VII LOCALIZATION OF BOUND STATES

We have seen: in asymptotically complete systems, the Hilbert space can be decomposed into a direct sum of bound states and scattering states, $\mathcal{H} = \mathcal{H}_B \oplus \operatorname{ran} \Omega_+$,
where $\mathcal{H}_B$ = closure of $\{\varphi \in D(H) : H\varphi = E\varphi\}$. eigenvectors

Scattering states behave like free states: particle flies away and disperses.

Eigenvectors (bound states) have trivial time evolution:

if $H = H^*$, $\sigma(H) \subset \mathbb{R}$, so $E \in \mathbb{R}$.

$$H\psi = E\psi \quad \Rightarrow \quad e^{-iHt}\psi = e^{-iEt}\psi.$$

The probability to find a particle near position $x \in \mathbb{R}^n$:

$$|(e^{-iHt}\psi)(x)|^2 = |\psi(x)|^2 \qquad \text{indep. of time.}$$

Goal: Show that $|\psi(x)|^2 \simeq e^{-c|x|}$ for large $|x|$.

PROP.: (IMS localization formula)

Let $V : \mathbb{R}^n \to \mathbb{R}$ measurable and such that $H = -\frac{\Delta}{2} + V$ is closed with domain $H^2(\mathbb{R}^n)$.

Let $f \in C^\infty(\mathbb{R}^n)$, real-valued and $\partial^\alpha f \in L^\infty(\mathbb{R}^n)$ $\forall |\alpha| \leq 2$.

Then on $H^2(\mathbb{R}^n)$ we have

$$2fHf = f^2 H + Hf^2 + |\nabla f|^2.$$

PROOF: We only show $2fHf\varphi = (f^2H + Hf^2 + |\nabla f|^2)\varphi$ $\forall \varphi \in \underline{C_0^\infty(\mathbb{R}^n)}$.

The identity for $\varphi \in H^2(\mathbb{R}^n)$ follows by an approximation argument in the graph norm of H.

(A priori it is not clear that $-\Delta = \mathcal{F}^{-1} p^2 \mathcal{F}$ satisfies a product rule; only when applied to C^2-functions, where it agrees with the classical derivatives.)

Straightforward calculation:

$$2f\left(-\frac{\Delta}{2} + \cancel{V}\right)f\varphi = f^2\left(-\frac{\Delta}{2} + \cancel{V}\right)\varphi + \left(-\frac{\Delta}{2} + \cancel{V}\right)f^2 V + |\nabla f|^2\varphi.$$

(because $f\varphi \in D(V) \cap D(-\frac{\Delta}{2})$; and $fVf\varphi$ can be written out pointwise almost everywhere.)

Use product rule for Laplacian:

LHS: $f\Delta(f\varphi) = f\nabla(\nabla f\,\varphi + f\nabla\varphi)$

$$= f(\Delta f)\varphi + f(\nabla f)(\nabla\varphi) + f(\nabla f)(\nabla\varphi) + f^2(\Delta\varphi).$$

RHS: $\frac{1}{2}f^2(\Delta\varphi) + \frac{1}{2}\nabla(\nabla(f^2\varphi)) - |\nabla f|^2\varphi$ Check it!

$= \dots = \text{LHS}$. ■

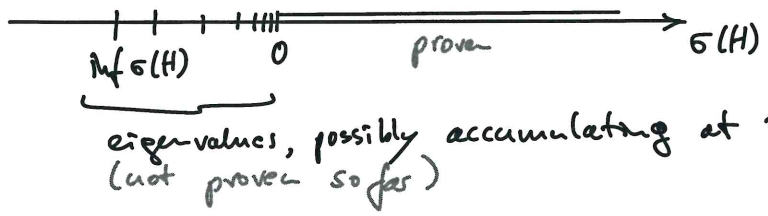
THM.: (Exp. localization of eigenvectors, Agmon)

Let $V \in L^2_{loc}(\mathbb{R}^n)$ and $n \leq 3$, or $V \in L^\infty(\mathbb{R}^n)$.
Let V real-valued and $V(x) \longrightarrow 0 \quad (|x| \to \infty)$.
Let $H = -\frac{\Delta}{2} + V$.

