zur Strahlungstheorie, sondern auch zur molekularen[2] Konstitution der Materie ..."

A. Sommerfeld, in: "Das Plancksche Wirkungsqu. & seine allg. Bedeutung für die Molekularphysik"

[1] in quantum theory

[2] ≃ atomistic (constitution)

1. Atomism & Quantization

"Interstellar dust": Class. cont. medium - states given by mass density

$$M f(x,p)\,dx\,dp$$

on $\mathbb{R}^3 \times \mathbb{R}^3$, with

$$\int f(x,p)\,dx\,dp = \nu \quad (\#\text{moles})$$

Time-dependence given by

Vlasov Equation

(A model of matter as a continuous medium)

Hamilton op. $\hat{\mathcal{H}}_V := :\mathcal{H}_V(a_N^*, a_N):$

Schrödinger Eq.

$$i N^{-1} \partial_t \Psi_t = \hat{\mathcal{H}}_V \Psi_t , \quad \Psi_t \in \mathcal{F}_V$$

$\Leftrightarrow$ Hamiltonian Eqs. of motion for symm. n-particle densities $f_n = \bar{\varphi}_n \cdot \varphi_n$, on $\Gamma^{(n)}$, 2-body potential $\frac{1}{N}\phi$, $n = 0, 1, 2, 3, \cdots$

Apparently, atomistic Newtonian mech. of pt. part $=$ "quantization" of cont. th. given by Vlasov

"

"classical lim of Newton"

Hartree & Hartree-Fock:

Replace $f(x,p) = \overline{\alpha(x,p)} \cdot \alpha(x,p)$ by

$$(2)\quad f_\hbar(x,p) := \frac{1}{(2\pi)^3} \int dy\, e^{-iyp}\, \overline{\psi\left(x - \frac{\hbar y}{2}\right)}\, \psi\left(x + \frac{\hbar y}{2}\right),$$

$f_\hbar$ = Wigner trsf. of ψ

Dynamics of ψ

$$(3)\quad i\hbar \partial_t \psi_t = \left[-\frac{\hbar^2}{2m} \Delta_x + V\right] \psi_t + \left[|\psi_t|^2 * \phi\right] \psi_t$$

Hartree Equation

If solu. ψ_t of (3) plugged into (2) then

$$\lim_{\hbar \downarrow 0} f_{\hbar,t}(x,p)$$

solves Vlasov Eq. (Na-Se)