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Generation of converging Regge-pole bounds for arbitrary rational fraction scattering potentials

C R Handy, A Z Msezane and Z Yan

Department of Physics and Center for Theoretical Studies of Physical Systems, Clark Atlanta University, Atlanta, GA 30314, USA

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Abstract
We expand upon the Regge-pole bounding formalism previously presented by Handy and Msezane (2001 *J. Phys. A: Math. Gen.* **34** L531), by analysing in greater detail several important *singular* potentials, including the $V(r) = \frac{\alpha^2}{r^3}$ potential, the polarization potential, $V(r) = \frac{\alpha^2}{r^4}$, and the Lennard-Jones class $V(r) = \frac{\alpha^2}{r^m} - \frac{\beta^2}{r^n}$, for $(m, n) = (6, 4), (12, 6)$. With respect to the polarization potential, our bounds enable one to assess the accuracy of the turning point based, asymptotic formula of Avdonina *et al* (Avdonina N B, Belov S, Felfli Z, Msezane A Z and Naboko S N 2001 *CAU Preprint* (2002 *Phys. Rev.* A **65** at press). We also extend the method to the *non-singular* Coulomb case, $V_{\mathrm{eff}}(r) = -\frac{1}{r} + \frac{l(l+1)}{r^2}$, which represents a more challenging class of problems (within the present bounding formalism) due to the nature of the underlying boundary conditions.

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1. Introduction

The exploitation of Regge-pole analysis facilitates the description of many quantum scattering problems (Frautschi 1963, Newton 1982), particularly for atomic and molecular processes, as documented in the works by Connor (1990), Amaha and Thylwe (1991, 1994), Andersson (1993), Germann and Kais (1997), Sofianos *et al* (1999), Sokolovski *et al* (1998), Vrinceanu *et al* (2000a, 2000b), and references therein. Most of these works focus on the intricacies of turning point contributions and Stokes line topologies. The ensuing numerical analysis has yielded very good results. Nevertheless, it is desirable to develop alternative, analytically simple, high precision computational methods for determining the Regge poles. One novel approach is to generate converging bounds to the Regge poles, as proposed by Handy and Msezane (2001). Their particular formulation originates from recent, and related, works in applying the eigenvalue moment method (EMM) for generating converging bounds to complex eigenenergies of non-Hermitian, rational fraction Hamiltonians (i.e. Handy 2001a, 2001b, Handy and Wang 2001, Handy *et al* 2001).

In their work, Handy and Msezane adapted this type of EMM analysis for generating converging bounds to the Regge-pole values of rational fraction scattering potentials. The particular formulation presented in their work yielded very good bounds for the case examined by them, that of the Lennard-Jones effective potential $V_{\rm eff}(r) = \frac{\alpha^2}{r^m} - \frac{\beta^2}{r^n} + \frac{l(l+1)}{r^2}$, for $(m, n) = (6, 4)$. However, the tightness of their bounds is not as impressive as those obtained in the above referenced works concerning complex eigenenergies. Still, the EMM–Regge-pole analysis by Handy and Msezane marks an unprecedented first step towards a new type of computational methodology capable of yielding highly accurate Regge poles, through the generation of rapidly converging lower and upper bounds to the real and imaginary parts of the Regge pole, $l = (l_r, l_i)$. The ability to generate complex Regge poles through converging bounds portends a significant new computational development complementing available numerical integration schemes and delicate analytic continuation methods. It is the near term objective of our continued efforts to identify alternate representations within which the generation of tight bounds becomes more efficient. To this end, as a benchmark, it is important to ascertain the limits of the present (simple) complex rotation based framework.

In this work we expand upon the abbreviated presentation by Handy and Msezane. We start our analysis by considering, for theoretical reasons, the $V(r) = \frac{\alpha^2}{r^3}$ potential. We then examine the case of the polarization potential problem, $V(r) = \frac{\alpha^2}{r^4}$, as well as the Lennard-Jones class $V(r) = \frac{\alpha^2}{r^m} - \frac{\beta^2}{r^n}$, for $(m, n) = (6, 4)$ and $(12, 6)$. These types of potentials correspond to 'singular' differential equations of non-Fuchsian type, where the effective potential diverges at the origin faster than r^{-2} (i.e. the solutions involve essential singularities, etc). However, despite these complexities, the boundary condition for the physical, Regge-pole solution, in such cases, demands that

$$\lim_{r\to 0^+} \Psi_{r.p.}(r) = 0 \qquad \text{if} \quad \lim_{r\to 0} r^2 V_{\rm eff}(r) = \infty \tag{1}$$

and r restricted to the real axis, $\mathcal{R}$.

This is actually a much simpler boundary condition than that for 'non-singular' (Coulomb-like) effective potentials, $V_{\rm eff}(r)$, which diverge no faster than r^{-2} at the origin. In such cases, the Regge-pole solutions are of the Fuchsian type and the required boundary condition is

$$\Psi_{r.p.}(r) \to \mathcal{N} r^{l+1} \qquad \text{as} \quad r \to 0^+ \quad \text{if} \quad \lim_{r\to 0} r^2 V_{\rm eff}(r) < \infty \tag{2}$$

and $r \in \mathbb{R}$. The parameter l corresponds to the complex Regge pole. If $\mathbb{R}(l) < 0$, the boundary condition diverges at the origin. This is the case for the Coulomb (and related) problem. As such, it requires a more delicate EMM analysis than that for which the boundary condition vanishes at the origin. The last section of this work extends the Handy and Msezane formalism to such cases.

Three important independent results make the Regge-pole bounding formulation possible. The first of these results from the original work by Handy (2001a), and subsequent reformulations by Handy and Wang (2001), Handy (2001b) and Handy *et al* (2001), which show how the Schrödinger equation, extended to any complex contour in the complex-r plane, $r(\xi) : \mathbb{R} \to \mathcal{C}_r$ (i.e. $-\left(\frac{d\xi}{dr}\frac{d}{d\xi}\right)^2\Psi(\xi) + V_{\rm eff}(\xi)\Psi(\xi) = E\Psi(\xi)$), can be transformed into an equivalent fourth-order, linear differential equation for the probability density $S(\xi) = |\Psi(r(\xi))|^2$. This result is independent of the Hermitian/non-Hermitian (complex) nature of the Hamiltonian. The advantage of the $S(\xi)$ representation is that the physical solutions are non-negative (for $\xi \in \mathbb{R}$) and thus fulfil the first requirement towards an EMM analysis.

The second important result is that for any linear differential equation, with rational fraction function coefficients involving unknown parameters (i.e. eigenvalues, Regge poles, etc), for which the desired configuration solutions are uniquely non-negative and bounded (i.e. in the L^1 sense), one can employ EMM in order to determine the physical parameter values in terms of converging lower and upper bounds. The EMM formalism was developed more than 15 years ago by Handy and Bessis (1985) and Handy *et al* (1988a, 1988b). It exploits well-known theorems within the classic moment problem (Shohat and Tamarkin 1963) and makes use of a linear programming (Chvatal 1983) based *cutting algorithm*.

As noted above, in addition to the requirement that the transformed Schrödinger equation involves rational fraction function coefficients, we must confirm that the physical solutions are uniquely bounded. As explained below, the nature of the Regge-pole problem is such that in order to achieve this, one must work within the rotated complex plane.

The Regge-pole wavefunction, $\Psi_{r.p.}(r)$, along the real axis, must satisfy the asymptotic condition:

$$\Psi_{r.p.}(r) \to \mathcal{A}\,\mathrm{e}^{\mathrm{i}kr} \qquad \text{as} \quad r \to \infty \tag{3}$$

corresponding to an outgoing wave of wave number k. At the origin, the Regge-pole wavefunction must take on the form of the physical (bound state) wavefunction when l is analytically continued to non-negative integer values. This results in the boundary conditions specified in equations (1) and (2), for the Regge-pole solutions.

In order to make use of the EMM procedure, the underlying configurations must have finite moments (for the physical solutions). This is clearly impossible for Regge-pole solution along the real axis. One must then work within the complex-r plane, $r = \rho\,\mathrm{e}^{\mathrm{i}\theta}$. This is the third result required for full implementation of EMM.

We will work with fixed θ-values, and $\rho \geqslant 0$. This is a very simple, although unprecedented, complex rotation formalism for studying the Regge-pole problem. For $0 < \theta < \pi$, the Regge-pole wavefunction will be asymptotically zero, as $\rho \to \infty$. This follows from equation (3):

$$\Psi_{r.p.}(\rho,\theta) \to \mathcal{A}\,\mathrm{e}^{k\rho(\mathrm{i}\cos(\theta)-\sin(\theta))} \to 0 \qquad \text{as} \quad \rho \to \infty. \tag{4}$$

It is the origin, $\rho = 0, \theta =$ fixed, that presents the major challenges. Let us rewrite the wavefunction as

$$\Psi(\rho,\theta) = |\Psi(\rho,\theta)|\exp(\mathrm{i}\Phi(\rho,\theta)). \tag{5}$$

In most Regge-pole problem cases, the phase factor becomes singular at the origin (Handy and Msezane 2001):

$$\lim_{\rho\to 0^+} |\Phi(\rho,\theta)| = \infty. \tag{6}$$

One significant contribution of working with $S(\rho,\theta) = |\Psi(\rho,\theta)|^2$ is that much of the rapidly oscillating (non-analytic) contributions of Ψ phase are factored out. Thus, $S(\rho,\theta)$ is a much better behaved expression to work with.

One may use the preceding observation as an incentive in developing a *non-negativity quantization representation* (NQR) formalism, in which the Schrödinger equation for Ψ is transformed into the S representation. As noted, another compelling argument supporting this is that an S-differential representation is straightforward to derive and possesses all the necessary features allowing for implementation of EMM.

As previously noted, it is possible to transform the Schrödinger equation into a fourth-order, linear differential equation for S (Handy 2001a); however, depending on the nature of the problem being considered, the subsequent generation of the required *moment equation* for

S can become quite complicated. It is better to work with an equivalent representation (Handy and Wang 2001), reviewed below, which makes the generation of the desired S-moment equation much easier, particularly with regards to understanding the underlying *missing moment* structure.

The Schrödinger equation, along the θ ray direction, becomes

$$A(\rho)\Psi''(\rho) + B(\rho)\Psi'(\rho) + C(\rho)\Psi(\rho) = 0 \tag{7}$$

where $A(\rho) = 1$, $B(\rho) = 0$ and $C(\rho) = \mathrm{e}^{2\mathrm{i}\theta}(E - V(\rho\,\mathrm{e}^{\mathrm{i}\theta})) - \frac{l(l+1)}{\rho^2}$.

Define the four configurations $S(\rho) = |\Psi(\rho)|^2$, $P(\rho) = |\Psi'(\rho)|^2$, $J(\rho) = \mathrm{Im}(\Psi(\rho)\partial_\rho\Psi^*(\rho))$ and $T(\rho) = \mathrm{Im}\big(\partial_\rho\Psi(\rho)\partial_\rho^2\Psi^*(\rho)\big)$. These correspond to important physical quantities. The first two are non-negative functions corresponding to the probability density and the 'momentum density', while $J(\xi)$ is proportional to the probability flux.

The Schrödinger equation is then equivalent to the following set of coupled differential equations (i.e. $A = A_R + \mathrm{i}A_I$, etc):

$$(S''(\rho) - 2P(\rho))A_{R,I}(\rho) + S'(\rho)B_{R,I}(\rho) + 2S(\rho)C_{R,I}(\rho) \pm 2(B_{I,R}(\rho) + A_{I,R}(\rho)\partial_\rho)J(\rho) = 0 \tag{8}$$

and

$$P'(\rho)A_{R,I}(\rho) \pm 2T(\rho)A_{I,R}(\rho) + 2P(\rho)B_{R,I}(\rho) + S'(\rho)C_{R,I}(\rho) \mp 2J(\rho)C_{I,R}(\rho) = 0. \tag{9}$$

We have specified the most general form for the above, for completeness. Under the simpler assumptions indicated above (i.e. $A = 1$, $B = 0$, etc), these coupled equations reduce to three (the second relation of equation (9) defines T):

$$P(\rho) = \tfrac{1}{2}S''(\rho) + S(\rho)C_R(\rho) \tag{10}$$

$$\partial_\rho J(\rho) = S(\rho)C_I(\rho) \tag{11}$$

$$P'(\rho) + S'(\rho)C_R(\rho) - 2J(\rho)C_I(\rho) = 0. \tag{12}$$

Upon substituting the first two relations in the last equation, one obtains a fourth-order linear differential equation for S. We do not give its explicit form here (refer to Handy (2001a)).

