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Inverse Spectral Analysis with Partial Information on the Potential, I. The Case of an A.C. Component in the Spectrum

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Dedicated to Klaus Hepp and Walter Hunziker on the occasion of their sixtieth birthdays

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Abstract We consider operators $-\frac{d^2}{dx^2} + V$ in $L^2(\mathbb{R})$ with the sole hypothesis that V is limit point at $\pm\infty$ and that $-\frac{d^2}{dx^2} + V$ in $L^2((0,\infty))$ has some absolutely continuous component S_+ in its spectrum. We prove that V on $(-\infty, 0)$ is completely determined by knowledge of V on $(0,\infty)$ and by the reflection coefficient $R_+(\lambda)$ for scattering from right incidence and energies $\lambda \in S$, where $S \subseteq S_+$ has positive Lebesgue measure.

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It is well known [15] that knowledge of the reflection coefficient at positive energies does not determine the potential V of a Schrödinger operator $-\frac{d^2}{dx^2}+V$ ($V(x)\to 0$ sufficiently rapidly as $|x|\to\infty$), but that one also needs bound state energies and associated norming constants. This is most dramatically seen in one-soliton potentials where $R_+(\lambda)\equiv 0$, $\lambda\geq 0$, even though there is a two-parameter family of such potentials parametrized by the center and width of the soliton.

There has been a recent rash of papers [2, 3, 4, 6, 12, 18, 19] showing that if V is known a.e. on a half-line and vanishes sufficiently fast as $|x|\to\infty$ in the sense that at least its first moment on $\mathbb{R}$ exists, then the norming constants and even the bound state energies are not needed (some of these papers are limited to the case where V is assumed to vanish on the right half-line). Our goal here is to note that this is a special case of a very general and very elementary phenomenon: It is not required that V has simple asymptotics as $|x|\to\infty$. Rather, all that is significant is that V be known a.e. on $(0,\infty)$ and the Schrödinger operator H_+ associated with $-\frac{d^2}{dx^2}+V$ in $L^2((0,\infty))$ and any self-adjoint boundary condition at 0, has some absolutely continuous (a.c.) component in its spectrum. Also, rather than require detailed manipulation of the machinery of inverse problems and/or trace formulas, all that is required is a uniqueness result to go from a Weyl m-function to a potential. In particular, our m-function technique allows one to consider impurity (defect) scattering in (half) crystals, scattering off potentials with different spatial asymptotics at left and right including asymptotically periodic potentials, potential steps, and potentials diverging to $+\infty$ as $x\to-\infty$.

More subtle and deep is a comparison problem concerning knowledge of the potential on a half-line where the spectrum is purely discrete rather than having an absolutely continuous component. Here the paradigmal result is the remarkable theorem of Hochstadt and Lieberman [13] that a knowledge of all the eigenvalues of $-\frac{d^2}{dx^2}+V$ in $L^2((0,1);dx)$ with (for example) Neumann boundary conditions $u'(0)=u'(1)=0$ and knowledge of the potential on $(0,\frac{1}{2})$, uniquely determine V a.e. on all of $(0,1)$. We will study these problems in two forthcoming papers [8, 9]. Typical of our results is that a knowledge of V on $(0,\frac{3}{4})$ and of strictly more than half the eigenvalues uniquely determines V a.e. on all of $(0,1)$.

Suppose that $V\in L^1_{\text{loc}}(\mathbb{R})$ is real-valued such that the differential expression $-\frac{d^2}{dx^2}+V(x)$ is in the limit point case at $\pm\infty$. Then for any z with $\text{Im}\,(z)>0$, there is a unique (up to constant multiples) solution of

$$-u''+Vu=zu \tag{1}$$

which is L^2 at $+\infty$. Call it $\tilde\psi_+(z,x)$. Similarly, there is a solution $\tilde\psi_-(z,x)$ which is L^2 at $-\infty$. The Weyl m-functions $m_\pm$ are defined by

$$m_\pm(z)=\pm\frac{\tilde\psi'_\pm(z,0)}{\tilde\psi_\pm(z,0)}.$$

It is a fundamental result of Marchenko [17] that $m_\pm(z)$ uniquely determines V a.e. on $(0,\pm\infty)$. General principles (see, e.g., [14], Sect. III.1; [16], Sect. 2.4; [20]) imply that for a.e. $\lambda\in\mathbb{R}$, $\lim_{\epsilon\downarrow 0}m_\pm(\lambda+i\epsilon):=m_\pm(\lambda+i0)$ exists and is finite. For such $\lambda\in\mathbb{R}$, we'll define

