# Rank One Perturbations at Infinite Coupling\*

#### F. Gesztesy<sup>†</sup>

Department of Mathematics, University of Missouri, Columbia, Missouri 65211

#### AND

#### B. SIMON

Division of Physics, Mathematics, and Astronomy, California Institute of Technology, 253-37, Pasadena, California 91125

Communicated by L. Gross

Received February 7, 1994

We discuss rank one perturbations  $A_x = A + \alpha(\varphi, \cdot)\varphi$ ,  $\alpha \in \mathbb{R}$ ,  $A \ge 0$  self-adjoint. Let  $d\mu_x(x)$  be the spectral measure defined by  $(\varphi, (A_x - z)^{-1} \varphi) = \int d\mu_x(x)/(x - z)$ . We prove there is a measure  $d\rho_\infty$  which is the weak limit of  $(1 + \alpha^2) d\mu_x(x)$  as  $\alpha \to \infty$ . If  $\varphi$  is cyclic for A, then  $A_\infty$ , the strong resolvent limit of  $A_x$ , is unitarily equivalent to multiplication by x on  $L^2(\mathbb{R}, d\rho_\infty)$ . This generalizes results known for boundary condition dependence of Sturm-Liouville operators on half-lines to the abstract rank one case. © 1995 Academic Press, Inc.

# 1. Introduction

This paper is a contribution to the theory of rank one perturbations which in its natural format involves a self-adjoint operator  $A \ge 0$  in a complex separable Hilbert space  $\mathscr H$  and a vector,  $\varphi \in \mathscr H_{-1}(A)$ , with  $\mathscr H_s(A)$  the scale of spaces associated to A. Then  $q_{\varphi}(\psi,\eta) = (\psi,\varphi)(\varphi,\eta)$  defines a quadratic form on  $\mathscr H_{+1}(A)$  with  $q_{\varphi}$  a form-bounded perturbation of A with relative bound zero. Accordingly,  $A_x \equiv A + \alpha(\varphi,\cdot)\varphi$ ,  $\alpha \in \mathbb R$  defines a self-adjoint operator with  $\mathscr H_s(A_\alpha) = \mathscr H_s(A)$  for  $|s| \le 1$ .

We will suppose that  $\varphi$  is cyclic for A, in which case it is easy to see that  $\varphi$  is also cyclic for each  $A_{\alpha}$ . If  $d\mu_{\alpha}$  is the spectral measure for  $\varphi$  associated

<sup>\*</sup> This material is based on work supported by the National Science Foundation under Grant DMS-9101715. The government has certain rights in this material.

<sup>†</sup> E-mail: mathfg@mizzou1.missouri.edu.

to  $A_{\alpha}$ , then  $A_{\alpha}$  is unitarily equivalent to multiplication by x on  $L^{2}(\mathbb{R}, d\mu_{\alpha})$ . Define

$$F_{\alpha}(z) = \int_{\mathbb{R}} \frac{d\mu_{\alpha}(x)}{x - z},$$

where  $\varphi \in \mathcal{H}_{-1}(A_{\alpha})$  implies that

$$\int_{\mathbb{R}} \frac{d\mu_{\alpha}(x)}{|x|+1} < \infty$$

so that the integral defining F converges. One has the basic formula (with  $F(z) \equiv F_{\alpha=0}(z)$ )

$$F_{\alpha}(z) = \frac{F(z)}{1 + \alpha F(z)}. (1)$$

We are interested here in the case  $\alpha = \infty$ . By the monotone convergence theorem for forms [3, 6], we have that  $s - \lim_{\alpha \to \infty} (A_{\alpha} - z)^{-1}$  exists (the existence also follows from the explicit formula for  $(A_{\alpha} - z)^{-1}$ , Eq. (6) below) and can be described as follows. Let

$$\mathcal{H}_{+1}(A_{\infty}) = \left\{ \psi \in \mathcal{H}_{+1} \mid (\varphi, \psi) = 0 \right\}$$

