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## LETTER TO THE EDITOR

# Generation of converging Regge-pole bounds: a new formulation of complex rotation quantization

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## Abstract

We propose an unprecedented bounding theory which generates converging bounds to the Regge poles of rational fraction scattering potentials. This is made possible by the recent work of Handy (2001 *J. Phys. A: Math. Gen.* **34** L271) and Handy and Wang (2001 *J. Phys. A: Math. Gen.* **34** 8297) which transforms the Schrödinger equation into an equivalent fourth-order, *linear* differential equation for the probability density. This new representation is better suited for numerical considerations, since the rapid oscillations of the Regge-pole wavefunction are factored out. More importantly, the moments of the probability density can be constrained (and thereby the underlying complex angular momentum parameter of the effective potential function) through appropriate *moment problem* theorems, as incorporated within the eigenvalue moment method of Handy and Bessis (1985 *Phys. Rev. Lett.* **55** 931) and Handy *et al* (1988 *Phys. Rev. Lett.* **60** 253).

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## 1. Introduction

The complex angular momentum representation (Connor 1990), involving Regge-pole calculations, has proved very successful in the analysis of atomic, molecular, and electronic collision problems, as demonstrated in the recent works by 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, especially for singular potentials (i.e. potentials diverging faster than  $r^{-2}$  at the origin).

The development of new and reliable methods for calculating accurate Regge-pole trajectories is particularly important because of the difficulty in implementing WKB approximation methods (Connor 1990). Such approaches require a good understanding of the behavior of the relevant complex turning points, and the attendant problem of identifying the correct Stokes line topology.

Numerical integration methods are important because analytical approaches may not be readily forthcoming for varied types of problems. Within the framework of the complex rotation formalism (Connor 1990), which treats the Regge-pole problem as a bound state problem, numerical analysis must deal with the intricacy of the Regge-pole wavefunction's rapidly oscillating behavior near the origin of the complex- $r$  plane. That is, taking  $r \equiv \rho e^{i\theta}$ , the wavefunction,

$$\Psi(\rho, \theta) = |\Psi(\rho, \theta)| \exp(i\Phi(\rho, \theta)) \quad (1)$$

has a phase factor that goes as

$$\lim_{\rho \rightarrow 0^+} |\Phi(\rho, \theta)| = \infty. \quad (2)$$

We propose an alternative representation, based on the recent work by Handy (2001a), which avoids these complications. It transforms the Schrödinger equation into an equivalent linear differential representation for the probability density. Within this *nonnegativity* quantization representation (NQR) formulation the anomalous phase function is factored out.

In addition, if we apply the NQR formulation to the important class of rational fraction potentials (or those that can be transformed into such form), one can generate converging (lower and upper) bounds to the individual Regge poles. This is because NQR defines a natural framework within which to apply the eigenvalue moment method (EMM) of Handy and Bessis (1985) and Handy *et al* (1988a, 1988b).

This is an unprecedented achievement which can dramatically impact the generation of high accuracy Regge-pole trajectory calculations. Such bounding theories can provide very stringent tests for assessing the accuracy of other (faster) estimation methods; thereby defining a valuable tool in the calculation of Regge-pole trajectories. Although the numerical examples given here are modest, there is every expectation (based on the well established computational achievements of EMM theory) that further refinements of the present formalism will generate more robust, EMM-based, Regge-pole bounding algorithms.

The generation of converging bounds follows from the fact that the NQR formalism leads to a recursive equation for the moments of the nonnegative probability density,  $S(\rho) \equiv |\Psi(r(\rho, \theta(\rho)))|^2$ , along any (suitably chosen) contour in the complex- $r$  plane. Since  $S$  is uniquely nonnegative and bounded (i.e. in the sense that all, or almost all, of its power moments are finite) for the physical Regge-pole values, the imposition of the well known Moment Problem constraints (Shohat and Tamarkin 1963) leads to the generation of converging lower and upper bounds to the complex- $(l_R, l_I)$ , Regge poles. This is the basic philosophy of EMM (Handy and Bessis 1985, Handy *et al* 1988a, 1988b).

The following discussion assumes the simplest contour, that corresponding to a straight *ray* originating at  $\rho = 0$ , and with  $\theta$  having (an appropriate) constant value.

