2008.02.25

Recall that, if T is a closed operator in $\mathcal{H}$ and λ is a spectral value that is not an eigenvalue of T and is not in the residual spectrum of T, then $\exists$ a sequence $\{v_n\}$ from $\mathcal{H}$ such that

$$\|v_n\| = 1,$$
$$\|(\lambda I - T)v_n\| \to 0.$$

We have also mentioned that a self-adjoint operator T does not have residual spectrum, so that, for $\lambda \in \sigma(T)$, either λ is an eigenvalue or a sequence as described above exists. There is actually more that can be said for self-adjoint operators about such a sequence.

<u>Defn</u> A sequence $\{v_n\}$ from $\mathcal{H}$ is a <u>Weyl sequence</u> for the pair (T, λ) if

- $\|v_n\| = 1$
- $\|(\lambda I - T)v_n\| \to 0 \quad (n \to \infty)$
- $v_n \to 0$ weakly $(n \to \infty)$

New! →

<u>Theorem</u> If T is a self-adjoint operator in a Hilbert space $\mathcal{H}$ and $\lambda \in \sigma(T)$, then either λ is an eigenvalue of T or there exists a Weyl sequence for the pair (T, λ).

See Gustafson/Sigal p. 35-36

Weyl sequences for Δ on $\mathbb{R}$.

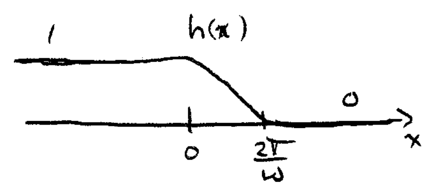
We know from the spectral representation of Δ ($\hat{\Delta} = T_{-\omega^2}$) that $\sigma(\Delta) = [-\infty, 0]$ and that Δ has no point spectrum. Let us find Weyl sequences for Δ on $\mathbb{R}$ for $\lambda = -\omega^2$.

Notice that $(\partial_{xx} + \omega^2) f = 0$ has no L^2 solutions f (otherwise $-\omega^2$ would be an eigenvalue of Δ. However, there are solutions that are bounded, for example we may take $\sin \omega x$, $\cos \omega x$, $e^{i\omega x}$, or $e^{-i\omega x}$. Let us use $\sin \omega x$ to construct a Weyl sequence. We have

$$(\partial_{xx} + \omega^2) \sin \omega x = 0$$

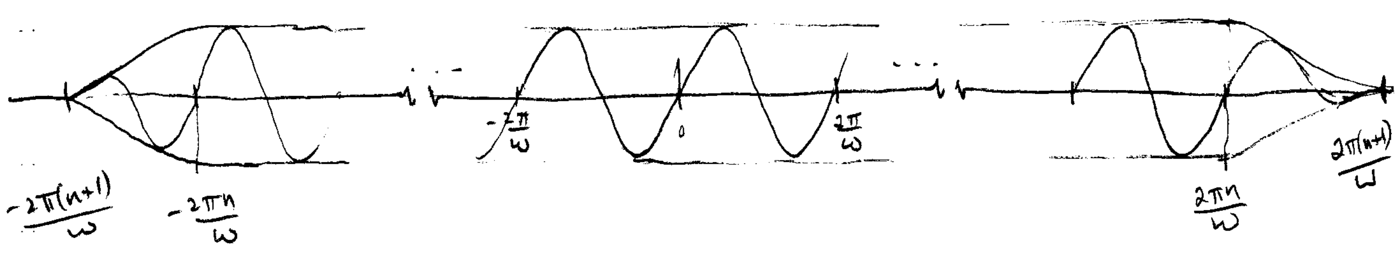
Let $h(x)$ be a smooth function on $\mathbb{R}$ such that

$$\begin{aligned} h(x) &= 1 , && x \le 0 \\ 0 \le h(x) &\le 1 , && 0 < x < \tfrac{2\pi}{\omega} \\ h(x) &= 0 , && \tfrac{2\pi}{\omega} \le x \end{aligned}$$



and define

$$f_n(x) = n^{-1/2} \sin \omega x \; h\left(|x| - \frac{2\pi n}{\omega}\right)$$



Notice that

$$f_n''(x) + \omega^2 f_n(x) = 0 \quad \text{for} \quad \begin{cases} |x| > \frac{2\pi(n+1)}{\omega} \\ |x| < \frac{2\pi n}{\omega} \end{cases}.$$

