Revista Brasileira de Física, Vol. 11, Nº 4, 1981

An Approximation Scheme for One-Dimensional Inverse Scattering

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Recebido em 13 de Outubro de 1981

An algorithm is proposed for reconstructing the potential $q(x)$ in the one-dimensional stationary Schrödinger operator $E\equiv -d^2/dx^2 + q(x)$, $-\infty<x<\infty$, with the reflection coefficient and the other scattering data as input. Preliminary experiments have indicated computing time savings of order as high as 10:1, as compared to the direct solution of Marchenko equations. Some open problems within this context are posed.

Propomos um algoritmo para, a partir do coeficiente de reflexão e dos outros dados de espalhamento, reconstruir o potential $q(x)$ associado ao operador de Schrödinger estacionário em uma dimensão $E \equiv -d^2/dx^2 + q(x)$, $-\infty<x<\infty$. Em testes realizados, obtivemos uma economia computacional da ordem de 10:1 relativamente à solução direta das equações de Marchenko. Mencionamos também alguns problemas em aberto nesta área.

1. INTRODUCTION

The one-dimensional scattering problem has been a source of deep investigation lately. This renewed interest partly results from the discovery[1] of the connection between that problem and the Korteweg-de Vries (KdV) model for long waves. The latter is a non-linear equation with a wealth of properties, some of which quite unexpected,[2,3,4] like its relationship with inverse scattering (IS) itself: it lets one trade a non-linear operator (viz, the solution of an initial value problem assigned to a non-linear partial differential equation) for a sequence of linear transformations (the solution of the IS problem via Marchenko equations). A more precise description of such a link follows:

Let $u(x,t)$ satisfy the KdV equation

$$u_t - uu_x + u_{xxx} = 0 \quad , \quad -\infty < x < \infty, \ t \geq 0 \tag{1}$$

and consider $u/6$ as potentials for the Schrödinger equations:

$$-\frac{d^2}{dx^2} y + \frac{u(x,t)}{6} y = k^2 y \ , \qquad t \geq 0 \quad . \tag{2}$$

Then the time evolution of the scattering data[5] associated to (2) is extremely simple, Cf. Ref. 6:

i) The reflection coefficients[5] satisfy

$$r^-(k,t) = r^-(k,0)\exp(-i8k^3t) \tag{3}$$

while

ii) The transmission coefficients are time invariant and so are the point spectrum and the normalization constants[5] $\{\lambda_j(t), m_j(t)\}_{1 \leq j \leq N(t)}$:

$$\lambda_j(t) = \lambda_j(0) \ , \quad m_j(t) = m_j(0) \ , \ j = 1,\ldots,N(t) = N(0) \ .$$

Consequently, to solve (1) subject to

$$u(x,0) = \phi(x) \ , \quad -\infty < x < \infty \tag{4}$$

the following path is pointed out by the above result:

a) first get the scattering data in correspondence with $u(x,0)$;

b) follow their time evolution according to (i) and (ii);

c) for any instant $t>0$ at which $u(x,t)$ is sought, solve the inverse scattering problem associated to the data found through (b).

We emphasize that steps (a) and (b) are straightforward and even step (c) may be considered as an easy one when compared to the subtleties involved in the direct solution of (1) and (4). Indeed, a quite natural way to deal with (c) is to call the Marchenko equations for help, and in this way a family of *linear* integral equations is brought in. Observe that their kernels are variable and so are their interval of integration (which, by the way, are irifinite). Each problem is neverthless a linear one.

This discovery led to a whole stream of search for "inverse transforms", see Ref. 7,8.

Efforts spent in seeking an efficient algorithm to solve the Marchenko equations would be fully justified even if the relationship KdV-IS were the only use of those equations. Nonetheless, a long list of other contexts where IS - and thus Marchenko equations - shows up is well known[9].

In the next section we present a numerical algorithm developed with this aim, while in Section 3 we point out some topics considered to be worth studying.