Utilizing the above set of differential equations, we can generate the necessary moment equation for S, as required for implementation of EMM.

In each of the following sections, we detail the implementation of the above formalism for representative scattering problems.

2. The $V(r) = \frac{\alpha^2}{r^3}$ potential

We first consider the $V(r) = \frac{\alpha^2}{r^3}$ potential in order to introduce our basic formalism. It also defines one of the lowest (missing moment) dimensional problems, within our approach, with interesting properties in the complex-r plane. In particular, we can work along the positive imaginary axis.

The relevant Schrödinger equation is (we adopt a more general representation in order to accomodate problems discussed in the following sections)

$$-\Psi''(r) + \left[\frac{\alpha^2}{r^m} + \frac{l(l+1)}{r^2}\right]\Psi(r) = E\Psi(r) \tag{13}$$

for $m = 3$.

Around the origin, the dominant potential term goes as $\frac{\alpha^2}{r^m}$ $(m > 2)$. Because of its non-Fuchsian nature (i.e. the origin is an irregular singular point (Bender and Orszag 1978)), application of WKB asymptotic analysis yields for the general solution

$$\Psi(r) \approx \frac{A}{(V_{\rm eff}(r) - E)^{\frac{1}{4}}} \exp(-Q(r)) + \frac{B}{(V_{\rm eff}(r) - E)^{\frac{1}{4}}} \exp(+Q(r)) \tag{14}$$

where (to lowest order) $Q(r) = \frac{\alpha}{(\frac{m}{2}-1)} r^{1-\frac{m}{2}}$ and $V_{\rm eff}(r) = V(r) + \frac{l(l+1)}{r^2}$. We note that this result is, essentially, independent of the (complex) Regge-pole angular momentum parameter, l. Since the (true) bound state solutions (for l analytically continued onto the positive real axis) must be zero at the origin (i.e. for $r \to 0^+$, along the real axis), the Regge-pole solutions must satisfy, at $r \approx 0$,

$$\Psi_{r.p.}(r) \approx \frac{A}{(V_{\rm eff}(r) - E)^{\frac{1}{4}}} \exp(-Q(r)). \tag{15}$$

The analytic continuation of this gives

$$\Psi_{r.p.}(\rho, \theta) \approx \mathcal{N} \rho^{-\frac{m}{4}} \exp\left(-\frac{\alpha}{\left(\frac{m}{2} - 1\right)} \rho^{1-\frac{m}{2}} \exp\left({\rm i} \left(1 - \frac{m}{2} \right) \theta \right) \right). \tag{16}$$

So long as $\cos\left(\left(1 - \frac{m}{2}\right)\theta\right) > 0$, or

$$0 < \theta < \frac{\pi}{m-2} \tag{17}$$

the Regge-pole wavefunction vanishes as $\rho \to 0$, and $\theta =$ fixed. It will also be bounded on $\rho \in (0, \infty)$, due to equation (4).

From equation (7), we have $C(\rho) = C_R(\rho) + {\rm i}C_I(\rho)$, where

$$C_R(\rho) = -\frac{\alpha^2 c_1(\theta)}{\rho^3} - \frac{\Lambda_R}{\rho^2} + E c_2(\theta) \tag{18}$$

and

$$C_I(\rho) = \frac{\alpha^2 s_1(\theta)}{\rho^3} - \frac{\Lambda_I}{\rho^2} + E s_2(\theta) \tag{19}$$

involving the expressions $c_n(\theta) \equiv \cos(n\,\theta)$, $s_n(\theta) \equiv \sin(n\,\theta)$ and $\Lambda = \Lambda_R + {\rm i}\Lambda_I \equiv l(l+1)$ (hence $\Lambda_R = l_R^2 - l_I^2 + l_R$ and $\Lambda_I = 2l_R l_I + l_I$).

Let us now define the moments for the three configurations, S, P and J as $\mu_p \equiv \int_0^\infty {\rm d}\rho\, \rho^p S(\rho)$, $\nu_p \equiv \int_0^\infty {\rm d}\rho\, \rho^p P(\rho)$ and $\omega_p \equiv \int_0^\infty {\rm d}\rho\, \rho^p J(\rho)$, respectively. For the problem under consideration, the Regge-pole configuration's decaying (essential singularity) structure at the origin allows the moments to exist for all values of p: $-\infty < p < +\infty$.

Applying $\int_0^\infty {\rm d}\rho \rho^p$ to both sides of the (corresponding) coupled equations in equations (10)–(12) and integrating by parts results in the coupled moment equations

$$\nu_p = E c_2(\theta) \mu_p + \left(\frac{p(p-1)}{2} - \Lambda_R \right) \mu_{p-2} - \alpha^2 c_1(\theta) \mu_{p-3} \tag{20}$$

$$(p+1)\omega_p = -E s_2(\theta) \mu_{p+1} + \Lambda_I \mu_{p-1} - \alpha^2 s_1(\theta) \mu_{p-2} \tag{21}$$

and

$$\begin{aligned} &p\nu_{p-1} + [E c_2(\theta) p \mu_{p-1} - \Lambda_R (p-2) \mu_{p-3} - \alpha^2 c_1(\theta)(p-3)\mu_{p-4}] \\ &\quad + 2[E s_2(\theta) \omega_p - \Lambda_I \omega_{p-2} + \alpha^2 s_1(\theta) \omega_{p-3}] = 0. \end{aligned} \tag{22}$$

We see that equation (21) does not yield a relation for ω_{-1}, when $p = -1$. Instead, it gives the constraint

$$-Es_2(\theta)\mu_0 + \Lambda_I\mu_{-2} - \alpha^2 s_1(\theta)\mu_{-3} = 0. \tag{23}$$

We can rewrite equation (21) as

$$\omega_p = \Delta(p+1)(-Es_2(\theta)\mu_{p+1} + \Lambda_I\mu_{p-1} - \alpha^2 s_1(\theta)\mu_{p-2}) + \delta_{p,-1}\omega_{-1} \tag{24}$$

where

$$\Delta(p) = \begin{cases} 0 & p = 0 \\ \frac{1}{p} & p \neq 0. \end{cases} \tag{25}$$

Substituting equations (20) and (24) in equation (22) results in the *moment equation*

$$\begin{aligned}(2\alpha^2 s_1\delta_{p,2} - 2\Lambda_I\delta_{p,1} + 2Es_2\delta_{p,-1})\omega_{-1} - 2\alpha^4 s_1^2\Delta(p-2)\mu_{p-5} \\ + (\alpha^2 c_1(3-2p) + 2\alpha^2\Lambda_I s_1(\Delta(p-2) + \Delta(p-1)))\mu_{p-4} \\ + \left(2\Lambda_R(1-p) + \frac{p(p-1)(p-2)}{2} - 2\Lambda_I^2\Delta(p-1)\right)\mu_{p-3} \\ + (-2\alpha^2 Es_1s_2(\Delta(p-2) + \Delta(p+1)))\mu_{p-2} + (2c_2Ep + 2\Lambda_I Es_2(\Delta(p-1) \\ + \Delta(p+1)))\mu_{p-1} - 2E^2s_2^2\Delta(p+1)\mu_{p+1} = 0.\end{aligned} \tag{26}$$

We are particularly interested in the case where $\sin(2\theta) = 0$, or $\theta = \frac{\pi}{2}$. From equations (4) and (17) we see that along the positive imaginary axis we retain the bounded nature of the Regge-pole wavefunction. Furthermore, for this special direction, the order of the above moment equation significantly reduces. Along this direction, the moment equation becomes ($s_2 = 0, c_2 = -1, s_1 = 1, c_1 = 0$)

$$\begin{aligned}(2\alpha^2\delta_{p,2} - 2\Lambda_I\delta_{p,1})\omega_{-1} - 2\alpha^4\Delta(p-2)\mu_{p-5} + (2\alpha^2\Lambda_I(\Delta(p-2) + \Delta(p-1)))\mu_{p-4} \\ + \left(2\Lambda_R(1-p) + \frac{p(p-1)(p-2)}{2} - 2\Lambda_I^2\Delta(p-1)\right)\mu_{p-3} - 2Ep\mu_{p-1} = 0.\end{aligned} \tag{27}$$

Correspondingly, equation (23) becomes

$$\mu_{-3} = \frac{\Lambda_I}{\alpha^2}\mu_{-2}. \tag{28}$$

The above moment equation (27) and constraint (28) have a relatively complicated structure. The four moments, $\{\mu_{-2}, \mu_{-1}, \mu_0, \mu_1\}$, referred to as the *missing moments*, generate all of the other moments, including ω_{-1}. The order of this is important. Thus, for $p \geqslant 3$, all of the moments $\{\mu_{p\geqslant 2}\}$ are linearly dependent on the missing moments. The $p = 2$ moment equation determines ω_{-1}, whereas the above constraint determines μ_{-3}. Finally, for $p \leqslant 1$, the moment equation generates all the moments $\{\mu_{p\leqslant -4}\}$.

We can represent the above generation process as follows. First, it is clear that all of the moments are linearly dependent on the missing moments. We can express this by the relation

$$\mu_p = \sum_{\ell=-2}^{1} M_{p,\ell}(\Lambda_R, \Lambda_I)\mu_\ell \tag{29}$$

where

$$M_{\ell_1,\ell_2}(\Lambda_R, \Lambda_I) = \delta_{\ell_1,\ell_2} \tag{30}$$

for $-2 \leqslant \ell_{1,2} \leqslant 1$. These are referred to as the *initialization* conditions. The $M_{p,\ell}$ coefficients must satisfy the moment equation with respect to the p-index, for each fixed value of the missing moment index, ℓ. They can be generated by making use of the initialization conditions combined with the previously described process for generating the moments.

One final ingredient is the requirement of a normalization prescription. Since we will be imposing the positivity requirements of the underlying S-representation configuration, we can choose the condition

$$\sum_{\ell=-2}^{1} \mu_\ell = 1 \tag{31}$$

and solve for the μ_{-2} moment. We thus obtain the *normalized* relation

$$\mu_p = \hat{M}_{p,-2}(\Lambda_R, \Lambda_I) + \sum_{\ell=-1}^{1} \hat{M}_{p,\ell}(\Lambda_R, \Lambda_I)\mu_\ell \tag{32}$$

where

$$\hat{M}_{p,\ell} = \begin{cases} M_{p,-2} & \ell = -2 \\ M_{p,\ell} - M_{p,-2} & \ell \neq -2. \end{cases} \tag{33}$$

The unconstrained, normalized, missing moments are restricted to values within the unit cube: $(\mu_{-1}, \mu_0, \mu_1) \in [0, 1]^3$.

The EMM algorithm involves determining the Regge-pole values $l = (l_R, l_I)$, that satisfy the Hankel–Hadamard inequalities (Handy *et al* 1988a, 1988b)

$$\int_0^\infty \mathrm{d}\rho\, \rho^s \left(\sum_{j=-J_1}^{J_2} C_j \rho^j \right)^2 S(\rho) > 0 \tag{34}$$

or

$$\sum_{j_1=-J_1}^{J_2} \sum_{j_2=-J_1}^{J_2} C_{j_1} \mu_{s+j_1+j_2} C_{j_2} > 0 \tag{35}$$

for arbitrary C_j (not all identically zero) and $s = -1, 0, 1$.

Upon inserting the moment/missing moment relation, the above inequalities become linear programming inequalities with respect to the unconstrained missing moments:

$$\sum_{\ell=-1}^{1} \left(- \sum_{j_1=-J_1}^{J_2} \sum_{j_2=-J_1}^{J_2} C_{j_1} \hat{M}_{s+j_1+j_2,\ell}(E, \Lambda(l)) C_{j_2} \right) \mu_\ell$$
$$< \left(\sum_{j_1=-J_1}^{J_2} \sum_{j_2=-J_1}^{J_2} C_{j_1} \hat{M}_{s+j_1+j_2,0}(E, \Lambda(l)) C_{j_2} \right). \tag{36}$$

The physical Regge-pole value, l, uniquely satisfies these inequalities for arbitrary C ($J_{1,2} < \infty$). That is, at a given expansion order $J_{1,2}$, the feasible Regge-pole values $l = (l_R, l_I)$ are those for which there exists a missing moment solution set, $\mathcal{U}^{(J_1,J_2)}(l)$, necessarily convex, satisfying the above inequalities for arbitrary C. As the expansion order approaches infinity, the set of feasible Regge-pole values reduces to the set of isolated points corresponding to the physical Regge-pole values. The missing moment solution set, $\mathcal{U}^{(\infty,\infty)}(l_{r.p.})$, for each physical Regge-pole value, $l_{r.p.}$, also reduces to an $m_s(=3)$ dimensional vector (i.e. a point, geometrically).