In this case, the relevant moments are defined by  $\mu_p \equiv \int_0^\infty d\rho \rho^p S(\rho)$ , and satisfy a recursive *moment equation*, dependent on the complex angular momentum parameter,  $l \equiv (l_R, l_I)$ . Along the *ray* contour, the desired Regge-pole configuration asymptotically vanishes, exponentially. For the case of 'singular potentials' (i.e. irregular-singular Sturm–Liouville (SL) potential functions), as defined earlier,  $S(\rho)$  becomes  $L^1$ , with all of its power moments finite. For the case of non-singular potentials (i.e. regular-singular SL potential functions), the same holds for all the power moments satisfying,  $\{\mu_p | p + 2(l_R + 1) > -1\}$ , where  $S(\rho) \approx O(\rho^{2(l_R+1)})$ , as  $\rho \rightarrow 0$ .

A related development is the recent application of EMM–NQR in the discrete state analysis of non-Hermitian Schrödinger operators. The combination of EMM with NQR allows one to generate converging bounds to the complex eigenenergies of certain PT-symmetry breaking

Hamiltonians (Handy 2001b, Handy *et al* 2001). In this work, we exploit this same basic philosophy for bounding Regge poles.

## 2. The NQR formulation

### 2.1. The singular phase factor

Consider the (normalized) radial Schrödinger equation:

$$-\Psi''(r) + \left( V(r) + \frac{l(l+1)}{r^2} \right) \Psi(r) = E\Psi(r). \quad (3)$$

The Regge-pole configurations, for complex values of the angular momentum,  $l \equiv l_R + il_I$ , must satisfy certain boundary conditions. The first of these is that the analytic continuation in  $l$ , into the physical angular momentum domain, must yield an  $r$  dependence consistent with the physical solutions. This means that

$$\lim_{r \rightarrow 0} \Psi(r) = \begin{cases} r^{l+1} & \text{for non-singular potentials} \\ 0 & \text{for singular potentials.} \end{cases} \quad (4)$$

The other boundary condition is

$$\lim_{r \rightarrow \infty} \Psi(r) = \mathcal{N} \exp(ik(E)r) \quad (5)$$

where  $k(E) = \sqrt{E} > 0$ . These conditions are imposed along the real axis. From equation (5), for sufficiently small and positive angles,  $\theta > 0$ , the Regge-pole configuration must be bounded in the asymptotic- $\rho$  direction:

$$\lim_{\rho \rightarrow \infty} |\Psi(\rho, \theta)| = |\mathcal{N}| \exp(-k(E) \sin(\theta)\rho). \quad (6)$$

For the case of 'non-singular' potentials (i.e.  $\lim_{r \rightarrow 0} r^2 V(r) = 0$ ), the wavefunction's behavior near the origin is determined by the Fuchsian relation

$$\Psi(r) = r^{l+1} A(r) \quad (7)$$

involving the analytic function,  $A(r)$ . The explicit form for the above is

$$\Psi(r) = \exp((l_R + il_I + 1)(\ln \rho + i\theta)) A(r). \quad (8)$$

For fixed  $\theta$ , the Regge-pole configuration behaves as

$$\Psi_{r.p.}(\rho) \approx (\rho^{l_R+1} e^{-\theta l_I}) \exp(i[l_I \ln \rho + \theta(l_R + 1)]). \quad (9)$$

Along constant- $\theta$  ray, as  $\rho \rightarrow 0^+$ , rapid oscillations will be exhibited by the wavefunction. This makes (conventional) numerical approaches very difficult, near the origin, in the complex- $r$  plane.

For the case of singular potentials, where  $\lim_{r \rightarrow 0} V(r) = \alpha^2/r^{2q}$ , and  $q > 1$ , the non-Fuchsian nature of the associated Schrödinger differential equation yields the essential singularity structure for the wavefunction:

$$\Psi(r) \approx \frac{1}{(V(r))^{1/4}} \exp\left(\pm \frac{\alpha}{q-1} r^{-(q-1)}\right) \quad (10)$$

obtainable from standard JWKB theory (Bender and Orszag 1978). In terms of the complex- $r$  plane representation, this becomes

$$\Psi(\rho, \theta) \approx \frac{1}{(V(r))^{1/4}} \exp\left(\pm \frac{\alpha}{q-1} \rho^{-(q-1)} (c_{q-1}(\theta) - is_{q-1}(\theta))\right) \quad (11)$$

for  $\rho \rightarrow 0$ , where  $c_n(\theta) \equiv \cos(n\theta)$ , and  $s_n(\theta) \equiv \sin(n\theta)$ .