We can now compute that $\|(\Delta + \omega^2) f_n\| \to 0$ as $n \to \infty$:

$$\int_{\mathbb{R}} |f_n''(x) + \omega^2 f(x)|^2 dx = 2\int_{\frac{2\pi n}{\omega}}^{\frac{2\pi(n+1)}{\omega}} [f_n''(x) + \omega^2 f_n(x)]^2 dx$$

$$= 2n^{-1} \int_{\frac{2\pi n}{\omega}}^{\frac{2\pi(n+1)}{\omega}} [(\partial_{xx} + \omega^2)(\sin \omega x \, h(x - \tfrac{2\pi n}{\omega}))]^2 dx$$

$$= 2n^{-1} \int_0^{\frac{2\pi}{\omega}} [(\partial_{yy} + \omega^2)(\sin \omega y \, h(y))]^2 dy = 2n^{-1} \cdot \text{const} \to 0$$

On the other hand, we compute

$$\int_{\mathbb{R}} |f_n(x)|^2 dx > \int_{-\frac{2\pi n}{\omega}}^{\frac{2\pi n}{\omega}} n^{-1} \sin \omega x \, dx = \frac{2\pi}{\omega} = \text{const.} > 0$$

In fact, one can see that $\|f_n\|_2^2 \to \frac{2\pi}{\omega}$ as $n \to \infty$

To see that $f_n \to 0$ weakly in $L^2(\mathbb{R})$, we let $g \in L^2(\mathbb{R})$ and $\varepsilon > 0$ be given. Let M_ε be such that

$$\int_{\mathbb{R} \setminus [-M, M]} |g(x)|^2 dx < \varepsilon,$$

and recall that, since $g \in L^2(\mathbb{R})$, $\int_{-M_\varepsilon}^{M_\varepsilon} |g| < \infty$.
Now observe that

$$\left|\int_{\mathbb{R}} f_n g\right| = \left|\int_{-M_\varepsilon}^{M_\varepsilon} f_n g\right| + \left|\int_{\mathbb{R} \setminus [-M_\varepsilon, M_\varepsilon]} f_n g\right| \le n^{-1/2} \int_{-M_\varepsilon}^{M_\varepsilon} |g| + \|f_n\|_{L^2} \varepsilon$$

Since ε is arbitrary, n can be chosen such that $|\int f_n g|$ is arbitrarily small.

Let us take another point of view on constructing Weyl sequences for Δ through its spectral representation $\hat{\Delta} = T_{-\omega^2}$ in $L^2(\mathbb{R}, d\omega)$. Let ω_0 be given, and let f_n be such that

$$\hat{f}_n(\omega) = n^{1/2} e^{-n^2(\omega-\omega_0)^2}$$

We show that $\{\hat{f}_n\}$ is a Weyl sequence for $(\hat{\Delta}, -\omega_0^2)$ so that $\{f_n\}$ is a Weyl sequence for $(\Delta, -\omega_0^2)$. ← up to const.