The EMM algorithmic structure uses linear programming to determine the existence, or non-existence, of $\mathcal{U}^{(J_1,J_2)}(l)$ for arbitrary l. It does this through implementation of a fast *cutting (bisection) method* that generates a bounding polytope (i.e. a convex set bounded by

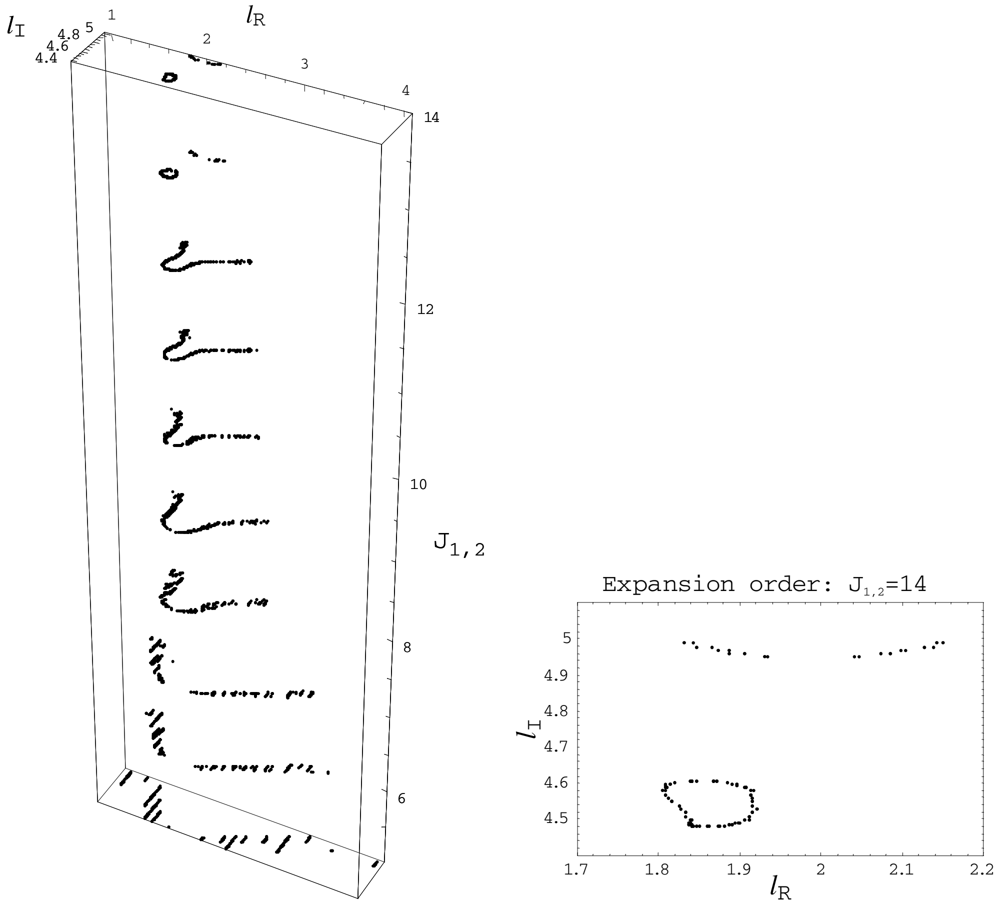

Figure 1. The formation of the bounding region for the first Regge pole of the $\frac{2}{r^3}$ potential.

Table 1. The bounds for the low-lying Regge pole of the $V(r) = \frac{2}{r^3}$ potential ($\theta = \frac{\pi}{2}$).

$(-J_1, J_2)$	$l_R^{(L)} < l_R < l_R^{(U)}$	$l_I^{(L)} < l_I < l_I^{(U)}$
$(-14, 14)$	$1.807 < l_R < 1.920$	$4.48 < l_I < 4.63$
$(-16, 16)$	$1.832 < l_R < 1.880$	$4.53 < l_I < 4.58$
$(-18, 18)$	$1.8426 < l_R < 1.8645$	$4.5533 < l_I < 4.5667$
$(-20, 20)$	$1.8538 < l_R < 1.8584$	$4.5553 < l_I < 4.5647$

intersecting hyperplanes), $\mathcal{P}$, within which the missing moment solution set must lie (if it exists): $\mathcal{U}^{(J_1,J_2)}(l) \subset \mathcal{P}^{(J_1,J_2)}(l)$. If the solution set does not exist, then the cutting method quickly reduces the initial (missing moment) unit hypercube to the null set.

The determination of the feasible l values, to given expansion order, requires a two-dimensional partitioning search within the complex $\mathcal{C}_l$ plane.

In table 1, we cite a few results for the $\frac{2}{r^3}$ potential. In figure 1 we depict the formation of the bounding region for the first Regge pole, for various expansion order values (i.e. $14 \leqslant J_1 = J_2 \leqslant 20$).

3. The $V(r) = \frac{\alpha^2}{r^4}$ polarization potential

The polarization potential problem $V(r) = \frac{\alpha^2}{r^4}$ has received much attention in the recent works by Vrinceanu *et al* (2000a) and Avdonina *et al* (2001). From the EMM–Regge analysis perspective, it defines a low dimension missing moment problem capable of generating tight Regge-pole bounds.

The relevant Schrödinger equation is

$$-\Psi''(r) + \left[\frac{\alpha^2}{r^4} + \frac{l(l+1)}{r^2}\right]\Psi(r) = E\Psi(r). \tag{37}$$

From equation (7), we have

$$C_R(\rho) = -\frac{\alpha^2 c_2(\theta)}{\rho^4} - \frac{\Lambda_R}{\rho^2} + Ec_2(\theta) \tag{38}$$

and

$$C_I(\rho) = \frac{\alpha^2 s_2(\theta)}{\rho^4} - \frac{\Lambda_I}{\rho^2} + Es_2(\theta). \tag{39}$$

Applying $\int_0^\infty \mathrm{d}\rho\, \rho^p$ to both sides of the (corresponding) coupled equations in equations (10)–(12) and integrating by parts results in the coupled moment equations

$$\nu_p = Ec_2(\theta)\mu_p + \left(\frac{p(p-1)}{2} - \Lambda_R\right)\mu_{p-2} - \alpha^2 c_2(\theta)\mu_{p-4} \tag{40}$$

$$(p+1)\omega_p = -Es_2(\theta)\mu_{p+1} + \Lambda_I\mu_{p-1} - \alpha^2 s_2(\theta)\mu_{p-3} \tag{41}$$

and

$$\begin{aligned} &p\nu_{p-1} + [Ec_2(\theta)p\mu_{p-1} - \Lambda_R(p-2)\mu_{p-3} - \alpha^2 c_2(\theta)(p-4)\mu_{p-5}] \\ &\quad + 2[Es_2(\theta)\omega_p - \Lambda_I\omega_{p-2} + \alpha^2 s_2(\theta)\omega_{p-4}] = 0. \end{aligned} \tag{42}$$

Two sets of equations ensue for the $p = even/odd$ cases. Either one can be used. The easier one corresponds to the $p = even$ case, since no zero denominators are encountered in solving for ω_p. The $p = odd$ case is discussed in the following section.

Implicitly assuming that $p = even$, we can substitute in equation (42) for ν_p and ω_p, obtaining the *moment equation*

$$\begin{aligned} &\left[\frac{2s_2^2E^2}{p+1}\right]\mu_{p+1} - \left[2c_2Ep + 2\Lambda_I s_2 E\left(\frac{1}{p+1} + \frac{1}{p-1}\right)\right]\mu_{p-1} + \left[-\frac{p}{2}((p-1)(p-2)\right. \\ &\quad \left. - 2\Lambda_R) + (p-2)\Lambda_R + 2\frac{\Lambda_I^2}{p-1} + 2s_2^2\alpha^2 E\left(\frac{1}{p+1} + \frac{1}{p-3}\right)\right]\mu_{p-3} \\ &\quad + \left[2\alpha^2 c_2(p-2) - 2\Lambda_I\alpha^2 s_2\left(\frac{1}{p-3} + \frac{1}{p-1}\right)\right]\mu_{p-5} + 2\left[\frac{\alpha^4 s_2^2}{p-3}\right]\mu_{p-7} = 0 \end{aligned} \tag{43}$$

where $p = even$!

Adopting the notation $p = 2\eta$, where $-\infty < \eta < +\infty$, we note that the odd-order moments, $\mu_{2\eta+1}$, correspond to the moments of the function $\Upsilon(\xi) \equiv \frac{1}{2}S(\sqrt{\xi})$, where $\xi \equiv \rho^2$. We denote the moments of $\Upsilon(\xi)$ by $u_\eta \equiv \int_0^\infty \mathrm{d}\xi\, \xi^\eta \Upsilon(\xi) = \mu_{2\eta+1}$.

The new moment equation becomes

$$\begin{aligned}\left[2s_2^2E^2D(\eta)\right]u_\eta &- [4c_2E\eta + 2\Lambda_I s_2E(D(\eta) + D(\eta-1)]u_{\eta-1}\\ &+[-2\eta((2\eta-1)(\eta-1) - \Lambda_R) + 2(\eta-1)\Lambda_R + 2\Lambda_I^2D(\eta-1)\\ &+2s_2^2\alpha^2E(D(\eta) + D(\eta-2)]u_{\eta-2} + [4\alpha^2c_2(\eta-1) - 2\Lambda_I\alpha^2s_2(D(\eta-1)\\ &+D(\eta-2))]u_{\eta-3} + 2\left[\alpha^4s_2^2D(\eta-2)\right]u_{\eta-4} = 0 \end{aligned} \tag{44}$$

where $D(\eta) \equiv \frac{1}{2\eta+1}$.

This corresponds to a finite difference equation of order 4, since specification of the missing moments $\{u_0, u_1, u_2, u_3\}$ is required before all of the other moments can be generated (i.e. take $\eta \geqslant 4$, thereby generating $u_{\geqslant 4}$ and $\eta \leqslant 3$, generating $u_{\leqslant -1}$).

The linear dependence on the missing moments can be expressed in terms of the relation

$$u_\eta = \sum_{\ell=0}^{3} M_{\eta,\ell}(E, \Lambda(l))u_\ell \tag{45}$$

where the $M_{\eta,\ell}(E, \Lambda(l))$ coefficients satisfy the above moment equation with respect to the η-index, and in addition must satisfy the initialization conditions

$$M_{\ell_1,\ell_2} = \delta_{\ell_1,\ell_2} \tag{46}$$

for $0 \leqslant \ell_{1,2} \leqslant 3$.

A normalization condition is required. One can impose $\sum_{\ell=0}^{m_s=3} u_\ell = 1$. Solving for u_0 yields the relation

$$u_\eta = \hat{M}_{\eta,0}(E, \Lambda(l)) + \sum_{\ell=1}^{3} \hat{M}_{\eta,\ell}(E, \Lambda(l))u_\ell \tag{47}$$

where

$$\hat{M}_{\eta,\ell}(E, \Lambda(l)) = \begin{cases} M_{\eta,0}(E, \Lambda(l)) & \text{for} \quad \ell = 0 \\ M_{\eta,\ell}(E, \Lambda(l)) - M_{\eta,0}(E, \Lambda(l)) & \text{for} \quad \ell = 1, 2, 3. \end{cases} \tag{48}$$

As in the previous problem, the unconstrained, normalized, missing moments are always constrained to assume values within the unit hypercube: $(u_1, \ldots, u_{m_s}) \in [0, 1]^{m_s}$.

The EMM algorithm involves determining the Regge-pole values $l = (l_R, l_I)$, that satisfy the Hankel–Hadamard inequalities

$$\int_0^\infty \mathrm{d}\xi\, \xi^s \left(\sum_{j=-J_1}^{J_2} C_j \xi^j\right)^2 \Upsilon(\xi) > 0 \tag{49}$$

or

$$\sum_{j_1=-J_1}^{J_2} \sum_{j_2=-J_1}^{J_2} C_{j_1} u_{s+j_1+j_2} C_{j_2} > 0 \tag{50}$$

for arbitrary C_j (not all identically zero) and $s = -1, 0, 1$.