If $\varphi \in H^2(\mathbb{R}^n)$ and $H\varphi = E\varphi$, then

$$e^{\beta |x|}\varphi \in L^2(\mathbb{R}^n) \qquad \forall \beta > 0 \text{ with } E + \frac{\beta^2}{2} < 0.$$

RMK: $\sigma(-\frac{\Delta}{2}) \subset \sigma(H)$ if $\Omega_\pm$ exist. $\sigma(-\frac{\Delta}{2}) = [0, \infty)$.



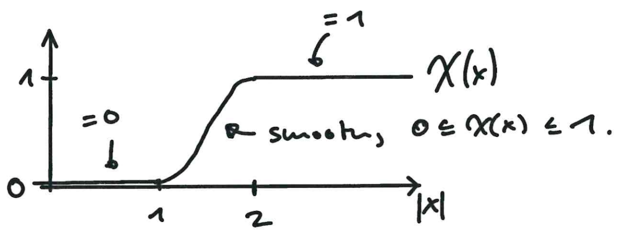
This means for the decay of eigenvectors, $H\varphi = E\varphi$:

$$\varphi(x) \sim e^{-\beta|x|} \quad \text{for } |x| \longrightarrow \infty,$$

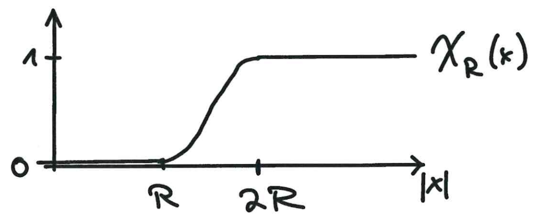
but rate of decay β smaller and smaller for E closer and closer to zero.

PROOF (of exp. localization):

Let $\chi \in C^\infty(\mathbb{R}^n)$:



Let $\chi_R(x) := \chi\left(\frac{x}{R}\right)$:
(for $R > 0$)



Let $f(x) := \dfrac{\beta|x|}{1 + \varepsilon|x|}$

(for $\varepsilon > 0$ this is a regularization of $\beta|x|$).

Properties (check!):

$|f| \le \frac{\beta}{2}$, and for $x \neq 0$: $|\nabla f(x)| \le \beta$.

(forgetting $+1$ in denominator) (growth is slower than of $\beta|x|$, and the growth of $\beta|x|$ is proportional to β)

Let $G := \chi_R e^f$. Then $G \in C^\infty(\mathbb{R}^n) \cap L^\infty(\mathbb{R}^n)$,

$$(*) \qquad \nabla G = (\nabla\chi_R)e^f + \chi_R e^f(\nabla f) = (\nabla \chi_R)e^f + G(\nabla f) \in L^\infty(\mathbb{R}^n),$$

and $\partial_i\partial_j G \in L^\infty(\mathbb{R}^n)$ $\forall i,j \in \{1,\dots,n\}$.

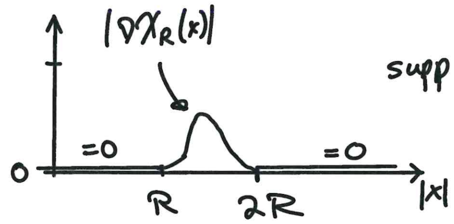
Now: $$\langle G\varphi, (H-E)G\varphi\rangle \overset{\text{IMS}}{=} \langle \varphi, \left(\tfrac{1}{2}\left[G^2H + HG^2 + |\nabla G|^2\right] - E\right)\varphi\rangle$$

$$\overset{H^*=H,\ H\varphi = E\varphi}{=} \langle \varphi, \tfrac{1}{2}|\nabla G|^2 \varphi\rangle$$

$$\overset{(*)}{=} \tfrac{1}{2}\langle \varphi, \left(|\nabla\chi_R|^2 e^{2f} + 2\nabla\chi_R\cdot\nabla f\, e^f G + \underbrace{G^2|\nabla f|^2}_{\text{to the other side.}}\right)\varphi\rangle$$

$$\Rightarrow \langle G\varphi, (H - E - \tfrac{|\nabla f|^2}{2})G\varphi\rangle \le \sup_{x\in\mathbb{R}^n}\left(|\nabla\chi_R|^2 e^{2\beta|x|} + 2|\nabla\chi_R|\beta e^{2\beta|x|}\right)\|\varphi\|_{L^2}^2.$$

Notice:



$\operatorname{supp}|\nabla\chi_R(x)| \subset \{x\in\mathbb{R}^n : R \le |x| \le 2R\}$.