$\psi_\pm(\lambda,x)$ by requiring that $\psi_\pm$ satisfies (1) (with $z=\lambda$) and the boundary conditions

$$\psi_\pm(\lambda,0)=1, \qquad \psi'_\pm(\lambda,0)=\pm m_\pm(\lambda+i0). \tag{2}$$

Example. $V=0$. Then $m_\pm(z)=i\sqrt{z}$, choosing the square root branch with $\mathrm{Im}\,(\sqrt{z})>0$ for $z\in\mathbb{C}\backslash[0,\infty)$ and $\psi_\pm(\lambda,x)=e^{\pm i\sqrt{\lambda}x}$ (where $\sqrt{\lambda}>0$) if $\lambda\geq 0$ and $\psi_\pm(\lambda,x)=e^{\mp\sqrt{-\lambda}x}$ if $\lambda\leq 0$.

It is also known [16, 20] that if H_+ is associated with $-\frac{d^2}{dx^2}+V$ in $L^2((0,\infty))$ and Dirichlet boundary conditions $u(0)=0$ (or equivalently, any other self-adjoint boundary condition at 0 of the type $u'(0)+\beta u(0)=0$, $\beta\in\mathbb{R}$), then the essential support of the a.c. spectrum of H_+ is precisely $S_+ := \{\lambda\in\mathbb{R}\mid \mathrm{Im}\,[m_+(\lambda+i0)]>0\}$. For $\lambda\in S_+$, $\psi_+(\lambda,x)$ is not a multiple of a real solution, so $\overline{\psi_+(\lambda,x)}$ is always a linearly independent solution of (1). As a result we can expand,

$$\psi_-(\lambda,x)=A(\lambda)\,\overline{\psi_+(\lambda,x)}\;+B(\lambda)\psi_+(\lambda,x),\ \lambda\in S_+. \tag{3}$$

Definition. For $\lambda\in S_+$, $R_+(\lambda):=B(\lambda)/A(\lambda)$ denotes the (relative) reflection coefficient (from right incidence).

Remarks. 1. Suppose that $V=0$ on $(0,\infty)$ so $\psi_+(\lambda,x)=e^{i\lambda^{1/2}x}$ and that for some $\epsilon>0$, $V=0(|x|^{-1-\epsilon})$ at $-\infty$ so $\psi_-(\lambda,x)\sim Ce^{-i\lambda^{1/2}x}$ near $-\infty$. Then the usual reflection coefficient is B/A and the usual transmission coefficient C/A. Thus, this very general definition agrees with the usual one if $V=0$ on $(0,\infty)$.

2. If $V=0(|x|^{-1-\epsilon})$ at $\pm\infty$, then $\psi_+(\lambda,x)\sim D(\lambda)e^{i\lambda^{1/2}x}$ at $+\infty$ (note we chose a particular normalization of $\psi_+(\lambda,x)$ in (2)). In this case, the usual reflection coefficient is *not* B/A but is $(B/A)(D/\overline{D})=\tilde{R}_+$. However, if V is explicitly known on $[0,\infty)$, so is D, and thus knowing R_+ is the same as knowing $\tilde{R}_+$.

3. (2) and (3) let us solve for A, B and R in terms of $m_\pm$, viz.,

$$\begin{aligned} A(\lambda)&=\frac{m_+(\lambda+i0)+m_-(\lambda+i0)}{2i\,\mathrm{Im}(m_+(\lambda+i0))},\\ B(\lambda)&=-\frac{\overline{m}_+(\lambda+i0)+m_-(\lambda+i0)}{2i\,\mathrm{Im}(m_+(\lambda+i0))},\\ R_+(\lambda)&=-\frac{\overline{m}_+(\lambda+i0)+m_-(\lambda+i0)}{m_+(\lambda+i0)+m_-(\lambda+i0)},\quad \lambda\in S_+, \end{aligned} \tag{4}$$

(see also the corresponding discussions in [11]). In particular, since $\mathrm{Im}\,(m_+)$, $\mathrm{Im}\,(m_-)\geq 0$, we have $|R_+(\lambda)|\leq 1$. Also, since $\mathrm{Im}\,[m_+(\lambda+i0)]>0$ for a.e. $\lambda\in S_+$, the essential support of $\sigma_{\mathrm{ac}}(H_+)$,

$$R_+(\lambda)\neq -1 \quad \text{for a.e. } \lambda\in S_+. \tag{5}$$

Theorem. *Assume that $V \in L^1_{\text{loc}}(\mathbb{R})$ is real-valued and $-\frac{d^2}{dx^2} + V(x)$ is in the limit point case at $\pm\infty$. Suppose that V is known a.e. on $(0, \infty)$ and that $R_+(\lambda)$ is known a.e. on a set $S \subseteq S_+$ of positive Lebesgue measure inside the essential support S_+ of $\sigma_{\text{ac}}(H_+)$. Then V is uniquely determined a.e. on $(-\infty, 0)$ and hence a.e. on $\mathbb{R}$.*