If  $\alpha > 0$ , then the physical Regge-pole solution must have a decaying essential singularity behavior at the origin (for  $\theta = 0$ ), and this must persist for sufficiently small, positive angles, in the complex- $r$  plane. Thus

$$\Psi(\rho, \theta) \rightarrow \begin{cases} 0 & \rho \rightarrow 0 \\ 0 & \rho \rightarrow \infty \end{cases} \quad (12)$$

for  $\theta_{\min} < \theta < \theta_{\max}$  and  $\alpha > 0$ . An immediate estimate for the extremum angles are  $\theta_{\min} = 0$ , and

$$\theta_{\max} = \frac{\pi}{2(q-1)} < \pi. \quad (13)$$

If  $\alpha = ia$ , and  $a > 0$ , then although the physical Regge-pole solution will satisfy the boundary condition at the origin, along the real axis, it need not do so for  $\theta \neq 0$ .

In all the above cases, the validity of equation (2) is very clear. Thus, the presence of very rapid oscillations near the origin of the complex- $r$  plane is a significant anomaly complicating any numerical or analytical investigations. One could work within the  $|\Psi(\rho, \theta)|$ ,  $\Phi(\rho, \theta)$  representation; however, this would involve nonlinear differential equations.

## 2.2. The NQR differential equations

One can factor out the anomalous phase function,  $e^{i\Phi(\rho, \theta)}$ , by working with the NQR formulation. In general, for any complex effective potential,  $V_{\text{eff}}(r) \equiv V(r) + l(l+1)/r^2$ , on the real axis, the NQR formalism transforms the Schrödinger equation into an equivalent, fourth-order, linear differential equation for the probability density  $S(r) \equiv |\Psi(r)|^2$ . Since we are interested in working within the complex- $r$  plane contour corresponding to the semi-infinite, ray, contour we adopt the more general formalism discussed in the work of Handy and Wang (2001).

In the present work, we are concerned with those cases where  $\theta$  is held fixed at some small positive value, and the Regge-pole configuration,  $\Psi_{\text{r.p.}}(\rho)$  (the  $\theta$  dependence is implicit) is of  $L^2$  type, vanishing at the origin and at infinity,  $\Psi_{\text{r.p.}}(0) = 0$ ,  $\Psi_{\text{r.p.}}(\infty) = 0$ . We assume this case, for simplicity. Thus, we do not discuss here the singular potential case corresponding to  $\alpha = ia$ .

The Schrödinger equation, along the  $\theta$  ray direction, becomes

$$A(\rho) \Psi''(\rho) + B(\rho) \Psi'(\rho) + C(\rho) \Psi(\rho) = 0 \quad (14)$$

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

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

The Schrödinger equation is then equivalent to the following set of coupled differential equations (i.e.  $A = A_{\text{R}} + iA_{\text{I}}$ , etc):

$$(S''(\rho) - 2P(\rho))A_{\text{R,I}}(\rho) + S'(\rho)B_{\text{R,I}}(\rho) + 2S(\rho)C_{\text{R,I}}(\rho) \pm 2(B_{\text{I,R}}(\rho) + A_{\text{I,R}}(\rho)\partial_\rho)J(\rho) = 0 \quad (15)$$

and

$$P'(\rho)A_{\text{R,I}}(\rho) \pm 2T(\rho)A_{\text{I,R}}(\rho) + 2P(\rho)B_{\text{R,I}}(\rho) + S'(\rho)C_{\text{R,I}}(\rho) \mp 2J(\rho)C_{\text{I,R}}(\rho) = 0. \quad (16)$$

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 (16) generates  $T$ ):

$$P(\rho) = \frac{1}{2}S''(\rho) + S(\rho)C_R(\rho) \quad (17)$$

$$\partial_\rho J(\rho) = S(\rho)C_I(\rho) \quad (18)$$

$$P'(\rho) + S'(\rho)C_R(\rho) - 2J(\rho)C_I(\rho) = 0. \quad (19)$$

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).

In light of the nonnegative character of  $S$  (and  $P$ ), and the fact that one is interested in  $L^1$  physical (Regge-pole) solutions (i.e. the  $L^2$  requirement for  $\Psi_{r.p.}$  becomes equivalent to  $L^1$  conditions for the  $S_{r.p.}$  counterpart), the above equations easily lend themselves to an EMM analysis.