- First, we show $\|\hat{f}_n\|$ is constant:

$\sigma = n(\omega-\omega_0)$
$$\int_{\mathbb{R}} |\hat{f}_n(\omega)|^2 d\omega = n\int_{\mathbb{R}} e^{-2(n(\omega-\omega_0))^2} d\omega = \int_{\mathbb{R}} e^{-2\sigma^2} d\sigma = \sqrt{\frac{\pi}{2}}.$$

- Next we show that $\|(\hat{\Delta}+\omega_0^2)\hat{f}_n(\omega)\| \to 0$:

$\sigma = n(\omega-\omega_0)$
$$\int_{\mathbb{R}} \left((\hat{\Delta}+\omega_0^2)\hat{f}_n(\omega)\right)^2 d\omega = n\int_{\mathbb{R}} (\omega_0^2-\omega^2)^2 e^{-2n^2(\omega-\omega_0)^2} d\omega$$
$$= \int_{\mathbb{R}} \left(-\frac{\sigma^2}{n^2} - \frac{2\sigma\omega_0}{n}\right) e^{-2\sigma^2} d\sigma \longrightarrow 0 \quad \text{as } n\to\infty.$$

- One can also prove that $\{\hat{f}_n\}$ converges weakly to 0 in L^2.

Finally, we find $f_n(x) = \mathcal{F}^{-1}(\hat{f}_n(\omega))$:

$$f_n(x) = \frac{1}{\sqrt{2n}} e^{i\omega_0 x} e^{-\frac{x^2}{4n^2}},$$

using $\mathcal{F}\left[e^{-\alpha x^2/2}\right] = \frac{1}{\sqrt{\alpha}} e^{-\omega^2/2\alpha}$

and $\mathcal{F}\left[e^{i\omega_0 x} f(x)\right] = \hat{f}(\omega-\omega_0)$

[See Folland or Reed/Simon, for example.]

Let us find eigenfunctions and Weyl sequences for $-\Delta + T_V$, with V equal to a "square potential well"

$$V(x) = \begin{cases} 0, & x \notin [-L,L] \\ -M, & x \in [-L,L] \end{cases}.$$

First let's find the eigenfunctions. These are known as "bound states" in quantum mechanics.

Let $\lambda = -\sigma^2 < 0$ be given. We seek solutions $f \in L^2$ of the equation

$$-f'' + (V(x) - \lambda) f = 0,$$

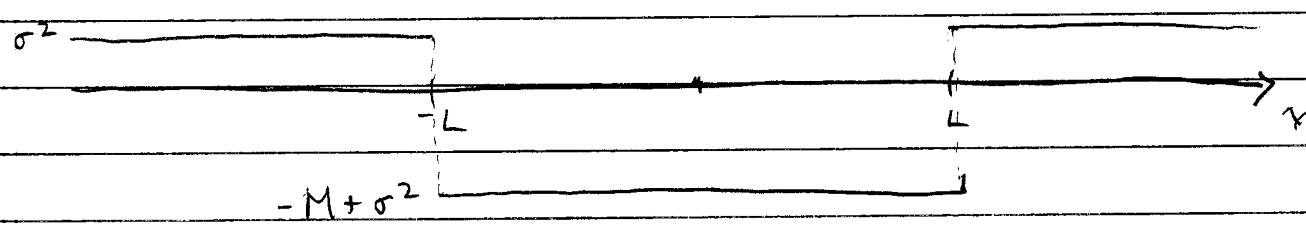
where

$$V(x) - \lambda = \begin{cases} \sigma^2, & x \notin [-L,L] \\ -M + \sigma^2, & x \in [-L,L] \end{cases}.$$

So we must solve

$$\begin{cases} f'' - \sigma^2 f = 0, & x \notin [-L,L] \\ f'' + (M - \sigma^2) f = 0, & x \in [-L,L] \end{cases}.$$

Picture of $V(x) - \lambda$:



Let's assume that $\sigma^2 < M$ (otherwise there are no L^2-solutions).
The general solution of

$$f'' - \sigma^2 f = 0 \qquad (|x| > L)$$

is $C_1 e^{\sigma x} + C_2 e^{-\sigma x}$, so this is the form of f for $x < -L$ and for $x > L$. Now, we want f to be in $L^2(\mathbb{R})$, so we need to seek solutions such that

$$f(x) = C_1 e^{\sigma x}, \quad x < -L \qquad (*)$$

$$f(x) = C_2 e^{-\sigma x}, \quad x > L \qquad (**)$$

For $|x| < L$, we have

$$f'' + (M - \sigma^2) f = 0 \qquad (|x| < L)$$

Let us set $M - \sigma^2 = \rho^2 > 0$. The general soln is

$$f(x) = A e^{i\rho x} + B e^{-i\rho x}, \quad |x| < L \qquad (***)$$

Now, in order that f, satisfying $(*)$, $(**)$, and $(***)$ be a global solution on $\mathbb{R}$, the values of the forms given in the three regions must match at $-L$ and at L. The derivatives must also match at $-L$ and L:

$$\left.\begin{aligned} C_1 e^{-\sigma L} &= A e^{-i\rho L} + B e^{i\rho L} \\ C_1 \sigma e^{-\sigma L} &= i\rho \left[A e^{-i\rho L} - B e^{i\rho L} \right] \end{aligned}\right\} \text{ conditions at } x = L$$

$$\left.\begin{aligned} C_2 e^{-\sigma L} &= A e^{i\rho L} + B e^{-i\rho L} \\ -C_2 \sigma e^{-\sigma L} &= i\rho \left[A e^{i\rho L} - B e^{-i\rho L} \right] \end{aligned}\right\} \text{ conditions at } x = -L$$

We can put these equations in matrix form and solve for A & B:

$$\begin{bmatrix} A \\ B \end{bmatrix} = \begin{bmatrix} e^{-i\rho L} & e^{i\rho L} \\ i\rho e^{-i\rho L} & -i\rho e^{i\rho L} \end{bmatrix}^{-1} \begin{bmatrix} e^{-\sigma L} \\ \sigma e^{-\sigma L} \end{bmatrix} \cdot C_1$$

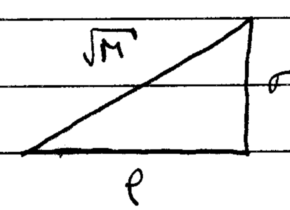
$$\begin{bmatrix} A \\ B \end{bmatrix} = \begin{bmatrix} e^{i\rho L} & e^{-i\rho L} \\ i\rho e^{i\rho L} & -i\rho e^{-i\rho L} \end{bmatrix}^{-1} \begin{bmatrix} e^{-\sigma L} \\ -\sigma e^{-\sigma L} \end{bmatrix} \cdot C_2$$

This tells us that, in order that an L^2 solution f exist, the two vectors on the right-hand sides must be equal for some choice of C_1 and C_2. This is equivalent to saying that the determinant of the matrix whose columns are these two vectors (without the C_1 and C_2) is equal to zero. This is the result of the calculations (after factoring out $e^{-\sigma L}$):

$$0 = \begin{vmatrix} (\sigma + i\rho) e^{i\rho L} & -(\sigma - i\rho) e^{-i\rho L} \\ -(\sigma - i\rho) e^{-i\rho L} & (\sigma + i\rho) e^{i\rho L} \end{vmatrix} = (\sigma + i\rho)^2 e^{2i\rho L} - (\sigma - i\rho)^2 e^{-2i\rho L}$$