Upon inserting the moment/missing moment relation, the above inequalities become linear programming inequalities with respect to the unconstrained missing moments, as discussed previously.

In table 2, we cite a few results for the polarization problem. We compare our bounds to the results derived from Avdonina *et al*'s (2001) turning point analysis estimation formula for the nth Regge pole:

$$l_n \approx -\frac{1}{2} + (1 + \mathrm{i})(\alpha k)^{\frac{1}{2}} + \mathrm{i}\left(\sqrt{2}n + \frac{1}{\sqrt{2}}\right). \tag{51}$$

Table 2. The bounds for the low-lying Regge poles of the $V(r) = \frac{2}{r^4}$ polarization potential ($\theta = \frac{\pi}{4}$).

$(-J_1, J_2)$	$l_R^{(L)} < l_R < l_R^{(U)}$	$l_I^{(L)} < l_I < l_I^{(U)}$	l_n, equation (51)
(−12, 12)	$4.796 < l_R < 4.842$	$5.92 < l_I < 6.20$	
(−16, 16)	$4.826 < l_R < 4.832$	$5.976 < l_I < 6.060$	
(−20, 20)	$4.827\,14 < l_R < 4.829\,84$	$6.006\,24 < l_I < 6.026\,40$	
(−24, 24)	$4.828\,827 < l_R < 4.829\,081$	$6.012\,00 < l_I < 6.016\,12$	$(4.818\,296, 6.025\,403)_{n=0}$
(−12, 12)	$4.34 < l_R < 6.51$	$6.6 < l_I < 9.4$ (no bound[a])	
(−16, 16)	$4.89 < l_R < 5.98$	$6.9 < l_I < 9.4$ (no bound[a])	
(−24, 24)	$4.920 < l_R < 4.953$	$7.20 < l_I < 7.58$	$(4.818\,296, 7.439\,616)_{n=1}$

[a] The bound is artificial, due to its being the endpoint of the sampling interval in question.

Table 3. The tightness of polarization potential bounds for varying θ, where $(-J_1, J_2) = (-12, 12)$.

θ	$l_R^{(L)} < l_R < l_R^{(U)}$	$l_I^{(L)} < l_I < l_I^{(U)}$
0.3	$2.3 < l_R < 7.3$	$4.72 < l_I < 8$ (no bound[a])
0.4	$2.9 < l_R < 8.4$	$5.44 < l_I < 8$ (no bound[a])
0.5	$3.5 < l_R < 9.0$	$5.68 < l_I < 8$ (no bound[a])
0.6	$4.08 < l_R < 8.07$	$5.80 < l_I < 8$ (no bound[a])
0.7	$4.79 < l_R < 4.84$	$5.96 < l_I < 6.12$
$\frac{\pi}{4} = 0.785\,40$	$4.796 < l_R < 4.842$	$5.92 < l_I < 6.20$
0.8	$4.795 < l_R < 4.846$	$5.92 < l_I < 6.20$
0.9	$4.686 < l_R < 4.991$	$5.84 < l_I < 6.32$
1.0	$3.97 < l_R < 8.11$	$5.76 < l_I < 8$ (no bound[a])
1.1	$3.4 < l_R < 9.8$	$5.52 < l_I < 8$ (no bound[a])

[a] The bound is artificial, due to its being the endpoint of the sampling interval in question.

We take $k = 20$ and $\alpha^2 = 2$. Since $\theta < \frac{\pi}{2}$ from equation (17), we can take $\theta = \frac{\pi}{4}$, resulting in $s_2 = 1$, and eliminating the numerical problems associated with small denominators.

Our numerical results were implemented with rescaled moments, $\tilde{u}_\eta = \frac{u_\eta}{f^\eta}$, where we choose f so that the $\tilde{u}$-moment equation coefficients (obtainable from equation (44)) for the $\tilde{u}_\eta$ and $\tilde{u}_{\eta-4}$ terms are identical: $f = \frac{\alpha}{k}$.

In table 3 we compare the tightness of the bounds, with varying θ values, for the first Regge pole. Usually, tighter bounds are achieved when the associated wavefunction configuration decays faster. For singular potential problems, the decay characteristics near the origin, $\rho \approx 0$, and at infinity, $\rho \to \infty$, in accordance with the relations cited in equation (4) and equations (16) and (17), respectively, affect the tightness of the bounds. The fastest decay, near the origin, is along the real axis ($\theta = 0$). The fastest decay, at infinity, is along the imaginary axis $\left(\theta = \frac{\pi}{2}\right)$. Of course, we are limited by $0 < \theta < \frac{\pi}{2}$ for the polarization problem. The decay characteristics worsen at the origin, as θ becomes more positive. Similarly, the decay characteristics at infinity also become less rapid, as θ decreases.

For the case of the polarization potential, we have $S(\rho) \approx \mathcal{N}_1 \rho^2 \exp\left(-\frac{2\alpha\cos(\theta)}{\rho}\right)$, as $\rho \to 0$. Also, $S(\rho) \approx \mathcal{N}_2 \exp(-2k\sin(\theta)\rho)$, as $\rho \to \infty$. If we rescale in accordance with $\tilde{\rho} = \frac{\rho}{\sqrt{f}}$, we see that the coefficients within the arguments of the exponentials become $\frac{2\alpha\cos(\theta)}{\sqrt{f}}$ and $2k\sin(\theta)\sqrt{f}$. Thus, for this problem, we have identical (asymptotic) exponential decay (with respect to the $\frac{1}{\rho}$ and ρ variables, respectively) when both coefficients are equal to each other. Since $f \equiv \frac{\alpha}{k}$, where $E = k^2$, it follows that the tightest bounds are to be expected near $\theta \approx \frac{\pi}{4}$, as given in table 3.

Table 4. The improved bounds for the low-lying Regge poles of the $V(r) = \frac{2}{r^4}$ polarization potential ($\theta = \frac{\pi}{4}$).

k	$(-J_1, J_2)$	$l_R^{(L)} < l_R < l_R^{(U)}$	$l_I^{(L)} < l_I < l_I^{(U)}$	l_n, equation (51)
20	$(-12, 12)$	$4.8172 < l_R < 4.8388$	$5.992 < l_I < 6.048$	
20	$(-16, 16)$	$4.8275 < l_R < 4.8305$	$6.01 < l_I < 6.02$	
20	$(-20, 20)$	$4.828\,79 < l_R < 4.829\,11$	$6.012 < l_I < 6.016$	$(4.818\,296, 6.025\,403)_{n=0}$
20	$(-12, 12)$	$4.21 < l_R < 8.10$	$6.88 < l_I < 10.8$ (no bound[a])	
20	$(-20, 20)$	$4.92 < l_R < 4.94$	$7.20 < l_I < 7.43$	
24	$(-24, 24)$	$4.922 < l_R < 4.9302$	$7.25 < l_I < 7.34$	$(4.818\,296, 7.439\,616)_{n=1}$

[a] The bound is artificial, due to its being the endpoint of the sampling interval in question.

In the last section of this work we analyse the Bohr potential (a non-singular case), where the bounds do improve as $\theta \to \frac{\pi}{2}$. This is because the relevant EMM analysis does not involve any angular dependences associated with the origin. One is free to take $\theta \to \frac{\pi}{2}$.

3.1. Improving the tightness of the bounds

We can improve the previous results by also imposing the constraints corresponding to the non-negativity of the $P(\rho)$ configuration. Thus, from equation (40), taking $p = 2\eta + 1$ (so as to convert it into a moment equation involving the odd-order μ moments), we obtain

$$v_\eta = Ec_2(\theta)u_\eta + (\eta(2\eta+1) - \Lambda_R)u_{\eta-1} - \alpha^2 c_2(\theta)u_{\eta-2} \tag{52}$$

where $v_\eta \equiv \nu_{2\eta+1}$. We can then rescale this relation:

$$\tilde{v}_\eta = Ec_2(\theta)\tilde{u}_\eta + f^{-1}(\eta(2\eta+1) - \Lambda_R)\tilde{u}_{\eta-1} - f^{-2}\alpha^2 c_2(\theta)\tilde{u}_{\eta-2} \tag{53}$$

where $\tilde{v}_\eta \equiv \frac{v_\eta}{f^\eta}$, etc.

The normalized and rescaled $\tilde{u}$-moment equation can be written as $\tilde{u}_\eta = \hat{M}^{(f)}{}_{\eta,0} + \sum_{\ell=1}^{3} \hat{M}^{(f)}{}_{\eta,\ell}\tilde{u}_\ell$ (we omit the details of this obvious procedure). Substituting above, we can also rewrite the $\tilde{v}$-moment equation in an analogous form: $\tilde{v}_\eta = \hat{N}^{(f)}_{\eta,0} + \sum_{\ell=1}^{3} \hat{N}^{(f)}_{\eta,\ell}\tilde{u}_\ell$, and proceed to generate the moment problem constraints as before. The results of this analysis are given in table 4. It is evident that a few orders of magnitude improvement, in the generated bounds, are obtained.

Clearly, the generated bounds establish some important limitations in the accuracy of the asymptotic analysis by Avdonina *et al*. Their estimation formula is off by 0.2% and 2%, for the first and second Regge-pole values, respectively.

4. The $V(r) = \frac{\alpha^2}{r^6} - \frac{\beta^2}{r^4}$ scattering potential

In this section we expand upon the abbreviated discussion presented by Handy and Msezane (2001) with regards to the Lennard-Jones problem defined by (i.e. $\alpha > 0$)

$$-\Psi''(r) + \left[\frac{\alpha^2}{r^6} - \frac{\beta^2}{r^4} + \frac{l(l+1)}{r^2}\right]\Psi(r) = E\Psi(r) \tag{54}$$

previously investigated by Amaha and Thylwe (1991, 1994).

The relevant $C_{R,I}(\rho)$ functions become

$$C_R(\rho) = -\frac{\alpha^2 c_4(\theta)}{\rho^6} + \frac{\beta^2 c_2(\theta)}{\rho^4} - \frac{\Lambda_R}{\rho^2} + Ec_2(\theta) \tag{55}$$

and

$$C_I(\rho) = \frac{\alpha^2 s_4(\theta)}{\rho^6} - \frac{\beta^2 s_2(\theta)}{\rho^4} - \frac{\Lambda_I}{\rho^2} + E s_2(\theta) \tag{56}$$

involving the expressions $c_n(\theta) \equiv \cos(n\,\theta)$, $s_n(\theta) \equiv \sin(n\,\theta)$ and $\Lambda = \Lambda_R + \mathrm{i}\Lambda_I \equiv l(l+1)$ (hence $\Lambda_R = l_R^2 - l_I^2 + l_R$ and $\Lambda_I = 2l_R l_I + l_I$).

As in the polarization potential case, define the moments for the three configurations, S, P and J as $\mu_p \equiv \int_0^\infty \mathrm{d}\rho\, \rho^p S(\rho)$, $\nu_p \equiv \int_0^\infty \mathrm{d}\rho\, \rho^p P(\rho)$ and $\omega_p \equiv \int_0^\infty \mathrm{d}\rho\, \rho^p J(\rho)$. As before, Regge-pole configuration's decaying (essential singularity) structure at the origin allows the moments to exist for all values of p: $-\infty < p < +\infty$.

Applying $\int_0^\infty \mathrm{d}\rho\, \rho^p$ to both sides of the (corresponding) coupled equations in equations (10)–(12) and integrating by parts results in the coupled moment equations

$$\nu_p = E c_2(\theta)\mu_p + \left(\frac{p(p-1)}{2} - \Lambda_R\right)\mu_{p-2} + \beta^2 c_2(\theta)\mu_{p-4} - \alpha^2 c_4(\theta)\mu_{p-6} \tag{57}$$

$$p\omega_{p-1} = -E s_2(\theta)\mu_p + \Lambda_I \mu_{p-2} + \beta^2 s_2(\theta)\mu_{p-4} - \alpha^2 s_4(\theta)\mu_{p-6} \tag{58}$$

and

$$\begin{aligned} p\nu_{p-1} &+ [E c_2(\theta) p\mu_{p-1} - \Lambda_R(p-2)\mu_{p-3} + \beta^2 c_2(\theta)(p-4)\mu_{p-5} - \alpha^2 c_4(\theta)(p-6)\mu_{p-7}] \\ &+ 2[E s_2(\theta)\omega_p - \Lambda_I \omega_{p-2} - \beta^2 s_2(\theta)\omega_{p-4} + \alpha^2 s_4(\theta)\omega_{p-6}] = 0. \end{aligned} \tag{59}$$

We see that the second moment equation (58) determines all the ω-moments, in terms of the μ-moments, except for ω_{-1} (for $p = 0$). Adopting Handy and Msezane's (2001) notation, let us therefore rewrite this as ($p \to p+1$)

$$\omega_p = \Omega(p)(-E s_2(\theta)\mu_{p+1} + \Lambda_I \mu_{p-1} + \beta^2 s_2(\theta)\mu_{p-3} - \alpha^2 s_4(\theta)\mu_{p-5}) + \delta_{p,-1}\omega_{-1} \tag{60}$$

where

$$\Omega(p) = \begin{cases} \dfrac{1}{p+1} & p \neq -1 \\ 0 & p = -1 \end{cases} \tag{61}$$

and $\delta_{p,-1}$ is the Kronecker delta function (i.e. $\Omega(p) \equiv \Delta(p+1)$, in equation (24)).

