

Geometric convergence

Ref.: H Lewin: "Geometric methods for nonlinear many-body quantum systems",
JFA 260 (2011), p. 3535-3595.

Motivation: Have minimization problem $E = \inf_{\|\Psi\|=1} \langle \Psi, H\Psi \rangle$.

→ Want to use min. sequence (Ψ_n) to obtain ^{weak} estimates on E .

Problem: Only have weak-convergent subsequence (Ψ_{n_k}) and limit could even be 0.

Solution: Introduce a weaker concept of convergence.

→ Need appropriate language.

Second quantization

1) Underlying spaces

For (sep.) H -space $\mathcal{H} = L^2(\mathbb{R}^d)$, def. Schatten space $\mathcal{S}_p(\mathcal{H}) \subseteq \mathcal{K}(\mathcal{H})$ by req.

$$\|A\|_{\mathcal{S}_p(\mathcal{H})} = \text{Tr}_{\mathcal{H}} (|A|^p)^{\frac{1}{p}} < \infty$$

$p=1$: Trace class, $p=2$: HS. Have

$$\underbrace{(\mathcal{K}(\mathcal{H}))}_S = \underbrace{\mathcal{S}_1(\mathcal{H})}_T, \quad \mathcal{S}_1(\mathcal{H})' = \underbrace{\mathcal{L}(\mathcal{H})}_{\mathcal{L}^\infty}$$

\mathcal{H} sep. $\Rightarrow \mathcal{K}(\mathcal{H})$ sep. $\Rightarrow (\Gamma_n)_n \in (\mathcal{B}_1^{\mathcal{S}_1(\mathcal{H})})^{\mathbb{N}}$ has weak-* conv. subseq. i.e.,

$$\text{Tr}((\Gamma_n - \Gamma)k) \xrightarrow{n \rightarrow \infty} 0 \quad \forall k \in \mathcal{K}(\mathcal{H}).$$

Define many-particle spaces

$$\mathbb{H}_{a/s}^N := \left\{ \bigwedge \bigvee \right\}_1^N \mathbb{H} :=: \mathbb{H}^{\otimes_{a/s} N}$$

For the particle number may not be conserved (later), we introduce the graded algebra

$$\mathbb{F}_{a/s} := \mathbb{C} \oplus \bigoplus_{n \geq 1} \mathbb{H}_{a/s}^n, \text{ called } \underline{\text{Fock space}}.$$

→ becomes H-space when endowed w/

$$\langle \Psi_1, \Psi_2 \rangle_{\mathbb{F}_{a/s}} = \sum_{n \geq 0} \langle \Psi_1^{(n)}, \Psi_2^{(n)} \rangle_{\mathbb{H}_{a/s}^n}.$$

$\mathbb{H}_{a/s}^0 = \mathbb{C}$

Def. vacuum · $\mathcal{D} := (1, 0, \dots, 0) \in \mathbb{F}_{a/s}$. Introduce the truncated Fock space:

$$\mathbb{F}_{a/s}^{\leq N} := \mathbb{C} \oplus \bigoplus_{n=1}^N \mathbb{H}_{a/s}^n.$$

$\mathbb{F}_{a/s}$ becomes graded algebra if one defines for $\psi_i \in \mathbb{H}_{a/s}^{N_i}$

$$\psi_1 \bigwedge \bigvee \psi_2 (x_{1,1}, \dots, x_{N_1+N_2}) := \frac{1}{\sqrt{N_1! N_2! (N_1+N_2)!}} \sum_{\pi \in S_{N_1+N_2}} \left\{ \begin{matrix} \text{sign}(\pi) \\ 1 \end{matrix} \right\} \psi_1 \otimes \psi_2 (x_{\pi(1)}, \dots, x_{\pi(N_1+N_2)})$$

where we refer to $\{a\}$ in the $\left\{ \begin{matrix} \text{fermionic} \\ \text{bosonic} \end{matrix} \right\}$ case.