$$\iff \operatorname{Im}\left[(\sigma + i\rho)^2 e^{2i\rho L}\right] = 0$$

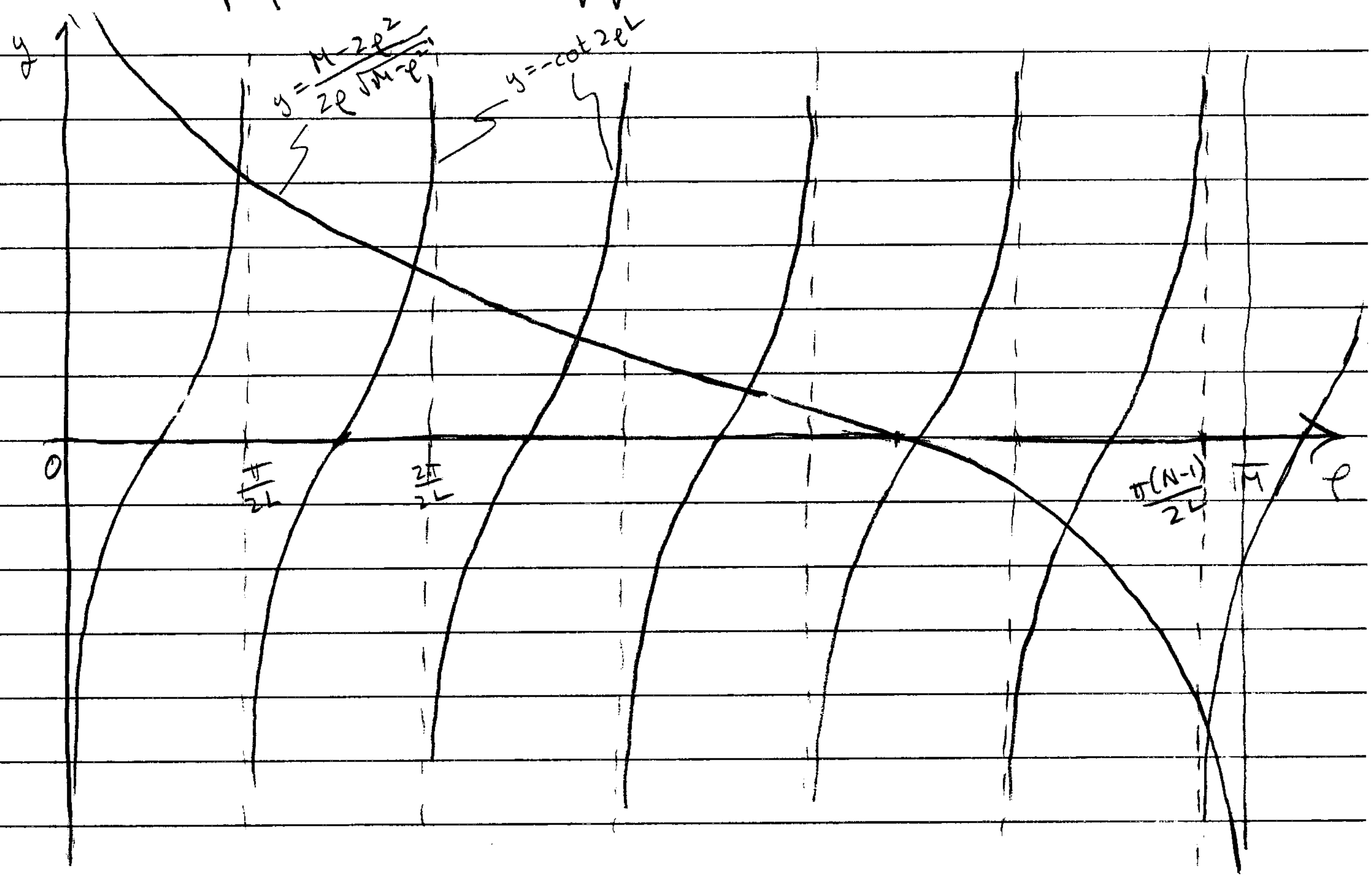
$$\iff (\sigma^2 - \rho^2)\sin 2\rho L + 2\sigma\rho\cos 2\rho L$$



$$\star \quad \iff -\cot 2\rho L = \frac{M - 2\rho^2}{2\rho\sqrt{M - \rho^2}}$$

Graphical interpretation of ✡.

Notice that both sides of ✡ are odd, so it suffices to find the values of $\rho \geq 0$ that satisfy it.



The number of positive intersections of the graphs $y = (M-2\rho^2)/(2\rho\sqrt{M-\rho^2})$ and $y = -\cot 2\rho L$ is the number of bound states. This number N is given by

$$\frac{\pi(N-1)}{2L} < \sqrt{M} \leq \frac{\pi N}{2L},$$

or, equivalently,

$$\boxed{N-1 < \frac{2L\sqrt{M}}{\pi} < N},$$

so N tends to ~~∞~~ as L and as $\sqrt{M}$.