and  $\mathscr{H}(A_{\infty}) = \overline{\mathscr{H}_{+1}(A_{\infty})}$ . This is all of  $\mathscr{H}$  if  $\varphi \notin \mathscr{H}$  and a codimension one subspace if  $\varphi \in \mathscr{H}$ . Let  $A_{\infty}$  be the self-adjoint operator on  $\mathscr{H}(A_{\infty})$  defined by the closed quadratic form  $\psi$ ,  $\eta \mapsto (\psi, A\eta)$  on  $\mathscr{H}_{+1}(A_{\infty})$ . If  $\mathscr{H}(A_{\infty}) \neq \mathscr{H}$ , extend  $(A_{\infty} - z)^{-1}$  to all of  $\mathscr{H}$  by setting it zero on  $\mathscr{H}(A_{\infty})^{\perp}$ . Then  $s - \lim(A_{\infty} - z)^{-1} = (A_{\infty} - z)^{-1}$ .

By (1),  $d\mu_{\alpha}(x) \to 0$  weakly as  $\alpha \to \infty$ , so we do not have any obvious spectral measure of  $A_{\infty}$ . Our main goal here is to prove that  $(1 + \alpha^2) d\mu_{\alpha}$  does have a weak limit as  $\alpha \to \infty$ , which is the spectral measure for a vector  $\eta \in \mathscr{H}_{-2}(A_{\infty})$ . Explicitly, define

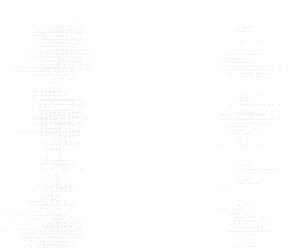
$$d\rho_{\alpha}(x) = (1 + \alpha^2) d\mu_{\alpha}(x). \tag{2}$$

Then we will prove that

Theorem 1. There exists a vector,  $\eta \in \mathcal{H}_{-2}(A_{\infty})$ , cyclic for  $A_{\infty}$  so that if  $d\rho_{\infty}(x)$  is the spectral measure for  $\eta$  with respect to  $A_{\infty}$ , then

$$\int_{\mathbb{R}} f(x) \, d\rho_{\alpha}(x) \to \int_{\mathbb{R}} f(x) \, d\rho_{\infty}(x) \tag{3}$$

for all continuous functions, f, of compact support.



Note that since  $\eta \in \mathcal{H}_{-2}(A_{\infty})$ ,

$$\int_{\mathbb{R}} \frac{d\rho_{\infty}(x)}{(|x|+1)^2} < \infty. \tag{4}$$

It may be that (4) fails if  $(|x|+1)^{-2}$  is replaced by  $(|x|+1)^{-1}$ . We will see explicit examples in Section 5 where the integral diverges for  $(|x|+1)^{-2+\epsilon}$ . The proof will show that (3) holds if  $f(x) = (|x|+1)^{-\alpha}$  with  $\alpha > 2$ . There will be examples when it fails if  $\alpha = 2$ .

Another major result we will prove is that

$$d\rho_{\infty}(x) = \lim_{\varepsilon \downarrow 0} \pi^{-1} [\operatorname{Im}((-F(x+i\varepsilon))^{-1}) dx].$$

The abstract theory appears in Section 2. We discuss boundary condition dependence of Schrödinger operators on the half-line in Section 3. In that case,  $d\rho_{\infty}$  is the Weyl spectral measure and  $d\rho_{\infty}$  is the Dirichlet spectral measure. In Section 4, we consider the case when A is bounded. In Section 5, we discuss a further example.

# 2. THE MAIN RESULTS

We begin by recalling some of the standard formulae for rank one perturbations [7]:

$$F_{x}(z) = F(z)/[1 + \alpha F(z)],$$

$$(A_{x} - z)^{-1} \varphi = (1 + \alpha F(z))^{-1} (A - z)^{-1} \varphi,$$

$$(A_{x} - z)^{-1} = (A - z)^{-1} - \frac{\alpha}{1 + \alpha F(z)}$$

$$\times ((A - \bar{z})^{-1} \varphi, \cdot)(A - z)^{-1} \varphi,$$

$$(6)$$

$$Tr[(A - z)^{-1} - (A_{x} - z)^{-1}] = \int_{E_{x}}^{\infty} (\lambda - z)^{-2} \xi_{x}(\lambda) d\lambda,$$

$$E_{x} = \min(0, \inf \operatorname{spec}(A_{x})),$$

where  $\xi_x$  is the Krein spectral shift [4] given by

$$\xi_{\alpha}(x) = \frac{1}{\pi} \operatorname{Arg}(1 + \alpha F(x + i0)). \tag{7}$$