2. THE ALGORITHM DESCRIPTION

In order to numerically solve the one-dimensional IS problem we have to:

a) Solve either one of the Fredholm integral equations (due to Marchenko)

$$\Omega_{\pm}(x+y) + B_{\mp}(x,y) \pm \int_0^{\pm\infty} \Omega_{\pm}(x+t+y) B_{\pm}(x,t)\,dt = 0 \ , \quad \pm y \geqslant 0 \qquad (5)_{\pm}$$

for $B_{\pm}(x,y)$ as functions of y, x being kept as a parameter;

b) differentiate $B_{\pm}(x,0)$ to obtain $q(x)$ from

$$q(x) = \mp \partial_1 B(x,0) \qquad (6)_{\pm}$$

Solving (approximately) either of equations $(5)_{\pm}$ by Nyström quadrature technique amounts to solving a finite linear algebraic system whose order depends on both the accuracy we need and the behaviorof the functions $\Omega_{\pm}$. Also we need to solve these equations for a large number of values of x, as numerical differentiation is known to be a rather unstable procedure.

In this section we shall describe a simpler algorithm forthis problem, using an idea originally suggested by V. Bargmann and carried out by I. Kay[10].

From now on we shall deal with Marchenko equations $(5)_{+}$ replacing B_{+} by the function K introduced as

$$K(x,y) \equiv B_{+}(x, \frac{y-x}{2}) / 2 ,$$

and taking instead of R+ the function

$$\omega(t) \equiv \Omega_{+}(t/2)/2 . \quad (7)$$

With these changes of variables, our working relations become:

$$\omega(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} r^{+}(k) e^{ikt}\, dk , \quad (8)$$

$$K(x,y) = \int_{x}^{\infty} \omega(t+y) K(x,t) dt + \omega(x+y) = 0 , \ x \leq y \quad (9)$$

and

$$q(x) = -\frac{1}{2} \frac{d}{dx} K(x,x) \quad (10)$$

The basis for the algorithm is the observation that when the reflection coefficient r^{-} is a rotational function of k with all its poles in the lower half plane, an explicit formula for $q(x)$ can be obtained. Observe that the analyticity of $r^{-}(k)$ for Im $k>0$ implies that q vanishes on the negative axis, if no eigenvalues exist.

Since r is rational and analytic for Im $k>0$, it has theform

$$r^-(k) \equiv r_0 \frac{\prod^{M} (k - \mu_j)}{\prod^{L} (k - \delta_j)} \tag{11}$$

with $M<L$, and $\mathrm{Im}\,\delta_j<0$. Now, basic properties of the scattering matrix imply that the relation

$$t(k)t(-k) = 1-r^-(k)r^-(-k)$$

holds on the real axis. Then denoting the roots of

$$1 - r^-(k)r^-(-k) = 0$$

located in the upper half plane by ρ_j and assuming that 0 , we get

$$t(k)t(-k) = \prod^{L} \frac{(k-\rho_j)}{(k-\delta_j)} \frac{(k+\rho_j)}{(k+\delta_j)} \tag{12}$$

for real k.

If there are no eigenvalues, $t(k)$ is a non-vanishing analytic function in the upper half-plane; as a consequence of (12), t must have the form

$$t(k) = \prod^{L} \frac{k + \rho_j}{k - \delta_j} .$$

It is known that on the real axis

$$r^+(k) = -r^-(-k)\,t(k)\,/\,t(-k) ,$$

so that

$$r^+(k) = (-1)^{L+M+1} r_0 \frac{\prod^{M}(k+\mu_j)\prod^{L}(k+\rho_j)}{\prod^{L}(k-\delta_j)\prod^{L}(k-\rho_j)}$$

Corisequently

$$r^+(k) = p(k) + \Sigma\, \tilde\rho_j/(k-\rho_j) \tag{13}$$

where $p(k)$ is analytic in the upper half-plane.