Substituting equations (57) and (60) in equation (59), one obtains the μ-moment equation

$$\begin{aligned} 2\alpha^4 s_4^2(\theta)\Omega(p-6)\mu_{p-11} &- 2\alpha^2\beta^2 s_2(\theta)s_4(\theta)[\Omega(p-6) + \Omega(p-4)]\mu_{p-9} \\ &+ \left[2\alpha^2 c_4(\theta)(p-3) - 2\alpha^2 s_4(\theta)\Lambda_I \Omega(p-6) + 2\beta^4 s_2^2(\theta)\Omega(p-4)\right. \\ &\left.- 2\alpha^2\Lambda_I s_4(\theta)\Omega(p-2)\right]\mu_{p-7} + [2\beta^2(c_2(\theta)(2-p) + \Lambda_I s_2(\theta)(\Omega(p-2) \\ &+ \Omega(p-4))) + 2\alpha^2 E s_2(\theta)s_4(\theta)(\Omega(p) + \Omega(p-6))]\mu_{p-5} \\ &+ \left[-2\Lambda_R - p + 2\Lambda_R p + \tfrac{3}{2}p^2 - \tfrac{1}{2}p^3 - 2\beta^2 E s_2^2(\theta)\Omega(p-4)\right. \\ &\left.+ 2\Lambda_I^2\Omega(p-2) - 2\beta^2 E s_2^2(\theta)\Omega(p)\right]\mu_{p-3} \\ &- 2E[c_2(\theta)p + \Lambda_I s_2(\theta)(\Omega(p-2) + \Omega(p))]\mu_{p-1} + 2E^2 s_2^2(\theta)\Omega(p)\mu_{p+1} \\ &+ 2[-\alpha^2 s_4(\theta)\delta_{p-6,-1} + \beta^2 s_2(\theta)\delta_{p-4,-1} + \Lambda_I\delta_{p-2,-1} - E s_2(\theta)\delta_{p,-1}]w_{-1} = 0. \end{aligned} \tag{62}$$

In addition, we also have from equation (58) (i.e. $p = 0$):

$$-E s_2(\theta)\mu_0 + \Lambda_I\mu_{-2} + \beta^2 s_2(\theta)\mu_{-4} - \alpha^2 s_4(\theta)\mu_{-6} = 0. \tag{63}$$

These equations split into two recursive relations, one for the even-order moments $\{\mu_{2\eta} | -\infty < \eta < +\infty\}$, the other for the odd moments $\{\mu_{2\eta+1} | -\infty < \eta < +\infty\}$. We can work either one of these. For completeness, we detail the form of both relationships.

The first set corresponds to the moments of the function $\Upsilon_e(\xi) \equiv \frac{1}{2\sqrt{\xi}} S(\sqrt{\xi})$, as is evident from the change of variables $\rho^2 = \xi$: $\mu_{2\eta} = \int_0^\infty d\rho\, \rho^{2\eta} S(\rho)$, or $\mu_{2\eta} = \int_0^\infty d\xi\, \xi^\eta \Upsilon_e(\xi)$. The odd-order moments, $\mu_{2\eta+1}$, are the moments of the function $\Upsilon_o(\xi) \equiv \frac{1}{2} S(\sqrt{\xi})$, through a similar argument. We will designate these moments as follows:

$$\mu_{2\eta+\sigma} = \begin{cases} u_\eta^e & \sigma = 0 \\ u_\eta^o & \sigma = 1. \end{cases} \tag{64}$$

The ensuing moment equations become (i.e. $p = 2\eta$)

$$\begin{aligned}
&2\alpha^4 s_4^2(\theta)\Omega(2\eta-6)u_{\eta-6}^o - 2\alpha^2\beta^2 s_2(\theta)s_4(\theta)[\Omega(2\eta-6)+\Omega(2\eta-4)]u_{\eta-5}^o \\
&\quad + \left[2\alpha^2 c_4(\theta)(2\eta-3) - 2\alpha^2 s_4(\theta)\Lambda_I\Omega(2\eta-6) + 2\beta^4 s_2^2(\theta)\Omega(2\eta-4)\right. \\
&\quad \left. - 2\alpha^2\Lambda_I s_4(\theta)\Omega(2\eta-2)\right] u_{\eta-4}^o + [2\beta^2(c_2(\theta)(2-2\eta) + \Lambda_I s_2(\theta)(\Omega(2\eta-2) \\
&\quad + \Omega(2\eta-4))) + 2\alpha^2 E s_2(\theta)s_4(\theta)(\Omega(2\eta)+\Omega(2\eta-6))]u_{\eta-3}^o \\
&\quad + \left[-2\Lambda_R - 2\eta + 4\Lambda_R\eta + \tfrac{3}{2}(2\eta)^2 - \tfrac{1}{2}(2\eta)^3 - 2\beta^2 E s_2^2(\theta)\Omega(2\eta-4)\right. \\
&\quad \left. + 2\Lambda_I^2\Omega(2\eta-2) - 2\beta^2 E s_2^2(\theta)\Omega(2\eta)\right] u_{\eta-2}^o - 2E[c_2(\theta)2\eta \\
&\quad + \Lambda_I s_2(\theta)(\Omega(2\eta-2)+\Omega(2\eta))]u_{\eta-1}^o + 2E^2 s_2^2(\theta)\Omega(2\eta)u_\eta^o = 0
\end{aligned} \tag{65}$$

and (i.e. $p = 2\eta + 1$)

$$\begin{aligned}
&2\alpha^4 s_4^2(\theta)\Omega(2\eta-5)u_{\eta-5}^e - 2\alpha^2\beta^2 s_2(\theta)s_4(\theta)[\Omega(2\eta-5)+\Omega(2\eta-3)]u_{\eta-4}^e \\
&\quad + \left[2\alpha^2 c_4(\theta)(2\eta-2) - 2\alpha^2 s_4(\theta)\Lambda_I\Omega(2\eta-5)\right. \\
&\quad \left. + 2\beta^4 s_2^2(\theta)\Omega(2\eta-3) - 2\alpha^2\Lambda_I s_4(\theta)\Omega(2\eta-1)\right] u_{\eta-3}^e \\
&\quad + [2\beta^2(c_2(\theta)(1-2\eta) + \Lambda_I s_2(\theta)(\Omega(2\eta-1)+\Omega(2\eta-3))) \\
&\quad + 2\alpha^2 E s_2(\theta)s_4(\theta)(\Omega(2\eta+1)+\Omega(2\eta-5))]u_{\eta-2}^e \\
&\quad + \left[-2\Lambda_R - (2\eta+1) + 2\Lambda_R(2\eta+1) + \tfrac{3}{2}(2\eta+1)^2 - \tfrac{1}{2}(2\eta+1)^3\right. \\
&\quad \left. - 2\beta^2 E s_2^2(\theta)\Omega(2\eta-3) + 2\Lambda_I^2\Omega(2\eta-1) - 2\beta^2 E s_2^2(\theta)\Omega(2\eta+1)\right] u_{\eta-1}^e \\
&\quad - 2E[c_2(\theta)(2\eta+1) + \Lambda_I s_2(\theta)(\Omega(2\eta-1)+\Omega(2\eta+1))]u_\eta^e \\
&\quad + 2E^2 s_2^2(\theta)\Omega(2\eta+1)u_{\eta+1}^e + 2[-\alpha^2 s_4(\theta)\delta_{\eta,2} + \beta^2 s_2(\theta)\delta_{\eta,1} \\
&\quad + \Lambda_I\delta_{\eta,0} - E s_2(\theta)\delta_{\eta,-1}]\omega_{-1} = 0
\end{aligned} \tag{66}$$

together with

$$-E s_2(\theta)u_0^e + \Lambda_I u_{-1}^e + \beta^2 s_2(\theta)u_{-2}^e - \alpha^2 s_4(\theta)u_{-3}^e = 0. \tag{67}$$

The moment equation for the u_η^e moments involves the ω_{-1} moment. Both moment equations are recursively generated in both the positive and negative asymptotic directions with respect to η, as described below.

The u_η^o moments satisfy a sixth-order finite difference equation. We can pick $\{u_{-5}^o, u_{-4}^o, \ldots, u_0^o\}$ as the initialization, or missing moments. All of the other moments are linearly dependent on them. We express this as

$$u_\eta^o = \sum_{\ell=-5}^{0} M_{\eta,\ell}^o(l_R, l_I)u_\ell^o \tag{68}$$

where $M_{\ell_1,\ell_2}^o = \delta_{\ell_1,\ell_2}$, for $-5 \leqslant \ell_{1,2} \leqslant 0$. In addition, the $M_{\eta,\ell}^o$ coefficients satisfy the corresponding u_η^o-moment equation with respect to the η-index. To generate the u^o (as well as the M^o coefficients) we take $\eta \geqslant 1$, and generate the positive-indexed moments $\{u_{\eta\geqslant 1}^o\}$, from equation (65) (i.e. using the $2E^2 s_2^2(\theta)\Omega(2\eta)u^o_\eta$ term). We then take $\eta \leqslant 0$ in equation (65), and use the first term (i.e. $2\alpha^4 s_4^2(\theta)\Omega(2\eta-6)u^o_{\eta-6}$) to generate all the remaining negative-indexed moments. We will generate the moments $\{u^o_{P_1}, \ldots, u^o_{P_2}\}$, where $P_1 \leqslant -6$ and $P_2 \geqslant 1$.

A similar, although more involved, process holds for the u^e_η moments. In particular, the ω_{-1} effectively becomes an inhomogeneous term. More precisely, from equation (66), it follows that knowledge of the initialization variables $\{\chi_\ell | -3 \leqslant \ell \leqslant 3\} \equiv \{u^e_{-3}, \ldots, u^e_2\} \bigcup \{\omega_{-1}\}$ generates all of the moments $\{u^e_{\leqslant -4} | \eta \leqslant 1$ in equation (66)$\} \bigcup \{u^e_{\geqslant 3} | \eta \geqslant 2$ in equation (66)$\}$. This linear dependence on the initialization variables can be represented as

$$u^e_\eta = \sum_{\ell=-3}^{3} M^e_{\eta,\ell}(l_R, l_I)\chi_\ell \tag{69}$$

for all $\eta \in (-\infty, +\infty)$, where $\{\chi_{-3}, \chi_{-2}, \ldots, \chi_3\} \equiv \{u^e_{-3}, u^e_{-2}, \ldots, u^e_2, \omega_{-1}\}$.

Care must be exercised in defining the appropriate initialization conditions. Specifically,

$$M^e_{\eta,\ell} = \delta_{\eta,\ell} \qquad -3 \leqslant \eta \leqslant 2, \quad -3 \leqslant \ell \leqslant 3. \tag{70}$$

However, one must now also incorporate the additional constraint from equation (67). Eliminating $\chi_{-3} \equiv u^e_{-3}$, or $u^e_{-3} = \sum_{\ell=-2}^{0} \Gamma_\ell u^e_\ell$ (where $\Gamma_{-2} = \frac{\beta^2 s_2(\theta)}{\alpha^2 s_4(\theta)}$, $\Gamma_{-1} = \frac{\Lambda_I}{\alpha^2 s_4(\theta)}$, $\Gamma_0 = -\frac{E s_2(\theta)}{\alpha^2 s_4(\theta)}$), yields a new linear relation:

$$u^e_\eta = \sum_{\ell=-2}^{3} \tilde{M}^e_{\eta,\ell}(l_R, l_I)\chi_\ell \tag{71}$$

where $\tilde{M}^e_{\eta,\ell}(l_R, l_I) = M^e_{\eta,\ell}(l_R, l_I) + M^e_{\eta,-3}(l_R, l_I)\Gamma_\ell$, for $-2 \leqslant \ell \leqslant 0$ and $\tilde{M}^e_{\eta,\ell}(l_R, l_I) = M^e_{\eta,\ell}(l_R, l_I)$, for $1 \leqslant \ell \leqslant 3$.