For  $\alpha > 0$  we have  $Arg(\cdot) \in [0, \pi]$  and hence  $0 \le \xi_{\alpha} \le 1$  in this case.

If  $\|\varphi\| = \infty$ , let P = 0, and if  $\|\varphi\| < \infty$ , let P be the projection onto  $\{c\varphi \mid c \in \mathbb{C}\}$ . Thus,  $\mathscr{H}(A_{\infty}) = \operatorname{Ran}(1 - P)$ .

PROPOSITION 2. There exists  $\eta \in \mathcal{H}_{-2}(A_{\infty})$  so that for all  $z \in \mathbb{C}$ :

$$(A_{\infty} - z)^{-1} \eta = \lim_{z \to \infty} \alpha (1 - P)(A_z - z)^{-1} \varphi.$$
 (8)

If  $\varphi$  is cyclic for A, then  $\eta$  is cyclic for  $A_{\infty}$ .

*Proof.* By (5), the limit on the right side of (8) exists, call it  $\psi(z)$ , and is given by

$$\psi(z) = F(z)^{-1} (1 - P)(A - z)^{-1} \varphi. \tag{9}$$

We have that

$$(A_{\alpha}-z)^{-1}\varphi - (A_{\alpha}-w)^{-1}\varphi = (z-w)(A_{\alpha}-z)^{-1}(A_{\alpha}-w)^{-1}\varphi.$$
 (10)

Multiply by  $\alpha$ , take  $\alpha \to \infty$ , and note that if  $\|\varphi\| < \infty$ , then  $P(A_{\infty} - w)^{-1} \varphi = 0$ . We conclude that

$$\psi(z) - \psi(w) = (z - w)(A_{\infty} - z)^{-1} \psi(w)$$

or

$$\psi(z) = \left[1 + (z - w)(A_{\infty} - z)^{-1}\right] \psi(w). \tag{11}$$

Note that  $\psi(z) \in \mathcal{H}(A_{\infty})$  (because of the 1-P) so we can define  $\eta(z) \equiv (A_{\infty} - z) \psi(z)$  in  $\mathcal{H}_{-2}(A_{\infty})$ . Equation (11) precisely says that  $\eta(z) = \eta(w)$ , that is, it is independent of z; call it  $\eta$ . Cyclicity follows from (9) since if  $\{(A-z)^{-1} \varphi\}$  is total in  $\mathcal{H}$ , then clearly  $\{(1-P)(A-z)^{-1} \varphi\}$  is total  $(1-P)\mathcal{H} = \mathcal{H}(A_{\infty})$ .

*Remark.* In Section 4, we will prove that when A is bounded, then  $\eta = -(1 - P) A \varphi$ .

Theorem 3. Let  $d\rho_{\infty}$  be the spectral measure for  $\eta$ . Then

$$\int_{\mathbb{R}} \frac{d\rho_{\infty}(x)}{(x-z)^2} = F(z)^{-2} \frac{dF}{dz} - \frac{1}{\|\varphi\|^2}.$$
 (12)

*Proof.* For simplicity, suppose z is real and negative. By definition of  $\eta$ 

$$\int_{\mathbb{R}} \frac{d\rho_{\infty}(x)}{(x-z)^{2}} \equiv (\eta, (A_{\infty}-z)^{-2} \eta)$$

$$= (\varphi, (A-z)^{-1} (1-P)(A-z)^{-1} \varphi)/F(z)^{2}$$

$$= \left[ (\varphi, (A-z)^{-2} \varphi) - \frac{1}{\|\varphi\|^{2}} \langle \varphi, (A-z)^{-1} \varphi \rangle^{2} \right] / F(z)^{2}$$

since  $P = \|\varphi\|^{-2} (\varphi, \cdot) \varphi$ . But this is precisely the right side of (12). Equation (12) for general z follows by analyticity.