Note that if $\{f_i\} \subseteq \mathbb{H}$ is an ONB, we have that

$$\left\{ \begin{aligned} \{f_{i_1, \dots, i_{N_1}}\}_{i_1, \dots, i_{N_1}} &\text{ is an ONB of } \mathbb{H}_a^{N_1} \\ \{f_{i_1, \dots, i_{N_2}}\}_{i_1, \dots, i_{N_2}} &\text{ is an orthogonal basis of } \mathbb{H}_s^{N_2} \\ &\text{(Have } f^{\vee N} = \sqrt{N!} f^{\otimes N}) \end{aligned} \right.$$

2) Annihilation and creation operators

Let $f \in \mathcal{H}$, $\mathcal{F}_{a/s}^{fin} = \bigcup_{N \geq 1} \mathcal{F}_{a/s}^N$.

Def. $a^+(f): \mathcal{F}_{a/s}^{fin} \rightarrow \mathcal{F}_{a/s}^{fin}$ by requiring:

$$(i) a^+(f) \mathcal{H}_{a/s}^N \subseteq \mathcal{H}_{a/s}^{N+1} \quad \forall N \geq 0$$

Abuse of notation: $0 \otimes \dots \otimes \mathcal{H}_{a/s}^N \otimes 0 \in \mathcal{F}_{a/s}$

$$(ii) \forall \psi \in \mathcal{H}_{a/s}^N \quad a^+(f)\psi := \begin{cases} f \wedge \psi & \text{fermions} \\ f \vee \psi & \text{bosons} \end{cases}$$

If $\{f_i\}$ is an ONB of \mathcal{H} , then $\left\{ \begin{array}{l} \prod_{k=1}^N a^+(f_k) \Omega \\ - \quad - \quad - \\ - \quad - \quad - \end{array} \right\}_{i_1, \dots, i_N, N \geq 0}$ is an $\left\{ \begin{array}{l} \text{ON} \\ \text{orthogonal} \end{array} \right\}$ basis of $\mathcal{F}_{a/s}$.

Def. $a(f): \mathcal{F}_{a/s}^{fin} \rightarrow \mathcal{F}_{a/s}^{fin}$ by requiring:

$$(i) a(f) \mathcal{H}_{a/s}^N \subseteq \mathcal{H}_{a/s}^{N-1} \quad \forall N \geq 1 \text{ and } a(f)\Omega = 0$$

$$(ii) \forall \psi \in \mathcal{H}_{a/s}^N \quad (a(f)\psi)(x_1, \dots, x_{N-1}) := \int \overline{f(x)} \psi(x, x_1, \dots, x_{N-1}) dx.$$

$a^+(f)$ is called creation operator, $a(f)$ annihilation operator. We abuse notation in the sense of

$$\left(a^+(f) \left((\psi^{(w)})_{w \in \mathcal{N}_s} \right)^{(j+1)} \right) = a^+(f) \psi^{(w)}$$

$$\left(a(f) \left((\psi^{(w)})_{w \in \mathcal{N}_s} \right)^{(j)} \right) = a(f) \psi^{(w)}$$

We have

$$\langle \Phi, a^+(f) \Psi \rangle_{\mathcal{F}_{a/s}} = \langle a(f) \Phi, \Psi \rangle_{\mathcal{F}_{a/s}} \quad \text{justifies notation.}$$

In the fermionic case have (CAR): $\begin{cases} \{a(f), a^+(g)\} = \langle g, f \rangle_{\mathcal{H}} \\ \{a(f), a^+(g)\} = \{a(f), a(g)\} = 0 \end{cases} \quad (\{A, B\} := AB + BA)$

In the bosonic case have (CCR): Exchange $\{, \cdot\}$ by $[, \cdot]$ where $[A, B] := AB - BA$.

3) Observables

Start w/ occupation number operator

$$\mathcal{N} = \bigoplus_{N \geq 0} \mathcal{N}; \quad \mathcal{D}(\mathcal{N}) = \left\{ (\psi^{(N)})_{N \geq 0} \in \mathbb{F}_{\text{Fock}} \mid \sum_{N \geq 0} N^2 \|\psi^{(N)}\|_{\mathbb{H}_N}^2 < \infty \right\}$$

For $A: \mathbb{H} \supseteq \mathcal{D}(A) \rightarrow \mathbb{H}$ s.a. def.

$$\hat{A} = A = d\Gamma(A) = 0 \oplus \bigoplus_{N \geq 1} \left(\sum_{i=1}^N A_{x_i} \right)$$

