Exact bounds to one-dimensional potential scattering amplitudes through the classical theory of moments

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A new method is described for solving the time-independent one-dimensional finite-range-potential scattering problem. The method utilizes positivity properties of the scattering wave function, implemented through the classical theory of moments. It is shown to provide exact narrow bounds to the scattering amplitudes. The method is particularly suited to treat the strong-interaction regimes, where perturbative approximations fail.

The solution of the time-independent scattering problem is of crucial importance in a wide spectrum of problems ranging from atomic collisions in fusion plasmas to particle physics. Given the complexity of a typical problem, exact solutions are usually unobtainable. Many methods are available to approximate the exact unknown solution.[1] Very often, however, the range of validity of these methods (Born perturbation series, Glauber semiclassical approximation, etc.) is very limited. Even more seriously, they do not provide exact error bounds to their approximations. The present work is an initial attempt at addressing these concerns.

We introduce a new method for solving the one-dimensional time-independent scattering problem, utilizing positivity properties of the wave function and implemented through the classical theory of moments.[2] This method (hereafter referred to as the *moments method*) recommends itself for two major reasons. Firstly, instead of looking for approximate scattering amplitudes, this approach computes exact bounds to their actual values. Secondly, yet equally important, the moments method is well suited to the strong-singular-perturbation-interaction regime which eludes many perturbative procedures.[3-6] Indeed, this work is motivated by the need to develop alternative and reliable computational schemes to understand the behavior of generalized oscillator strengths for low-energy-electron–atom forward inelastic scattering.[7] Although a definite answer to this problem is as yet unavailable, we are confident that "positivity," a universal notion, will be of significance in this regard. The crucial question for any system is how to recognize its positivity structure. In this work we outline an effective positivity framework by which to understand one-dimensional scattering problems.

The moment method developed here follows from previous investigations by Handy and Bessis on the determination of the bound-state energies of multidimensional bosonic Schrödinger operators.[3-6] Most of the terminology used here has been adapted from these works. The essence of the method is as follows: the unknown scattering amplitudes define an initial-value problem for a recursion relation involving the moments of $|\psi(x)|^2$, the modulus of the time-independent scattering wave function. The positivity of $|\psi(x)|^2$ then leads to a hierarchical set of linear inequalities which constrain the scattering amplitudes through rapidly converging bounds.

The starting point is a differential equation for $s \equiv \psi\psi^*$ which can be obtained as follows. Let us consider the one-dimensional rescaled Schrödinger equation

$$-\frac{d^2}{dx^2}\psi(x)+V(x)\psi(x)=E\psi(x) \ . \tag{1}$$

Multiply Eq. (1) by ψ^*. Then add the resulting equation to its complex conjugate, to obtain

$$-\frac{d^2s}{dx^2}+2\left|\frac{d\psi}{dx}\right|^2+2V(x)s(x)=2Es(x) \ . \tag{2}$$

We now need to eliminate the dependence on the derivative of ψ. This may be accomplished by a similar manipulation of Eq. (1) multiplied by ψ'^*. Taking the complex conjugate of the new equation, and adding as before, we obtain

$$-\frac{d}{dx}\left|\frac{d\psi}{dx}\right|^2+V(x)\frac{ds}{dx}=E\frac{ds}{dx} \ . \tag{3}$$

Differentiating Eq. (2) with respect to x and making use of Eq. (3) yields the required differential equation for s,

$$-\frac{1}{2}\frac{d^3s}{dx^3}+2V(x)\frac{ds}{dx}+\frac{dV}{dx}s(x)=2E\frac{ds}{dx} \ . \tag{4}$$

This equation is the basis of all further developments. An identical differential equation for ψ^2 (ψ real) was used in Ref. 8 to analyze bound states. Three scattering problems will be investigated: a finite square-well potential, a polynomial potential, and a truncated partial-wave atomic potential. We now detail the analysis of the first case.

The potential for the square well is defined by

$$V(x)=\begin{cases}-V_0 \ , & x\in(0,1)\\ 0 \ , & x\notin(0,1) \ .\end{cases} \tag{5}$$

In this case, the interaction region is limited to the finite interval (0,1). The *moments* of the positive function $s(x)$ over this region are the non-negative quantities

$$\mu_p \equiv \int_0^1 x^p s(x)dx \ , \quad p=0,1,\ldots \ . \tag{6}$$

A recurrence relation for the μ_p's may be obtained from Eq. (4) by multiplying it by x^p and integrating over the unit interval,

$$\int_0^1 x^p s'''(x)dx+\varepsilon\int_0^1 x^p s'(x)dx=0\ , \tag{7}$$

where $\varepsilon\equiv 4(V_0+E)$. We now integrate by parts the derivatives of s, obtaining

$$\begin{aligned}\varepsilon p\mu_{p-1}+p(p-1)(p-2)\mu_{p-3}&\\ =s''(x)x^p\,|_0^1-ps'(x)x^{p-1}\,|_0^1&\\ +s(x)[p(p-1)x^{p-2}+\varepsilon x^p]\,|_0^1\ .&\end{aligned} \tag{8}$$

