# Sturm–Liouville *M*-Functions in Terms of Green's Functions

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### **Appreciation:**

# CONGRATULATIONS, PETER!!!!



#### **1** Topics Discussed

**2** Basic Facts and Self-Adjoint L<sup>2</sup>-Realizations **T**<sub>A,B</sub> of S–L Operators

#### **M**-Functions and Separated Boundary Conditions

M-Functions and General (e.g., Coupled) Boundary Conditions

**5** Connecting  $M(\cdot)$  and the Spectral Projections  $E_{T_{A,B}}(\cdot)$ 

#### **Topics Discussed:**

- General three-coefficient Sturm-Liouville operators generated by  $\tau = r(x)^{-1}[-(d/dx)p(x)(d/dx) + q(x)], x \in (a, b)$ , and their self-adjoint  $L^2((a, b); rdx)$ -realizations, T.
- The traditional 2 × 2 matrix-valued *M*-functions associated with separated boundary conditions (if any) at the endpoints *a* and *b*.
- The connection of *M* to the Green's function in the separated b.c. case.
- *M* for general b.c.'s and its **Nevanlinna–Herglotz** property.
- The precise connection between the family of spectral projections E<sub>T</sub>(λ), λ ∈ ℝ, in L<sup>2</sup>((a, b); rdx) and the 2 × 2 matrix-valued spectral measure Ω in the Nevanlinna–Herglotz representation of *M* for general b.c.'s.

#### Hypothesis 1. (To be assumed throughout this talk.)

Let  $-\infty \leq a < b \leq \infty$ . Suppose that p, q, r are Lebesgue measurable on (a, b) with  $p^{-1}, q, r \in L^1_{loc}((a, b); dx)$  and real-valued a.e. on (a, b) with r > 0 and p > 0 a.e. on (a, b).

Introduce the differential expression au

$$au f = rac{1}{r}ig(-(pf')'+qfig)\in L^1_{loc}((a,b);r\,dx), \quad f\in\mathfrak{D}((a,b)),$$

where

$$\mathfrak{D}((a,b)) = ig\{ f \in \mathcal{AC}_{\mathit{loc}}((a,b)) \, \big| \, f^{[1]} \in \mathcal{AC}_{\mathit{loc}}((a,b)) ig\},$$

and

$$f^{[1]} = pf'$$

is the **first quasi-derivative** of f. The **Wronskian** of f and g is defined as usual by

$$W(f,g)(x) = f(x)g^{[1]}(x) - f^{[1]}(x)g(x), \quad x \in (a,b), \ f,g \in \mathfrak{D}((a,b)).$$

Basic Facts and Self-Adjoint  $L^2$ -Realizations  $T_{A,B}$  of S–L Operators

### Basic Facts and Self-Adjoint L<sup>2</sup>-Realizations (contd.)

Then W(f,g) is locally absolutely continuous on (a,b) and its derivative is

$$W(f,g)'(x) = \left[g(x)(\tau f)(x) - f(x)(\tau g)(x)\right]r(x), \quad x \in (a,b).$$

If  $z \in \mathbb{C}$ , then the **Wronskian** of two solutions  $u_j(z, \cdot) \in \mathfrak{D}((a, b))$ ,  $j \in \{1, 2\}$ , of  $(\tau - z)u = 0$  on (a, b) is constant. Moreover,  $W(u_1(\lambda, \cdot), u_2(\lambda, \cdot)) \neq 0$  if and only if  $u_1(\lambda, \cdot)$  and  $u_2(\lambda, \cdot)$  are **linearly independent**.

#### **Definition 2.**

The differential expression  $\tau$  is said to be **regular** on (a, b) if  $-\infty < a < b < \infty$  (i.e., *a* and *b* are finite) and  $p^{-1}$ ,  $q, r, s \in L^1((a, b); dx)$ ; otherwise,  $\tau$  is said to be **singular** on (a, b).

If  $\tau$  is **regular** on (a, b), then for all  $f \in \mathfrak{D}((a, b))$ ,  $f, \tau f \in L^2((a, b); rdx)$  (i.e., for all  $f \in \text{dom}(T_{max})$ ) the following limits exist and are finite:

$$f(a) := \lim_{x \downarrow a} f(x), \quad f^{[1]}(a) := \lim_{x \downarrow a} f^{[1]}(x),$$
  
$$f(b) := \lim_{x \uparrow b} f(x), \quad f^{[1]}(b) := \lim_{x \uparrow b} f^{[1]}(x).$$

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### Basic Facts and Self-Adjoint L<sup>2</sup>-Realizations (contd.)

Maximal,  $T_{max}$ , preminimal,  $T_{min}$ , and minimal  $T_{min}$ , operators are then defined in a standard manner,

 $T_{max}f = \tau f,$   $f \in \operatorname{dom}(T_{max}) = \left\{ g \in L^2((a, b); r \, dx) \mid g \in \mathfrak{D}((a, b)), \tau g \in L^2((a, b); r \, dx) \right\}.$   $T_{min}f = \tau f,$   $f \in \operatorname{dom}\left(\frac{\dagger}{T_{min}}\right) = \left\{ g \in \operatorname{dom}(T_{max}) \mid g \text{ has compact support in } (a, b) \right\}.$  $T_{min} = \overline{T_{min}} = T_{max}^*, \quad T_{min}^* = T_{max}.$ 

(Here  $\overline{S}$  denotes the operator closure of S.) The existence of **principal** and **nonprincipal** solutions is closely connected to oscillation theory for  $\tau - \lambda$ .

#### **Definition 3.**

Let  $\lambda \in \mathbb{R}$ . The differential expression  $\tau - \lambda$  is called **oscillatory at** *a* (resp., *b*) if some solution of  $(\tau - \lambda)u = 0$  has infinitely many zeros accumulating at *a* (resp., *b*); otherwise,  $\tau - \lambda$  is called **nonoscillatory at** *a* (resp., *b*).

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### Basic Facts and Self-Adjoint L<sup>2</sup>-Realizations (contd.)

#### Theorem 4 (Eckhardt-G-Nichols-Teschl 2013).

Let  $\lambda \in \mathbb{R}$  be fixed. If  $\tau - \lambda$  is **nonoscillatory** at *b*, then there exists a real-valued solution  $u_b(\lambda, \cdot)$  of  $(\tau - \lambda)u = 0$  satisfying the following properties (i)-(ii) in which  $\hat{u}_b(\lambda, \cdot)$  denotes an arbitrary real-valued solution of  $(\tau - \lambda)u = 0$  linearly independent of  $u_b(\lambda, \cdot)$ .

(i)  $u_b(\lambda, \cdot)$  and  $\widehat{u}_b(\lambda, \cdot)$  satisfy the limiting relation

$$\lim_{x\uparrow b}\frac{u_b(\lambda,x)}{\widehat{u}_b(\lambda,x)}=0.$$

(ii)  $u_b(\lambda, \cdot)$  and  $\widehat{u}_b(\lambda, \cdot)$  satisfy

$$\int^b dx \, |p(x)|^{-1} \widehat{u}_b(\lambda, x)^{-2} < \infty \text{ and } \int^b dx \, |p(x)|^{-1} u_b(\lambda, x)^{-2} = \infty$$

The analogous result holds if  $\tau - \lambda$  is **nonoscillatory** at *a*.

 $u_b(\lambda, \cdot)$  is called a **principal** solution (it is unique up to normalization, and the "smallest" solution),  $\hat{u}_b(\lambda, \cdot)$  are called **nonprincipal** solutions of  $(\tau - \lambda)u = 0$ .

#### Theorem 5 (Eckhardt-G-Nichols-Teschl 2013).

Suppose there exist  $\lambda_a, \lambda_b \in \mathbb{R}$  such that  $\tau - \lambda_a$  is **nonoscillatory** at a and  $\tau - \lambda_b$  is **nonoscillatory** at b. Then  $T_{min}$  and hence any self-adjoint extension of the minimal operator  $T_{min}$  is **lower semibounded**. In particular, if  $\tau$  is regular on (a, b), then  $T_{min}$  and hence every self-adjoint extension of  $T_{min}$  is bounded from below.

#### Definition 6.

The operator  $\overline{T}_{min}$  is said to be **bounded from below at** *a* if there exists  $c \in (a, b)$  and  $\lambda_a \in \mathbb{R}$  such that

$$(u, \overline{T}_{\min}u)_{L^2((a,b);r\,dx)} \ge \lambda_a(u, u)_{L^2((a,b);r\,dx)},$$
$$u \in \operatorname{dom}(\overline{T}_{\min}) \text{ such that } u \equiv 0 \text{ on } (c, b).$$

Analogously one introduces the notion that  $\overline{T}_{min}$  is said to be **bounded from** below at *b*.

The celebrated **Weyl alternative** then can be stated as follows:

#### Theorem 7 (Weyl's Alternative).

Assume Hypothesis 1. Then the following alternative holds: Either,

(i) for every  $z \in \mathbb{C}$ , all solutions  $\psi$  of  $(\tau - z)\psi = 0$  are in  $L^2((a, b); rdx)$  near b (resp., near a),

or,

(ii) for every  $z \in \mathbb{C}$ , there exists at least one solution  $\psi$  of  $(\tau - z)\psi = 0$  which is not in  $L^2((a, b); rdx)$  near b (resp., near a). In this case, for each  $z \in \mathbb{C} \setminus \mathbb{R}$ , there exists precisely one solution  $\psi_b$  (resp.,  $\psi_a$ ) of  $(\tau - z)\psi = 0$  (up to constant multiples) which lies in  $L^2((a, b); rdx)$  near b (resp., near a).