Extended states (or scattering states)

Now let $\lambda = \tau^2 > 0$ be given. We seek solutions of the equation

$$-f'' + (V(x) - \lambda) f = 0$$

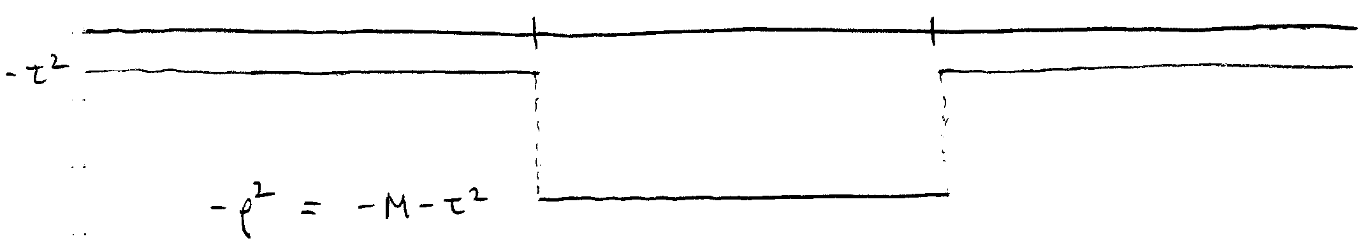
where

$$V(x) - \lambda = \begin{cases} -\tau^2 \,, & |x| > L \\ -M - \tau^2 \,, & |x| < L \,, \end{cases}$$

so we must solve

$$\begin{cases} f'' + \tau^2 f = 0 \,, & |x| > L \\ f'' + (M + \tau^2) f = 0 \,, & |x| < L \,. \end{cases}$$

Picture of $V(x) - \lambda$:



The form of the general solution in the three regions is

$$\begin{aligned} f(x) &= A_+ e^{i\tau x} + A_- e^{-i\tau x} \,, & x < -L \\ f(x) &= C_+ e^{i\rho x} + C_- e^{-i\rho x} \,, & |x| < L \\ f(x) &= B_+ e^{i\tau x} + B_- e^{-i\tau x} \,, & x > L \end{aligned}$$

As before, we have two matching conditions at each of $x=-L$ and $x=L$:

$$A_+ e^{-i\tau L} + A_- e^{i\tau L} = C_+ e^{-i\rho L} + C_- e^{i\rho L}$$
$$i\tau\left(A_+ e^{-i\tau L} - A_- e^{i\tau L}\right) = i\rho\left(C_+ e^{-i\rho L} - C_- e^{i\rho L}\right)$$

$$B_+ e^{i\tau L} + B_- e^{-i\tau L} = C_+ e^{i\rho L} + C_- e^{-i\rho L}$$
$$i\tau\left(B_+ e^{i\tau L} - B_- e^{-i\tau L}\right) = i\rho\left(C_+ e^{i\rho L} - C_- e^{-i\rho L}\right)$$

We can eliminate C_+ and C_- from these equations and obtain two equations for $A_+, A_-, B_+,$ and B_-. Ultimately, we can write them in either of two forms:

$$T\begin{bmatrix} A_+ \\ A_- \end{bmatrix} = \begin{bmatrix} B_+ \\ B_- \end{bmatrix},$$

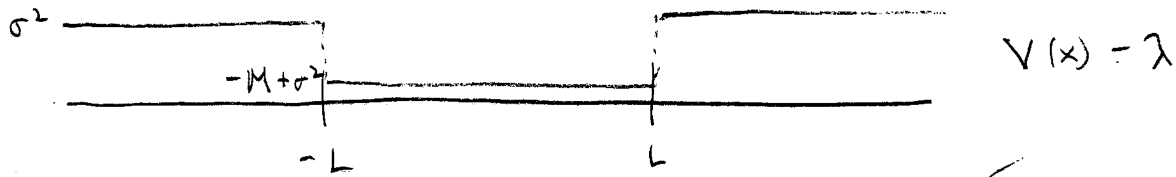
$$S\begin{bmatrix} A_+ \\ B_- \end{bmatrix} = \begin{bmatrix} A_- \\ B_+ \end{bmatrix}.$$