It is implicitly understood that the quantities $s''(0)$ and $s''(1)$ are to be taken as limits from the right and from the left, respectively, since ψ'' is discontinuous at these points. Equation (8) may be readily adapted to describe a scattering process by relating the boundary terms of s to the asymptotic form of the scattering states,

$$\begin{aligned}\psi^-(x)&=e^{ikx}+Re^{-ikx}\ ,\\ \psi^+(x)&=Te^{ikx}\ ,\end{aligned} \tag{9}$$

R and T being the reflection and transmission coefficients and $k^2=E$. Through Eq. (9), the boundary terms in Eq. (8) depend on $\mathrm{Re}R$, $\mathrm{Im}R$, $|T|^2$, and $|R|^2$. The latter may be eliminated through the relation $|R|^2+|T|^2=1$, which expresses probability conservation. As a consequence, the boundary terms depend *linearly* on the variables:

$$\begin{aligned}\nu_{-1}&\equiv \mathrm{Re}R\ ,\\ \nu_{-2}&\equiv \mathrm{Im}R\ ,\\ \nu_{-3}&\equiv |T|^2\ .\end{aligned} \tag{10}$$

It is to be noticed that we could have expressed ν_{-3} as a function of the other two variables. This would have involved a nonlinear relation, which we prefer to avoid in view of our intended use of linear programming.

The recursion relation in Eq. (8) may now be rewritten in the following form (where it is understood that μ_j for $j<0$ are set equal to zero):

$$\begin{aligned}\varepsilon p\mu_{p-1}+p(p-1)(p-2)\mu_{p-3}+\sum_{k=-3}^{-1}c_k^{(p)}\nu_k+C^{(p)}&\\ =0\ ,\quad p\geq 0\ .&\end{aligned} \tag{11}$$

The coefficients $c_{-k}^{(p)}$ (which depend on E and V_0) have been implicitly introduced, together with the inhomogeneous term $C^{(p)}$. Their form need not be explicitly presented here, as it may be recovered from Eqs. (8) and (9). We call attention to the structure of Eq. (11). Firstly, by setting $p=0$ it is simple to show that

$$\mathrm{Re}(R)=-(1+|T|^2)(1+2E/V_0)\ , \tag{12}$$

which permits the elimination of ν_{-1}. Accordingly, only ν_{-2} and ν_{-3} (pseudo-missing moments) need to be specified in order that the μ_j be determined through the recursion relation. In general, in addition to the ν's a finite number of so-called *proper missing moments* μ are also required to initialize the recursive relation. In the case of the square well, all the moments μ_p can be expressed as a linear combination of the pseudo-missing moments,

$$\mu_p=\sum_{k=-3}^{-2}g_k^{(p)}\nu_k+I^{(p)}\ ,\quad p=0,\ldots,\infty\ . \tag{13}$$

The coefficients $g_k^{(p)}$ and the inhomogeneous term $I^{(p)}$ may be determined recursively by substituting Eq. (13) into Eq. (11).

The next step in the moment method is the imposition of necessary and sufficient conditions on the quantities μ_p, $p\geq 0$ that guarantee that they be the moments of a positive measure s. The standard way of generating such constraints is to consider the set of inequalities[5]

$$\int_0^1 P_i(x)\left[\sum_{l=0}^N q_l x^l\right]^2 s(x)\,dx\geq 0\ ,\quad i=1,2,3\ . \tag{14}$$

In the above, q is any $(N+1)$-dimensional vector, and $P_i(x)=a_i x+b_i$, with

$$a_i=\begin{cases}0\ , & i=1\\ 1\ , & i=2\\ -1\ , & i=3\end{cases}\quad\text{and}\quad b_i=\begin{cases}1\ , & i=1\\ 0\ , & i=2\\ 1\ , & i=3\ .\end{cases} \tag{15}$$

We can now transform Eq. (14) into the quadratic form inequalities

$$\sum_{l,m=0}^N q_l q_m(a_i\mu_{l+m+1}+b_i\mu_{l+m})\geq 0\ , \tag{16}$$

which, together with Eq. (13), imply a set of linear inequalities in the pseudo-missing-moments space,

$$\begin{aligned}\sum_{k=-3}^{-2}\left[\sum_{l,m=0}^N q_l q_m(a_i g_k^{(l+m+1)}+b_i g_k^{(l+m)})\right]\nu_k&\\ +\sum_{l,m=0}^N q_l q_m(a_i I^{(l+m+1)}+b_i I^{(l+m)})\geq 0\ .&\end{aligned} \tag{17}$$

It has been proved elsewhere[5] that the infinite set of inequalities in Eq. (17) (for all the possible choices of q) defines a convex region with nonlinear boundaries in the pseudo-missing-moments space, which we will call the *feasibility region*. Such a region can be arbitrarily circumscribed by a polytope corresponding to a finite number of optimally chosen intersecting hyperplanes (defined by particular choices of q). This is the essence of a powerful "cutting" technique recently developed.[6] Through linear programming, the extent of the polytope can be easily determined, which in turn leads to bounds on the physical quantities of interest.[5,6] As N is increased, the bounds rapidly converge to the physical values.