This yields the **limit circle/limit point** classification of  $\tau$  at an interval endpoint and links self-adjointness of  $T_{min}$  (resp.,  $T_{max}$ ) and the **limit point** property of  $\tau$ at both endpoints as follows.

#### **Definition 8.**

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Assume Hypothesis 1.
In case (i) in Theorem 7, \tau is said to be in the limit circle case at b (resp., at a). (Frequently, \tau is then called quasi-regular at b (resp., a).)
In case (ii) in Theorem 7, \tau is said to be in the limit point case at b (resp., at a). If \tau is in the limit circle case at a and b then \tau is also called quasi-regular on (a, b).
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#### Theorem 9 (see, e.g., Eckhardt-G-Nichols-Teschl 2013).

If  $\overline{T}_{min}$  is bounded from below at *a*, then there exists  $\alpha \in \mathbb{R}$  such that for all  $\lambda < \alpha, \tau - \lambda$  is **nonoscillatory** at *a*. An analogous result holds at the endpoint *b*.

Assuming  $T_{min}$  is **lower semibounded** and in the **limit circle** case at *a*, and given **principal** and **nonprincipal** solutions  $u_a(\lambda_0, \cdot)$  and  $\hat{u}_a(\lambda_0, \cdot)$  of  $(\tau - \lambda_0)u = 0$ , one introduces generalized boundary values for functions  $g \in \text{dom}(T_{max})$  as follows:

$$\widetilde{g}(a) = \lim_{x \downarrow a} \frac{g(x)}{\widehat{u}_a(\lambda_0, x)}, \quad \widetilde{g}'(a) = \lim_{x \downarrow a} \frac{g(x) - \widetilde{g}(a)\widehat{u}_a(\lambda_0, x)}{u_a(\lambda_0, x)}, \quad (*)$$

and similarly at the endpoint *b* (see, **G-Nichols-Littlejohn 2020**). **Note.** When  $\tau$  is regular at *a*, then the following boundary values re-emerge,

$$\widetilde{g}(a) = g(a), \quad \widetilde{g}'(a) = g^{[1]}(a) = \lim_{x \downarrow a} p(x)g'(x).$$

Hence  $\tilde{g}'(a)$  in (\*) represents the natural analog of the (quasi) difference quotient at x = a.

If  $\tau$  is in the limit circle case at a and b, then

 $T_{\min}f=\tau f,$ 

 $f \in \operatorname{dom}(\operatorname{\mathcal{T}_{min}}) = \big\{g \in \operatorname{dom}(\operatorname{\mathcal{T}_{max}}) \,\big|\, \widetilde{g}(a) = \widetilde{g}\,'(a) = 0 = \widetilde{g}(b) = \widetilde{g}\,'(b)\big\},$ 

and the Friedrichs (resp., Dirichlet) extension  $T_F$  of  $T_{min}$  is given by

 $T_{F}f = \tau f, \quad f \in \operatorname{dom}(T_{F}) = \big\{g \in \operatorname{dom}(T_{\max}) \,\big|\, \widetilde{g}(a) = 0 = \widetilde{g}(b)\big\}.$ 

Actually, at this point ALL self-adjoint extensions can be described as follows:

#### Theorem 10.

Assume Hypothesis 1 and that  $\tau$  is in the limit circle case at *a* and *b*. In addition, assume that  $v_j \in \text{dom}(T_{max})$ , j = 1, 2, are real-valued solutions  $v_j$ , j = 1, 2, of  $(\tau - \lambda)u = 0$  with  $\lambda \in \mathbb{R}$ , such that  $W(v_1, v_2) = 1$ . For  $g \in \text{dom}(T_{max})$  we introduce the generalized boundary values

$$egin{aligned} \widetilde{g}_1(a) &= -W(v_2,g)(a), & \widetilde{g}_1(b) &= -W(v_2,g)(b), \ \widetilde{g}_2(a) &= W(v_1,g)(a), & \widetilde{g}_2(b) &= W(v_1,g)(b). \end{aligned}$$

Then the following items (i)-(iv) hold:

#### Theorem 10 (contd.).

(i)  $T_{A,B}$  is a self-adjoint extension of  $T_{min}$  if and only if there exist 2 × 2 matrices A and B (with complex-valued entries) satisfying

$$\mathsf{rank}(m{A} \ \ m{B}) = 2, \quad m{AJA}^* = m{B}Jm{B}^*, \quad J = \begin{pmatrix} 0 & -1 \ 1 & 0 \end{pmatrix},$$

with  $T_{A,B}$  given by

$$T_{A,B}f = \tau f, \quad f \in \operatorname{dom}(T_{A,B}) = \left\{ g \in \operatorname{dom}(T_{\max}) \middle| \begin{array}{c} A\left(\widetilde{g}_1(a) \\ \widetilde{g}_2(a) \end{array}\right) = B\left(\widetilde{g}_1(b) \\ \widetilde{g}_2(b) \end{array}\right) \right\}.$$

(ii) All self-adjoint extensions  $T_{\gamma,\delta}$  of  $T_{min}$  with separated boundary conditions are of the form

$$T_{\gamma,\delta}f = \tau f, \quad \gamma, \delta \in [0,\pi),$$
  
$$f \in \operatorname{dom}(T_{\gamma,\delta}) = \left\{ g \in \operatorname{dom}(T_{\max}) \mid \sin(\gamma)\widetilde{g}_2(a) + \cos(\gamma)\widetilde{g}_1(a) = 0; \\ \sin(\delta)\widetilde{g}_2(b) + \cos(\delta)\widetilde{g}_1(b) = 0 \right\}.$$

#### Theorem 10 (contd.).

(iii) All self-adjoint extensions  $T_{\varphi,R}$  of  $T_{min}$  with coupled boundary conditions are of the type

$$T_{\varphi,R}f = \tau f,$$
  
$$f \in \operatorname{dom}(T_{\varphi,R}) = \left\{ g \in \operatorname{dom}(T_{\max}) \middle| \begin{pmatrix} \widetilde{g}_1(b) \\ \widetilde{g}_2(b) \end{pmatrix} = e^{i\varphi} R \begin{pmatrix} \widetilde{g}_1(a) \\ \widetilde{g}_2(a) \end{pmatrix} \right\},$$

where  $\varphi \in [0, 2\pi)$ , and R is a real 2 × 2 matrix with det(R) = 1 (i.e.,  $R \in SL(2, \mathbb{R})$ ). (*iv*) Every self-adjoint extension of  $T_{min}$  is either of type (*ii*) (i.e., separated) or of type (*iii*) (i.e., coupled).

In the lower semibounded case this can be rewritten as follows:

#### Theorem 11.

Assume Hypothesis 1 and that  $\tau$  is in the **limit circle** case at *a* and *b*. In addition, assume that  $T_{min} \ge \lambda_0 I$  for some  $\lambda_0 \in \mathbb{R}$ , and denote by  $u_a(\lambda_0, \cdot)$  and  $\hat{u}_a(\lambda_0, \cdot)$  (resp.,  $u_b(\lambda_0, \cdot)$  and  $\hat{u}_b(\lambda_0, \cdot)$ ) principal and nonprincipal solutions of  $\tau u = \lambda_0 u$  at *a* (resp., *b*), satisfying

$$W(\widehat{u}_{a}(\lambda_{0}, \cdot), u_{a}(\lambda_{0}, \cdot)) = W(\widehat{u}_{b}(\lambda_{0}, \cdot), u_{b}(\lambda_{0}, \cdot)) = 1.$$

Then the following items (i)-(iii) hold:

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### Basic Facts and Self-Adjoint L<sup>2</sup>-Realizations (contd.)

#### Theorem 11 (contd.).

(i) Introducing  $v_j \in \text{dom}(T_{max})$ , j = 1, 2, via

$$v_1(x) = \begin{cases} \widehat{u}_a(\lambda_0, x), & \text{for } x \text{ near } a, \\ \widehat{u}_b(\lambda_0, x), & \text{for } x \text{ near } b, \end{cases} \quad v_2(x) = \begin{cases} u_a(\lambda_0, x), & \text{for } x \text{ near } a, \\ u_b(\lambda_0, x), & \text{for } x \text{ near } b, \end{cases}$$

one obtains for all  $g \in \text{dom}(T_{max})$ ,

$$\begin{split} \widetilde{g}(a) &= -W(v_2,g)(a) = \widetilde{g}_1(a) = -W(u_a(\lambda_0, \cdot), g)(a) = \lim_{x \downarrow a} \frac{g(x)}{\widehat{u}_a(\lambda_0, x)}, \\ \widetilde{g}(b) &= -W(v_2,g)(b) = \widetilde{g}_1(b) = -W(u_b(\lambda_0, \cdot), g)(b) = \lim_{x \uparrow b} \frac{g(x)}{\widehat{u}_b(\lambda_0, x)}, \\ \widetilde{g}'(a) &= W(v_1,g)(a) = \widetilde{g}_2(a) = W(\widehat{u}_a(\lambda_0, \cdot), g)(a) = \lim_{x \downarrow a} \frac{g(x) - \widetilde{g}(a)\widehat{u}_a(\lambda_0, x)}{u_a(\lambda_0, x)}, \\ \widetilde{g}'(b) &= W(v_1,g)(b) = \widetilde{g}_2(b) = W(\widehat{u}_b(\lambda_0, \cdot), g)(b) = \lim_{x \uparrow b} \frac{g(x) - \widetilde{g}(b)\widehat{u}_b(\lambda_0, x)}{u_b(\lambda_0, x)}. \end{split}$$

In particular, the limits on the right-hand sides above exist.