The first form involves the "transfer matrix" T, which transfers coefficients on the left to coefficients on the right. The second involves the "scattering matrix" S, which gives the coefficients for "outgoing" fields, A_- and B_+, in terms of the coefficients of the "incoming" fields.

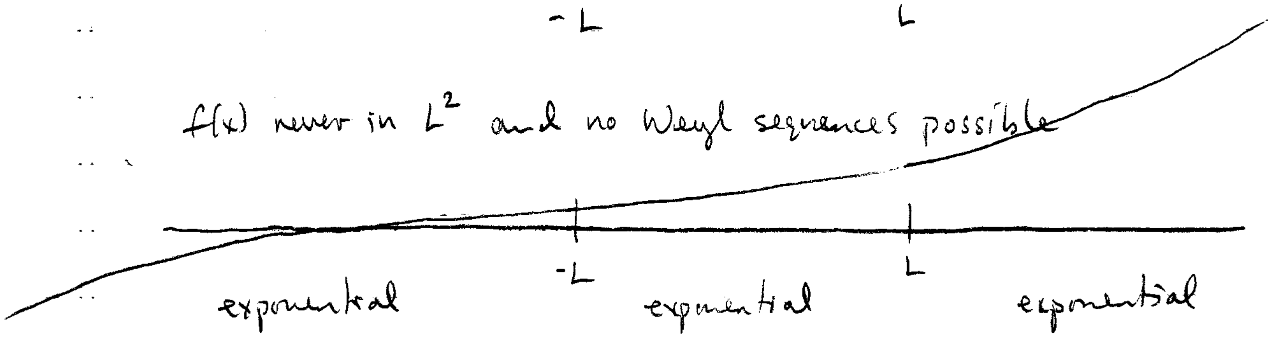
Notice that our solutions $f(x)$ are not in L^2, but that they are bounded in the sup norm. Therefore we can do similar analysis as we did for Δ to obtain Weyl sequences for $-\Delta + V$ for $\lambda > 0$.