Recall that  $d\rho_{\alpha}$  is defined by (2). Then

THEOREM 4.

(i) 
$$\lim_{\alpha \to \infty} \int_{\mathbb{R}} \frac{d\rho_{\alpha}(x)}{(x-z)^2} = \frac{1}{\|\varphi\|^2} + \int_{\mathbb{R}} \frac{d\rho_{\infty}(x)}{(x-z)^2}.$$

(ii) 
$$\lim_{\alpha \to \infty} \int_{\mathbb{R}} \frac{d\rho_{\alpha}(x)}{(x-z)^3} = \int_{\mathbb{R}} \frac{d\rho_{\infty}(x)}{(x-z)^3}.$$

(iii) For any continuous f of compact support

$$\lim_{\alpha \to \infty} \int_{\mathbb{R}} f(x) \, d\rho_{\alpha}(x) = \int_{\mathbb{R}} f(x) \, d\rho_{\infty}(x).$$

*Proof.* (ii) implies (iii) by a Stone-Weierstrass-type argument. (i) implies (ii) by using the fact that both sides are analytic in z on  $\mathbb{C}\setminus\mathbb{R}$  so their derivatives in z converge. To prove (i), use Theorem 3 and the calculation

$$\int_{\mathbb{R}} \frac{d\rho_{\alpha}(x)}{(x-z)^{2}} = (1+\alpha^{2})(\varphi, (A_{\alpha}-z)^{-2}\varphi)$$

$$= \frac{(1+\alpha^{2})}{(1+\alpha F)^{2}}(\varphi, (A-z)^{-2}\varphi)$$

$$= \frac{1+\alpha^{2}}{(1+\alpha F)^{2}} \frac{dF}{dz}.$$
(13)

Equation (13) follows from (5).

THEOREM 5.

$$d\rho_{\infty}(x) = \pi^{-1} \lim_{\epsilon \downarrow 0} \operatorname{Im} \left[ -\frac{1}{F(x+i\epsilon)} \right] dx.$$

*Proof.* We start with (12) and integrate, noting that  $F'/F^2 = (d/dz)(-1/F)$ , to get

$$\int_{\mathbb{R}} d\rho_{\infty}(x) \left( \frac{1}{x-z} - \frac{1}{x+1} \right) = -\frac{1}{F(z)} + \frac{1}{F(-1)} - (z+1) \frac{1}{\|\varphi\|^2}.$$

The theorem then follows by the standard relations between a measure and the boundary values of its Borel transform.

### 3. Variation of Boundary Condition

As an example of the general theory, we consider the case of boundary conditions variation for Schrödinger operators on  $L^2(0, \infty)$ . The formulae that result are well-known (see, e.g., [1, 2, 5, 8]). The point is that they fit into a more general framework. Let V be continuous and bounded below on  $[0, \infty)$ . Let  $H_{\theta}$  be the operator on  $L^2([0, \infty), dx)$  formally given by  $-d^2/dx^2 + V(x)$  with  $u(0)\cos\theta + u'(\theta)\sin\theta = 0$  boundary conditions. One defines the Weyl m-function,  $m_{\theta}(z)$ , and Weyl spectral measure,  $d\rho_{\theta}(x)$ , so that for  $\theta \neq 0$ 

$$m_{\theta}(z) = \cot(\theta) + \int_{\mathbb{R}} \frac{d\rho_{\theta}(x)}{x - z}$$
 (14)

and  $d\rho_{\theta} \rightarrow d\rho_{\theta=0}$  as  $\theta \downarrow 0$ . Moreover,

$$m_{\theta=0}(z) = -1/m_{\theta=\pi/2}(z).$$
 (15)