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Basic Facts and Self-Adjoint  $L^2$ -Realizations  $T_{A,B}$  of S–L Operators

#### Basic Facts and Self-Adjoint L<sup>2</sup>-Realizations (contd.) Theorem 11 (contd.).

(ii) All self-adjoint extensions  $T_{\gamma,\delta}$  of  $T_{min}$  with separated boundary conditions are of the form

$$egin{aligned} & T_{\gamma,\delta}f = au f, \quad \gamma,\delta \in [0,\pi), \ & f \in \operatorname{dom}(T_{\gamma,\delta}) = igg\{g \in \operatorname{dom}(T_{\max}) \ | \ \sin(\gamma)\widetilde{g}\,'(a) + \cos(\gamma)\widetilde{g}\,(a) = 0; \ & \sin(\delta)\widetilde{g}\,'(b) + \cos(\delta)\widetilde{g}\,(b) = 0 igg\}. \end{aligned}$$

Moreover,  $\sigma(T_{\gamma,\delta})$  is simple.

(iii) All self-adjoint extensions  $T_{\varphi,R}$  of  $T_{min}$  with coupled boundary conditions are of the type

$$\begin{aligned} T_{\varphi,R}f &= \tau f, \\ f &\in \operatorname{dom}(T_{\varphi,R}) = \left\{ g \in \operatorname{dom}(T_{\max}) \left| \begin{pmatrix} \widetilde{g}(b) \\ \widetilde{g}'(b) \end{pmatrix} = e^{i\varphi} R \begin{pmatrix} \widetilde{g}(a) \\ \widetilde{g}'(a) \end{pmatrix} \right\}, \end{aligned}$$

where  $\varphi \in [0, 2\pi)$ , and  $R \in SL(2, \mathbb{R})$ .

Note. For simplicity only, from now on we assume the lower semibounded case. Fritz Gesztesy (Baylor University) Weyl-Titchmarsh Theory July 5, 2022 18/43

#### **Classical** *M*-Function Theory

Throughout the following we assume Hypothesis 1 and fix  $\alpha \in [0, \pi)$ .

Associated with the differential expression  $\tau$  we consider the self-adjoint operator  $T_{\gamma,\delta}$  in  $L^2((a, b); rdx)$  corresponding to separated boundary conditions (if any) indexed by  $\gamma, \delta \in [0, \pi)$ , and the usual fundamental system of solutions  $\phi_{\alpha}(z, \cdot, x_0)$  and  $\theta_{\alpha}(z, \cdot, x_0)$ ,  $z \in \mathbb{C}$ , of  $\tau u = zu$ , with respect to a fixed reference point  $x_0 \in (a, b)$ , satisfying the initial conditions

$$\begin{split} \phi_{\alpha}(z, x_0, x_0) &= -\theta_{\alpha}^{[1]}(z, x_0, x_0) = -\sin(\alpha), \\ \phi_{\alpha}^{[1]}(z, x_0, x_0) &= \theta_{\alpha}(z, x_0, x_0) = \cos(\alpha), \quad \alpha \in [0, \pi), \ z \in \mathbb{C}, \ x_0 \in (a, b). \end{split}$$

Again we note that for any fixed  $x, x_0 \in (a, b)$ ,  $\phi_{\alpha}(z, x, x_0)$  and  $\theta_{\alpha}(z, x, x_0)$  are **entire** with respect to z and that

$$W( heta_{\alpha}(z,\,\cdot\,,x_0),\phi_{\alpha}(z,\,\cdot\,,x_0))(x)=1,\quad z\in\mathbb{C},\ x_0\in(a,b).$$

Particularly important solutions of  $\tau u = zu$  are the Weyl-Titchmarsh solutions  $\psi_{\alpha,b}(z, \cdot, x_0)$  or  $\psi_{\alpha,b,\delta}(z, \cdot, x_0)$  at *b* (resp.,  $\psi_{\alpha,a}(z, \cdot, x_0)$  or  $\psi_{\alpha,a,\gamma}(z, \cdot, x_0)$  at *a*) of  $\tau u = zu$ , uniquely characterized as follows:

(*i*) If  $\tau$  is in the **limit point** case at *b* (resp., *a*), one introduces  $\psi_{\alpha,b}(z, \cdot, x_0)$  (resp.,  $\psi_{\alpha,a}(z, \cdot, x_0)$ ) via the requirement

 $\psi_{\alpha,b}(z, \cdot, x_0) \in L^2([x_0, b); rdx), \quad (\text{resp.}, \ \psi_{\alpha,a}(z, \cdot, x_0) \in L^2((a, x_0]; rdx)),\\ \sin(\alpha)\psi_{\alpha,b}^{[1]}(z, x_0, x_0) + \cos(\alpha)\psi_{\alpha,b}(z, x_0, x_0) = 1$ 

 $(\text{resp., } \sin(\alpha)\psi_{\alpha,a}^{[1]}(z,x_0,x_0) + \cos(\alpha)\psi_{\alpha,a}(z,x_0,x_0) = 1), \quad z \in \mathbb{C} \setminus \mathbb{R}.$ 

The crucial condition is the  $L^2$ -property at b (resp., a), which uniquely determines  $\psi_{\alpha,b}(z, \cdot, x_0)$  (resp.,  $\psi_{\alpha,a}(z, \cdot, x_0)$ ) up to constant (possibly, z-dependent) multiples by the **limit point** case hypothesis of  $\tau$  at a and b. In particular, for  $\alpha, \beta \in [0, \pi)$ ,

$$\begin{split} \psi_{\alpha,b}(z,\cdot,x_0) &= C_b(z,\alpha,\beta,x_0)\psi_{\beta,b}(z,\cdot,x_0)\\ (\text{resp., }\psi_{\alpha,a}(z,\cdot,x_0) &= C_a(z,\alpha,\beta,x_0)\psi_{\beta,a}(z,\cdot,x_0))\\ \text{for some coefficients } C_b(z,\alpha,\beta,x_0) \in \mathbb{C}, \text{ (resp., } C_a(z,\alpha,\beta,x_0) \in \mathbb{C}). \end{split}$$

(ii) If  $\tau$  is in the **limit circle** case at *b* (resp., *a*), one introduces  $\psi_{\alpha,b,\delta}(z, \cdot, x_0)$  (resp.,  $\psi_{\alpha,a,\gamma}(z, \cdot, x_0)$ ) by requiring that

$$\begin{split} &\psi_{\alpha,b,\delta}(z,\cdot,x_0) \ (\text{resp.},\ \psi_{\alpha,a,\gamma}(z,\cdot,x_0)) \text{ satisfies the (separated) boundary condition} \\ &\text{ at } b \ (\text{resp.},\ a) \ \text{of the form, } \sin(\delta) \widetilde{\psi}'_{\alpha,b,\delta}(z,b,x_0) + \cos(\delta) \widetilde{\psi}_{\alpha,b,\delta}(z,b,x_0) = 0 \\ &(\text{resp.},\ \sin(\gamma) \widetilde{\psi}'_{\alpha,b,\gamma}(z,a,x_0) + \cos(\gamma) \widetilde{\psi}_{\alpha,b,\gamma}(z,a,x_0) = 0), \\ &\sin(\alpha) \psi^{[1]}_{\alpha,b,\delta}(z,x_0,x_0) + \cos(\alpha) \psi_{\alpha,b,\delta}(z,x_0,x_0) = 1 \\ &(\text{resp.},\ \sin(\alpha) \psi^{[1]}_{\alpha,a,\gamma}(z,x_0,x_0) + \cos(\alpha) \psi_{\alpha,a,\gamma}(z,x_0,x_0) = 1), \quad z \in \mathbb{C} \backslash \mathbb{R}. \end{split}$$

**Notational convention.** To minimize the case distinctions to be made in the following, we will adopt the notation of case (*ii*) and should the **limit point** case of  $\tau$  be present at *b* or *a* we simply ignore the extra  $\delta$ - or  $\gamma$ -dependence.