Unlike the u^e missing moments, ω_{-1}'s signature is arbitrary. One can proceed with an EMM analysis taking this into account. However, it is usually more convenient to work with non-negative linear programming variables. Thus, we can invert the $\eta = 2$ relation above and solve for ω_{-1} in terms of $\{u^e_{-2}, \ldots, u^e_3\}$. Thus, the final set of variables becomes $\{u^e_{-2}, \ldots, u^e_3\}$. Let us denote by $u^e_\eta = \sum_{\ell=-2}^{3} \tilde{\tilde{M}}_{\eta,\ell}(l_R, l_I)u^e_\ell$ the final linear relation, after substituting u^e_3 for ω_{-1}. We can then proceed to impose the normalization condition previously described, and implement the EMM algorithm.

Instead of the preceding circuitous analysis, we can achieve the same through a more direct approach. Let us symbolize equation (66), for $-\infty \leqslant \eta \leqslant +\infty$, as follows (we take $\Xi_{-5} \equiv 2\alpha^2 s_4^2(\theta)$ and $\Xi_1 \equiv 2E^2 s_2^2(\theta)$, and make use of $\Omega(-1) = 0$):

$$\begin{aligned}
&\Xi_{-5}\Omega(-9)u^e_{-7} + \cdots + \Xi_1\Omega(-3)u^e_{-1} = 0 && \text{for} \quad \eta = -2 \\
&\Xi_{-5}\Omega(-7)u^e_{-6} + \cdots + (\cdots)u^e_{-1} - 2Es_2(\theta)\omega_{-1} = 0 && \text{for} \quad \eta = -1 \\
&\Xi_{-5}\Omega(-5)u^e_{-5} + \cdots + \Xi_1\Omega(1)u^e_1 + 2\Lambda_I\omega_{-1} = 0 && \text{for} \quad \eta = 0 \\
&\Xi_{-5}\Omega(-3)u^e_{-4} + \cdots + \Xi_1\Omega(3)u^e_2 + 2\beta^2 s_2(\theta)\omega_{-1} = 0 && \text{for} \quad \eta = 1 \\
&(\cdots)u^e_{-2} + \cdots + \Xi_1\Omega(5)u^e_3 - 2\alpha^2 s_4(\theta)\omega_{-1} = 0 && \text{for} \quad \eta = 2 \\
&\Xi_{-5}\Omega(1)u^e_{-2} + \cdots + \Xi_1\Omega(7)u^e_4 = 0 && \text{for} \quad \eta = 3.
\end{aligned} \tag{72}$$

Combining these with equation (67), we see that we can use the $\eta = 2$ relation to determine ω_{-1} from $\{u^e_{-2}, \ldots, u^e_3\}$. Denote this relation by

$$\omega_{-1} = \sum_{\ell=-2}^{3} \mathcal{N}_\ell(l_R, l_I)u^e_\ell. \tag{73}$$

Table 5. The bounds for the first Regge pole of the $V(r) = \frac{\alpha^2}{r^6} - \frac{\beta^2}{r^4}$ scattering potential ($\theta = 0.3$).

$(-J_1, J_2)$	$l_R^{(L)} < l_R < l_R^{(U)}$	$l_I^{(L)} < l_I < l_I^{(U)}$
$(-14, 10)$	$97.4 < l_R < 97.7$	$12.3 < l_I < 12.6$
$(-16, 12)$	$97.48 < l_R < 97.56$	$12.36 < l_I < 12.45$
$(-18, 14)$	$97.4950 < l_R < 97.5400$	$12.3735 < l_I < 12.4185$

Amaha and Thylwe's (1994) result: (97.496 528 74, 12.396 371 67).

From equation (67), the same holds for u^e_{-3}. It then follows that for $\eta \leqslant 1$, we can generate the $u^e_{\leqslant -4}$ moments from the $\{u^e_{-2}, \ldots, u^e_3\}$. Similarly, for $\eta \geqslant 3$ we can generate the $u^e_{\geqslant 4}$ moments.

Having established that all of the moments, including ω_{-1}, are linearly dependent on the $\{u^e_{-2}, \ldots, u^e_3\}$ moments, we can write

$$u^e_\eta = \sum_{\ell=-2}^{3} \tilde{\tilde{M}}_{\eta,\ell}(l_R, l_I) u^e_\ell \tag{74}$$

for $-\infty < \eta < +\infty$. Self-consistency requires the initialization conditions:

$$\tilde{\tilde{M}}_{\eta,\ell} = \delta_{\ell_1,\ell_2} \tag{75}$$

for $-2 \leqslant \ell_1, \ell_2 \leqslant 3$.

Substituting the above linear relations (including that for ω_{-1}) into equations (66) and (67), we obtain new expressions valid for arbitrary $\{u^e_{-2}, \ldots, u^e_{-3}\}$; these in turn define the recursion relation for the $\tilde{\tilde{M}}_{\eta,\ell}(l_R, l_I)$. We can then impose the desired normalization condition, as before, and implement the necessary EMM analysis.

In order to test the validity of the above theoretical relations, we examine one of the examples considered by Amaha and Thylwe. Specifically, we take (in terms of their notation) $\alpha^2 = 2\frac{A^2}{K}$, $\beta^2 = 3\frac{A^2}{K}$, $E = A^2$, $A = 63.641$ and $K = 1.1489$.

In table 5 we only cite the numerical results for the u^o formulation. The numerical results achieved with the u^e formulation are comparable. The generation of bounds to the low-lying Regge pole manifests a clear convergent behaviour, with increasing moment order $J_{1,2}$, as defined in the previous section.

From equation (17), we see that $\theta_{\max} < \frac{\pi}{4}$. From equation (65), the generation of the negative-indexed moments involves the denominator expression $\sin^2(4\theta)$, whereas the generation of the positive-indexed moments involves $\sin^2(2\theta)$. If one takes $4\theta = \frac{\pi}{2}$, then equation (17) is satisfied, and no 'small denominator' numerical error generation is anticipated for the negative-indexed moments, since $\sin^2(4\theta) = 1$. The corresponding expression for the positive-indexed moments involves $\sin^2(2\theta) = \frac{1}{2}$, which is also not too small. Nevertheless, for $\theta = 0.4 \approx \frac{\pi}{8}$, the convergence rate of the Regge-pole bounds appeared to be very slow. For $\theta = 0.3$, faster convergence was noted. This is the case cited in table 5.

5. The $V(r) = \frac{\alpha^2}{r^{12}} - \frac{\beta^2}{r^6}$ scattering potential

We now consider the (12, 6) Lennard-Jones potential,

$$-\Psi''(r) + \left[\frac{\alpha^2}{r^{12}} - \frac{\beta^2}{r^6} + \frac{\Lambda}{r^2}\right]\Psi(r) = E\Psi(r) \tag{76}$$

rotated in the complex-r plane, $r = \rho\, e^{i\theta}$:

$$\Psi_\theta''(\rho) + \left[-\frac{\alpha^2\, e^{-10i\theta}}{\rho^{12}} + \frac{\beta^2\, e^{-4i\theta}}{\rho^6} - \frac{\Lambda}{\rho^2} + E\, e^{2i\theta}\right]\Psi_\theta(\rho) = 0 \tag{77}$$

where $\Psi_\theta(\rho) \equiv \Psi(\rho\, e^{i\theta})$.

All of the analytical results pertaining to the (6, 4) Lennard-Jones case considered in the previous section hold. In particular, the Regge-pole solution in the present case also vanishes, exponentially, at the origin, due to the underlying essential singularity. Relative to the coupled set of equations in equations (10)–(12), the relevant function coefficients become:

$$C_R(\rho) = -\frac{\alpha^2 c_{10}}{\rho^{12}} + \frac{\beta^2 c_4}{\rho^6} - \frac{\Lambda_R}{\rho^2} + c_2 E \tag{78}$$

and

$$C_I(\rho) = \frac{\alpha^2 s_{10}}{\rho^{12}} - \frac{\beta^2 s_4}{\rho^6} - \frac{\Lambda_I}{\rho^2} + s_2 E. \tag{79}$$

The coupled moment equations for the S, P, J configurations assume the form

$$\nu_p = c_2 E\mu_p + \left(\frac{p(p-1)}{2} - \Lambda_R\right)\mu_{p-2} + \beta^2 c_4 \mu_{p-6} - \alpha^2 c_{10}\mu_{p-12} \tag{80}$$

$$-(p+1)\omega_p = s_2 E\mu_{p+1} - \Lambda_I \mu_{p-1} - \beta^2 s_4 \mu_{p-5} + \alpha^2 s_{10}\mu_{p-11} \tag{81}$$

$$\begin{aligned} -\alpha^2 c_{10}(p-12)\mu_{p-13} + \beta^2 c_4(p-6)\mu_{p-7} - \Lambda_R(p-2)\mu_{p-3} + c_2 E p\mu_{p-1} \\ + p\nu_{p-1} + 2\alpha^2 s_{10}\omega_{p-12} - 2\beta^2 s_4\omega_{p-6} - 2\Lambda_I\omega_{p-2} + 2Es_2\omega_p = 0. \end{aligned} \tag{82}$$

As before, the odd/even μ-moments separate. We will only work with the odd case, since then one can use equation (81) to solve for all the even-order ω-moments, which are then substituted in equation (82). The first moment relation, equation (80), is used to substitute for the ν-moments in equation (82) as well. The moment equation for the odd-order moments, $u^o_\eta \equiv \mu_{2\eta+1}$, becomes

$$\sum_{j\in\mathcal{J}} C_j(\eta) u^o_{\eta-j} = 0 \tag{83}$$

where

$$\mathcal{J} = \{0, 1, 2, 3, 4, 6, 7, 9, 12\}. \tag{84}$$

Defining $D(\eta) \equiv \frac{1}{1+2\eta}$, the required coefficients are

$$C_j(\eta) = \begin{cases} -2\alpha^4 s_{10}^2 D(\eta-6) & j = 12 \\ 2(\alpha\beta)^2 s_{10}s_4(D(\eta-6) + D(\eta-3)) & j = 9 \\ 12\alpha^2 c_{10} - 4\alpha^2 c_{10}\eta + 2\alpha^2 s_{10}\Lambda_I(D(\eta-6) + D(\eta-1)) & j = 7 \\ -2\alpha^2 E s_{10}s_2(D(\eta) + D(\eta-6)) - 2\beta^4 s_4^2 D(\eta-3) & j = 6 \\ -6\beta^2 c_4 + 4\beta^2 c_4\eta - 2\beta^2\Lambda_I s_4(D(\eta-3) + D(\eta-1)) & j = 4 \\ 2\beta^2 E s_2 s_4(D(\eta) + D(\eta-3)) & j = 3 \\ 2\Lambda_R + 2\eta - 4\Lambda_R\eta - 6\eta^2 + 4\eta^3 - 2\Lambda_I^2 D(\eta-1) & j = 2 \\ 4c_2 E\eta + 2Es_2\Lambda_I(D(\eta-1) + D(\eta)) & j = 1 \\ -2s_2^2 E^2 D(\eta) & j = 0. \end{cases} \tag{85}$$

In principle, we can take the missing moments to be $\{u^o_0, \ldots, u^o_{11}\}$, which can be used to generate all the moments u^o_η, for $\eta \geqslant 12$ and $\eta \leqslant -1$. However, in generating these moments,

Table 6. The bounds for the first Regge pole of the $V(r) = \frac{\alpha^2}{r^{12}} - \frac{\beta^2}{r^6}$ scattering potential ($\theta = \frac{\pi}{20} \approx 0.157, \alpha^2 = 4\frac{A^2}{K^2} = \beta^2, E = A^2, A = 141.425, K = 5$).

$(-J_1, J_2)$	$l_R^{(L)} < l_R < l_R^{(U)}$	$l_I^{(L)} < l_I < l_I^{(U)}$
$(-10, 16)$	$174.45 < l_R < 184.28$	$20.06 < l_I < 23$[a]

[a] Search boundary (not an upper bound); Andersson's (1993) numerical result is (180.011 94, 21.218 92).

we will be dividing by small numbers corresponding to the inversion of the $C_{12}(\eta)$ coefficient. To make things more balanced (in generating both negative- and positive-indexed moments), we may take $\{u^o_{-6}, \ldots, u^o_5\}$ as the missing moments.