A is s.a. if

$$\mathcal{D}(A) = \left\{ (\psi^{(N)})_{N \geq 0} \in \bigoplus_{N \geq 0} \mathcal{D}\left(\sum_{j=1}^N A_{x_j}\right) \mid \sum_{N \geq 0} \left\| \left(\sum_{j=1}^N A_{x_j}\right) \psi^{(N)} \right\|_{\mathbb{H}_N}^2 < \infty \right\}$$

$A \text{ s.a.} \iff \bigwedge_{\psi \in \mathcal{D}(A)} \sum_{N \geq 0} \left\| \left(\sum_{j=1}^N A_{x_j}\right) \psi^{(N)} \right\|_{\mathbb{H}_N}^2 < \infty$

Note that $d\Gamma = d\Gamma(\text{Id}_{\mathbb{H}})$. Take $\{f_i\}_{i \geq 1} \in \mathcal{D}(A)$ to be an ONB of \mathbb{H} . Then we have

$$A = \sum_{j \geq 1} a^*(A f_j) a(f_j) = \sum_{j \geq 1} \underbrace{A_{j,j}}_{= \langle f_j, A f_j \rangle_{\mathbb{H}}} a^*(f_j) a(f_j)$$

For a two-body operator $W: \mathbb{H}_{\text{Fock}}^2 \rightarrow \mathbb{H}_{\text{Fock}}^2$ def.

$$W = 0 \oplus 0 \oplus \bigoplus_{N \geq 2} \left(\sum_{1 \leq i < j \leq N} \underbrace{W_{i,j}}_{\text{acting on } x_i \text{ and } x_j} \right)$$

Again w/ ONB $\{f_i\}$

$$W = \sum_{\substack{1 \leq k \leq l \\ 1 \leq i \leq j}} W_{ijkl} a^*(f_k) a^*(f_l) a(f_i) a(f_j)$$

$$w/ \quad W_{ijkl} = \begin{cases} \langle f_i, f_j, W f_k, f_l \rangle_{\mathbb{H}_2} & \text{fermions} \\ \frac{\langle f_i, f_j, W f_k, f_l \rangle_{\mathbb{H}_2}}{(1 + \delta_{ij})(1 + \delta_{kl})} & \text{bosons} \end{cases}$$

Example: $H^V(N) := \sum_{j=1}^N \left(\frac{-\Delta_{x_j}}{2} + V(x_j) \right) + \sum_{1 \leq k < l \leq N} W(x_k - x_l)$

2nd quant.

$$H^V = \sum_j h_{ij} a^\dagger(f_i) a(f_j) + \sum_{\substack{1 \leq k < l \\ 1 \leq i \leq j}} W_{i,j,k,l} a^\dagger(f_i) a^\dagger(f_j) a(f_l) a(f_k)$$

w/ $h_{ij} = \int \left(\frac{\nabla f_i(x) \cdot \nabla f_j(x)}{2} + V(x) \overline{f_i(x)} f_j(x) \right) dx$.

Physicists' notation: $a^\dagger(f) = \int_{\mathbb{R}^d} f(x) \varphi^*(x) dx \rightsquigarrow \varphi^*(x) = \sum_{i \geq 1} \overline{f_i(x)} a^\dagger(f_i)$ creation at position $x \in \mathbb{R}^d$

w/ $\{f_i\}_i \in \mathcal{H}$ an ONB.

$$\hookrightarrow H = \int_{\mathbb{R}^d} \left(\frac{1}{2} \nabla \varphi^*(x) \cdot \nabla \varphi(x) + V(x) \varphi^*(x) \varphi(x) \right) dx + \frac{1}{2} \int_{\mathbb{R}^d} W(x-y) \varphi^*(x) \varphi^*(y) \varphi(y) \varphi(x) dx dy$$

4) States, density matrices

\mathcal{X} H-sp.

Def. (State). $\Gamma \in \mathcal{O}_1(\mathcal{X})$ is a state iff $\Gamma \geq 0$ is s.a. and $\text{Tr}(\Gamma) = 1$.

Denote the set of all states by $S(\mathcal{X})$.