In either case (i) or (ii), the normalizations employed show that  $\psi_{\alpha, \underline{b}, \delta}(z, \cdot, x_0)$  are of the type

$$\psi_{\alpha,\underset{\mathbf{a},\gamma}{b,\delta}}(z,x,x_0) = \theta_{\alpha}(z,x,x_0) + m_{\alpha,\underset{\mathbf{a},\gamma}{b,\delta}}(z,x_0)\phi_{\alpha}(z,x,x_0), \quad z \in \mathbb{C} \setminus \mathbb{R}, \ x \in (\mathbf{a},b),$$

for some coefficients  $m_{\alpha,\frac{b,\delta}{a,\gamma}}(z,x_0)$ ,  $z \in \mathbb{C} \setminus \mathbb{R}$ , the Weyl–Titchmarsh *m*-functions associated with  $\tau$ ,  $\alpha$ ,  $\gamma$ ,  $\delta$ , and  $x_0$ , which contains (half-line) spectral information,

$$m_{\alpha,\underset{a,\gamma}{b,\delta}}(z,x_0) = \cos(\alpha)\psi_{\alpha,\underset{a,\gamma}{b,\delta}}^{[1]}(z,x_0,x_0) - \sin(\alpha)\psi_{\alpha,\underset{a,\gamma}{b,\delta}}(z,x_0,x_0), \quad z \in \mathbb{C} \setminus \mathbb{R}$$

One recalls the fundamental identities

$$\int_{x_0}^{b} r(x) dx \,\psi_{\alpha,b,\delta}(z_1, x, x_0) \psi_{\alpha,b,\delta}(z_2, x, x_0) = \frac{m_{\alpha,b,\delta}(z_1, x_0) - m_{\alpha,b,\delta}(z_2, x_0)}{z_1 - z_2},$$

$$\int_{a}^{x_0} r(x) dx \,\psi_{\alpha,a,\gamma}(z_1, x, x_0) \psi_{\alpha,a,\gamma}(z_2, x, x_0) = -\frac{m_{\alpha,a,\gamma}(z_1, x_0) - m_{\alpha,a,\gamma}(z_2, x_0)}{z_1 - z_2},$$

$$z_1, z_2 \in \mathbb{C} \setminus \mathbb{R}, \ z_1 \neq z_2,$$

and concludes

$$\overline{m_{\alpha,\underline{b},\delta}(z,x_0)} = m_{\alpha,\underline{b},\delta}(\overline{z},x_0), \quad z \in \mathbb{C} \setminus \mathbb{R}.$$

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-Functions and Separated Boundary Conditions

#### Classical *M*-Function Theory (contd.)

Choosing  $z_1 = z$ ,  $z_2 = \overline{z}$  one infers

$$egin{aligned} &\int_{x_0}^b r(x)dx\,|\psi_{lpha,b,\delta}(z,x,x_0)|^2 = rac{\mathrm{Im}(m_{lpha,b,\delta}(z,x_0))}{\mathrm{Im}(z)} > 0, \quad z\in\mathbb{C}ackslash\mathbb{R}, \ &\int_a^{x_0} r(x)dx\,|\psi_{lpha,a,\gamma}(z,x,x_0)|^2 = -rac{\mathrm{Im}(m_{lpha,a,\gamma}(z,x_0))}{\mathrm{Im}(z)} > 0, \quad z\in\mathbb{C}ackslash\mathbb{R}. \end{aligned}$$

In addition, since  $m_{\alpha, \frac{b}{a}, \gamma}(\cdot, x_0)$  are known to be analytic on  $\mathbb{C}\setminus\mathbb{R}$ , one obtains that  $\pm m_{\alpha, \frac{b}{a}, \gamma}(\cdot, x_0)$  are **Nevanlinna–Herglotz** functions. The Green's function  $G_{\gamma, \delta}(z, x, x')$ ,  $z \in \rho(T_{\gamma, \delta})$ ,  $x, x' \in (a, b)$ , of  $T_{\gamma, \delta}$  then reads

$$egin{aligned} & \mathcal{G}_{\gamma,\delta}(z,x,x') = rac{1}{W(\psi_{lpha,b,\delta}(z,\,\cdot\,,x_0),\psi_{lpha,a,\gamma}(z,\,\cdot\,,x_0))} \ & imes \left\{ egin{aligned} & \psi_{lpha,a,\gamma}(z,x,x_0)\psi_{lpha,b,\delta}(z,x',x_0), & a < x \leqslant x' < b, \ & \psi_{lpha,b,\delta}(z,x,x_0)\psi_{lpha,a,\gamma}(z,x',x_0), & a < x' \leqslant x < b, \end{aligned} 
ight. \ & z \in \mathbb{C} ackslash \mathbb{R}, \end{aligned}$$

with

$$W(\psi_{\alpha,b,\delta}(z,\,\cdot\,,x_0),\psi_{\alpha,a,\gamma}(z,\,\cdot\,,x_0))=m_{\alpha,a,\gamma}(z,x_0)-m_{\alpha,b,\delta}(z,x_0),\quad z\in\mathbb{C}\backslash\mathbb{R}.$$

Thus (given  $z \in \mathbb{C} \setminus \mathbb{R}$ ,  $x \in (a, b)$ ,  $f \in L^2((a, b); rdx)$ ), for separated bc's,

$$((T_{\gamma,\delta}-zI)^{-1}f)(x)=\int_a^b r(x')dx' G_{\gamma,\delta}(z,x,x')f(x')$$

For each  $x \in \mathbb{R}$ , the **diagonal Green's function** of  $T_{\gamma,\delta}$ , denoted by  $g_{\gamma,\delta}(z,x)$ , has the **Nevanlinna–Herglotz** property,

Given  $m_{\alpha, \frac{b}{a}, \gamma}(z, x_0)$ , introduce the 2 × 2 matrix-valued Weyl–Titchmarsh fct.

$$\begin{split} M_{\alpha,\gamma,\delta}(z,x_0) &= \left(M_{\alpha,\gamma,\delta,\ell,\ell'}(z,x_0)\right)_{\ell,\ell'=1,2} \\ &= \begin{pmatrix} \frac{1}{m_{\alpha,a,\gamma}(z,x_0) - m_{\alpha,b,\delta}(z,x_0)} & \frac{1}{2}\frac{m_{\alpha,a,\gamma}(z,x_0) + m_{\alpha,b,\delta}(z,x_0)}{m_{\alpha,a,\gamma}(z,x_0) - m_{\alpha,b,\delta}(z,x_0)} \\ \frac{1}{2}\frac{m_{\alpha,a,\gamma}(z,x_0) - m_{\alpha,b,\delta}(z,x_0)}{m_{\alpha,a,\gamma}(z,x_0) - m_{\alpha,b,\delta}(z,x_0)} & \frac{m_{\alpha,a,\gamma}(z,x_0) - m_{\alpha,b,\delta}(z,x_0)}{m_{\alpha,a,\gamma}(z,x_0) - m_{\alpha,b,\delta}(z,x_0)} \end{pmatrix}, \quad z \in \mathbb{C} \backslash \mathbb{R}, \end{split}$$

and notes that

 $\det_{\mathbb{C}^2}(M_{\alpha,\gamma,\delta}(z,x_0)) = -1/4, \quad M_{\alpha,\gamma,\delta}(z,x_0)^* = M_{\alpha,\gamma,\delta}(\overline{z},x_0), \quad z \in \mathbb{C} \setminus \mathbb{R}.$ By inspection,  $M_{\alpha,\gamma,\delta}(z,x_0)$  is a 2 × 2 matrix-valued **Nevanlinna–Herglotz** fct. since  $-m_{\alpha,a,\gamma}(\cdot,x_0)$  and  $m_{\alpha,b,\delta}(\cdot,x_0)$  are scalar **Nevanlinna–Herglotz** fcts. -Functions and Separated Boundary Conditions

### Classical *M*-Function Theory (contd.)

Turning to the connection between  $M_{\alpha,\gamma,\delta}(z,x_0)$  and the Green's function  $G_{\gamma,\delta}(z,\cdot,\cdot)$  of  $T_{\gamma,\delta}$ , still in the **separated b.c. case**, we introduce

$$\begin{split} & \left(\partial_{1}^{[1]}G_{\gamma,\delta}\right)(z,x_{0},x') = p(x_{1})\partial_{x_{1}}G_{\gamma,\delta}(z,x_{1},x')\big|_{x_{1}=x_{0}}, \\ & \left(\partial_{2}^{[1]}G_{\gamma,\delta}\right)(z,x,x_{0}) = p(x_{2})\partial_{x_{2}}G_{\gamma,\delta}(z,x,x_{2})\big|_{x_{2}=x_{0}}, \\ & \left(\partial_{1}^{[1]}\partial_{2}^{[1]}G_{\gamma,\delta}\right)(z,x_{0},x_{0}) = p(x_{1})\partial_{x_{1}}p(x_{2})\partial_{x_{2}}G_{\gamma,\delta}(z,x_{1},x_{2})\big|_{x_{1}=x_{0},x_{2}=x_{0}} \\ & = \left(\partial_{2}^{[1]}\partial_{1}^{[1]}G_{\gamma,\delta}\right)(z,x_{0},x_{0}), \text{ etc.} \end{split}$$

Then  $M_{\alpha,\gamma,\delta}(z,x_0)$  can be rewritten as

$$\begin{split} &\mathcal{M}_{\alpha,\gamma,\delta,1,1}(z,x_0) = \left(\left[\cos(\alpha) + \sin(\alpha)\partial_1^{[1]}\right]\left[\cos(\alpha) + \sin(\alpha)\partial_2^{[1]}\right]G_{\gamma,\delta}\right)(z,x_0,x_0), \\ &\mathcal{M}_{\alpha,\gamma,\delta,1,2}(z,x_0) = \mathcal{M}_{\alpha,\gamma,\delta,2,1}(z,x_0) \\ &= (1/2)\left(\left\{\left[\cos(\alpha) + \sin(\alpha)\partial_1^{[1]}\right]\left[-\sin(\alpha) + \cos(\alpha)\partial_2^{[1]}\right]\right] \\ &+ \left[-\sin(\alpha) + \cos(\alpha)\partial_1^{[1]}\right]\left[\cos(\alpha) + \sin(\alpha)\partial_2^{[1]}\right]\right\}G_{\gamma,\delta}\right)(z,x_0\pm 0,x_0\mp 0), \\ &\mathcal{M}_{\alpha,\gamma,\delta,2,2}(z,x_0) = \left(\left[-\sin(\alpha) + \cos(\alpha)\partial_1^{[1]}\right]\left[-\sin(\alpha) + \cos(\alpha)\partial_2^{[1]}\right]G_{\gamma,\delta}\right)(z,x_0,x_0), \\ &z \in \mathbb{C} \backslash \mathbb{R}. \end{split}$$

Thus,  $G_{\gamma,\delta}(z, x_0, x_0)$  and appropriate first quasi-derivatives of  $G_{\gamma,\delta}(z, \cdot, \cdot)$  at  $x_0$  uniquely determine  $M_{\alpha,\gamma,\delta}(z, x_0)$  in a straightforward fashion.