Specifically, for rational fraction potentials, or those that can be transformed into such form (although then one may have to deal with the full set of coupled  $S$ ,  $P$ ,  $J$ ,  $T$  equations), one can transform the above coupled equations into a coupled set of moment equations, which in turn (usually) reduce to a linear recursion relation for the moments of  $S$ . These in turn can be constrained to satisfy the positivity requirements ensuing from the classic moment problem (Shohat and Tamarkin 1963), leading to converging lower and upper bounds to the complex Regge-pole locations,  $l = l_R + il_I$ . In the next section we provide one example of this.

It is important to re-emphasize that working with the  $\{S, P, J\}$  set of configurations is equivalent to the original Schrödinger representation. Specifically, if we take  $\Psi(\rho) \equiv e^{Q(\rho)}$ , then  $S(\rho) = e^{2Q_R(\rho)} > 0$ ,  $P(\rho) = |Q'(\rho)|^2 S(\rho)$ , and  $J(\rho) = \text{Im}(\Psi\Psi^*) = -Q_I'(\rho)S(\rho)$ . Note also that  $S'(\rho) = 2\text{Re}(\Psi\Psi^*)' = 2Q_R'(\rho)S(\rho)$ . Therefore, knowledge of  $\{S, J\}$  determines  $Q$ , and in turn  $\Psi$ . We note that  $\{S, S', P, J\}$  form a closed system as well, under the conditions of  $A = 1$ ,  $B = 0$ :

$$\partial_\rho \begin{pmatrix} S(\rho) \\ S'(\rho) \\ P(\rho) \\ J(\rho) \end{pmatrix} = \begin{pmatrix} 0, 1, 0, 0 \\ -2C_R(\rho), 0, 2, 0 \\ 0, -C_R(\rho), 0, 2C_I(\rho) \\ C_I(\rho), 0, 0, 0 \end{pmatrix} \begin{pmatrix} S(\rho) \\ S'(\rho) \\ P(\rho) \\ J(\rho) \end{pmatrix}. \quad (20)$$

The numerical analysis of these equations is presently under investigation.

### 3. The $V(r) = \alpha^2/r^6 - \beta^2/r^4$ scattering potential

Consider an illustrative example corresponding to the scattering potential problem

$$-\Psi''(r) + \left[ \frac{\alpha^2}{r^6} - \frac{\beta^2}{r^4} + \frac{l(l+1)}{r^2} \right] \Psi(r) = E\Psi(r) \quad (21)$$

previously investigated by Amaha and Thylwe (1991, 1994). From equation (14), we have  $C(\rho) = C_R(\rho) + iC_I(\rho)$ , where

$$C_R(\rho) = -\frac{\alpha^2 c_4(\theta)}{\rho^6} + \frac{\beta^2 c_2(\theta)}{\rho^4} - \frac{\Lambda_R}{\rho^2} + E c_2(\theta) \quad (22)$$

and

$$C_I(\rho) = \frac{\alpha^2 s_4(\theta)}{\rho^6} - \frac{\beta^2 s_2(\theta)}{\rho^4} - \frac{\Lambda_I}{\rho^2} + E s_2(\theta) \quad (23)$$

where  $\Lambda = \Lambda_R + i\Lambda_I \equiv l(l+1)$ , 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  $\mu_p \equiv \int_0^\infty d\rho \rho^p S(\rho)$ ,  $\nu_p \equiv \int_0^\infty d\rho \rho^p P(\rho)$  and  $\omega_p \equiv \int_0^\infty d\rho \rho^p J(\rho)$ . 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  $\int_0^\infty d\rho \rho^p$  to both sides of the coupled equations in equations (17)–(19), and integrating by parts, results in the coupled moment equations

$$\nu_p = E c_2(\theta) \mu_p + \left( \frac{p(p-1)}{2} - \Lambda_R \right) \mu_{p-2} + \beta^2 c_2(\theta) \mu_{p-4} - \alpha^2 c_4(\theta) \mu_{p-6} \quad (24)$$

$$p \omega_{p-1} = -E s_2(\theta) \mu_p + \Lambda_1 \mu_{p-2} + \beta^2 s_2(\theta) \mu_{p-4} - \alpha^2 s_4(\theta) \mu_{p-6} \quad (25)$$

and

$$p \nu_{p-1} + \left[ E c_2(\theta) p \mu_{p-1} - \Lambda_R (p-2) \mu_{p-3} + \beta^2 c_2(\theta) (p-4) \mu_{p-5} - \alpha^2 c_4(\theta) (p-6) \mu_{p-7} \right] \\ + 2 \left[ E s_2(\theta) \omega_p - \Lambda_1 \omega_{p-2} - \beta^2 s_2(\theta) \omega_{p-4} + \alpha^2 s_4(\theta) \omega_{p-6} \right] = 0. \quad (26)$$