Note that $S(\mathcal{X})$ is c.w. and by the Spectral Thm, every state $\Gamma \in S(\mathcal{X})$ can be written as

$$\Gamma = \sum_{i \geq 1} u_i |\varphi_i\rangle \langle \varphi_i|, \quad \sum_{i \geq 1} u_i = 1.$$

$S(\mathcal{X})$ is not closed under weak-* limit: $\Gamma_n \xrightarrow{*} \Gamma, (\Gamma_n) \in S(\mathcal{X})^{\mathbb{N}} \Rightarrow \Gamma = \Gamma^* \geq 0 \omega /$

$$\text{Tr}_{\mathcal{X}}(\Gamma) \leq \liminf_{n \rightarrow \infty} \text{Tr}_{\mathcal{X}}(\Gamma_n) = 1$$

There are examples where \langle

holds: Take $\varphi_n := \varphi_1 \wedge \varphi_n$ for ONS $\{\varphi_n\}$. $\varphi_n \rightarrow 0 \Rightarrow |\varphi_n\rangle \langle \varphi_n| \xrightarrow{*} 0$.

Def. (density matrix) Let $\Gamma \in S(\mathcal{F}_{\mathbb{R}})$. Define $\Gamma^{(p,q)}, \mathbb{H}_{a|s}^q \rightarrow \mathbb{H}_{a|s}^p$ by

$$\langle g_1 | \hat{v} \rangle = \langle \hat{v} | g_1 \rangle \Gamma^{(p,q)} | \hat{v} \rangle = \langle \hat{v} | g_2 \rangle = \text{Tr}_{\mathcal{F}_{\mathbb{R}}} (\Gamma a^*(g_1) a(g_2) a(g_1) a(g_2)).$$

Write $\Gamma^{(p,p)} = \Gamma^{(p)}$. Have $\Gamma^{(0)} = \pi(\Gamma) = 1$.

Properties. (i) $\forall N \in \mathbb{N} \exists C_N > 0 \forall 0 \leq p, q \leq N \forall \Gamma \in S(\mathcal{F}_{\mathbb{R}}^{\leq N}), \|\Gamma^{(p,q)}\|_{\mathcal{O}_1(\mathbb{H}_{a|s}^p, \mathbb{H}_{a|s}^q)} \leq C_N$

Def. via singular values

(ii) $S(\mathcal{F}_{a|s}^{\leq N}) \ni \Gamma \mapsto \Gamma^{(p,q)} \in \mathcal{O}_1(\mathbb{H}_{a|s}^q, \mathbb{H}_{a|s}^p)$ is continuous but not weak-* continuous.

(iii) States fully determined by density matrices: $\Gamma_1^{(p,q)} = \Gamma_2^{(p,q)} \forall p, q \Rightarrow \Gamma_1 = \Gamma_2$
 $(\Gamma_1, \Gamma_2 \in S(\mathcal{F}_{a|s}^{\leq N}))$.

Rem. States in this context generalize the concept of states in QM ($= L^2$ -cas w/ $\|\cdot\|_2 = 1$)

Had: $E(\varphi) = \langle \varphi, H \varphi \rangle = \text{Tr}(H |\varphi\rangle \langle \varphi|)$

\Rightarrow Have $E(\Gamma) = \text{Tr}_{\mathcal{F}}(\underbrace{H}_{2^{\text{nd}} \text{ quant of } H} \Gamma)$ iff $\Gamma \in S(\mathcal{F}_{a|s}^{\text{fin}})$.

Geometric convergence

Def. (Geometric convergence)

Def. the geometric topology \mathcal{T}_g on $S(\mathcal{F}^{\leq N})$ to be the initial topology for the maps

$$S(\mathcal{F}^{\leq N}) \ni \Gamma \longmapsto \langle \Phi, \Gamma^{(p,q)} \Psi \rangle_{\mathbb{H}^p}.$$

We say $(\Gamma_n)_n \in S(\mathcal{F}^{\leq N})^{\mathbb{N}}$ converges geometrically to $\Gamma \in \mathcal{O}_1(\mathcal{F}^{\leq N})$ iff

$$\lim_{n \rightarrow \infty} \langle \Phi, \Gamma_n^{(p,q)} \Psi \rangle_{\mathbb{H}^p} = \langle \Phi, \Gamma^{(p,q)} \Psi \rangle_{\mathbb{H}^p} \quad \forall \Phi, \Psi, p, q.$$

In this case, we write $\Gamma_n \xrightarrow{g} \Gamma$.