In the particular case  $\alpha = 0$ , one obtains the remarkably simple formula

$$M_{0,\gamma,\delta}(z,x_0) = \begin{pmatrix} G_{\gamma,\delta}(z,x_0,x_0) & 2^{-1} \left( \left[ \partial_1^{[1]} + \partial_2^{[1]} \right] G_{\gamma,\delta} \right) (z,x_0 \pm 0,x_0 \mp 0) \\ \\ 2^{-1} \left( \left[ \partial_1^{[1]} + \partial_2^{[1]} \right] G_{\gamma,\delta} \right) (z,x_0 \pm 0,x_0 \mp 0) & \left( \partial_1^{[1]} \partial_2^{[1]} G_{\gamma,\delta} \right) (z,x_0,x_0) \end{pmatrix}, \\ z \in \mathbb{C} \setminus \mathbb{R}.$$

**Note.** (*i*) Above, one can of course replace  $z \in \mathbb{C} \setminus \mathbb{R}$  by  $z \in \rho(T_{\gamma,\delta})$ . (*ii*) It is possible to take the limit  $x_0 \downarrow a$  (resp.,  $x_0 \uparrow b$ ) as long as  $\tau$  is in the **limit circle** case at a (resp., b).

This summarizes the traditional approach to  $2 \times 2$  Weyl–Titchmarsh theory which focuses on separated boundary conditions at *a* and *b* (if any).

How about **coupled boundary conditions** at *a* and *b*? E.g., the **periodic** case?

### **General** *M*-Function Theory

Let  $T_{A,B}$  be a fixed self-adjoint extension of  $T_{min}$  with (separated or coupled) boundary conditions encoded in the 2 × 2 matrices  $A, B \in \mathbb{C}^{2\times 2}$ , and abbreviate the associated Green's function of  $T_{A,B}$  by  $G_{A,B}(z, \cdot, \cdot)$ ,  $z \in \mathbb{C} \setminus \sigma(T_{A,B})$ .

Inspired by the explicit form of  $M_{0,\gamma,\delta}(\cdot, x_0)$  in terms of the Green's function  $G_{\gamma,\delta}(\cdot, x_0, x_0)$  and some of its first quasi-derivatives, we now introduce the general *M*-function in exactly the same manner,

$$\begin{split} \mathsf{M}_{0,A,B}(z,x_0) &= \begin{pmatrix} \mathsf{G}_{A,B}(z,x_0,x_0) & 2^{-1} \left( \left[ \partial_1^{[1]} + \partial_2^{[1]} \right] \mathsf{G}_{A,B} \right) (z,x_0 + 0,x_0 - 0) \\ 2^{-1} \left( \left[ \partial_1^{[1]} + \partial_2^{[1]} \right] \mathsf{G}_{A,B} \right) (z,x_0 + 0,x_0 - 0) & \left( \partial_1^{[1]} \partial_2^{[1]} \mathsf{G}_{A,B} \right) (z,x_0,x_0) \end{pmatrix} \\ &= \begin{pmatrix} \mathsf{G}_{A,B}(z,x_0,x_0) & 2^{-1} \left( \left[ \partial_1^{[1]} + \partial_2^{[1]} \right] \mathsf{G}_{A,B} \right) (z,x_0 - 0,x_0 + 0) \\ 2^{-1} \left( \left[ \partial_1^{[1]} + \partial_2^{[1]} \right] \mathsf{G}_{A,B} \right) (z,x_0 - 0,x_0 + 0) & \left( \partial_1^{[1]} \partial_2^{[1]} \mathsf{G}_{A,B} \right) (z,x_0,x_0) \end{pmatrix}, \\ &z \in \mathbb{C}_+, \ x_0 \in (a,b). \end{split}$$

Eventually, we will (indicate how to) prove the **Nevanlinna–Herglotz** property of  $M_{0,A,B}(\cdot, x_0)$ .

**Note.** To simplify matters we restrict ourselves to the simplest case  $\alpha = 0$  only.

M-Functions and General (e.g., Coupled) Boundary Conditions

### General *M*-Function Theory (contd.)

Here we employed the abbreviations

$$\begin{split} & \left(\partial_{1}^{[1]}G_{A,B}\right)(z,x_{0}\pm0,x_{0}\mp0) = \lim_{\varepsilon\downarrow0} p(x)\partial_{x}G_{A,B}(z,x,x')\Big|_{\substack{x=x_{0}\pm\varepsilon,\\x'=x_{0}\mp\varepsilon}} \\ & \left(\partial_{2}^{[1]}G_{A,B}\right)(z,x_{0}\pm0,x_{0}\mp0) = \lim_{\varepsilon\downarrow0} p(x')\partial_{x'}G_{A,B}(z,x,x')\Big|_{\substack{x=x_{0}\pm\varepsilon,\\x'=x_{0}\mp\varepsilon}} \\ & \left(\partial_{1}^{[1]}\partial_{2}^{[1]}G_{A,B}\right)(z,x_{0},x_{0}) = p(x)\partial_{x}p(x')\partial_{x'}G_{A,B}(z,x,x')\Big|_{\substack{x=x'=x_{0}\\x'=x_{0}\pm\varepsilon}} \\ & = \left(\partial_{2}^{[1]}\partial_{1}^{[1]}G_{A,B}\right)(z,x_{0},x_{0}), \end{split}$$

and note the explicit formula (for  $z \in \rho(T_{A,B})$ ,  $x, x', x_0 \in (a, b)$ )

$$\begin{aligned} G_{A,B}(z,x,x') &= G_{A,B}(z,x_0,x_0)\theta_0(z,x,x_0)\theta_0(z,x',x_0) \\ &+ \left[ (\partial_1^{[1]} \partial_2^{[1]} G_{A,B})(z,x_0,x_0) \right] \phi_0(z,x,x_0) \phi_0(z,x',x_0) \\ &+ \left[ (\partial_2^{[1]} G_{A,B})(z,x_0 \pm 0,x_0 \mp 0) + \begin{pmatrix} -1, \\ 0, \end{pmatrix} \right] \theta_0(z,x,x_0) \phi_0(z,x',x_0) \\ &+ \left[ (\partial_1^{[1]} G_{A,B})(z,x_0 \pm 0,x_0 \mp 0) + \begin{pmatrix} 1, \\ 0, \end{pmatrix} \right] \phi_0(z,x,x_0) \theta_0(z,x',x_0) \\ &+ \left\{ \begin{smallmatrix} 0 \\ \theta_0(z,x,x_0) \phi_0(z,x',x_0) - \phi_0(z,x,x_0) \theta_0(z,x',x_0) \end{bmatrix}, \begin{array}{l} a < x \leq x' < b, \\ a < x \leq x < b. \end{split} \right. \end{aligned}$$

**Note.**  $\phi_0, \theta_0$  are **entire !!!!!** All possible spectral information sits in the **rest** !!!!!

### General *M*-Function Theory (contd.)

#### Theorem 12.

Assume Hypothesis 1, that  $T_{min}$  is bounded from below, and let  $z \in \mathbb{C}_+$ . Then, for each fixed  $x_0 \in (a, b)$ ,  $M_{0,A,B}(\cdot, x_0)$ , is a  $2 \times 2$  Nevanlinna–Herglotz matrix with strictly positive imaginary part,

$$\operatorname{Im}(M_{0,A,B}(z,x_0)) > 0, \quad z \in \mathbb{C}_+.$$

**Sketch of Proof.** (I will have to pull your leg badly, very sorry !!!!) Introduce the graph Hilbert space<sup>1</sup>  $H^2_{\tau}((a, b))$  associated with  $T_{max}$  as follows,

$$H^{2}_{\tau}((a,b)) = \operatorname{dom}(T_{max})$$
  
= { g \in L^{2}((a,b); rdx) | g, g^{[1]} \in AC\_{loc}((a,b)); \tau g \in L^{2}((a,b); rdx) }

with associated graph norm

$$\|f\|_{H^{2}_{\tau}((a,b))}^{2} = \|T_{\max}f\|_{L^{2}((a,b);rdx)}^{2} + \|f\|_{L^{2}((a,b);rdx)}^{2}, \quad f \in \operatorname{dom}(T_{\max}),$$

and scalar product

$$\frac{(f,g)_{H^2_{\tau}((a,b))} = (T_{\max}f, T_{\max}g)_{L^2((a,b);rdx)} + (f,g)_{L^2((a,b);rdx)}, \quad f,g \in \text{dom}(T_{\max}).$$
<sup>1</sup>We chose the notation  $H^2_{\tau}((a,b))$  since in the special case  $p = r = 1, q = 0, \tau_0 = -d^2/dx^2$ ,

 $H^2_{\tau_0}((a,b))$  coincides with the standard Sobolev space  $H^2((a,b)) = W^{2,2}((a,b))$ .