For  $\theta \neq 0$ , the Green's function,  $G_{\theta}(0,0;z)$  is related to  $m_{\theta}(z)$  by

$$G_{\theta}(0,0;z) = \sin^2(\theta) \left[ -\cot \theta + m_{\theta}(z) \right]. \tag{16}$$

This fits into the general framework by taking  $A = H_{\theta = \pi/2}$  and  $\varphi = \delta_0$ , the delta function at 0. Then for  $\theta \neq 0$ ,

$$H_{\theta} = A - \cot(\theta)(\varphi, \cdot)\varphi$$

and  $F_{-\cot(\theta)}(z) = G_{\theta}(0, 0; z)$ . By (14) and (16),  $d\rho_{\theta}$  is just  $(1 + \alpha^2) d\mu_{\alpha}$  where  $\alpha = -\cot \theta$  and  $\lim_{\theta \to 0} d\rho_{\theta} = d\rho_{0}$  is just what we found in the last section. Equation (15) is just Theorem 5.

We want to identify the vector  $\eta$ . Let  $\psi_+(x, z)$  be the solution of  $(-d^2/dx^2 + V(x) - z)\psi = 0$  which is  $L^2$  at infinity normalized any way that is convenient. Then, from the Wronskian formula for  $G_{\theta = \pi/2}$ , we get

$$((A-z)^{-1}\varphi)(x) = \frac{\psi_{+}(x,z)}{\psi'_{+}(0,z)}$$

and

$$F(z) = -\psi_{+}(0, z)/\psi'_{+}(0, z).$$

It follows that

$$F(z)^{-1} (A-z)^{-1} \varphi = \psi_{\perp}(x,z)/\psi_{\perp}(0,z)$$

which, by the Wronskian formula for  $G_{\theta=0}$ , is just

$$(A_{\infty}-z)^{-1}\delta'(x);$$

that is,  $\eta$  is  $\delta'$  (note that P=0 in this case) and  $d\rho_{\infty}$  is the spectral function for the vector  $\delta'$ .

We note that it is well-known that  $\int_0^\mu d\rho_\infty(x) \sim C\mu^{3/2}$  as  $\mu \to \infty$  so that  $\int_0^\infty (d\rho_\infty(\lambda)/(1+|\lambda|)^k) < \infty$  if and only if k > 3/2. In particular,  $\eta \notin \mathcal{H}_{-1}(A_\infty)$ .

## 4. BOUNDED OPERATORS

One gets insight into the general theory by considering the case where A is bounded. Since  $\|\varphi\|$  is then finite, we will suppose  $\|\varphi\| = 1$ . We will also get a better understanding of the  $1/\|\varphi\|^2$  term in Theorem 4(i). We first note:

THEOREM 6. If A is bounded and  $\|\varphi\| = 1$ , then  $\eta = -(1 - P) A\varphi$ .

*Proof.* If A is bounded, then  $A_{\infty}$  is just (1-P) A(1-P). Thus

$$\eta = F(z)^{-1} (1 - P)(A - z)(1 - P)(A - z)^{-1} \varphi$$

$$= F(z)^{-1} (1 - P)(A - z)(A - z)^{-1} \varphi$$

$$- F(z)^{-1} [(1 - P)(A - z)\varphi] F(z).$$

The first term is zero since  $(1-P)\varphi = 0$ . The second is  $-(1-P)A\varphi$  since  $(1-P)z\varphi = 0$ .

Since  $\|\varphi\| = 1$ ,  $(\varphi, \cdot)\varphi$  is just a projection P. Instead of  $A + \alpha P$ , look at

$$P + \alpha^{-1}A = B_{\alpha}.$$

*P* has an isolated simple eigenvalue at 1 with eigenvector  $\varphi$ . Thus by regular perturbation theory [3],  $B_{\alpha}$  has the eigenvalue at  $1 + (\varphi, A\varphi) \alpha^{-1} + O(\alpha^{-2})$  with eigenvector

$$\psi_{\alpha} = \varphi + \alpha^{-1}(1-P)A\varphi + O(\alpha^{-2}) = \varphi + \alpha^{-1}\eta + O(\alpha^{-2}).$$

The first order term is standard perturbation theory where the reduced resolvent  $(H_0 - E)^{-1} (1 - P)$  is just -(1 - P) since  $H_0$  is P and hence 0 on Ran(1 - P).