Properties. (i) $\mathcal{T}_g \subseteq \mathcal{T}_{\mathcal{O}_1}$ ^{coarser}: $\Gamma_n \rightarrow \Gamma$ in $\mathcal{O}_1(\mathcal{F}^{\leq N}) \Rightarrow \Gamma_n \xrightarrow{g} \Gamma$

(ii) $\Gamma_n \xrightarrow{g} \Gamma$ in $S(\mathcal{F}^{\leq N}) \Leftrightarrow \Gamma_n^{(p,q)} \xrightarrow{*} \Gamma^{(p,q)}$ weakly-* in $\mathcal{O}_1(\mathcal{F}^{\leq N}) \quad \forall 0 \leq p, q \leq N$.

(iii) Note that $S(\mathcal{F}^{\leq N}) \subseteq \mathcal{O}_1(\mathcal{F}^{\leq N})$ is closed under \mathcal{T}_g but not under the weak-* topology.

Example: $\{\varphi_n\}_n \subseteq \mathbb{H}$ ONB. Def. $\varphi_n := \varphi_1 + \varphi_n \mapsto \Gamma_n := 0 \oplus \langle \varphi_n | \varphi_n \rangle \langle \varphi_n | \cdot \rangle \in S(\mathcal{F}_0^{\leq 1})$.

Have $\Gamma_n \xrightarrow{*} 0$ weakly-* but $\Gamma_n \xrightarrow{g} 0 \oplus \langle \varphi_1 | \cdot \rangle \langle \varphi_1 | \cdot \rangle$.

(iv) Even more: $(S(\mathcal{F}^{\leq N}), \mathcal{T}_g)$ is compact, i.e., $(\Gamma_n)_n \in S(\mathcal{F}^{\leq N})^{\mathbb{N}}$ has a conv. subseq $\Gamma_{n_k} \xrightarrow{g} \Gamma$

\rightsquigarrow Follows from \mathcal{T}_g being the restriction of a topology on the CCR (CCP) algebra generated by $\{a(p), a(p)^*\}$.

(v) $\left(\begin{array}{l} \text{Average particle number conservation} \\ + \\ \text{geometric convergence} \end{array} \right) \Leftrightarrow \text{strong convergence:}$ Geometric ISC: $\Gamma_n \xrightarrow{g} \Gamma \Rightarrow \mathcal{T}_g(\mathcal{K}(\Gamma))$
Strong \mathcal{T}_g $\mathcal{K}(\Gamma)$
 $n \rightarrow \infty$
 $w/ \text{ " " } \Leftrightarrow \Gamma_n \rightarrow \Gamma$

Application: HVZ Theorem

Recall:
$$H^V(k) = \sum_{j=1}^k \left(-\frac{\Delta_{x_j}}{2} + V(x_j) \right) + \sum_{1 \leq k' < l \leq N} W(x_{k'} - x_l)$$

and
$$H^V = 0 \oplus \bigoplus_{k \geq 1} H(k).$$

For a big class of V, W have

$$(1-\varepsilon) \left(\sum_{j=1}^N -\Delta_{x_j} \right) - C \leq H^V(N) \leq (1+\varepsilon) \left(\sum_{j=1}^N -\Delta_{x_j} \right) + C.$$

Assume this. If $\text{Tr} \left((-\Delta)^{\frac{1}{2}} \Gamma^{(1)} (-\Delta)^{\frac{1}{2}} \right) < \infty$ define

$$\mathcal{E}^V(\Gamma) = \text{Tr}_{\mathbb{R}^2} (H^V \Gamma) = \text{Tr}_{\mathbb{R}^2} \left[\left(-\frac{1}{2} \Delta + V \right) \Gamma^{(1)} \right] + \text{Tr}_{\mathbb{R}^2} (W \Gamma^{(2)}).$$

Motivation: $\Psi \mapsto \langle \Psi, H(N) \Psi \rangle$ is not weak lsc. Indeed, defining

$$E^V(N) := \inf_{\mathbb{R}^2} e(H^V(N)), \quad \Sigma^V(N) := \inf_{\mathbb{R}^2} e_{\Sigma}(H^V(N)).$$

typically have $\Sigma^V(N) < 0$, i.e., \exists singular Weyl sequence $\Psi_n \rightarrow 0$ w/ $\langle \Psi_n, H^V(N) \Psi_n \rangle \rightarrow \Sigma^V(N) < 0$.