M-Functions and General (e.g., Coupled) Boundary Conditions

### General *M*-Function Theory (contd.)

We also introduce the scale of Hilbert spaces corresponding to the self-adjoint operator  $T_{A,B}$ , assuming, for simplicity only, that  $T_{A,B} \ge 0$ . Hence, one obtains the chain of strict inclusions,

$$\begin{aligned} \mathcal{H}_2(\mathcal{T}_{A,B}) &\subsetneqq \mathcal{H}_{\tau}^2((a,b)) \lneq \mathcal{H}_0(\mathcal{T}_{A,B}) = \mathcal{H} = \mathcal{H}^* = \mathcal{H}_0(\mathcal{T}_{A,B})^* \\ & \subsetneqq \mathcal{H}_{\tau}^2((a,b))^* \subsetneqq \mathcal{H}_2(\mathcal{T}_{A,B})^* = \mathcal{H}_{-2}(\mathcal{T}_{A,B}), \end{aligned}$$

with

 $\|\cdot\|_{\mathcal{H}_2(T_{A,B})^*}\leqslant\|\cdot\|_{H^2_\tau((a,b))^*}\leqslant\|\cdot\|_{L^2((a,b);rdx)}\leqslant\|\cdot\|_{H^2_\tau((a,b))}\leqslant\|\cdot\|_{\mathcal{H}_2(T_{A,B})}.$ 

At this point we introduce the map

$$\mathsf{F}_{\mathsf{x}_0} \colon \begin{cases} \mathsf{H}^2_\tau((a,b)) \to \mathbb{C}^2, \\ u \mapsto \begin{pmatrix} u(x_0) \\ u^{[1]}(x_0) \end{pmatrix}, \qquad x_0 \in (a,b), \end{cases}$$

and record its properties in the following.

M-Functions and General (e.g., Coupled) Boundary Conditions

#### General *M*-Function Theory (contd.)

#### Lemma 13.

Assume Hypothesis 1 and that  $T_{A,B} \ge 0$ . Then

 $\Gamma_{\mathbf{x}_0} \in \mathcal{B}(H^2_{\tau}((a, b)), \mathbb{C}^2)$ 

#### and

$$\Gamma^*_{\mathbf{x}_0} \colon \begin{cases} \mathbb{C}^2 \to H^2_{\tau}((a,b))^* \\ \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} \mapsto c_1 \delta_{\mathbf{x}_0} - c_2 p \delta'_{\mathbf{x}_0}, \qquad \Gamma^*_{\mathbf{x}_0} \in \mathcal{B}(\mathbb{C}^2, H^2_{\tau}((a,b))^*), \end{cases}$$

where

$$\begin{split} \delta_{x_0}(u) &= {}_{H^2_\tau((a,b))^*} \langle \delta_{x_0}, u \rangle_{H^2_\tau((a,b))} = u(x_0), \\ p \delta'_{x_0}(u) &= {}_{H^2_\tau((a,b))^*} \langle p \delta'_{x_0}, u \rangle_{H^2_\tau((a,b))} = -u^{[1]}(x_0), \quad u \in H^2_\tau((a,b)). \end{split}$$

#### General *M*-Function Theory (contd.)

Using mapping properties of resolvents of  $T_{A,B}$  in connection with the chain of Hilbert spaces  $\mathcal{H}_s(T_{A,B})$ ,  $s \in \mathbb{R}$ , more precisely, using the special cases,

$$\begin{split} & (\widetilde{T_{A,B}} + \widetilde{I})^{-1} \colon L^2((a,b); rdx) = \mathcal{H}_0(T_{A,B}) \to \mathcal{H}_2(T_{A,B}) \text{ is an isomorphism,} \\ & (\widetilde{T_{A,B}} + \widetilde{I})^{-1} \colon \mathcal{H}_2(T_{A,B})^* = \mathcal{H}_{-2}(T_{A,B}) \to L^2((a,b); rdx) \text{ is an isomorphism,} \\ & (\widetilde{T_{A,B}} + \widetilde{I})^{-2} \colon \mathcal{H}_2(T_{A,B})^* = \mathcal{H}_{-2}(T_{A,B}) \to \mathcal{H}_2(T_{A,B}) \text{ is an isomorphism,} \end{split}$$

with  $\tilde{I}$  appropriate inclusion maps, one introduces

$$N_{A,B}(z,x_0) = \begin{pmatrix} \mathsf{Im}(G_{A,B}(z,x_0,x_0)) & \partial_2^{[1]}\mathsf{Im}(G_{A,B}(z,x_0,x_0)) \\ \partial_1^{[1]}\mathsf{Im}(G_{A,B}(z,x_0,x_0)) & \partial_1^{[1]}\partial_2^{[1]}\mathsf{Im}(G_{A,B}(z,x_0,x_0)) \end{pmatrix}, \quad z \in \mathbb{C}_+,$$

and computes as follows:

#### General *M*-Function Theory (contd.)

$$\begin{aligned} (c, N_{A,B}(z, x_{0})c)_{\mathbb{C}^{2}} \\ &= \left( \begin{pmatrix} c_{1} \\ c_{2} \end{pmatrix}, \begin{pmatrix} \operatorname{Im}(G_{A,B}(z, x_{0}, x_{0})) & \partial_{2}^{[1]}\operatorname{Im}(G_{A,B}(z, x_{0}, x_{0})) \\ \partial_{1}^{[1]}\operatorname{Im}(G_{A,B}(z, x_{0}, x_{0})) & \partial_{1}^{[1]}\partial_{2}^{[1]}\operatorname{Im}(G_{A,B}(z, x_{0}, x_{0})) \end{pmatrix} \begin{pmatrix} c_{1} \\ c_{2} \end{pmatrix} \right)_{\mathbb{C}^{2}} \\ &= \left( c, (2i)^{-1}\Gamma_{x_{0}} \left[ \left( \overline{T_{A,B}} - z\tilde{I} \right)^{-1} - \left( \overline{T_{A,B}} - \overline{z}\tilde{I} \right)^{-1} \right] \Gamma_{x_{0}}^{*}c \right)_{\mathbb{C}^{2}} \\ &= \operatorname{Im}(z) \left( c, \Gamma_{x_{0}} \left( \overline{T_{A,B}} - z\tilde{I} \right)^{-1} \left( \overline{T_{A,B}} - \overline{z}\tilde{I} \right)^{-1} \Gamma_{x_{0}}^{*}c \right)_{\mathbb{C}^{2}} \\ &= \operatorname{Im}(z) \left( \left( \overline{T_{A,B}} - \overline{z}\tilde{I} \right)^{-1} \Gamma_{x_{0}}^{*}c, \left( \overline{T_{A,B}} - \overline{z}\tilde{I} \right)^{-1} \Gamma_{x_{0}}^{*}c \right)_{L^{2}((a,b);rdx)} \\ &= \operatorname{Im}(z) \| \left( \overline{T_{A,B}} - \overline{z}\tilde{I} \right)^{-1} \Gamma_{x_{0}}^{*}c \|_{L^{2}((a,b);rdx)}^{2} \geqslant 0. \end{aligned}$$

Thus,

$$\mathrm{Im}(M_{0,A,B}(z,x_{0})) = 2^{-1} [N_{A,B}(z,x_{0}) + N_{A,B}(z,x_{0})^{\top}] \ge 0, \quad z \in \mathbb{C}_{+}.$$

Finally, proving strict inequality is elementary and hence omitted here.  $\Box$ 

Connecting  $M(\cdot)$  and the Spectral Projections  $E_{T_A}$ ,  $p(\cdot)$ 

### Connecting $M_{0,A,B}(\cdot, x_0)$ and $E_{T_{A,B}}(\cdot)$

Since  $M_{0,A,B}(\cdot, x_0)$  is a 2 × 2 matrix-valued Nevanlinna–Herglotz function, it permits the representation,

$$\mathcal{M}_{0,\mathcal{A},\mathcal{B}}(z,\mathsf{x}_0) = C_{0,\mathcal{A},\mathcal{B}}(\mathsf{x}_0) + \int_{\mathbb{R}} d\Omega_{0,\mathcal{A},\mathcal{B}}(\lambda,\mathsf{x}_0) igg(rac{1}{\lambda-z} - rac{\lambda}{1+\lambda^2}igg), \quad z\in\mathbb{C}ackslash\mathbb{R},$$

where

$$C_{0,A,B}(x_0) = C_{0,A,B}(x_0)^* = \operatorname{Re}(M_{0,A,B}(i, x_0)), \quad \int_{\mathbb{R}} \frac{\|d\Omega_{0,A,B}(\lambda, x_0)\|}{1 + \lambda^2} < \infty.$$

The **Stieltjes inversion formula** for the 2 × 2 nonnegative matrix-valued measure  $d\Omega_{0,A,B}(\cdot, x_0)$  then reads

$$\begin{split} \Omega_{0,A,B}((\lambda_1,\lambda_2],x_0) &= \pi^{-1} \lim_{\delta \downarrow 0} \lim_{\varepsilon \downarrow 0} \int_{\lambda_1+\delta}^{\lambda_2+\delta} d\lambda \operatorname{Im}(\mathcal{M}_{0,A,B}(\lambda+i\varepsilon,x_0)), \\ \lambda_1,\lambda_2 \in \mathbb{R}, \; \lambda_1 < \lambda_2, \end{split}$$

and hence we are now after the connection between  $\Omega_{0,A,B}(\cdot, x_0)$  and  $E_{T_{A,B}}(\cdot)$ .