Substitution of (13) into (8) gives

$$\omega(t) = i \sum_j^L \tilde\rho_j\, e^{i\rho_j t}, \qquad t\geq 0 . \tag{14}$$

Using this relation in (9) we get that for $0\leq x\leq y$

$$K(x,y) + i \sum_j^L \tilde\rho_j \{\int_x^\infty e^{i\rho_j t} K(x,t)dt\} e^{i\rho_j y}$$

$$+ i \prod_j^L \{\tilde\rho_j e^{i\rho_j x}\} e^{i\rho_j y} = 0 . \tag{15}$$

Therefore, in the range $0\leq x\leq y$, K is a kernel of Pincherle-Goursat type, that is, it has the form

$$K(x,y) = \sum_j^L f_j(x)\, e^{i\rho_j y} , \tag{16}$$

and thus, suhstituting (16) into (15) we get the $L\times L$ system

$$f_j(x) - \tilde\rho_j \sum_m^L \frac{e^{i(\rho_j+\rho_m)x}}{\rho_j + \rho_m} f_m(x) = -i\tilde\rho_j e^{i\rho_j x} . \tag{17}$$

By using Cramer's rule and (10), one obtains from (17) the expression

$$q(x) = -2 \frac{d^2}{dx^2} \log \det[I-A(x)] , \tag{18}$$

where $A = (a_{jm})$ is the matrix associated to the system (17), namely

$$a_{jm}(x) \equiv \tilde\rho_j \frac{e^{i(\rho_j+\rho_m)x}}{\rho_j + \rho_m}$$

Observe that the order of this matrix equals the number of poles of $r^-(k)$.

Although (18) is theoretically simpler than (17), this latter formula has more computational interest than the former. This can be seen as follows: setting $y=x$ in (16) and differentiating, we have

$$\frac{d}{dx} K(x,x) = \Sigma \{f'_j(x) + i\rho_j\} e^{i\rho_j x} , \qquad (19)$$

for $x \geqslant 0$. To compute the values of $f'_j(x)$ we differentiate (9) and (16) with respect to x and obtain

$$\partial_1 K(x;y) + \int_x^\infty \omega(t+y)\partial_1 K(x,t) - \omega(x+y)K(x,x) +$$

$$\omega'(x+y) = 0 , \qquad (20)$$

and

$$\partial_1 K(x,y) = \Sigma f'_j(x) e^{i\rho_j y}$$

If we now use this last expression and (16) in (20) we get the following system for $f'_j(x)$:

$$f'_j(x) - \tilde{\rho}_j \sum_m \frac{e^{i(\rho_j+\rho_m)x}}{\rho_j + \rho_m} f'_m(x) =$$

$$= \tilde{\rho}_j e^{i\rho_j x} \{\rho_j + i \sum_m f_m(x) e^{i\rho_m x} \} . \qquad (21)$$

Notice thet the coefficient matrix in (21) is again $I-A(x)$, so that to get the solution for this system after having solved (17) is a computationally cheap task. Moreover it avoids having to numerically carry out the differentiation in (10).

We observe that passing from r^- to r^+ makes it possible to obtain (18) and also makes the derivation of (17) quite simple. Nevertheless, a system analogous to (17) can be obtained by making use of r^- only, Cf. Ref. 11.

We have solved numerically the inverse scattering problem by implementing both (9) and (17), for some rational coefficients r^-. In dealing with Marchenko equations directly, we discretized (9) by using Simpson's formula and we needed a 60-point mesh to obtain an accuracy of 10^{-5} in the average. The second method, even for $L=8$, was ten times faster than the first.

As it stands, we can use the second method only for rational reflection coefficients. When solving the inverse problern for a reflection coefficient r^- which is analytic in the upper half-plane, and if there are no eigenvalues, we can use the following numerical rnethod:

(a) approximate r^- by a rational reflection coefficient r_ε, which is analytic in the upper half plane,

(b) solve the inverse problern for r_ε by using the algorithrn described in (10), (17), (19) and (21).

Theorem 3 in Ref. 9 gives us the conditions on the approximation r_ε under which we can expect the potential q_ε to be close tothe potential q we are seeking. The main difficulty is that the common techniques for approximating a given function by a rational one, e.g. the Rehmes algorithm, can be applied only for real functions, while the requirement that all poles of r_ε lie in the lower half-plane prevents us from approximating the real and the imaginary parts of r separately.