Pictures of solutions of $-f'' + (V(x) - \lambda) f = 0$

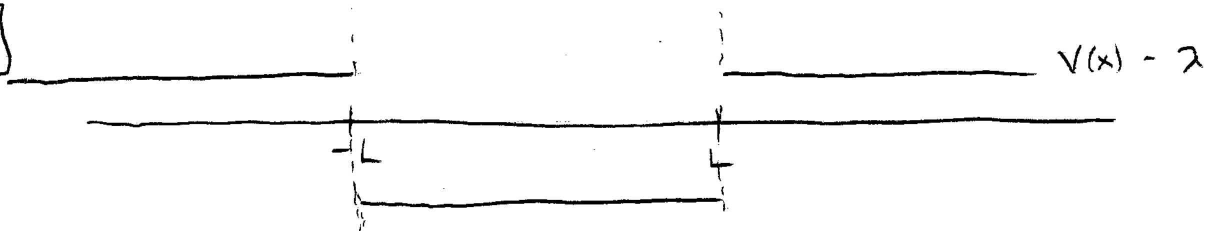
$\boxed{\lambda = -\sigma^2 < -M}$

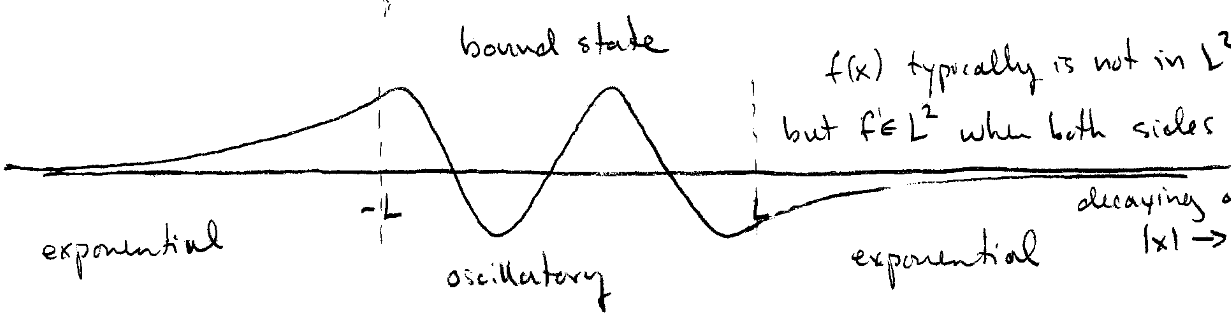


$f(x)$ never in L^2 and no Weyl sequences possible



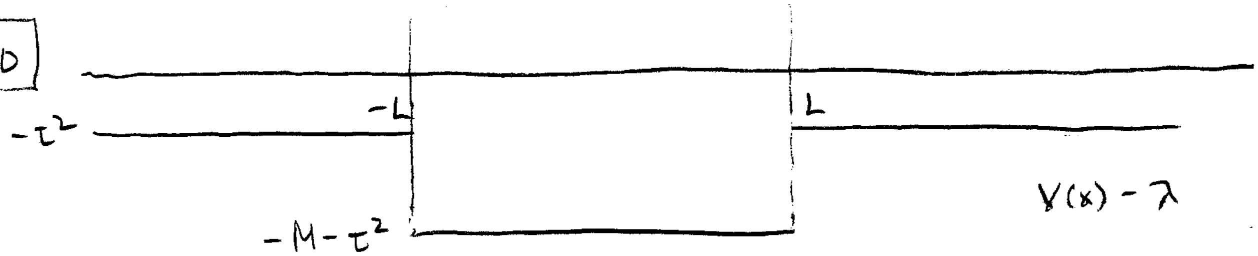
$\boxed{-M < \lambda = -\sigma^2 < 0}$

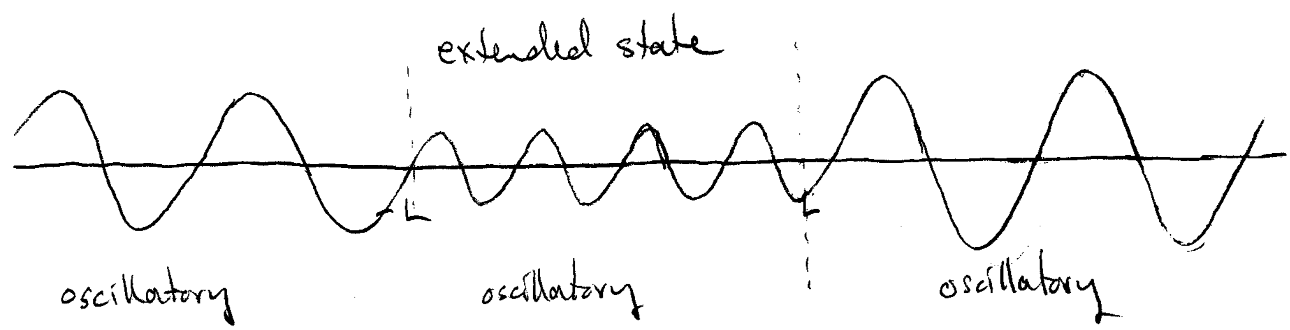




$f(x)$ typically is not in L^2, but $f \in L^2$ when both sides are decaying as $|x| \to \infty$.

$\boxed{\lambda = \tau^2 > 0}$





Multiply by a cutoff function $h(|x| - n)$ to get Weyl sequences.