Connecting  $M(\cdot)$  and the Spectral Projections  $E_{T_A}$ 

# Connecting $M_{0,A,B}(\cdot, x_0)$ and $E_{T_{A,B}}(\cdot)$ (contd.)

#### Theorem 14.

Assume Hypothesis 1 and  $T_{min}$  is bounded from below. In addition, suppose that  $f, g \in C_0^{\infty}((a, b)), F \in C(\mathbb{R}), x_0 \in (a, b)$ , and  $\lambda_1, \lambda_2 \in \mathbb{R}, \lambda_1 < \lambda_2$ . Then,

$$f, F(T_{A,B})E_{T_{A,B}}((\lambda_1, \lambda_2])g)_{L^2((a,b);rdx)}$$
  
=  $(\widehat{f_0}(\cdot, x_0), M_F M_{\chi_{(\lambda_1, \lambda_2]}}\widehat{g_0}(\cdot, x_0))_{L^2(\mathbb{R}; d\Omega_{0,A,B}(\cdot, x_0))}$   
=  $\int_{(\lambda_1, \lambda_2]} \overline{\widehat{f_0}(\lambda, x_0)^\top} d\Omega_{0,A,B}(\lambda, x_0) \widehat{g_0}(\lambda, x_0)F(\lambda),$ 

where we introduced the notation (generalized Fourier coefficients)

$$\begin{split} \widehat{h}_{0,1}(\lambda, x_0) &= \int_a^b r(x) dx \, \theta_0(\lambda, x, x_0) h(x), \\ \widehat{h}_{0,2}(\lambda, x_0) &= \int_a^b r(x) dx \, \phi_0(\lambda, x, x_0) h(x), \\ \widehat{h}_0(\lambda, x_0) &= \left(\widehat{h}_{0,1}(\lambda, x_0), \widehat{h}_{0,2}(\lambda, x_0)\right)^\top, \quad \lambda \in \mathbb{R}, \ h \in C_0^\infty((a, b)). \end{split}$$

Connecting  $M(\cdot)$  and the Spectral Projections  $E_{T,a,p}$ 

## Connecting $M_{0,A,B}(\cdot, x_0)$ and $E_{T_{A,B}}(\cdot)$ (contd.)

Here  $M_G$  represents the maximally defined operator of multiplication by the  $d\Omega_{0,A,B}^{tr}(\cdot, x_0)$ -measurable function G in the Hilbert space  $L^2(\mathbb{R}; d\Omega_{0,A,B}(\cdot, x_0))$ ,

$$(M_{G}\widehat{h})(\lambda) = G(\lambda)\widehat{h}(\lambda) = (G(\lambda)\widehat{h}_{1}(\lambda), G(\lambda)\widehat{h}_{2}(\lambda))^{\top} \text{ for } d\Omega_{0,A,B}^{tr}(\cdot, x_{0})\text{-a.e. } \lambda \in \mathbb{R},$$
  
 
$$\widehat{h} \in \operatorname{dom}(M_{G}) = \{\widehat{k} \in L^{2}(\mathbb{R}; d\Omega_{0,A,B}(\cdot, x_{0})) \mid G\widehat{k} \in L^{2}(\mathbb{R}; d\Omega_{0,A,B}(\cdot, x_{0}))\},$$

and

 $d\Omega^{tr} = d\Omega_{1,1} + d\Omega_{2,2}$ 

denotes the trace measure of a 2 × 2 matrix-valued nonnegative measure  $d\Omega = (d\Omega_{\ell,\ell'})_{\ell,\ell'=1,2}$  on  $\mathbb{R}$ .

The proof of Theorem 14 involves, **Stone's formula** relating the family of spectral projections  $E_T(\cdot)$  with nontangential boundary values of the resolvent  $(T - zI)^{-1}$ , the explicit structure of the Green's function  $G_{A,B}(z, \cdot, \cdot)$ ,  $z \in \mathbb{C} \setminus \sigma(T_{A,B})$ , the **Stieltjes inversion formula**, and essentially every other trick in the book on (matrix-valued) **Nevanlinna–Herglotz** functions. Here is a sketch of the proof:

Connecting  $M(\cdot)$  and the Spectral Projections  $E_{T_A}$   $(\cdot)$ 

# Connecting $M_{0,A,B}(\cdot, x_0)$ and $E_{T_{A,B}}(\cdot)$ (contd.)

The points of departure are **Stone's formula** and the explicit expression for the Green's function  $G_{A,B}(z, x, x')$ ,  $z \in \rho(T_{A,B})$ ,  $x, x' \in (a, b)$ , of  $T_{A,B}$  in terms of  $\phi_0(z, x, x_0)$  and  $\theta_0(z, x, x_0)$ ,

$$f, F(T_{A,B})E_{T_{A,B}}((\lambda_{1},\lambda_{2}])g)_{L^{2}((a,b);rdx)}$$

$$= \lim_{\delta \downarrow 0} \lim_{\varepsilon \downarrow 0} \frac{1}{2\pi i} \int_{\lambda_{1}+\delta}^{\lambda_{2}+\delta} d\lambda F(\lambda) [(f, (T_{A,B} - (\lambda + i\varepsilon)I)^{-1}g)_{L^{2}((a,b);rdx)} - (f, (T_{A,B} - (\lambda - i\varepsilon)I)^{-1}g)_{L^{2}((a,b);rdx)}]$$

$$= \lim_{\delta \downarrow 0} \lim_{\varepsilon \downarrow 0} \frac{1}{2\pi i} \int_{\lambda_{1}+\delta}^{\lambda_{2}+\delta} d\lambda F(\lambda) \int_{a}^{b} r(x)dx \int_{a}^{b} r(x')dx' \overline{f(x)}g(x')$$

$$\times \left\{ \left[ G_{A,B}(\lambda + i\varepsilon, x_{0}, x_{0})\theta_{0}(\lambda + i\varepsilon, x, x_{0})\theta_{0}(\lambda + i\varepsilon, x', x_{0}) + (\partial_{1}^{[1]}\partial_{2}^{[1]}G_{A,B})(\lambda + i\varepsilon, x_{0}, x_{0})\phi_{0}(\lambda + i\varepsilon, x, x_{0})\phi_{0}(\lambda + i\varepsilon, x', x_{0}) + (\partial_{1}^{[1]}G_{A,B})(\lambda + i\varepsilon, x_{0} \pm 0, x_{0} \mp 0)\theta_{0}(\lambda + i\varepsilon, x, x_{0})\theta_{0}(\lambda + i\varepsilon, x', x_{0}) \right\}$$

Connecting  $M(\cdot)$  and the Spectral Projections  $E_{T, \epsilon}$ 

# Connecting $M_{0,A,B}(\cdot, x_0)$ and $E_{T_{A,B}}(\cdot)$ (contd.)

 $- \quad \mbox{terms with } \lambda + i \varepsilon \mbox{ replaced by } \lambda - i \varepsilon \\$ 

+ terms entire in z taken at  $\lambda + i\varepsilon$  minus them taken at  $\lambda - i\varepsilon$ .