Proof. By (4),

$$m_-(\lambda + i0) = -\frac{m_+(\lambda + i0)R_+(\lambda) + \overline{m_+(\lambda + i0)}}{(1 + R_+(\lambda))} \quad \text{for a.e. } \lambda \in S. \tag{6}$$

By (5), m_- is well defined for a.e. $\lambda \in S$. Thus knowing $R_+(\lambda)$ a.e. on S and knowing m_+ a.e. on S (since we know V a.e. on $(0, \infty)$), we know $m_-(\lambda + i0)$ a.e. on S. But m_- is the boundary value of a Herglotz function and such functions are determined uniquely by their boundary values on any set of positive Lebesgue measure, and so on S. By Marchenko's uniqueness theorem [17], m_- uniquely determines V a.e. on $(-\infty, 0)$. □

Remarks. 1. The principal strategy behind our theorem and the results in [8, 9] is extremely simple and may be summarized as follows: Consider a Schrödinger operator $-\frac{d^2}{dx^2} + V$ on an interval $(a, b) \subseteq \mathbb{R}$ with fixed separated boundary conditions (if any) at a and b. Suppose $x_0 \in (a, b)$ and denote by m_{+,x_0} and m_{-,x_0} the Weyl m-functions associated with the intervals (x_0, b) and (a, x_0), respectively. By Marchenko's uniqueness theorem [17], m_{+,x_0} and m_{-,x_0} uniquely determine V a.e. on (x_0, b) and (a, x_0). Hence, if V (and thus m_{+,x_0}) is known on (x_0, b), one only needs to specify m_{-,x_0} in order to determine V uniquely a.e. on (a, b). The issue thus becomes determination of m_{-,x_0} from knowledge of m_{+,x_0} and additional spectral (e.g., scattering) data associated with $-\frac{d^2}{dx^2} + V$ on (a, b). For instance, if $(a, b) = \mathbb{R}$, $x_0 = 0$, and $-\frac{d^2}{dx^2} + V$ restricted to $(0, \infty)$ has an a.c. component in its spectrum as considered in this paper, the reflection coefficient R_+ from right incidence together with m_+ determine m_- and hence V on $\mathbb{R}$. If, on the other hand, $-\frac{d^2}{dx^2} + V$ on (a, b) has purely discrete spectrum as considered in [8], then a certain portion of the eigenvalues of $-\frac{d^2}{dx^2} + V$ on (a, b), the portion depending on x_0, together with m_{+,x_0} will again determine m_{-,x_0} and hence V on all of (a, b) as long as the size of the interval (x_0, b) is "sufficiently large" compared to the size of (a, x_0). The fact that $m_{\pm,x_0}$ are Herglotz functions (and in the discrete spectrum case also meromorphic) then considerably aids in determining m_{-,x_0}. This comment also underscores that our approach is by no means restricted to Schrödinger operators on $\mathbb{R}$. It applies as well to one-dimensional Dirac-type operators, second-order finite difference (Jacobi) operators [9], and $n \times n$ matrix-valued Schrödinger operators [1] (in this case $m_{\pm,x_0}$, R_+, etc., are $n \times n$ matrices) on arbitrary intervals (a, b). In particular, it applies to three-dimensional Schrödinger operators with spherically symmetric potentials $v(x) = V(|x|)$, $x \in \mathbb{R}^3$ upon decomposition with respect to angular momenta and restriction to the angular momentum channel $\ell = 0$.

2. In some cases, one only needs to know $m_-(\lambda + i0)$ on a smaller set than one of positive measure. For example, if it is known a priori that for some $\alpha > 0$, $|V(x)| \leq e^{-\alpha|x|}$ near $x = -\infty$, then m_- is known to be analytic in a neighborhood of $\mathbb{R}$, and so it suffices that

$R_+(\lambda)$ (and so $m_-(\lambda + i0)$) is known on a set of points with a finite limit point. Or if the restriction of V to $(-\infty, 0]$ is known to have compact support, then m_- is a ratio of entire functions of order $\frac{1}{2}$ and known type (depending on the size of the support in $(-\infty, 0]$), so m_- is uniquely determined by a sequence of values $\lambda_j \to \infty$ of sufficient density.

3. All the results of [2, 3, 4, 6, 12, 18, 19] are consequences of our theorem save that in [18], which follows from the extension indicated at the end of Remark 1. (For those results where one only supposes $V(x)$ vanishes in (b, ∞) rather than $(0, \infty)$, we use the fact that b can be determined from R_+ [2], and then the problem can be translated to one with V vanishing on $(0, \infty)$.)