In $\operatorname{supp}|\nabla\chi_R(x)|$: $e^{2\beta|x|} \le e^{4\beta R} < \infty$.

$$\Rightarrow \langle G\varphi, (H - E - \tfrac{|\nabla f|^2}{2})G\varphi\rangle \le C_R\|\varphi\|_{L^2}^2, \quad C_R < \infty. \quad (i)$$

On the other hand:

$$\langle \psi, (-\Delta)\psi\rangle = \int dp\, |\hat{\psi}(p)|^2 p^2 \geq 0.$$

$$\langle G\varphi, (H - E - \tfrac{|\nabla f|^2}{2}) G\varphi\rangle \geq \langle G\varphi, (V - E - \tfrac{|\nabla f|^2}{2}) G\varphi\rangle$$

$$\overset{|\nabla f| \leq \beta}{\geq} \langle G\varphi, (V - E - \tfrac{\beta^2}{2}) G\varphi\rangle$$

$$\overset{\operatorname{supp} G \subset \mathbb{R}^n \setminus B_R(0)}{\geq} \underbrace{\Big(\inf_{|x|\geq R} V(x) - E - \tfrac{\beta^2}{2}\Big)}_{\substack{>0 \text{ for some } R>0 \\ \text{because } V(x)\to 0\ (|x|\to\infty).}} \|G\varphi\|_{L^2}^2$$

Recall: $E<0$.

$$\geq \delta_R \|G\varphi\|_{L^2}^2. \qquad (ii)$$

Combining (i) & (ii) $\Rightarrow$ $\|G\varphi\|_{L^2}^2 \leq \underbrace{\frac{C_R}{\delta_R} \|\varphi\|_{L^2}^2}_{\text{estimate uniform in } \varepsilon>0!}.$

$$\Rightarrow \int_{|x|\geq 2R} e^{2\beta|x|} |\varphi(x)|^2\, dx = \int_{|x|\geq 2R} \lim_{\varepsilon\downarrow 0} e^{2f(x)} |\varphi(x)|^2\, dx$$

$$\overset{\text{Lebesgue monotone convergence}}{=} \lim_{\varepsilon\downarrow 0} \int_{|x|\geq 2R} e^{2f(x)} |\varphi(x)|^2\, dx$$

$$\leq \lim_{\varepsilon\downarrow 0} \int \underbrace{\chi_R^2(x)\, e^{2f(x)}}_{=G(x)^2} |\varphi(x)|^2 dx$$

charact. fct. of the ball $B_{2R}(0)$ is bounded by $\chi_R(x)^2$ (look at the pictures above).

$$\leq \lim_{\varepsilon\downarrow 0} \frac{C_R}{\delta_R} \|\varphi\|^2 = \frac{C_R}{\delta_R} \|\varphi\|^2.$$

$$\int_{|x|\leq 2R} e^{2\beta|x|} |\varphi(x)|^2 dx \leq \int_{|x|\leq 2R} e^{4R\beta} |\varphi(x)|^2 dx$$

$$\leq e^{4R\beta} \|\varphi\|_{L^2}^2 < \infty.$$

$$\Rightarrow \quad e^{\beta|x|}\varphi \in L^2(\mathbb{R}^4). \qquad \blacksquare$$

RMK: One can strengthen the result to

$$|\varphi(x)| \leq C_\beta \, e^{-\beta|x|} \quad \text{almost everywhere.}$$

<u>Lemma 7.3:</u> Let $u \in L^2(\mathbb{R}^n)$ with $\hat{u} \in L^1(\mathbb{R}^n)$ and $\int |p| \, \hat{u}(p) \, dp < +\infty$. Then $u \in C^1(\mathbb{R}^n)$ and

$$\partial_k u(x) = (2\pi)^{-n/2} \int e^{ip\cdot x} (ip_k) \, \hat{u}(p) \, dp.$$