Lemma: Assume $W \geq 0$, $(\Gamma_n)_n \in S(\mathbb{F}^{\leq N})^N$, $\Gamma_n \xrightarrow{f} \Gamma$. Then

$$\mathcal{E}^V(\Gamma) \leq \liminf_{n \rightarrow \infty} \mathcal{E}^V(\Gamma_n).$$

Thm (Huzariker-Vu-Winter-Zhishan in lsc case)

Let $W \geq 0$. Then $E^0(N) = 0 \forall N \geq 0$ and $\Sigma^V(N) = E^V(N-1)$

In particular, $E^V(N)$ is an isolated ev iff

$$E^V(N) < E^V(N-1) = \min \{ E^V(N-k) + E^0(k), k \in \{1, \dots, N\} \}.$$

Remark: For $\Gamma \in S(\mathbb{F}^{\leq N})$ def. $G_{inn} := \Pi_{in} \Gamma \Pi_n : H_{1/s}^n \rightarrow H_{1/s}^m$.

If $[\Gamma, d] = 0$, then

$$\Gamma = \begin{bmatrix} G_{11} & & 0 \\ & \ddots & \\ 0 & & G_{NN} \end{bmatrix}$$

Now take $\Gamma_n \rightarrow \Gamma$ w/ $[\Gamma_n, d] = 0$. Then $\Gamma_n^{(pq)} = 0$ for $p \neq q$ and thus $\Gamma^{(pq)} = 0$ for $p \neq q$.

Thus $[\Gamma, d] = 0$.

Proof of Thm. $\sum^v(N) \leq E^v(N-1)$ is shown by a std argument constructing an appropriate singular Weyl sequence, using a Weyl sequence for $E^v(N-1)$.

Now notice $E^v(N) \leq \sum_{\substack{\uparrow \\ \text{inf over}}}^v(N) \leq E^v(N-1) \Rightarrow N \mapsto E^v(N-1)$ non-increasing.

For $v=0$, $E^0(N) \geq 0$ ($w \geq 0$), $E^0(1) = 0 \Rightarrow E^0(N) = 0 \forall N$.

Take a singular Weyl sequence $(\Psi_n)_n \in (H^N)^N$ for $\sum^v(N)$.

$$(H^v(N) - \sum^v(N)) \Psi_n \xrightarrow{n \rightarrow \infty} 0, \quad \|\Psi_n\| = 1, \quad \Psi_n \rightarrow 0 \text{ weakly in } H^N.$$

Def. $\Gamma_n = 0 \oplus \dots \oplus 0 \oplus |\Psi_n\rangle\langle\Psi_n| \in S(\mathbb{F}^{\leq N})$.

Up to taking a subsequence, may assume $\Gamma_n \rightarrow \Gamma \in S(\mathbb{F}^{\leq N})$. By the above remark have

$$\Gamma = \begin{bmatrix} G_{11} & & 0 \\ & \ddots & \\ 0 & & G_{NN} \end{bmatrix}$$

Here $G_{NN} = G_{NN}^{(N)}$ is weak-* limit of $|\Psi_n\rangle\langle\Psi_n|$, thus $G_{NN} = 0$ for $\Psi_n \rightarrow 0$.

$$\text{Then: } \sum^v(N) \stackrel{\text{why?}}{\leq} \lim_{n \rightarrow \infty} \mathcal{E}^v(\Gamma_n) \stackrel{\text{Lemma}}{\geq} \mathcal{E}^v(\Gamma) = \sum_{j=0}^{N-1} \text{Tr}_{H^1} (H^v(j) G_{jj}) \stackrel{\text{var. char. of EV}}{\geq} \sum_{j=0}^{N-1} \frac{E^v(j)}{\geq E^v(N-1)} \text{Tr}_{H^1} (G_{jj}) \stackrel{\geq 0}{\geq 0}$$

$$\geq E^v(N-1).$$

$$\sum_{j=0}^{N-1} \text{Tr}_{H^1} (G_{jj}) = \text{Tr } \Gamma = 1.$$