Table I gives the data for a square-well potential. The scattering amplitudes obtained by the moments method

TABLE I. Values of the transmission probability $|T|^2$ and of the imaginary part of the reflection coefficient R in the case of the square-well potential, for different scattering energies E. N is the number of moments utilized in the linear inequalities (see text). Upper and lower bounds for these quantities are shown, together with the exact value of $|T|^2$.

E	N	$\|T\|^2$ (exact)	$\|T\|^2_{(-)}$	$\|T\|^2_{(+)}$	$\mathrm{Im}R_{(-)}$	$\mathrm{Im}R_{(+)}$
10	6	0.999 931 085	0.980 01	1.031 82	0	2.241
10	10	0.999 931 085	0.999 808 8	1.000 018 4	6.79×10^{-3}	1.669×10^{-2}
10	14	0.999 931 085	0.999 931 03	0.999 931 13	8.1742×10^{-3}	8.1787×10^{-3}
0.1	6	0.369 315 23	0.3687	0.3716	0.2397	0.2414
0.1	10	0.369 315 23	0.369 315 21	0.369 315 32	0.240 635 905	0.240 635 962
10^{-4}	10	0.000 564 614 42	0.000 564 614 40	0.000 564 614 54	0.012 833 831 1	0.012 833 832 3

are compared to their exact values. We see that even using relatively few moments, the scattering probabilities are determined up to significant precision, particularly for low energies.

In order to illustrate the versatility of our method, we briefly turn to a more complicated example. Let the scattering potential be defined by the following:

$$V(x)=\begin{cases}\alpha(2x-1)^2+(2x-1)^4+V_0\ , & x\in(0,1)\\ 0\ , & x\notin(0,1)\end{cases} \tag{18}$$

where α is a real constant and $V_0=-(\alpha+1)$.

Proceeding in the same way as before, we find the moment recursion relation,

$$\begin{aligned}p(p-1)(p-2)\mu_{p-3}-4pE\mu_{p-1}+(16+8\alpha)(2p+1)\mu_p-(p+1)(16\alpha+96)\mu_{p+1}+64(2p+3)\mu_{p+2}\\ -64(p+2)\mu_{p+3}+4\delta_{p,2}\nu_{-1}-4k\delta_{p,1}\nu_{-2}+[2(\delta_{p,2}+2k^2\delta_{p,0})+p(p-1)+4k^2](1-\nu_{-3})\\ +2(\delta_{p,2}+2k^2\delta_{p,0})-p(p-1)-4k^2=0\ .\end{aligned} \tag{19}$$

As usual, we introduced $k^2=E$ and $\delta_{i,j}$, the Kronecker δ. Here, the *proper* missing moments μ_j, $j=0,1,2$, and the pseudo-missing moments ν_l, $l=-3,-2,-1$, are the necessary and sufficient quantities needed to generate all other moments μ_i, $i=3,\ldots,\infty$. The space spanned by them is called an *extended*-missing-moments space. Apart from this generalization, the same linear-programming procedure described above can be applied. Table II shows the bounds to the value of $|R|^2$, the square modulus of the reflection coefficient. Bounds for all the other extended missing moments are also obtainable. In Table II we make a comparison with the results given by the first- and second-order terms in the Born series. The undesirable features of the low-energy behavior of the Born series are not present in our method.

As a last example of the moments method, we consider the partial-wave equation for Coulomb scattering,

$$-\frac{d^2}{dr^2}\phi(r)+\frac{l(l+1)}{r^2}\phi(r)-\frac{Z}{r}\phi(r)=E\phi(r)\ , \tag{20}$$

where Z is the nuclear charge. ϕ is the so-called *normalized solution* of Eq. (20), satisfying the boundary condition $\phi(0)=0$. After multiplication of Eq. (20) by r^3, the differential equation for s becomes

TABLE II. Reflection probability in the case of the polynomial potential with $\alpha=1$, for different energies E. The bounds obtained by linear inequalities involving 18 moments are compared to perturbative calculations of first and second order. The latter is numerically nonsensical at $E=0.01$.

