We heuristically discuss stationary scattering theory.

This is the typical approach of physics books & more convenient to calculate transition probabilities.

But conceptually not so clear & mathematically complicated to make sense of (but see, e.g., Reed & Simon Vol. 3).

STATIONARY SCATTERING THEORY (heuristic!)

$H_0 = -\frac{\Delta}{2}$ has formal "eigenfunctions" $\varphi_k(x) := e^{ik\cdot x}$ (plane waves).

Formally "$H_0 \varphi_k = \frac{k^2}{2}\varphi_k$", even though strictly speaking $H_0\varphi_k$ is not defined since $\varphi_k \notin L^2$!

(Of course $|e^{-iHt}\varphi_k(x)|^2 = |\varphi_k(x)|^2$ time-independently, so it is unclear how to think of this as a "flying particle". Nevertheless we think of it as a particle flying with momentum $k \in \mathbb{R}^n$; the fact that we cannot assign it a position is related to the Heisenberg uncertainty principle.)

We construct formal eigenfct. for H, that "for $t \to -\infty$" look like plane waves,
by trying to formally (!) make sense of "$\varphi := \Omega_- \varphi_k$":

By intertwining we expect: $H\varphi = H\Omega_-\varphi_k = \Omega_- H_0 \varphi_k = \frac{k^2}{2}\varphi$.

Recall: for all ψ: $\Omega_-\psi = \lim_{t \to -\infty} e^{iHt} e^{-iH_0 t}\psi$.

So $\Omega_-^* \psi = \lim_{t \to -\infty} e^{iH_0 t} e^{-iHt}\psi$.

Using the abelian limit formula (see Assignment 2):

$$\Omega_-^*\psi = \lim_{\varepsilon \downarrow 0} \varepsilon \int_{-\infty}^{0} e^{\varepsilon t} e^{iH_0 t} e^{-iHt}\psi \, dt$$

Duhamel formula

$$= \lim_{\varepsilon \downarrow 0} \varepsilon \int_{-\infty}^{0} e^{\varepsilon t} \left[\psi + \int_0^t \frac{d}{ds}\left(e^{iH_0 s} e^{-iHs}\psi\right) ds \right] dt$$

$$= \psi + \lim_{\varepsilon \downarrow 0} \varepsilon \int_{-\infty}^{0} \int_0^t e^{\varepsilon t} e^{iH_0 s}(-iV) e^{-iHs}\psi \, ds \, dt$$

$$= \psi + \lim_{\varepsilon \downarrow 0} \varepsilon \int_{-\infty}^{0} \underbrace{\int_s^{-\infty} e^{\varepsilon t}}_{\text{integral over } t: \; = -\frac{1}{\varepsilon} e^{\varepsilon s}} e^{iH_0 s}(-iV) e^{-iHs}\psi \, dt \, ds$$

$$\rightsquigarrow \Omega_-^* \psi = \psi + i \lim_{\varepsilon \downarrow 0} \int_{-\infty}^{0} ds\, e^{\varepsilon s} e^{iH_0 s} V e^{-iHs} \psi.$$

Take $\psi = \Omega_- \varphi_k$ (recall that Ω_-^* is the left-inverse).

$$\rightsquigarrow \varphi_k = \psi + i \lim_{\varepsilon \downarrow 0} \int_{-\infty}^{0} ds\, e^{\varepsilon s} e^{iH_0 s} V \underbrace{e^{-iHs} \Omega_- \varphi_k}_{\text{intertwining} \; = e^{-i\frac{k^2}{2}s} \Omega_- \varphi_k}$$

resolvent identity

$$= \psi + i \lim_{\varepsilon \downarrow 0} \int_{-\infty}^{0} ds\, e^{i(H_0 - \frac{k^2}{2} - i\varepsilon) s} V \psi$$

$$= \psi + i \lim_{\varepsilon \downarrow 0} \left(H_0 - \frac{k^2}{2} - i\varepsilon \right)^{-1} V \psi.$$

$$\rightsquigarrow \psi = \varphi_k - i \lim_{\varepsilon \downarrow 0} \left(H_0 - \frac{k^2}{2} - i\varepsilon \right)^{-1} V \psi$$

The resolvent of H_0 is given by the Yukawa potential (see Assignment 1):

$$\longrightarrow \boxed{\psi(x) = e^{ik\cdot x} - \frac{1}{2\pi} \int \frac{e^{i|k||x-y|}}{|x-y|} V(y)\, \psi(y)\, dy}$$

<u>Lippmann–Schwinger equation</u> often taken as the "obvious" starting point in physics.