The following is a possible strategy for solving the approximation problem:

Restricting ourselves to reflection coefficients r that die out like

$$r(k) = O(|k|^{-1}) \quad , \quad |k| \sim \infty \quad , \tag{22}$$

define

$$R(k) \equiv (k+i)r(k)$$

and, for $\omega = e^{i\theta}$, the Cayley-transforrn type change of variables

$$s(\omega) \equiv R\left(\frac{1}{i}\,\frac{\omega+1}{\omega-1}\right)$$

By (22) s is continuous at $\omega=1$. Thus, obtain trigonometric approximations

$$s(\omega) \sim \Sigma\, a_n \omega^n = \Sigma\, a_n e^{in\theta}$$

for s and define

$$r_\varepsilon(k) \equiv \frac{1}{k+i} \sum^{m-1} a_n \left(\frac{k-i}{k+i}\right)$$

as the sought approximations.

3. SOME WORTH SOLVING PROBLEMS

It is our opinion that the following questions deserve investigation.

. Can the algorithm described in Section 2 give better approximation results if instead of defining r_ε with an m-th order pole one gets its poles spread out in the lower half plane? How to achieve such an approximation scheme?

. Stability results for direct and inverse scattering are rather scanty in the literature. In particular, some of them, like the one by Lundina and Marchenko[12], suffer from the following ailment we often have found in the treatment of many questions related to inverse problems - see also Ref. 13: the general setting is to investigate a mapping from accessible data $\{\phi\}$ into sought data $\{f\}$. Hypotheses are then made on $\{f\}$ without knowing how these can be read out from the informations on $\{\phi\}$ one has at hand. Of course, results gotten in this way are barely useful.

In Ref. 9 two stability results were presented, one for direct and the other for inverse scattering in the one-dimensional case. By no means was that a thorough treatment for the problem, and thus the questions below are naturally raised.

i) Particular distances were introduced inorder to reach those results, namely, for the direct mapping

$$\|q\|_d \equiv \sup_x |q(x)| + \int_{-\infty}^{\infty} |xq(x)|dx + \sup_x x^2|q(x)| \ , \tag{23a}$$

$$\|r^+\|_d \equiv \int_{-\infty}^{\infty} |r^+(k)|^2 \ dk \tag{23b}$$

were taken, while for the inverse mapping we used

$$\|q\|_i \equiv \sum_{n=1}^{\infty} 2^{-n} \sup_{-n\leqslant x\leqslant n} |q(x)| \tag{24a}$$

(that is, uniform convergence on compact sets) and

$$\|r^+\|_i \equiv \sup_t |F_+'(t)| + \int_{-\infty}^{\infty} |tF_+'(t)|dt \tag{24b}$$

where

$$F_+(t) \equiv \frac{1}{\pi} \int_{-\infty}^{\infty} r^+(k) \ e^{2ikt} \ dk \tag{25}$$

Are there other metrics better suited to the problem? In particular, can one deal with the same pair of metrics for both direct and inverse problems? (In other words, does a homeomorphism between the set of potential and of scattering data exist?) Must one definiteiy get rid of more familiar norms within this context, that is, which negative stability results hold?

ii) The above mentioned continuity properties were only shown to hold for some sets of potentials and of scattering data, while both direct and inverse mappings are defined on nuch bigger sets. This is another way in which such results may be improved.

. Deift and Trubowitz[14] exhibitted another approach to one--dimensional scattering. Is their treatment amenable to nurnerical studies and to deduce more stúbility facts?

. As far as we know, no stability results exist for the three-dimensional case, in which some light was recently shed by the discoveries of R. Newton[15].

. We close this section recalling that a list of other important questions were posed during a meeting of the American Mathematical Society in Bloomington, April 1980, Cf. 16, page 526.

Section 2 is part of a Ph.D. thesis[17] written at the Courant Institute, under the guidance of P.D. Lax (NYU) and Jerry Goldstein (Tulane), for whose encouragement the author is indebted.

The computational tests wave carried out on a CDC-6600 of the Energy Research and Development Administration computer facilities at NYU.

Financial support granted to the author at different stages of the research by CNPq, M.R. Exteriores, UnB and NYU is also acknowledged.

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An Approximation Scheme for One-dimensional Inverse Scattering - C. A. Moura - Added in proof: A very thorough numerical treatment** - both theoretical and computational - for a different inverse scattering problem, the so-called Chudov problem, has just caught up our attention. The author accomplishes quite a deep analysis of the proposed algorithm and states that his approach may also be employed for the radial inverse spectral problem and is suitable for some higher dimension generalizations.

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