We see that the second moment equation (25) determines all the  $\omega$ -moments, in terms of the  $\mu$ -moments, except for  $\omega_{-1}$  (for  $p = 0$ ). Let us therefore rewrite this as ( $p \rightarrow p+1$ )

$$\omega_p = \Omega(p) \left( -E s_2(\theta) \mu_{p+1} + \Lambda_1 \mu_{p-1} + \beta^2 s_2(\theta) \mu_{p-3} - \alpha^2 s_4(\theta) \mu_{p-5} \right) + \delta_{p,-1} \omega_{-1} \quad (27)$$

where

$$\Omega(p) = \begin{cases} \frac{1}{p+1} & p \neq -1 \\ 0 & p = -1. \end{cases} \quad (28)$$

and  $\delta_{p,-1}$  is the Kronecker delta function.

A detailed analysis of the above moment relations will be presented in a forthcoming work. For the immediate purposes of this brief communication, we note that upon making the appropriate substitutions, we can reduce the above to one moment equation relation for the  $\mu_p$ 's. This moment equation in turn separates into two distinct moment equations: one for the even moments,  $\mu_{2\eta}$ , and the other for the odd moments,  $u_\eta^o \equiv \mu_{2\eta+1}$ .

The odd order moments are themselves moments of an appropriate Stieltjes measure:  $u_\eta^o = \int_0^\infty d\xi \xi^\eta \Upsilon_o(\xi)$ , where  $\Upsilon_o(\xi) \equiv \frac{1}{2} S(\sqrt{\xi})$ , and  $\xi \equiv \rho^2$ . The relevant  $u_\eta^o$  moment equation becomes

$$2\alpha^4 s_4^2(\theta) \Omega(2\eta-6) u_{\eta-6}^o - 2\alpha^2 \beta^2 s_2(\theta) s_4(\theta) \left[ \Omega(2\eta-6) + \Omega(2\eta-4) \right] u_{\eta-5}^o \\ + \left[ 2\alpha^2 c_4(\theta) (2\eta-3) - 2\alpha^2 s_4(\theta) \Lambda_1 \Omega(2\eta-6) + 2\beta^4 s_2^2(\theta) \Omega(2\eta-4) \right. \\ \left. - 2\alpha^2 \Lambda_1 s_4(\theta) \Omega(2\eta-2) \right] u_{\eta-4}^o \\ + \left[ 2\beta^2 \left( c_2(\theta) (2-2\eta) + \Lambda_1 s_2(\theta) \left( \Omega(2\eta-2) + \Omega(2\eta-4) \right) \right) \right. \\ \left. + 2\alpha^2 E s_2(\theta) s_4(\theta) \left( \Omega(2\eta) + \Omega(2\eta-6) \right) \right] u_{\eta-3}^o \\ + \left[ -2\Lambda_R - 2\eta + 4\Lambda_R \eta + \frac{3}{2} (2\eta)^2 - \frac{1}{2} (2\eta)^3 - 2\beta^2 E s_2^2(\theta) \Omega(2\eta-4) \right. \\ \left. + 2\Lambda_1^2 \Omega(2\eta-2) - 2\beta^2 E s_2^2(\theta) \Omega(2\eta) \right] u_{\eta-2}^o \\ - 2E \left[ c_2(\theta) 2\eta + \Lambda_1 s_2(\theta) \left( \Omega(2\eta-2) + \Omega(2\eta) \right) \right] u_{\eta-1}^o + 2E^2 s_2^2(\theta) \Omega(2\eta) u_\eta^o \\ = 0. \quad (29)$$

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

$$u_\eta^o = \sum_{\ell=-5}^0 M_{\eta,\ell}^o(l_R, l_1) u_\ell^o \tag{30}$$

where  $M_{\ell_1,\ell_2}^o = \delta_{\ell_1,\ell_2}$ , for  $-5 \leq \ell_{1,2} \leq 0$ . In addition, the  $M_{\eta,\ell}^o$  coefficients satisfy the corresponding  $u_\eta^o$  moment equation with respect to the  $\eta$ -index.