<u>Proof:</u> Recall

$$u(x) = (2\pi)^{-n/2} \int e^{ip\cdot x} \, \hat{u}(p) \, dp \quad \text{a.e.}$$

We use the following standard corollary of Lebesgue's dominated convergence:

Let $f : \mathbb{R}^n \times \mathbb{R} \longrightarrow \mathbb{C}$ such that $\partial_t f(x,t)$ exists and there exists $g \in L^1(\mathbb{R}^n)$ such that $|\partial_t f(x,t)| \leq g(x) \quad \forall x \in \mathbb{R}^n, t \in \mathbb{R}$.

Then $\int f(x,t)\, d^n x$ is differentiable in t and

$$(*) \qquad \frac{d}{dt}\int f(x,t)\, dx = \int \partial_t f(x,t)\, dx .$$

We take $f(p,x) := e^{ip\cdot x}\hat{u}(p)$.

Then $\partial_x f(p,x) = e^{ipx}(ip)\hat{u}(p)$

exists and

$$|\partial_x f(p,x)| = |p|\,|\hat{u}(p)| =: g(p)$$

which is by assumption an integrable dominating function.

By $(*)$ the partial derivatives exist and are given by

$$\partial_k u(x) = (2\pi)^{-n/2}\int e^{ip\cdot x}(ip_k)\,\hat{u}(p)\, dp .$$

Continuity w.r.t. x follows also by dominated convergence. ∎

Theorem 7.4: (Sobolev lemma)

Let $u \in H^s(\mathbb{R}^n)$, where $s > \frac{n}{2} + k$ for some $k \in \mathbb{N}$. Then:

(i) $u \in C^k(\mathbb{R}^n)$ and

$$\partial^\alpha u(x) \longrightarrow 0 \quad (|x| \to \infty) \text{ for } |\alpha| \leq k.$$

(ii) $$\sup_{|\alpha| \leq k} \|\partial^\alpha u\|_{L^\infty} \leq C_{s,n,k} \|u\|_{H^s}.$$

Proof: By induction, we generalize Lemma 7.3 to more than one derivative: Let $\alpha = (\alpha_1, \dots \alpha_n)$

If $|p|^k \hat{u} \in L^1(\mathbb{R}^n)$ and $|\alpha| = \alpha_1 + \dots + \alpha_n \leq k$

then $$\partial^\alpha u(x) = (2\pi)^{-n/2} \int e^{ip\cdot x} \underbrace{(ip)^\alpha}_{=(ip_1)^{\alpha_1}(ip_2)^{\alpha_2}\dots(ip_n)^{\alpha_n}} \hat{u}(p)\, dp.$$

Now let $u \in H^s(\mathbb{R}^n)$, with $s > \frac{n}{2} + k$. Then $u \in L^2(\mathbb{R}^n)$ and

$$\int |\hat{u}(p)| (1+p^2)^{k/2}\, dp$$

$$= \int |\hat{u}(p)| \, (1+p^2)^{s/2} (1+p^2)^{\frac{k}{2} - \frac{s}{2}}\, dp$$

$$\overset{C.S.}{\leq} \left(\int |\hat{u}(p)|^2 (1+p^2)^s\, dp \right)^{1/2} \left(\int \frac{1}{(1+p^2)^{s-k}}\, dp \right)^{1/2}$$

$$= \|u\|_{H^s} \qquad\qquad \text{finite because } 2(s-k)>n$$

finite by assumption

(go to spherical coordinates)

So $|p|^k \hat{u} \in L^1(\mathbb{R}^n)$ as had to be shown.

The Riemann-Lebesgue lemma implies $\partial^\alpha u(x) \longrightarrow 0 \quad (|x| \to +\infty)$.

This concludes (i)

By the same Cauchy-Schwarz as above:

$$|\partial^\alpha u(x)| \leq (2\pi)^{-n/2} \int |e^{ip\cdot x} (ip)^\alpha \hat{u}(p)| dp$$

$$\leq \|u\|_{H^s} (2\pi)^{-n/2} \left(\int \frac{1}{(1+p^2)^{s-k}} dp \right)^{1/2}.$$

This concludes (ii).

$\blacksquare$