In addition, from equation (17) we know that (i.e. $m = 12$) $0 < \theta < \frac{\pi}{10}$. The theta dependence of the $C_{12}(\eta)$ will be largest at $\theta = \frac{\pi}{20}$. Note that we do not want θ to be too small (i.e. ≈ 0) since then the corresponding Regge-pole solution dies off more slowly as $\rho \to \infty$. If we make $\theta \approx \frac{\pi}{10}$, then the exponential decay of the Regge-pole solution is affected, for $\rho \to 0$. Thus, somewhere in the middle $\left(\theta \approx \frac{\pi}{20}\right)$ would be the ideal position.

Table 6 compares the results of our EMM analysis with those of Andersson (1993). Our numerical analysis also involves rescaled moments, $\tilde{u}_\eta = \frac{u_\eta}{f^\eta}$, where f is chosen so that the coefficients of the $\tilde{u}^o_{\eta-12}$ and $\tilde{u}^o_\eta$ moments, in the $\tilde{u}$-moment equation (derivable from equation (85)), are equal: $f = \left(\frac{s_2(\theta)E}{\alpha^2 s_{10}(\theta)}\right)^{\frac{1}{6}}$.

Because of the smaller angle, the convergence rate of the bounds is very slow, as suggested by the result in table 6. Nevertheless, the results are consistent with the result of Andersson's numerical calculations (1993), as well as those of Vrinceanu *et al* (2000a).

6. Non-singular scattering problems: the Bohr potential

For the case of 'non-singular' potentials, corresponding to scattering differential equations where the origin is a regular singular point (Bender and Orszag 1978), if the sought for Regge pole has a positive real part, $l_R > 0$, then we can implement the previous formalism. If not, as is the case for the Coulomb potential, a different approach is required. This is presented here.

Another important point concerns the convergence rate of the bounds. There is a strong correlation between the rate at which the bounds converge, and how fast the associated configuration dies off asymptotically. Evidence of this was presented in the polarization potential case examined earlier. Also, in the recent work by Yan and Handy (2001), they show how the convergence rate of the bounds significantly increases along the anti-Stokes lines. With respect to the complex rotation of the Regge-pole Schrödinger equation, as θ increases, the rate of decay of the configuration also decreases faster, as $\rho \to \infty$ (i.e. equation (4)). However, for singular potentials, equation (17) limits us (within the present EMM formulation, as defined in the preceding sections). It is possible to take different (nonlinear) paths in the complex-r plane that should increase the convergence rate of the bounds; however, this is not discussed here.

For non-singular potentials, we are not limited by equation (17), thus we can take $0 < \theta \leqslant \frac{\pi}{2}$. That is, non-singular problems will usually display faster convergent bounds than singular problems.

For the case of the Bohr potential,

$$-\Psi''(r) + \left[-\frac{Z}{r} + \frac{\Lambda}{r^2}\right]\Psi(r) = E\Psi(r) \tag{86}$$

and other ‘non-singular’ potentials, the Regge-pole boundary condition at the origin significantly complicates the analysis.

From the theory of differential equations, the basic solutions have the form $r^\sigma A(r)$, where $A(r)$ is analytic at the origin ($A(0) \equiv 1$), and the indicial exponent satisfies $\sigma(\sigma-1) = \Lambda = l(l+1)$, or $\sigma = l+1, -l$. Thus, at the origin we have

$$\Psi(r) = r^{l+1}\mathcal{N}_1 A_1(r) + r^{-l}\mathcal{N}_2 A_2(r). \tag{87}$$

The Regge-pole solution has $\mathcal{N}_2 = 0$, or $\Psi_{r.p.}(r) = r^{l+1}\mathcal{N} A_1(r)$. In turn, it follows that $S_{r.p}(\rho) = \rho^{2(l_R+1)}\,\mathrm{e}^{-2l_I\theta}|\mathcal{N} A_1(\rho\,\mathrm{e}^{\mathrm{i}\theta})|^2$.

In order for EMM to yield bounds within the NQR ‘S’-representation (equations (10)–(12)), we must have that the physical solutions be uniquely bounded and non-negative. If the Regge-pole, complex angular momentum has a positive real part, $l_R > 0$, then it is the unique solution which is both bounded and non-negative. This is because the other mode becomes singular at the origin, and thus unbounded (i.e. the ρ^{-2l_R} factor becomes singular, yielding no finite moments, for $l_R \geqslant \frac{1}{2}$).

However, if $l_R < 0$, as is the case for the Coulomb potential, then within the NQR representation, the Regge-pole solution is no longer uniquely non-negative. This is because the Schrödinger equation will always admit solutions which decay along the $\theta =$ const ray (i.e. $0 < \theta < \frac{\pi}{2}$), as $\rho \to \infty$. These same solutions, when continued in the $\rho \to 0$ direction, will display the behaviour given in equation (87). The corresponding S-representation configuration will automatically be non-negative, and also satisfy the Regge-pole condition at the origin (asymptotically), since the non-physical mode (r^{-l}) is subdominant relative to the physical mode (r^{l+1}).

Clearly, we must define some other condition that uniquely singles out the desired, physical, Regge-pole solution. Obviously, we must exploit the fact that the Regge-pole boundary condition at the origin is that the Regge-pole configuration becomes exactly the r^{l+1} mode. We must develop an EMM formulation that only involves the physical mode in equation (87), that is, $A_1(r)$. The only way to do this is to develop a moment equation representation within the interval $[\rho_s, \infty)$, and match it to the power series approximation for A_1 at ρ_s.

Taking $\Psi_{r.p.}(r) = r^{l+1}A_1(r)$ and substituting in the original Schrödinger equation give

$$\left[E + \frac{Z}{r}\right]A_1(r) + \frac{2(l+1)}{r}A_1'(r) + A_1''(r) = 0. \tag{88}$$

The power series expansion, $A_1(r) = \sum_{j=0}^{\infty} a_j r^j$, yields the recursion relation

$$a_1 = -\frac{Z}{2(l+1)}a_0 \tag{89}$$

$$a_{j+1} = -\left(\frac{Za_j + Ea_{j-1}}{(j+1)(2(l+1)+j)}\right) \qquad j \geqslant 1. \tag{90}$$

We now perform a complex rotation on equation (88), using the notation $A_1(\rho\,\mathrm{e}^{\mathrm{i}\theta}) \equiv A_\theta(\rho)$:

$$\left[E\,\mathrm{e}^{2\mathrm{i}\theta} + \frac{Z\,\mathrm{e}^{\mathrm{i}\theta}}{\rho}\right]A_\theta(\rho) + \frac{2(l+1)}{\rho}A_\theta'(\rho) + A_\theta''(\rho) = 0. \tag{91}$$

Of course, A_θ vanishes exponentially in the asymptotic limit $\rho \to \infty$.

We can transform the above into an NQR formulation by using equations (8) and (9). In terms of the notation adopted there, $A_R = 1$, $A_I = 0$, $B_R = \frac{2(l_R+1)}{\rho}$, $B_I = \frac{2l_I}{\rho}$, $C_R = Ec_2 + \frac{Zc_1}{\rho}$ and $C_I = Es_2 + \frac{Zs_1}{\rho}$. The $\{S, P, J\}$ coupled equations become

$$S''(\rho) - 2P(\rho) + B_R(\rho)S'(\rho) + 2C_R(\rho)S(\rho) + 2B_I(\rho)J(\rho) = 0 \tag{92}$$

$$B_I(\rho)S'(\rho) + 2C_I(\rho)S(\rho) - 2(B_R(\rho) + \partial_\rho)J(\rho) = 0 \tag{93}$$

and

$$P'(\rho) + 2B_R(\rho)P(\rho) + C_R(\rho)S'(\rho) - 2C_I(\rho)J(\rho) = 0. \tag{94}$$

In order to single out the physical mode (particularly in the case that $l_R < 0$), we must develop a moment equation over the interval $[\rho_s, \infty)$, where ρ_s is sufficiently small so that a power series expansion for $\{S, P, J\}$ converges rapidly. We need to multiply each of the above equations by ρ^{p+1} and integrate over $[\rho_s, \infty)$. The ensuing moment equations involve the various boundary values for $\{S, P, J\}$. We note that

$$\int_{\rho_s}^{\infty} \mathrm{d}\rho\, \rho^p S'(\rho) = -\rho_s^p S(\rho_s) - p\mu_{p-1} \tag{95}$$

and

$$\int_{\rho_s}^{\infty} \mathrm{d}\rho\, \rho^p S''(\rho) = -\rho_s^p S'(\rho_s) + p\rho_s^{p-1} S(\rho_s) + p(p-1)\mu_{p-2} \tag{96}$$

where

$$\mu_p \equiv \int_{\rho_s}^{\infty} \mathrm{d}\rho\, \rho^p S(\rho) \tag{97}$$

and likewise for ν_p and ω_p.

The corresponding moment equations are

$$\begin{aligned} 2Ec_2\mu_{p+1} + 2Zc_1\mu_p + p(p-(2l_R+1))\mu_{p-1} + \rho_s^p[p-(2l_R+1)]S(\rho_s) \\ - \rho_s^{p+1}S'(\rho_s) - 2\nu_{p+1} + 4l_I\omega_p = 0 \end{aligned} \tag{98}$$

$$((2l_R+1)-p)\omega_p = Es_2\mu_{p+1} + Zs_1\mu_p - l_I p\mu_{p-1} - l_I\rho_s^p S(\rho_s) + \rho_s^{p+1}J(\rho_s) \tag{99}$$

$$\begin{aligned} [4l_R+3-p]\nu_p = Ec_2(p+1)\mu_p + Zc_1 p\mu_{p-1} + \rho_s^p(Zc_1 + Ec_2\rho_s)S(\rho_s) \\ + \rho_s^{p+1}P(\rho_s) + 2Es_2\omega_{p+1} + 2Zs_1\omega_p. \end{aligned} \tag{100}$$

All for $p \geqslant 0$.

Since $A_\theta(\rho) = \sum_{j=0}^{\infty} a_j\, \mathrm{e}^{ij\theta}\rho^j$ depends only on a_0, all of the quantities $\{S(\rho_s), S'(\rho_s), P(\rho_s), J(\rho_s)\}$ depend, linearly, on $|a_0|^2 = S(0)$. Recall from the discussion following equation (7) that $S(\rho) = |A_\theta(\rho)|^2$, $S'(\rho) = \partial_\rho S(\rho) = 2\,\mathrm{Re}(A_\theta(\rho)\partial_\rho A_\theta^*(\rho))$, $P(\rho) = |\partial_\rho A_\theta(\rho)|^2$ and $J(\rho) = \mathrm{Im}(A_\theta(\rho)\partial_\rho A_\theta^*(\rho))$. All of these quantities can be calculated very precisely at ρ_s, from the power series expansion given by equations (89) and (90). Therefore, the above quantities can be written as $S(\rho_s) = f_1 S(0)$, $S'(\rho_s) = f_2 S(0)$, $P(\rho_s) = f_3 S(0)$, $J(\rho_s) = f_4 S(0)$. The f_n factors are numerically determined, to high accuracy, from the power series expansion, for given θ.