4. An example of a totally new result is a situation where $V(x) \to \infty$ as $x \to -\infty$ in which case $|R_+(\lambda)| = 1$. By a result of Borg [5], it suffices, for example, to consider $V(x) = 0$, $x > 0$, $V(x) \geq 0$ for $x < 0$, $V(x) \to \infty$ at $-\infty$ and to then know those energies λ_j with $R_+(\lambda_j) = -1$ and those λ_k with $R_+(\lambda_k) = +1$.

5. Other situations of interest in physics, covered by our theorem but not addressed by previous results in this context, concern impurity (defect) scattering in (half) crystals and charge transport in mesoscopic quantum-interference devices associated with (possibly different) asymptotically periodic potentials as $x \to \pm\infty$. The interested reader might consult [7, 10, 11] and the literature cited therein.

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Dedication. It is an enormous pleasure to dedicate this paper in honor of the sixtieth birthdays of Klaus Hepp and Walter Hunziker. During his mathematical physics phase, Klaus made important contributions to quantum field theory. Walter has been a major figure in multiparticle quantum theory for more than thirty years, and we have learned much from him.

References

1. Z.S. Agranovich and V.A. Marchenko, *The Inverse Problem of Scattering Theory*, Gordon and Breach, New York, 1963.

2. T. Aktosun, *Bound states and inverse scattering for the Schrödinger equation in one dimension,* J. Math. Phys. **35** (1994), 6231–6236.

3. T. Aktosun, *Inverse Schrödinger scattering on the line with partial knowledge of the potential,* SIAM J. Appl. Math. **56** (1996), 219–231.

4. T. Aktosun, M. Klaus, and C. van der Mee, *On the Riemann-Hilbert problem for the one-dimensional Schrödinger equation,* J. Math. Phys. **34** (1993), 2651–2690.

5. G. Borg, *Uniqueness theorems in the spectral theory of* $y'' + (\lambda - q(x))y = 0$, Proc. 11th Scandinavian Congress of Mathematicians, Johan Grundt Tanums Forlag, Oslo, 1952, 276–287.

6. M. Braun, S. Sofianos, and R. Lipperheide, *One-dimensional Marchenko inversion in the presence of bound states,* Inverse Problems **11** (1995), L1–L3.

7. E.B. Davies and B. Simon, *Scattering theory for systems with different spatial asymptotics on the left and right,* Commun. Math. Phys. **63** (1978), 277–301.

8. F. Gesztesy and B. Simon, *Inverse spectral analysis with partial information on the potential, II. The case of discrete spectrum*, in preparation.

9. F. Gesztesy and B. Simon, *m-functions and inverse spectral analysis for finite and semi-infinite Jacobi matrices*, in preparation.

10. F. Gesztesy, H. Holden, and B. Simon, *Absolute summability of the trace relation for certain Schrödinger operators,* Commun. Math. Phys. **168** (1995), 137–161.

11. F. Gesztesy, R. Nowell, and W. Pötz, *One-dimensional scattering theory for quantum systems with nontrivial spatial asymptotics*, Adv. Diff. Eqs., to appear.

12. B. Grebert and R. Weder, *Reconstruction of a potential on the line that is a priori known on the half-line,* SIAM J. Appl. Math. **55** (1995), 242–254.

13. H. Hochstadt and B. Lieberman, *An inverse Sturm-Liouville problem with mixed given data,* SIAM J. Appl. Math. **34** (1978), 676–680.

14. Y. Katznelson, *An Introduction to Harmonic Analysis*, 2nd corr. ed., Dover, New York, 1976.

15. I. Kay and H.E. Moses, *Reflectionless transmission through dielectrics and scattering potentials,* J. Appl. Phys. **27** (1956), 1503–1508.

16. B.M. Levitan and I.S. Sargsjan, *Sturm-Liouville and Dirac Operators*, Kluwer, Dordrecht, 1991.

17. V.A. Marchenko, *Some questions in the theory of one-dimensional linear differential operators of the second order, I*, Trudy Moskov. Mat. Obšč. **1** (1952), 327–420 (Russian); English transl. in Amer. Math. Soc. Transl. (2) **101** (1973), 1–104.

18. W. Rundell and P. Sacks, *On the determination of potentials without bound state data,* J. Comp. Appl. Math. **55** (1994), 325–347.

19. P. Sacks, *Reconstruction of steplike potentials,* Wave Motion **18** (1993), 21–30.

20. B. Simon, *Spectral analysis of rank one perturbations and applications* in CRM Proc. Lecture Notes Vol. 8 (J. Feldman, R. Froese, and L. Rosen, eds.), pp. 109–149, Amer. Math. Soc., Providence, RI, 1995.