E	$\|R\|^2_{(-)}$	$\|R\|^2_{(+)}$	First-order Born	Second-order Born
7	$2.910\,37\times10^{-4}$	$2.910\,42\times10^{-4}$	3.150×10^{-4}	2.937×10^{-4}
6	$4.474\,20\times10^{-4}$	$4.474\,27\times10^{-4}$	4.822×10^{-4}	4.519×10^{-4}
5	$6.975\,87\times10^{-4}$	$6.975\,96\times10^{-4}$	7.491×10^{-4}	7.057×10^{-4}
4	$1.191\,39\times10^{-3}$	$1.191\,45\times10^{-3}$	1.198×10^{-3}	1.137×10^{-3}
3	$1.894\,30\times10^{-3}$	$1.894\,31\times10^{-3}$	2.023×10^{-3}	2.042×10^{-3}
2	$3.570\,41\times10^{-3}$	$3.570\,42\times10^{-3}$	3.811×10^{-3}	2.004×10^{-2}
1.5	$5.314\,615\times10^{-3}$	$5.314\,617\times10^{-3}$	5.676×10^{-3}	6.007×10^{-1}
0.01	$5.251\,560\times10^{-1}$	$5.251\,561\times10^{-1}$	1.171	

$$-\frac{r^3}{2}s'''+2[l(l+1)r-Zr^2]s'-[2l(l+1)-Zr]s = 2Es' . \quad (21)$$

By leveling the potential at $r=R$ [that is, $V(r>R)=V(R)$], the moment analysis may be carried over in the range $r\in(0,R)$, with the obvious modification $P_3(r)=R-r$ in Eq. (15). This is analogous to the boundary terms treatment in the R-matrix formulation of Berrington *et al.*[9] Indeed, the moment method allows for the precise determination of $\phi'(R)/\phi(R)$ which is central to the R-matrix method. Hence follows the equation

$$2E(p+1)\mu_{p+1}+\frac{Z}{R}(2p+1)\mu_p+\frac{p}{R^2}[(p^2-1)/2-2l(l+1)]\mu_{p-1} = \frac{R}{2}s''(R)-\frac{p+1}{2}s'(R)+\left[\frac{p(p+1)}{2R}-\frac{2l(l+1)}{R}+2Z+2ER\right]s(R) . \quad (22)$$

After this is done, the asymptotic scattering states can be chosen in the form

$$\phi^+(r)=e^{-ikr}+e^{i(kr-\Delta)} , \quad (23)$$

where probability conservation has been imposed once more. We remark that our method needs only this asymptotic information in order to be implemented, and no particular solution of the differential equation for s in the inner region is required. The relation between the boundary terms and Δ then becomes

$$\begin{aligned} s(R)&=2(1+C\cos\Delta+S\sin\Delta) , \\ s'(R)&=-4k(S\cos\Delta-C\sin\Delta) , \\ s''(R)&=-8k^2(C\cos\Delta+S\sin\Delta) , \end{aligned} \quad (24)$$

where

$$\begin{aligned} C&\equiv\cos(2kR) , \\ S&\equiv\sin(2kR) , \\ k^2&\equiv E-V(R) . \end{aligned} \quad (25)$$

By following exactly the same procedures as in the two previous cases we solve now for the pseudo-missing moments $\cos\Delta$ and $\sin\Delta$. In Table III we exhibit the bounds for $\cos\Delta$.

TABLE III. Partial-wave ($l=1$) scattering by Coulomb potential, leveled at $r=R$. The energy E has been kept fixed at a low value. Bounds for $\cos\Delta$ are shown as a function of the number of moments used, N, and of the cutoff R.

R	E	N	$\cos\Delta_{(-)}$	$\cos\Delta_{(+)}$
20	0.1	30	−0.391 39	−0.391 35
20	0.1	32	−0.391 385	−0.391 365
30	0.1	30	0.496 41	0.496 81
36	0.1	36	0.496 57	0.496 61
50	0.1	43	0.969 82	0.969 86
75	0.1	42	0.2119	0.2135

It is clear that the application of the moments method to the $R\to\infty$ case is impossible, since it would entail working with infinitely large moments. The numerical results quoted manifest this fact. In the case of the Bohr atom we attempted a mapping of the problem from $[0,\infty)$ to $[0,1)$ through the transformation

$$y=\frac{r}{r_0+r} . \quad (26)$$

The results were not as good as expected, partly because of the presence of simple-pole singularities near the $[0,1)$ domain which affect convergence rates. Some other transformation may perhaps remedy this difficulty, such as working in Fourier space. In any case, bearing in mind how large R is in Table III, one should be able to use the present moments-method formulation within an inner region of strong interaction, together with an asymptotic matching to an outer solution provided, for instance, by Wentzel-Kramers-Brillouin analysis.

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