To generate the  $u^o$ 's (as well as the  $M^o$  coefficients) we take  $\eta \geq 1$ , and generate the positive index moments  $\{u_{\eta \geq 1}^o\}$ , from equation (29) (i.e. using the  $2E^2 s_2^2(\theta)\Omega(2\eta)u_\eta^o$  term). We then take  $\eta \leq 0$  in equation (29), and use the first term (i.e.  $2\alpha^4 s_4^2(\theta)\Omega(2\eta - 6)u_{\eta-6}^o$ ) to generate all the remaining negative index moments. We will generate the moments  $\{u_{P_1}^o, \dots, u_{P_2}^o\}$ , where  $P_1 \leq -5$ , and  $P_2 \geq 1$ .

The required moment problem constraints, within the EMM procedure, correspond to

$$\int_0^\infty d\xi \xi^s \left( \sum_{j=J_1}^{J_2} C_j \xi^j \right)^2 \Upsilon_0(\xi) \geq 0 \tag{31}$$

for  $s = 0, 1$ , and arbitrary  $C$ 's. The  $J_{1,2}$  indices satisfy  $-\infty < J_1 < J_2 < +\infty$ . These become quadratic-form inequality constraints, upon inserting the previous linear relations:

$$\sum_{\ell=m_1}^{m_2} u_\ell^o \left( \sum_{j_1=J_1}^{J_2} \sum_{j_2=J_1}^{J_2} C_{j_1} M_{j_1+j_2+s,\ell}(l_R, l_1) C_{j_2} \right) > 0 \tag{32}$$

where  $(m_1, m_2) = (-5, 0)$ . Of course, the  $J_{1,2}$  must be consistent with the previously defined moment order indices  $P_{1,2}$ . That is, for a given  $s$  value, the corresponding  $J$ 's must satisfy  $P_1 \leq 2J_1 + s < 2J_2 + s \leq P_2$ .

An appropriate choice of normalization is required. One may take  $\sum_{\ell=m_1}^{m_2} u_\ell^o = 1$ . Upon constraining  $u_0^o$  in terms of  $\{u_\ell^o | -5 \leq \ell \leq -1\}$ , and substituting in equation (32), there ensues the linear programming inequality constraints that must be satisfied by the physical Regge-pole solution, and which form the core of EMM's algorithmic structure.

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)  $\alpha^2 = 2A^2/K$ ,  $\beta^2 = 3A^2/K$ ,  $E = A^2$ ,  $A = 63.641$ , and  $K = 1.1489$ .

In table 1 we cite the numerical results for the  $u^o$  formulation, since this involves fewer missing moment (initialization) variables. The generation of bounds to the low-lying Regge pole manifests a clear convergent behavior, with increasing moment order  $P_{1,2}$ .

**Table 1.** Bounds for the first Regge pole of the  $V(r) = \alpha^2/r^6 - \beta^2/r^4$  scattering potential ( $\theta = 0.3$ ). Cf. Amaha and Thylwe's (1994) result:(97.496 528 74,12.396 371 67).

$(P_1, P_2)$	$l_R^{(L)} < l_R < l_R^{(U)}$	$l_1^{(L)} < l_1 < l_1^{(U)}$
(-14, 10)	97.4 < $l_R$ < 97.7	12.3 < $l_1$ < 12.6
(-16, 12)	97.48 < $l_R$ < 97.56	12.36 < $l_1$ < 12.45
(-18, 14)	97.4950 < $l_R$ < 97.5400	12.3735 < $l_1$ < 12.4185

#### 4. Conclusion

The objective of this work is not necessarily to produce rapidly converging Regge-pole bounds, but instead to confirm the validity of the general theoretical formalism, which



is an unprecedented accomplishment. Handy (1996) has shown that through appropriate transformations, the generation of eigenenergy bounds to singular potentials can be dramatically accelerated. The adaptation of these, and related, methods to the present problem requires applying EMM on a more complicated set of moment equations than those given here. We anticipate a much faster Regge-pole EMM formulation in the near future, capable of generating rapidly converging bounds for many of the Regge poles (for moderate  $l$  values), at a given, arbitrary, energy. This work is ongoing.

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## References

- Bender C M and Orszag S A 1978 *Advanced Mathematical Methods for Scientists and Engineers* (New York: McGraw-Hill)
- 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
- Connor J N L 1990 *J. Chem. Soc. Faraday Trans.* **86** 1627
- 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 Xiao-Qian and Tymczak C J 2001 *J. Phys. A: Math. Gen.* **34** 5593
- Handy C R and Wang Xiao-Qian 2001 *J. Phys. A: Math. Gen.* 34 8297 (this issue)
- 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