Freely interchanging the dx and dx' integrals with the limits and the  $d\lambda$  integral (since all integration domains are finite and all integrands are continuous) and introducing the notation

$$\begin{split} \Phi_{0}(z,x,x_{0}) &= \begin{pmatrix} \theta_{0}(z,x,x_{0}) \\ \phi_{0}(z,x,x_{0}) \end{pmatrix}, \quad x \in (a,b), \ z \in \mathbb{C}, \\ \widetilde{M}_{0,A,B}(z,x_{0}) &= \begin{pmatrix} G_{A,B}(z,x_{0},x_{0}) & (\partial_{2}^{[1]}G_{A,B})(z,x_{0}\pm 0,x_{0}\mp 0) \\ (\partial_{1}^{[1]}G_{A,B})(z,x_{0}\pm 0,x_{0}\mp 0) & (\partial_{1}^{[1]}\partial_{2}^{[1]}G_{A,B})(z,x_{0},x_{0}) \end{pmatrix} \\ &z \in \mathbb{C} \backslash \mathbb{R}, \ x_{0} \in (a,b), \end{split}$$

then yield

Connecting  $M(\cdot)$  and the Spectral Projections  $E_{T,\epsilon,p}$ 

## Connecting $M_{0,A,B}(\cdot, x_0)$ and $E_{T_{A,B}}(\cdot)$ (contd.)

$$\begin{split} (f, F(T_{A,B})E_{T_{A,B}}((\lambda_{1},\lambda_{2}])g)_{L^{2}((a,b);rdx)} \\ &= \int_{a}^{b} r(x)dx\,\overline{f(x)}\int_{a}^{b} r(x')dx'\,g(x')\lim_{\delta\downarrow 0}\lim_{\varepsilon\downarrow 0}\frac{1}{2\pi i}\int_{\lambda_{1}+\delta}^{\lambda_{2}+\delta}d\lambda\,F(\lambda) \\ &\times \Big[\Phi_{0}(\lambda+i\varepsilon,x,x_{0})^{T}\widetilde{M}_{0,A,B}(\lambda+i\varepsilon,x_{0})\Phi_{0}(\lambda+i\varepsilon,x',x_{0}) \\ &\quad -\Phi_{0}(\lambda-i\varepsilon,x,x_{0})^{T}\widetilde{M}_{0,A,B}(\lambda-i\varepsilon,x_{0})\Phi_{0}(\lambda-i\varepsilon,x',x_{0})\Big]. \end{split}$$

With  $\bullet$  abbreviating d/dz, one obtains

$$\Phi_0(\lambda \pm i\varepsilon, x, x_0) \underset{\varepsilon \downarrow 0}{=} \Phi_0(\lambda, x, x_0) \pm i\varepsilon \Phi_0(\lambda, x, x_0) + O(\varepsilon^2),$$

with  $O(\varepsilon^2)$  being uniform with respect to  $(\lambda, x)$  as long as  $\lambda$  and x vary in compact subsets of  $\mathbb{R} \times (a, b)$  (recall that f, g have compact support right now!). We also note that for some  $C(\lambda_1, \lambda_2, \varepsilon_0, x_0) \in (0, \infty)$ ,

$$\begin{split} \varepsilon |M_{0,A,B,\ell,\ell'}(\lambda + i\varepsilon, x_0)| &\leq C(\lambda_1, \lambda_2, \varepsilon_0, x_0), \quad \lambda \in [\lambda_1, \lambda_2], \ 0 < \varepsilon \leqslant \varepsilon_0, \ \ell, \ell' = 1, 2, \\ \varepsilon |\text{Re}(M_{0,A,B,\ell,\ell'}(\lambda + i\varepsilon, x_0))| \underset{\varepsilon \downarrow 0}{=} o(1), \quad \lambda \in \mathbb{R}, \ \ell, \ell' = 1, 2, \end{split}$$

Thus, one arrives at

Connecting  $M(\cdot)$  and the Spectral Projections  $E_{T_A, P}(\cdot)$ 

# Connecting $M_{0,A,B}(\cdot, x_0)$ and $E_{T_{A,B}}(\cdot)$ (contd.)

$$(f, F(T_{A,B})E_{T_{A,B}}((\lambda_{1},\lambda_{2}])g)_{L^{2}((a,b);rdx)} = \int_{a}^{b} r(x)dx \overline{f(x)} \int_{a}^{b} r(x')dx' g(x')$$

$$\times \lim_{\delta \downarrow 0} \lim_{\varepsilon \downarrow 0} \frac{1}{\pi} \int_{\lambda_{1}+\delta}^{\lambda_{2}+\delta} d\lambda F(\lambda)\Phi_{0}(\lambda,x,x_{0})^{T} \operatorname{Im}(M_{0,A,B}(\lambda+i\varepsilon,x_{0}))\Phi_{0}(\lambda,x',x_{0})$$

$$\times \lim_{\delta \downarrow 0} \frac{1}{\pi} \int_{\lambda_{1}+\delta}^{\lambda_{2}+\delta} F(\lambda)\Phi_{0}(\lambda,x,x_{0})^{T} d\Omega_{0,A,B}(\lambda,x_{0}) \Phi_{0}(\lambda,x',x_{0})$$

$$= \int_{(\lambda_{1},\lambda_{2}]} \overline{\widehat{f_{0}}(\lambda,x_{0})^{T}} d\Omega_{0,A,B}(\lambda,x_{0}) \widehat{g_{0}}(\lambda,x_{0})F(\lambda).$$

Here we interchanged the dx, dx' and  $d\Omega_{0,A,B}(\cdot, x_0)$  integrals once more, and employed the generalized Fourier coefficient

$$\widehat{h}_0(\lambda, x_0) = \int_a^b r(x) dx \, \Phi_0(\lambda, x, x_0) h(x), \quad \lambda \in \mathbb{R}, \ h \in C_0^\infty((a, b)).$$

Connecting  $M(\cdot)$  and the Spectral Projections  $E_{T_A}$ 

### Connecting $M_{0,A,B}(\cdot, x_0)$ and $E_{T_{A,B}}(\cdot)$ (contd.)

One removes the compact support restrictions on f and g in a standard manner: Introduce the unitary map

$$\begin{aligned} \boldsymbol{\mathcal{F}}_{0,A,B}(\mathbf{x}_{0}) &: \begin{cases} L^{2}((a,b); rdx) \rightarrow L^{2}(\mathbb{R}; d\Omega_{0,A,B}(\cdot, \mathbf{x}_{0})) \\ h \mapsto \widehat{h}_{0}(\cdot, \mathbf{x}_{0}) &= (\widehat{h}_{0,1}(\cdot, \mathbf{x}_{0}), \widehat{h}_{0,2}(\cdot, \mathbf{x}_{0}))^{\top}, \end{cases} \\ \widehat{h}_{0}(\cdot, \mathbf{x}_{0}) &= \begin{pmatrix} \widehat{h}_{0,1}(\cdot, \mathbf{x}_{0}) \\ \widehat{h}_{0,2}(\cdot, \mathbf{x}_{0}) \end{pmatrix} = \underset{c \downarrow a, d \uparrow b}{\operatorname{s-lim}} \begin{pmatrix} \int_{c}^{d} r(x) dx \, \theta_{0}(\cdot, \mathbf{x}, \mathbf{x}_{0}) h(x) \\ \int_{c}^{d} r(x) dx \, \phi_{0}(\cdot, \mathbf{x}, \mathbf{x}_{0}) h(x) \end{pmatrix}, \end{aligned}$$

where s-lim refers to the  $L^2(\mathbb{R}; d\Omega_{0,A,B}(\cdot, x_0))$ -limit. The associated inverse operator is then given by

$$\begin{aligned} \boldsymbol{\mathcal{F}}_{0,A,B}(\mathbf{x}_{0})^{-1} \colon \begin{cases} L^{2}(\mathbb{R}; d\Omega_{0,A,B}(\cdot, \mathbf{x}_{0})) \to L^{2}((a, b); rd\mathbf{x}) \\ \widehat{h} \mapsto h_{0}, \end{cases} \\ h_{0}(\cdot) &= \underset{\mu_{1}\downarrow-\infty,\mu_{2}\uparrow\infty}{\text{s-lim}} \int_{\mu_{1}}^{\mu_{2}} (\theta_{0}(\lambda, \cdot, \mathbf{x}_{0}), \phi_{0}(\lambda, \cdot, \mathbf{x}_{0})) \, d\Omega_{0,A,B}(\lambda, \mathbf{x}_{0}) \, \widehat{h}(\lambda), \end{aligned}$$

where s-lim now refers to the  $L^2((a, b); rdx)$ -limit.

Connecting  $M(\cdot)$  and the Spectral Projections  $E_{T, r, p}$ 

# Connecting $M_{0,A,B}(\cdot, x_0)$ and $E_{T_{A,B}}(\cdot)$ (contd.)

Thus, with  $d\Omega_{0,A,B}^{tr}(\cdot,x_0) = d\Omega_{0,A,B,1,1}(\cdot,x_0) + d\Omega_{0,A,B,2,2}(\cdot,x_0)$  representing the **trace measure** of  $d\Omega_{0,A,B}(\cdot,x_0)$ , and with  $M_F$  denoting the operator of multiplication by the function  $F \in C(\mathbb{R})$  in  $L^2(\mathbb{R}; d\Omega_{0,A,B}(\cdot,x_0))$ , one obtains the following result.

#### Theorem 15.

Assume Hypothesis 1 and  $T_{min}$  is bounded from below. In addition, let  $F \in C(\mathbb{R})$ , and  $x_0 \in (a, b)$ . Then, the "diagonalization,"

$$\mathcal{F}_{0,A,B}(x_0)F(\mathcal{T}_{A,B})\mathcal{F}_{0,A,B}(x_0)^{-1}=M_F,$$

holds in  $L^2(\mathbb{R}; d\Omega_{0,A,B}(\cdot, x_0))$ . Moreover,

 $\sigma(T_{A,B}) = \operatorname{supp} \left( d\Omega_{0,A,B}(\cdot, x_0) \right) = \operatorname{supp} \left( d\Omega_{0,A,B}^{tr}(\cdot, x_0) \right).$ 

**Note.** (*i*) While we focused on the case  $\alpha = 0$  for simplicity, the general case  $\alpha \in [0, \pi)$  is handled in the same manner.

(*ii*) Again, boundedness from below of  $T_{min}$  is convenient, but not essential. (Krein-type resolvent formulas exist independently of boundedness from below.)

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Thank you!