Given the above, we can reduce the coupled set of moment equations to just one moment equation for the μ_p and $S(0)$. In doing this, we assume that l_R takes on values such that the quantities

$$\Delta_j[p] = \begin{cases} 2l_R + 1 - p & j = 1 \\ 2l_R - p & j = 2 \\ 2l_R - 1 - p & j = 3 \\ 4l_R + 2 - p & j = 4 \end{cases} \tag{101}$$

do not become non-negative integers. We can then use equation (99) to solve for ω_p and equation (100) to solve for ν_p. These are then substituted in equation (98). The resulting μ-moment equation becomes

$$\left(T_e(p) - \frac{2T_\nu(p+1)}{\Delta_4(p)} + \frac{4l_I T_\omega(p)}{\Delta_1(p)} - \frac{4s_1 Z T_\omega(p+1)}{\Delta_2(p)\Delta_4(p)} - \frac{4Es_2T_\omega(p+2)}{\Delta_3(p)\Delta_4(p)}\right) S(0)$$
$$- \left(\frac{p\left(4l_I^2 + (\Delta_1(p))^2\right)}{\Delta_1(p)}\right)\mu_{p-1} + \left(2c_1 Z\left(1 - \frac{p+1}{\Delta_4(p)}\right) + \frac{4l_I s_1 Z}{\Delta_1(p)}\right.$$
$$\left. + \frac{4l_I s_1 Z(1+p)}{\Delta_2(p)\Delta_4(p)}\right)\mu_p \left(2c_2 E\left(1 - \frac{(p+2)}{\Delta_4(p)}\right) + \frac{4El_I s_2}{\Delta_1(p)}\right.$$
$$\left. + \frac{4El_I s_2(2+p)}{\Delta_3(p)\Delta_4(p)} - \frac{4s_1^2 Z^2}{\Delta_2(p)\Delta_4(p)}\right)\mu_{p+1}$$
$$- \frac{4Es_1s_2Z}{\Delta_4(p)}\left(\frac{1}{\Delta_3(p)} + \frac{1}{\Delta_2(p)}\right)\mu_{p+2} - \frac{4E^2s_2^2}{\Delta_3(p)\Delta_4(p)}\mu_{p+3} = 0 \qquad (102)$$

where

$$T_\ell(p) = \begin{cases} \rho_s^p[p - (2l_R+1)]f_1 - \rho_s^{p+1} f_2 & \ell = e \\ -l_I\rho_s^p f_1 + \rho_s^{p+1} f_4 & \ell = \omega \\ \rho_s^p (Zc_1 + Ec_2\rho_s) f_1 + \rho_s^{p+1} f_3 & \ell = \nu. \end{cases} \qquad (103)$$

The moments are linearly dependent on the missing moments $\{\mu_0, \mu_1, \mu_2\}$ and $S(0)$. We denote these by $\{\chi_\ell | 0 \leqslant \ell \leqslant 3\}$, respectively. This is expressed by

$$\mu_p = \sum_{\ell=0}^{3} M_{p,\ell}(l_R, l_I)\chi_\ell \qquad (104)$$

$p \geqslant 0$, satisfying the initialization conditions:

$$M_{\ell_1,\ell_2} = \delta_{\ell_1,\ell_2} \qquad 0 \leqslant \ell_{1,2} \leqslant 2 \qquad (105)$$

and

$$M_{\ell_1,3} = 0 \qquad 0 \leqslant \ell_1 \leqslant 2. \qquad (106)$$

The M satisfy the moment equation (equation (102)) with respect to the p-index. Thus we have

$$\frac{4E^2s_2^2}{\Delta_3(p)\Delta_4(p)}M_{p+3,\ell} = -\left(\frac{p\left(4l_I^2 + (\Delta_1(p))^2\right)}{\Delta_1(p)}\right)M_{p-1,\ell} + \left(2c_1 Z\left(1 - \frac{p+1}{\Delta_4(p)}\right)\right.$$
$$\left. + \frac{4l_I s_1 Z}{\Delta_1(p)} + \frac{4l_I s_1 Z(1+p)}{\Delta_2(p)\Delta_4(p)}\right)M_{p,\ell}\left(2c_2 E\left(1 - \frac{(p+2)}{\Delta_4(p)}\right) + \frac{4El_I s_2}{\Delta_1(p)}\right.$$
$$\left. + \frac{4El_I s_2(2+p)}{\Delta_3(p)\Delta_4(p)} - \frac{4s_1^2Z^2}{\Delta_2(p)\Delta_4(p)}\right)M_{p+1,\ell}$$
$$- \frac{4Es_1s_2Z}{\Delta_4(p)}\left(\frac{1}{\Delta_3(p)} + \frac{1}{\Delta_2(p)}\right)M_{p+2,\ell} \qquad (107)$$

for $0 \leqslant \ell \leqslant 2$, and

$$\frac{4E^2s_2^2}{\Delta_3(p)\Delta_4(p)}M_{p+3,3} = \left(T_e(p) - \frac{2T_\nu(p+1)}{\Delta_4(p)} + \frac{4l_I T_\omega(p)}{\Delta_1(p)} - \frac{4s_1 Z T_\omega(p+1)}{\Delta_2(p)\Delta_4(p)}\right.$$
$$\left. - \frac{4Es_2T_\omega(p+2)}{\Delta_3(p)\Delta_4(p)}\right) - \left(\frac{p\left(4l_I^2 + (\Delta_1(p))^2\right)}{\Delta_1(p)}\right)M_{p-1,3} + \left(2c_1 Z\left(1 - \frac{p+1}{\Delta_4(p)}\right)\right.$$

$$+ \frac{4l_I s_1 Z}{\Delta_1(p)} + \frac{4l_I s_1 Z(1+p)}{\Delta_2(p)\Delta_4(p)}\Bigg) M_{p,3} \left(2c_2 E\left(1 - \frac{(p+2)}{\Delta_4(p)}\right) + \frac{4El_I s_2}{\Delta_1(p)}\right.$$
$$\left. + \frac{4El_I s_2(2+p)}{\Delta_3(p)\Delta_4(p)} - \frac{4s_1^2 Z^2}{\Delta_2(p)\Delta_4(p)}\right) M_{p+1,3}$$
$$- \frac{4Es_1 s_2 Z}{\Delta_4(p)}\left(\frac{1}{\Delta_3(p)} + \frac{1}{\Delta_2(p)}\right) M_{p+2,3}. \tag{108}$$

The normalization condition is

$$S(0) + \sum_{\ell=0}^{2} \mu_\ell = 1. \tag{109}$$

We can solve for μ_0 in terms of the other variables $\{\chi_\ell | 1 \leqslant \ell \leqslant 3\}$. Substituting back into equation (104) gives

$$\mu_p = \hat{M}_{p,0} + \sum_{\ell=1}^{3} \hat{M}_{p,\ell}\chi_\ell \tag{110}$$

where

$$\hat{M}_{p,\ell} = \begin{cases} M_{p,0} & \ell = 0 \\ M_{p,\ell} - M_{p,0} & 1 \leqslant \ell \leqslant 3. \end{cases} \tag{111}$$

Finally, the moment problem constraints become

$$\int_{\rho_s}^{\infty} \mathrm{d}\rho\, F_n(\rho)\left(\sum_{j=0}^{J} C_j \rho^j\right)^2 S(\rho) > 0 \tag{112}$$

for arbitrary C_j (not all identically zero), $J < \infty$, and

$$F_n(\rho) = \begin{cases} 1 & n = 0 \\ \rho & n = 1 \\ (\rho - \rho_s) & n = 2. \end{cases} \tag{113}$$

These in turn become the quadratic form inequalities

$$\sum_{j_1, j_2=0}^{J} C_{j_1}\left(\Omega_{n,1}\mu_{j_1+j_2} + \Omega_{n,2}\mu_{j_1+j_2+1}\right) C_{j_2} > 0 \tag{114}$$

where

$$(\Omega_{n,1}, \Omega_{n,2}) = \begin{cases} (1, 0) & n = 0 \\ (0, 1) & n = 1 \\ (-\rho_s, 1) & n = 2. \end{cases} \tag{115}$$

Substituting equation (110) defines the linear programming problem which is solved through the EMM algorithm:

$$\sum_{\ell=1}^{3} \chi_\ell \left(- \sum_{j_1, j_2=0}^{J} C_{j_1}\left[\Omega_{n,1}\hat{M}_{j_1+j_2,\ell}(l_R, l_I) + \Omega_{n,2}\hat{M}_{j_1+j_2+1,\ell}(l_R, l_I)\right] C_{j_2}\right)$$
$$< \sum_{j_1, j_2=0}^{J} C_{j_1}\left[\Omega_{n,1}\hat{M}_{j_1+j_2,0}(l_R, l_I) + \Omega_{n,2}\hat{M}_{j_1+j_2+1,\ell}(l_R, l_I)\right] C_{j_2} \tag{116}$$

which must be satisfied for all C (not identically zero) and all $J \geqslant 0$, by the correct physical (l_R, l_I) Regge-pole value. Note that if $P_{\max}$ is the maximum moment order generated, then $1 + 2J \leqslant P_{\max}$.

Table 7. The bounds for the first two Regge poles of the, $V(r) = -\frac{Z}{r}$, Coulomb potential $(Z = 1, k = 1)$. The expansion order in equation (90) is 40.

$P_{\max}$	ρ_s	θ	$l_R^{(L)} < l_R < l_R^{(U)}$	$l_I^{(L)} < l_I < l_I^{(U)}$
30	1	$\frac{\pi}{4}$	$-1.001\,23 < l_R < -0.997\,93$	$0.4990 < l_I < 0.5005$
30	1	$\frac{\pi}{4}$	$-2.06 < l_R < -1.88$	$0.3 < l_I < 0.56$
40	1	$\frac{\pi}{4}$	$-2.03 < l_R < -1.96$	$0.42 < l_I < 0.53$
30	2	1	$-1.000\,0013 < l_R < -0.999\,9990$	$0.499\,999\,88 < l_I < 0.500\,000\,30$
30	2	1	$-2.000\,11 < l_R < -1.999\,95$	$0.4993 < l_I < 0.5004$

The results of our analysis, for the $Z = 1$ Bohr potential problem, are given in table 7. Note that the exact formula is (Frautschi 1963, equations (8)–(11), p 121, Newton 1982, chapter 13)

$$l_{\text{Bohr–Regge pole}} = -(1+n) + \frac{\mathrm{i}Z}{2k} \tag{117}$$

where $E = k^2$, and for $n = 0, 1, 2, \ldots$.

7. Conclusion

We have presented in greater detail the EMM–Regge-pole bounding formalism first communicated by Handy and Msezane (2001). The present results confirm the benefits of this type of analysis in assessing the theoretical/numerical accuracy of other methods. We have presented the formalism on various types of rational fraction potentials, focusing on the essentials of each type. These included both irregular singular point potentials (i.e. *singular potentials*) and regular singular point potentials (i.e. *regular potentials*). Presently, we are investigating alternate representations capable of making the previous formalism more efficient (i.e. tighter bounds).

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References

Amaha A and Thylwe K E 1991 *Phys. Rev.* A **44** 4203
Amaha A and Thylwe K E 1994 *Phys. Rev.* A **50** 1420
Andersson N 1993 *J. Phys. A: Math. Gen.* **26** 5085
Avdonina N B, Belov S, Felfli Z, Msezane A Z and Naboko S N 2001 *CAU Preprint* (2002 *Phys. Rev.* A **65** at press)
Bender C M and Orszag S A 1978 *Advanced Mathematical Methods for Scientists and Engineers* (New York: McGraw-Hill)
Chvatal V 1983 *Linear Programming* (New York: Freeman)
Connor J N L 1990 *J. Chem. Soc. Faraday Trans.* **86** 1627
Frautschi S C 1963 *Regge Poles and S-Matrix Theory* (New York: Benjamin)

Germann T C and Kais S 1997 *J. Chem. Phys.* **106** 599
Handy C R 1996 *Phys. Lett.* A **216** 15
Handy C R 2001a *J. Phys. A: Math. Gen.* **34** L271
Handy C R 2001b *J. Phys. A: Math. Gen.* **34** 5065
Handy C R and Bessis D 1985 *Phys. Rev. Lett.* **55** 931
Handy C R, Bessis D and Morley T D 1988a *Phys. Rev.* A **37** 4557
Handy C R, Bessis D, Sigismondi G and Morley T D 1988b *Phys. Rev. Lett* **60** 253
Handy C R, Khan D, Wang X-Q and Tymczak C J 2001 *J. Phys. A: Math. Gen.* **34** 5593
Handy C R and Msezane A Z 2001 *J. Phys. A: Math. Gen.* **34** L531
Handy C R and Wang X-Q 2001 *J. Phys. A: Math. Gen.* **34** 8297
Newton R G 1982 *Scattering Theory of Waves and Particles* 2nd edn (New York: Springer)
Shohat J A and Tamarkin J D 1963 *The Problem of Moments* (Providence, RI: American Mathematical Society)
Sofianos S A, Rakityansky S A and Massen S E 1999 *Phys. Rev.* A **60** 337
Sokolovski D, Tully C and Crothers D S F 1998 *J. Phys. A: Math. Gen.* **31** 1
Vrinceanu D, Msezane A Z and Bessis D 2000a *Phys. Rev.* A **62** 022719
Vrinceanu D, Msezane A Z, Bessis D, Connor J N L and Sokolovski D 2000b *Chem. Phys. Lett.* **324** 311
Yan Z and Handy C R 2001 *J. Phys. A: Math. Gen.* **34** 9907