Thus with respect to  $A + \alpha P = \alpha B_{\alpha}$ , the measure  $(1 + \alpha^2) d\mu_{\alpha}$  has a pole of weight  $(1 + \alpha^2)$  at  $E_{\alpha} = \alpha + (\varphi, A\varphi) + O(\alpha^{-1})$  plus the spectral measure of  $\eta$  for the operator  $A_{\infty}$  plus an error of order  $\alpha^{-1}$ . If  $\nu > 2$ , the pole at

 $E_{\alpha}$  makes no asymptotic contribution to  $\int_{\mathbb{R}} (d\rho_{\alpha}(x)/|x-z|^{\gamma})$  as  $\alpha \to \infty$  but for  $\nu = 2$ , it makes a contribution of  $(1 + \alpha^2)/E_{\alpha}^2 \to 1 = 1/\|\varphi\|^2$ .

## 5. A FURTHER EXAMPLE

Let  $0 < \gamma < 1$ . Let  $d\mu_0(x) = \pi^{-1} |x|^{-\gamma} \sin(\pi \gamma) dx$  on  $[0, \infty)$ . Let A be multiplication by x on  $L^2([0, \infty), d\mu_0(x))$  and  $\varphi \equiv 1$ . Then  $\int_0^\infty (d\mu_0(x)/(|x|+1)) < \infty$  so  $\varphi \in \mathscr{H}_{-1}(A_\infty)$ .

$$F(z) = \int_0^\infty \frac{d\mu_0(x)}{x - z} = (-z)^{-\gamma}$$

(the easiest way to see this is to compute the imaginary part of  $(-z)^{-\gamma}$  for  $z = x + i\varepsilon$  with  $\varepsilon \to 0$ ). Then, by Theorem 5,

$$d\rho_{\infty}(x) = \pi^{-1} |x|^{\gamma} \sin(\pi \gamma) dx.$$

It follows that  $\int_0^\infty d\rho_\infty(x)/(|x|+1)^k < \infty$  only if  $k > 1 + \gamma$ . Thus, we cannot conclude in general that  $\int_0^\infty d\rho_\infty(x)/(|x|+1)^k < \infty$  for any k < 2.

#### ACKNOWLEDGMENT

F. G. is indebted to the Department of Mathematics at Caltech for its hospitality and support during the summer of 1993 where some of this work was done.

#### REFERENCES

- E. A. CODDINGTON AND N. LEVINSON, "Theory of Ordinary Differential Equations," Krieger, Malabar, 1985.
- 2. E. HILLE, "Lectures on Ordinary Differential Equations," Addison-Wesley, New York, 1969.
- 3. T. KATO, "Perturbation Theory for Linear Operators," 2nd ed., Springer, Berlin, 1980.
- M. G. Krein, Perturbation determinants and a formula for the traces of unitary and self-adjoint operators, Soviet. Math. Dokl. 3 (1962), 707-710.
- B. M. LEVITAN AND I. S. SARGSJAN, "Introduction to Spectral Theory," Amer. Math. Soc. Transl., Vol. 39, Amer. Math. Soc., Providence, RI, 1975.
- B. Simon, A canonical decomposition for quadratic forms with applications to monotone convergence theorems, J. Funct. Anal. 28 (1978), 377-385.
- 7. B. Simon, Spectral analysis of rank one perturbations and applications, lecture given at the 1993 Vancouver Summer School, in "Proceedings on Mathematical Quantum Theory II: Schrödinger Operators (CRM Proceedings and Lecture Notes)" (J. Feldman, R. Froese, and L. M. Rosen, Eds.), to appear.
- 8. E. C. TITCHMARSH, "Eigenfunction Expansions," 2nd ed., Oxford Univ. Press, Oxford, 1962.

Printed in Belgium Uitgever: Academic Press, Inc. Verantwoordelijke uitgever voor België: Hubert Van Maele Altenastraat 20, B-8310 Sint-Kruis