But: RHS still depends on ψ $\rightsquigarrow$ How do you solve the eqn.?
Like with the Duhamel formula, we can try to iterate to obtain a series expansion. There are many smart ways to do this (with angular momentum decomposition), see physics books. We just do a naive expansion now:

First Born approximation: We iterate by plugging in
$$\psi(x) = e^{ik\cdot x} + \mathcal{O}(V)$$

$$\Rightarrow \quad \psi(x) = e^{ik\cdot x} \underbrace{- \frac{1}{2\pi} \int \frac{e^{i|k||x-y|}}{|x-y|} V(y)\, e^{ik\cdot y}\, dy}_{} + \mathcal{O}(V^2).$$

in the 1. Born approx. this is an explicit Fourier transform that can be calculated, depending on V, k and observation position x.

Physical interpretation of the Lippmann-Schwinger equation:

Think of y as small (inside supp V, ~ scale of "size of an atom") and x as large (macroscopically far away, ~ scale "meters")

Do an <u>expansion</u>!

$$|x-y| = |x| \left| \frac{x}{|x|} - \frac{y}{|x|} \right|, \quad \text{Taylor expansion in } \frac{|y|}{|x|}:$$

$$\frac{e^{i|k||x-y|}}{|x-y|} = \frac{e^{i|k||x|}}{|x|} e^{-ik'\cdot y} + \mathcal{O}\left(\frac{|y|}{|x|}\right)$$

where $k' := |k| \frac{x}{|x|}$ is the "wave vector" in the direction of the observation.

Then the Lippmann-Schwinger equation takes the following form:

$$\psi(x) \approx \underbrace{e^{ik\cdot x}}_{\text{ingoing plane wave}} + \underbrace{f(k,k')}_{\text{scattering amplitude}} \underbrace{\frac{e^{i|k||x|}}{|x|}}_{\text{outgoing spherical wave}}$$

Interpretation: If we shoot a particle at the target potential V with energy $|k|^2/2$ from direction k, then $|f(k,k')|^2$ is the probability to detect it later far away in the direction of k'.
(The energy is of course conserved, $|k'|^2/2 = |k|^2/2$.)

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.

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

Eigenvectors (bound states) have trivial time evolution:

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

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 $V : \mathbb{R}^n \longrightarrow \mathbb{R}$ 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 $\partial^\alpha f \in L^\infty(\mathbb{R}^n)$ $\forall |\alpha| \le 2$.

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

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

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

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:

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

(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!

$= \dots = \text{LHS}.$ ∎

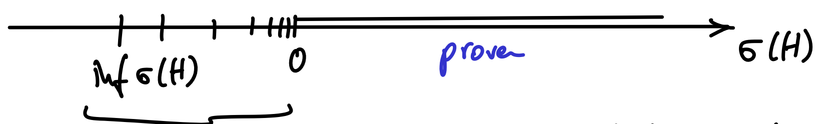
THM.: (Exp. localization of eigenvectors, Agmon)

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 $V(x) \to 0$ $(|x| \to \infty)$.
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. $\sigma(-\frac{\Delta}{2}) = [0,\infty)$.



eigenvalues, possibly accumulating at zero.
(not proven so far)

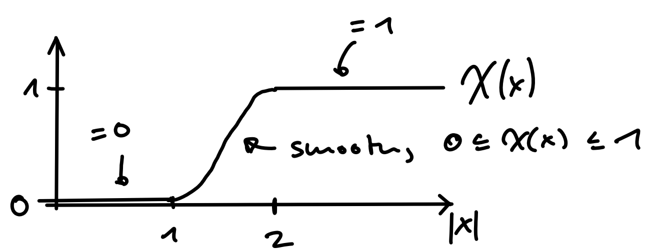
This means for the decay of eigenvectors, $H\varphi = E\varphi$:

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

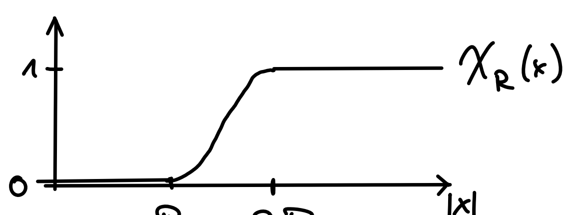
but rate of decay β smaller and smaller for E closer and closer to zero.

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

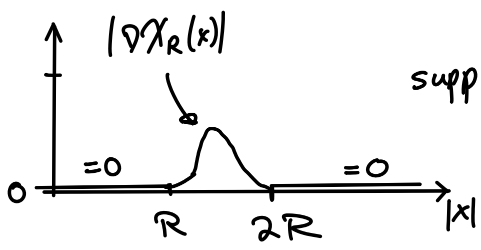
Now: $$\langle G\varphi, (H-E)G\varphi\rangle \overset{\text{IMS}}{=} \langle \varphi, \left(\tfrac{1}{2}\left[G^2 H + HG^2 + |\nabla G|^2\right] - E\right)\varphi\rangle$$

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

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

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

Notice:



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

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

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

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).

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

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

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

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

$\blacksquare$

RMK: One can strengthen the result to

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